CALPHAD 2026

53rd International Conference on Computer Coupling of Phase Diagrams and Thermochemistry

June 7 – 12, 2026

Centre des congrès de Québec, Québec City, Canada

Preface

Dear colleagues and friends,

It is with great pleasure that we welcome you to Quebec City for the 53rd International Conference on Computer Coupling of Phase Diagrams and Thermochemistry. We are honoured to host the CALPHAD community in this remarkable city, whose four centuries of history, French-rooted culture, and UNESCO-listed Vieux-Québec offer a fitting setting for a week of scientific exchange.

Since its first edition more than half a century ago, CALPHAD has brought together those who develop and apply thermodynamic and phase-diagram modelling to advance our understanding of materials. The 2026 edition continues this tradition with roughly 86 oral presentations and 53 posters, covering fundamental thermodynamic modelling, DFT-informed approaches, applications to metallic and oxide systems, machine-learning methods in CALPHAD, and the design of materials for energy and process industries. We are particularly pleased to see strong participation from junior researchers, whose work will shape the field in the years to come.

A conference of this scope is the product of many hands. We wish to thank the members of the Organizing and Scientific Committees for their dedication, our sponsors for their generous support, the staff of the Centre for Research in Computational Thermochemistry (CRCT) at Polytechnique Montréal, and the team at the Quebec Convention Centre. Above all, we thank each of you — speakers, poster presenters, and participants — for making the journey to Quebec City.

We invite you to make the most of the scientific programme, to renew old collaborations and to build new ones, and also to step outside and enjoy what the city has to offer: the cobblestone streets of the Petit-Champlain, the ramparts of the Citadelle, and the view of the St. Lawrence from Château Frontenac. *Bon congrès et bienvenue à Québec.*

Patrice Chartrand & Jean-Philippe Harvey
Conference Chairs, CALPHAD 2026

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Organizing Committee

Conference Chairs

Patrice Chartrand, Polytechnique Montréal
Jean-Philippe Harvey, Polytechnique Montréal

Organizing Committee Members

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Sponsors

CALPHAD 2026 gratefully acknowledges the support of our sponsors.

Program at a Glance

June 7 (Sun)	Registration from 12:00 | 18:30 (310 Hall)					13:00 | 17:00 **Workshop FactSage Laval University** ADJ-2320	13:00 | 17:00 **Workshop Pandat Laval University** ADJ-2300	13:00 | 17:00 **Workshop PyCalphad Laval University** ADJ-4512	18:30 | 20:00 **Welcome reception (pink coupon)** Espace Urbain		
June 8 (Mon)	7:15 **Breakfast** Espace Urbain	8:00 | 10:00 **Fundamental Thermo Modelling – 1** 306AB	10:00 | 10:20 **Break**	10:20 | 12:00 **CALPHAD Assisted Material Design of Metallic Systems – 1** 306AB	12:00 | 13:30 **Lunch** Espace Urbain	13:30 | 15:30 **Fundamental Thermo Modelling – 2** 306AB	15:30 | 15:50 **Break**	15:50 | 17:50 **DFT in CALPHAD** 306AB	17:50 | 19:20 **Dinner (blue coupon)** Espace Urbain	19:30 | 21:00 **Poster Session #1 (red coupon)** 308AB	21:00 | 22:30 **Young Calphadian Night** 306AB
June 9 (Tue)	7:15 **Breakfast** Espace Urbain	8:00 | 10:00 **Fundamental Thermo Modelling – 3** 306AB	10:00 | 10:20 **Break**	10:20 | 12:00 **CALPHAD Assisted Material Design of Metallic Systems – 2** 306AB	12:00 | 13:30 **Lunch** Espace Urbain	13:30 | 15:30 **Calphad Application - 1** 306AB	15:30 | 15:50 **Break**	15:50 | 17:50 **Calphad Application - 2** 306AB	17:50 | 19:30 **Dinner** Espace Urbain	19:30 | 21:00 **Poster Session #2 (orange coupon)** 309AB	20:30 | 22:30 **CALPHAD AGA (Board members only)** Room 311
June 10 (Wed)	7:15 **Breakfast** Espace Urbain	8:00 | 10:00 **Software and New Models** 306AB	10:00 | 10:20 **Break**	10:20 | 12:00 **CALPHAD for Aluminum Alloys** 306AB	12:00 | 13:30 **Lunch** Espace Urbain	13:30 | 14:00 **Group picture** Promenade Desjardins	15:30 | 17:30 Huron Traditional site	17:45 | 20:15 Cocktail and Meal at *La Sagamité*	18:15 Wendat Nation Conference & Wendat Song	20:30 | 21:00 Myths & Legends at Onhwa' Lumina	21:00 | 22:15 Onhwa' Lumina night walk
							Social excursion Wendake (Bus departure - **14:45** from the Delta Hotel)				
June 11 (Thu)	7:15 **Breakfast** Espace Urbain	8:20 | 10:20 **Diffusion, Microstructure, Properties** 306AB	10:20 | 10:40 **Break**	10:40 | 12:00 **CALPHAD for Oxides – 1** 306AB	12:00 | 13:30 **Lunch** Espace Urbain	13:30 | 14:50 **CALPHAD for Nuclear Applications** 306AB	14:50 | 15:10 **Break**	15:10 | 16:30 **CALPHAD for Salts** 306AB	18:00 | 22:30 Boarding 18:00 | Departure 19:00 Banquet Cruise (Awards announcement) Buses leave the Delta Hotel at **17:30** Chouinard Wharf, 10 Dalhousie Street, Québec, QC G1K 8L8		
June 12 (Fri)	7:15 **Breakfast** Espace Urbain	8:00 | 10:20 **CALPHAD Applications to Metallic Systems** 306AB	10:20 | 10:40 **Break**	10:40 | 12:00 **CALPHAD for Oxides – 2** 306AB	12:00 | 13:30 **Lunch boxes** 308-309 corridor						

Venue




Conference venue

Centre des congrès de Québec
1000 boulevard René-Lévesque Est
Québec, QC G1R 5T8, Canada

Conference hotel

Hôtel Delta Québec
690 boulevard René-Lévesque Est
Québec, QC G1R 5A8, Canada

Transportation

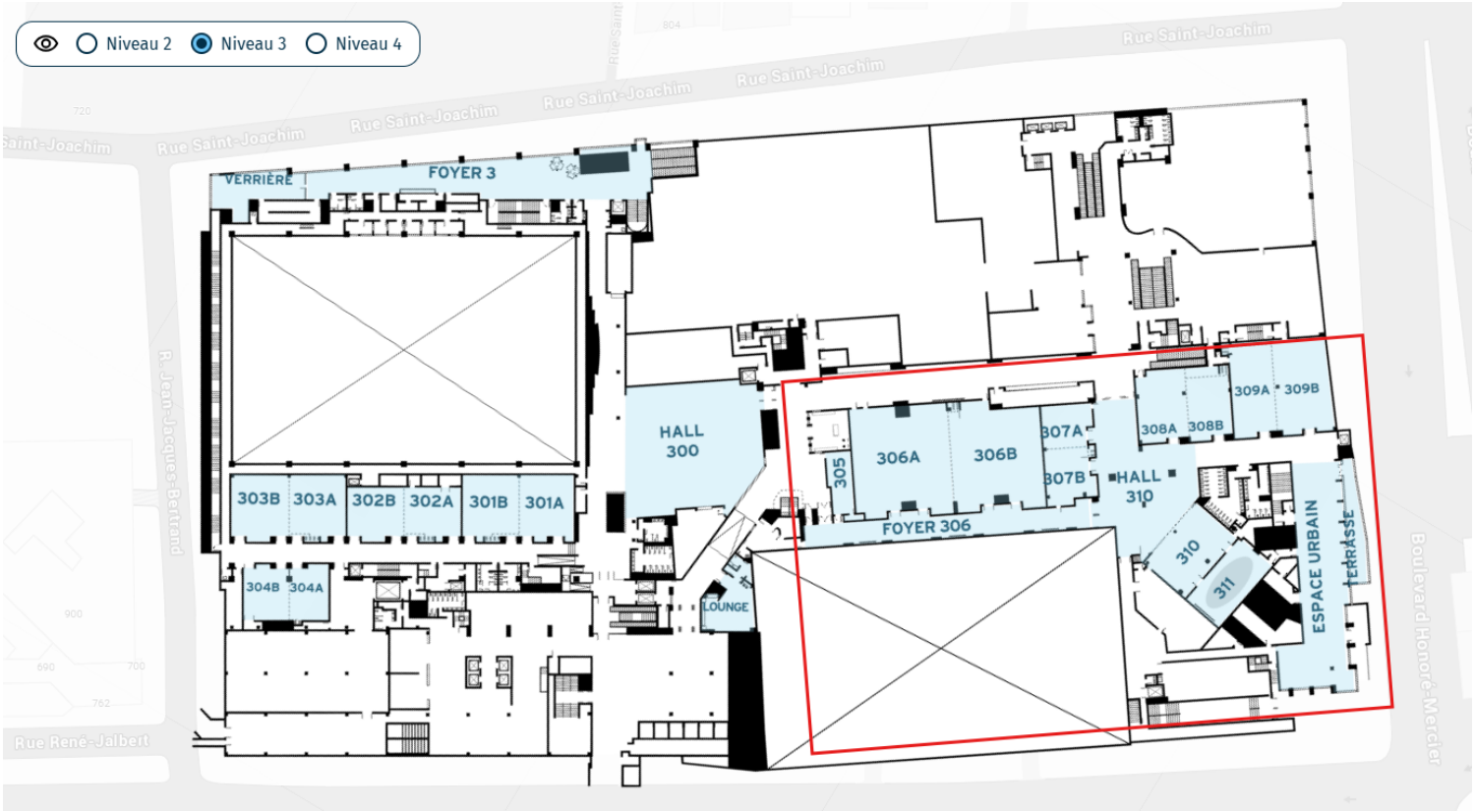
Taxis Coop 418-525-5191, Taxi Laurier 418-651-2727, Quebec City is also well deserved by Uber and Lyft.

Enjoy Your Badge Program

Throughout your stay, your CALPHAD 2026 badge unlocks exclusive offers at participating restaurants, museums, cultural attractions, boutiques and entertainment venues across Québec City. Simply present your badge at the point of purchase. A few establishments have specific conditions or codes – the full list of partners and offers is available at:

https://www.convention.qc.ca/en/plan-visit/enjoy-your-badge-program/

Floor map



Emergencies: each room has an emergency plan and a QR code that allows you to contact the Center's staff, who serve as first responders. The direct number is: **418-644-8796**.

City map

See the Official Calphad 2026 website for an interactive map with points of interest for the Calphad Conference.

Pre-conference Workshops

Three pre-conference workshops will be held on Sunday, June 7, 2026, at Université Laval (Pavillon Alphonse-Desjardins). All three sessions run from 13:00 to 17:00 and require.

Workshop | FactSage

FactSage is a fully integrated thermochemical database and software system widely used to calculate phase equilibria and thermodynamic properties of alloys, slags, salts, ceramics and aqueous solutions. This workshop presents practical and advanced uses of FactSage 8.4 together with ChemApp, the CALPHAD Optimizer, ThermML and database optimization examples, and closes with a FactFlow demonstration linking equilibrium calculations to process-level simulation. A short look at the new FactSage 9.0 installation approach is also included.

When: Sunday, June 7, 2026
Time: 13:00 – 17:00
Location: Université Laval, Pavillon Alphonse-Desjardins, Room ADJ-2320
Organizer: GTT-Technologies / CRCT
Instructors: Jean-Philippe Harvey, Christopher W. Bale, Kyota Poëti & Kentaro Oishi (CRCT, Polytechnique Montréal) — Moritz to Baben, Florian Tang & GTT team (GTT-Technologies)
Full program: FactSage_Workshop_Calphad_2026.pdf

A FactSage workshop version will be provided to registered participants before the workshop; installation instructions and any preparation steps will be sent in advance. Participants who wish to follow selected demonstrations on their own machines should bring a laptop; the session is also accessible to attendees who prefer not to run the software during the workshop.

Who should attend

- CALPHAD researchers, database developers, and materials scientists working with phase equilibria, high-temperature processes, alloy design, or process chemistry.
- Process-modelling researchers and industrial users connecting thermodynamic calculations with process-level analysis.
- Students, postdoctoral researchers, and new users seeking a structured introduction to FactSage, ChemApp, and FactFlow.
- Current FactSage users interested in the new FactSage 9.0 installation approach and recent additions to the suite.

Agenda

- Opening — FactSage, CRCT, and GTT-Technologies (13:00 – 13:15).
- FactSage 8.4 today — current capabilities and practical workflows (13:15 – 14:15).
- ChemApp, CALPHAD Optimizer, ThermML, and database optimization examples (14:15 – 15:05).
- Advanced equilibrium calculation example and FactFlow process-simulation demonstration (15:15 – 16:30).
- FactSage 9.0 installation approach, discussion and attendee feedback (16:30 – 17:00).

Workshop | Pandat

This workshop, organized by CompuTherm LLC, introduces Pandat as an integrated CALPHAD platform for materials design and process simulation. Participants will see how Pandat supports phase diagram calculations, thermodynamic analysis, precipitation and recrystallization modelling, diffusion simulation, and solidification analysis, with examples that emphasise practical workflows for research and accelerated materials development.

When: Sunday, June 7, 2026
Time: 13:00 – 17:00
Location: Université Laval, Pavillon Alphonse-Desjardins, Room ADJ-2300
Organizer: CompuTherm LLC
Instructors: Dr. Shuanglin Chen (CompuTherm LLC) — Prof. Rainer Schmid-Fetzer (TU Clausthal)
Full program: Pandat_Workshop_Calphad_2026.pdf

No advanced Pandat experience is required. Basic familiarity with materials thermodynamics, phase diagrams and heat-treatment or solidification concepts is helpful. Participants are encouraged to install the Pandat education version (Pandat_2026_Education_Setup.exe) before the workshop.

Who should attend

- Researchers, engineers, and industry practitioners using computational thermodynamics, alloy design, phase transformation, or process modelling.
- Graduate students, postdoctoral researchers, and new users seeking a practical introduction to Pandat.
- Current Pandat users interested in recent features and broader applications.

Agenda

- Introduction — development of Pandat software.
- Pandat overview — interface, workflow, modules, and databases.
- Live demonstration — Pandat simulation and result interpretation.
- Discussion — questions, applications, and more.

Workshop | Open-source CALPHAD tools (PyCalphad, ESPEI, Kawin)

This workshop gives a detailed introduction to CALPHAD-type computational thermodynamics and kinetics software within the PyCalphad ecosystem. It features hands-on exercises in an interactive cloud environment that enables attendees to calculate phase diagrams, simulate solid-state precipitation in alloys, and propagate uncertainty in thermodynamic calculations. Attendees are encouraged to bring a laptop or computing device to follow along interactively. Tables, power outlets, and Wi-Fi will be provided.

When: Sunday, June 7, 2026
Time: 13:00 – 17:00
Location: Université Laval, Pavillon Alphonse-Desjardins, Room ADJ-4512
Components: PyCalphad — ESPEI — Kawin
Audience: Engineers and practitioners interested in open-source materials-design tools.
Full program: PyCalphad_Workshop_Calphad_2026.pdf

Agenda

13:00 | Opening and introductions
13:15 | PyCalphad
14:15 | ESPEI
15:15 | Break
15:30 | Kawin
16:30 | Discussion and Q&A
17:00 | Closing

Social activities

Excursion | Wendake, La Sagamité & Onhwa' Lumina night walk

The Wendat — historically called Huron in French colonial records — are a First Nation whose ancestral homeland includes Wendake, a community located just minutes north of Quebec City. This excursion immerses participants in their culture: the Huron-Wendat Traditional Site introduces ancestral knowledge and daily life; dinner is served at *La Sagamité*, a restaurant named after a traditional Wendat corn-and-bean stew; and the evening concludes with *Onhwa' Lumina*, an outdoor night walk through the forest celebrating Wendat stories, song, and connection to the land.

When: Wednesday, June 10, 2026
Cost: Included
Starting point: Delta Hotel
Destination: Wendake

14:45 | Departure

Private bus transfer to the Huron Traditional Site.

15:30 – 17:30 | Huron Traditional Site

Activities: walk through a reconstructed 17th-century Wendat village including a traditional longhouse, smokehouse, and sweat lodge; observe demonstrations of ancestral knowledge such as traditional transportation (canoes, snowshoes), hunting techniques, and traditional medicine; enjoy a hands-on experience of Wendat daily life, taking in the wood smoke, traditional furs, and village architecture.

17:30 | Private bus transfer to La Sagamité restaurant

17:45 – 20:15 | Dinner at La Sagamité

A refined three-course dinner inspired by traditional Wendat cuisine, served in a warm and welcoming atmosphere. The evening includes a presentation by the Wendat Nation and a traditional song.

18:15 | Wendat Nation Conference & Wendat Song

20:15 | Private bus transfer to Onhwa' Lumina

20:30 – 21:00 | Myths & Legends at Onhwa' Lumina

An intimate storytelling experience by the fire in the Ekionkiestha' Longhouse, where traditional stories about the creation of Mother Earth, the Pleiades, and other ancestral myths offer a unique insight into Huron-Wendat culture.

21:00 – 22:15 | Onhwa' Lumina Night Walk

An enchanting night walk celebrating the Huron-Wendat Nation. Under the stars, experience ancestral rhythm and song within the Great Circle, fostering a sense of connection with all living things.

22:15 | Private bus transfer to the Delta Hotel

Accompanying Persons | Monday June 8: Culture & Green Space

When: Monday, June 8, 2026
Cost: Free
Starting point: Québec Convention Centre
Destination: Grande Allée, Plains of Abraham, Old Québec, Château Frontenac
Theme: History, scenery, and iconic Québec landmarks. Timing may vary based on the group's pace and energy levels.

08:30 | Departure from Québec Convention Centre

Begin on foot toward Grande Allée.

08:35 – 09:00 | Grande Allée (25 min)

Highlights: Historic façades, cafés, and lively atmosphere.
Experience: Quick coffee or light breakfast stop.

09:05 – 10:15 | Plains of Abraham (1 h 10)

Must-visit: Joan of Arc Garden, Martello Towers, river viewpoints.
Highlights: Historic 1759 battlefield, scenic walking paths, panoramic views.
Experience: Relaxing walk combining history and nature.

10:15 – 10:30 | Walk to Old Québec

Scenic downhill route with views of the fortifications.

10:30 – 11:15 | Old Québec (45 min)

Must-visit: Place d'Armes, city walls, Terrasse Dufferin.
Highlights: UNESCO World Heritage Site with European charm.
Experience: Explore cobblestone streets and the historic ambiance.

11:15 – 11:45 | Château Frontenac & Dufferin Terrace (30 min)

Must-visit: Château exterior / lobby, terrace boardwalk.
Highlights: Iconic landmark, river views, photography spots.
Experience: Enjoy views, take photos, optional short break.

12:00 | Return to Québec Convention Centre

Accompanying Persons | Tuesday June 9: Nature & Excursion

When: Tuesday, June 9, 2026
Cost: Free
Starting point: Québec Convention Centre
Destination: Montmorency Falls Park, Île d'Orléans
Theme: Nature, countryside scenery, and local flavours. Timing may vary depending on pace and traffic.

Morning program — Montmorency Falls Park (08:30 – 11:30)

08:30 | Departure from Québec Convention Centre

08:50 – 10:50 | Montmorency Falls Park

Address: 5300 Boulevard Sainte-Anne, Québec, QC
Highlights: 83 m waterfall (higher than Niagara Falls), suspension bridge, cable car, scenic trails.
Must-visit: Main lookout, suspension bridge, cable car station.

11:30 | Return to Québec Convention Centre

Afternoon program — Île d'Orléans scenic tour (13:30 – 17:30)

Reference: https://www.quebec-cite.com/en/what-to-do-quebec-city/tour-ile-orleans

13:30 | Departure from Québec Convention Centre

14:00 – 14:50 | Vignoble Ste-Pétronille

Address: 8705 Chemin Royal, Sainte-Pétronille, QC
Highlights: Panoramic Québec City views, wine / cider tasting, group photos.

15:00 – 15:45 | Chocolaterie de l'Île d'Orléans

Address: 1505 Chemin Royal, Saint-Pierre, QC
Highlights: Handmade chocolates, relaxing indoor stop.

15:45 – 16:15 | Church of Saint-Jean de l'Île d'Orléans

Address: 4623 Chemin Royal, Saint-Jean-de-l'Île-d'Orléans, QC G0A 3W0
Highlights: Historic village church.

16:15 – 16:50 | Mauvide-Genest Manor, lighthouse and Saint-Jean-de-l'Île-d'Orléans

Address: 2 Chemin du Quai, Saint-Jean-de-l'Île-d'Orléans, QC
Highlights: Traditional houses, authentic Québec charm.

17:30 | Return to Québec Convention Centre

Accompanying Persons | Thursday June 11: Family Activity and Parliament of Quebec

When: Thursday, June 11, 2026
Cost: Free
Starting point: Québec Convention Centre
Destination: National Museum of Fine Arts of Quebec (MNBAQ), Parliament of Quebec

Morning program — National Museum of Fine Arts of Quebec (MNBAQ)

09:00: Departure from Québec Convention Centre.

09:30 – 11:30 | National Museum of Fine Arts of Quebec (MNBAQ)

Quebec and Canadian art collections.
Contemporary exhibitions.

Afternoon program — Parliament of Quebec

14:00 – 15:30 | Parliament of Quebec

Historic government building.
13:30: Departure from Québec Convention Centre.
14:00: Arrival at the Parliament (security, registration, coat check, etc.).
14:30: Guided visit.
15:30: End of the visit.

Oral Presentations

Monday

Fundamental Thermo Modelling – 1

Chairs: J.-M. Joubert & A. Jacob

8:00-8:20 O1.1

A Unified Thermodynamic Framework: From Equilibrium and Nonequilibrium to Zentropy, Cross Phenomena, and Artificial Intelligence

Z.-K. Liu
Pennsylvania State University, United States of America

8:20-8:40 O1.2

Recursive entropy in thermodynamics: establishing the statistical-physics basis of the zentropy approach

L. Myers, N. Hew, S. Shang, Z. Liu
Pennsylvania State University, United States of America

8:40-9:00 O1.3

Thermodynamic Entropy as Information - A compression-based demonstration of the Shannon—Boltzmann equivalence in condensed matter

D. Fisher, Q.-J. Hong
Arizona State University, United States of America

9:00-9:20 O1.4

CALPHAD Coupled Integrated Computational Materials Engineering (ICME) Framework for Microstructure Evolution and Property Optimization

K. L. M. Elder, S. M. Peters, J. Kaipainen, G. E. Isitman, S. A. Khairallah, M. R. Tupek, B. Bocklund, D. A. Tortorelli, J. D. Roehling, S. Watts, J. L. Fattebert, J. T. McKeown, T. Andersson, A. Laukkanen, T. Pinomaa, A. Perron, H. Villanueva
Lawrence Livermore National Laboratory, United States of America

9:20-9:40 O1.5

High-throughput calculation of eutectic compositions

K. E. Borowski, K. Firdova, G. Deffrennes, J.-M. Joubert
Université Paris-Est Créteil, France

9:40-10:00 O1.6

The Calfateria

N. Dupin, S. G. Fries
Calcul Thermodynamique, France

CALPHAD Assisted Material Design of Metallic Systems – 1

Chairs: W. Xiong & R. Schmid-Fetzer

10:20-10:40 O1.7

Development of Thermodynamic Databases Coupled to Alloy Design of Metallic Materials

K. Frisk
Innomat AB, Sweden

10:40-11:00 O1.8

Model Development and Design of High Strength, High Toughness Naval Steels: 10Ni-150

Y. N. Lee, C. C. Tasan, G. B. Olson
Massachusetts Institute of Technology, United States of America

11:00-11:20 O1.9

CALPHAD-assisted design of high-performance titanium alloys and refractory materials for melting

H. Zhu, Q. Feng, P. Gao, G. Chen, C. Li
Shanghai University, China

11:20-11:40 O1.10

Constrained Target Function for Alloy Design

S. Chen, C. Zhang, W. Cao, F. Zhang
CompuTherm, LLC, United States of America

11:40-12:00 O1.11

Revisiting the Fe-Mo System: Structural Investigation and Thermodynamic Modeling of Frank-Kasper Phases

A. Flores, S. Chatain, P. Fossati, J.-M. Joubert
CEA Paris-Saclay, France

Fundamental Thermo Modelling – 2

Chairs: N. Dupin & B. Bocklund

13:30-13:50 O1.12

Optimization and Uncertainty Quantification of CALPHAD Model Parameters via the No-U-Turn Sampler

C. Kunselman, B. Bocklund, R. Otis, R. Arroyave
Texas A&M University, United States of America

13:50-14:10 O1.13

Efficient CALPHAD coupling of quasi-equilibrium thermodynamics using a hash-table-based extrapolation scheme

H. H. Y. Craven, N. Warnken
University of Birmingham, United Kingdom

14:10-14:30 O1.14

Calphad assessment strategy and unexpected liquid miscibility gaps

R. Schmid-Fetzer, C.-H. Ho, H.-C. Huang, S.-W. Chen
Clausthal University of Technology, Germany

14:30-14:50 O1.15

Comparison of different model equations for size- and shape-dependent integral and partial molar Gibbs energies of nano-phases to screen out the incorrect ones

G. Kaptay
University of Miskolc, Hungary

14:50-15:10 O1.16

A modified Scheil approach for nucleation-dependent solidification pathways

S. Y. Kwon, Y. Yang, A. Plotkowski, M. Rolchigo, A. Shyam, S. Bahl, N. A. Richter, J. A. Haynes
Oak Ridge National Laboratory, United States of America

15:10-15:30 O1.17

Developing reliable Calphad descriptions: lessons from the Fe-Ni system

Z. He, Q. Chen, M. Selleby
Swerim, Sweden

DFT in CALPHAD

Chairs: B. Hallstedt & Y. Zhong

15:50-16:10 O1.18

Using Universal Machine Learning Potential to Accelerate the Thermodynamic Database Development

A. Saengdeejing, R. Sahara, H. Kino, T. Chkyow
National Institute for Materials Science, Japan

16:10-16:30 O1.19

A hybrid methodology based on first-principles calculations and Calphad to predict the Ni-Co phase diagram incorporating configurational, vibrational and magnetic contributions

C. Shi, W. Shao, J. LLorca
Fundación IMDEA Materiales, Spain

16:30-16:50 O1.20

Overestimation of Silica Melting at Ambient Pressure in DFT and High-Accuracy MLIPs: Tackling Unreachable Relaxation Timescales

L.-F. Zhu, F. Körmann, A. Forslund, J. Neugebauer, B. Grabowski
University of Stuttgart, Germany

16:50-17:10 O1.21

Application of an uncertainty quantification method based on a heterogeneous ensemble of pretrained Universal machine learning interatomic potentials applied to steels with tramp elements

N. K. Mohandas, K. Liu, M. H. F. Sluiter
University of Technology Delft, Netherlands

17:10-17:30 O1.22

Ab Initio Prediction of the Magnetic Thermodynamics of LaCoO3 Perovskite Based on the Zentropy Theory

S. Yang, Y. Zhong
Worcester Polytechnic Institute, United States of America

17:30-17:50 O1.23

Automated computation of ab initio bulk and defect phase diagrams

A. Tehranchi, P. Mathews, J. Janßen, T. Hickel, J. Neugebauer
Max Planck Institute for Sustainable Materials, Germany

Tuesday

Fundamental Thermo Modelling – 3

Chairs: B.J. Lee & A. Saengdeejing

8:00-8:20 O2.1

Bayesian Design of Experiments for Calphad Modeling

B. Bocklund, I. R. Crystal, E. Sobalvarro Converse
Lawrence Livermore National Laboratory, United States of America

8:20-8:40 O2.2

Utilizing CALPHAD databases for alloy microstructure prediction via phase-field modeling

T. Morino, M. Ode, S. Hirosawa
Yokohama National University, Japan

8:40-9:00 O2.3

Toward Defect Phase Diagrams by Integrating Constraints into CALPHAD

M. to Baben, P. Matthews, K. Rejiba, T. Hickel, U. Kerzel, A. Walnsch
GTT Technologies, Germany

9:00-9:20 O2.4

Thermodynamic Modeling of Pure Elements with Quantitative Model Selection and Uncertainty Quantification using PyCalphad and ESPEI

A. Richter, I. Roslyakova, A. M. Beese, Z-K. Liu
The Pennsylvania State University, United States of America

9:20-9:40 O2.5

A Cluster-Based Computational Thermodynamics Framework with Intrinsic Chemical Short-Range Order: New Developments and Implications for Precipitate Nucleation Kinetics

H. Chen, B.-C. Zhou
University of Virginia, United States of America

9:40-10:00 O2.6

Calphad models for the liquid phase

B. Sundman, A. Flores, L. Kjellqvist, C. Guéneau
OpenCalphad, Sweden

CALPHAD Assisted Material Design of Metallic Systems – 2

Chairs: K. Frisk & M. Sluiter

10:20-10:40 O2.7

Combinatorial Additive Manufacturing–Enabled Materials Discovery and Modeling of W–Re–Os Alloys

W. Chen
University at Buffalo, United States of America

10:40-11:00 O2.8

Development of a high-throughput approach to assess oxidation resistance using chemically graded Ni-based superalloys

S. Ghanes, M. Degeiter, E. Epifano, T. Vaubois, F. Fossard, J. S. Mérot, N. Horezan, M. Perrut, D. Monceau
ONERA, France

11:00-11:20 O2.9

Evaluation of the Cu-Ti phase diagram and thermodynamic prediction of continuous and discontinuous precipitation

I. Ohnuma, T. Suzuki, H. Ohtani
National Institute for Materials Science, Japan

11:20-11:40 O2.10

Phase diagrams of Bi-Cu-Sn-Te quaternary system

C.-H. Ho, H.-C. Huang, C. Y. Chuang, Y.-C. Tsai, C.-Y. Hsieh, S.-W. Chen
National Tsing Hua University, Taiwan

11:40-12:00 O2.11

Materials design of high-strength, ultra-pure copper alloys for the next-generation detectors to unravel the nature of dark matter

D. Spathara, P. Knights, K. Nikolopoulos
University of Birmingham, United Kingdom

CALPHAD Applications – 1

Chairs: M. to Baben & B. Davis

13:30-13:50 O2.12

Thermodynamic and Kinetic Modelling of Oxide-Metal Reactions During Casting of Reactive Alloys

J. Moses, N. Warnken
University of Birmingham, United Kingdom

13:50-14:10 O2.13

Schaeffler diagram – a CALPHAD-view on an established application tool

A. Schneider
Thermo-Calc Software AB, Sweden

14:10-14:30 O2.14

Deoxidation Equilibria in Liquid Alloys

M.-K. Paek, G. Hils, Y.-B. Kang, I.-H. Jung
Clausthal University of Technology, Germany

14:30-14:50 O2.15

Integration of thermodynamics with process development in ferroalloy production

B. Davis, J.-P. Harvey
Kingston Process Metallurgy Inc., Canada

14:50-15:10 O2.16

An assessment of hydrogen-induced NiTi martensite transition

G. Pollini, E. Alvares, B. Bocklund, M. Palumbo, P. Jarebek, C. Pistidda
University of Turin, Italy

15:10-15:30 O2.17

Investigation of the effects of tramp elements on the pearlitic transformation for a sustainable steelmaking industry

A. Maille, J. Bouquerel, P. Antoine, M. Bonvalet Rolland
Centrale lille institut, France

CALPHAD Applications – 2

Chairs: I.H. Jung & T. Morino

15:50-16:10 O2.18

Thermodynamic Modelling of Protective Coating for Solid Oxide Electrolysis Cells

M. Saab, C. Guéneau, S. Chatain, P. V. B. Pinho
Commissariat énergie atomique et alternatives, France

16:10-16:30 O2.19

Modelling and probing solid solution-aqueous solution equilibria of aqueous nickel iron sulfate at 6 °C

J. Self, E. D. D. Da Silva, K. Oishi, J.-P. Harvey
Polytechnique Montréal, Canada

16:30-16:50 O2.20

Unexpected Cracking in WAAM Cu-Ni Deposited on Steel Base Plates: Understanding the Role of Fe

T. Avey, E. Holcombe, J. Norkett, J. Semple, C. Fisher
NSWC Carderock, United States of America

16:50-17:10 O2.21

Blast Furnace Simulation Using a CASCADE Framework and ChemApp for Python

A. Mansy, K. H. Spitzer, M. K. Paek
Technical University of Clausthal, Germany

17:10-17:30 O2.22

Modelling of inorganic solid phases formed during pyrogasification of biomass

D. A. Pinto Huanaco, J. H. Ferrasse, O. Boutin, L. M. Romero Millan, M. Hervy, Y. Kara
Aix Marseille University, France

17:30-17:50 O2.23

Machine learning-assisted crystal plasticity modeling of microcrack behavior in gradient-structured steels

X. X. Luo, C. K. Liu, S. Y. Wen, H. Mao, L. Y. Liu, X. Y. Zheng, Y. Du
Central South University, China

Wednesday

Software and New Models

Chairs: B. Sundman & C. Bale

8:00-8:20 O3.1

Thermodynamic Modeling of Metal Hydrides: Workflows, Software, and Applications to Multicomponent Databases

P. Hannappel, G. H. Gu, M. T. Curnan, Ł. Gondek, J. Czub, F. Heubner, M. Balcerzak, T. Weißgärber
TUD Dresden University of Technology, Germany

8:20-8:40 O3.2

PhaseForge: Automated CALPHAD-Compatible Phase Diagram Generation Using Universal Machine Learning Potentials

D. Sarıtürk, S. Zhu, R. Arróyave
Texas A&M University, United States of America

8:40-9:00 O3.3

Web-Based APIs for Automated Thermodynamic Property Generation: MAPP and SLUSCHI

Q.-J. Hong
Arizona State University, United States of America

9:00-9:20 O3.4

Building Interoperable CALPHAD Workflows: ThermML and Calphad Optimizer 3.0

F. Tang, B. Reis, M. to Baben
GTT Technologies, Germany

9:20-9:40 O3.5

FactFlow-Assisted Optimization of Aluminum Recycling Processing Balancing Economic Performance, Product Quality, and Environmental Impact

K. Poëti, D. Wei, K. Oishi, J-P. Harvey
Polytechnique Montréal, Canada

9:40-10:00 O3.6

Development of a Modified Polyhedron Model for Improved Estimation of Thermodynamic Properties of Mixed Oxides

E. Moosavi-Khoonsari, J. Arias Hernandez, S.-Y. Kwon
École de technologie supérieure, Canada

CALPHAD for Aluminum Alloys

Chairs: A. Kroupa & E. Povoden

Special Focus on Canadian Aluminum Research and Innovation

This session highlights CALPHAD applications for aluminum alloy development and acknowledges the valued support of **CQRDA** and **Hatch** in promoting aluminum research, innovation, and industrial collaboration in Canada.

10:20-10:40 O3.7

CALPHAD-driven discovery and rapid experimental validation of low-cost, high-strength, Al-alloys for additive manufacturing

B. Glaser, A. J. Hart, S. M. Taheri-Mousavi
Carnegie Mellon University, United States of America

10:40-11:00 O3.8

Thermodynamic modeling of the Al-rich Al-B system with LIBS/DSC Liquidus measurements

J.-R. Castillo-Sánchez, A. Vázquez Prudencio, P. Lafaye, J.-P. Harvey, K. Leosson, G. Salloum-Abou-Jaoude
Polytechnique Montréal, Canada

11:00-11:20 O3.9

Comparative Assessment of Crack Susceptibility Criteria Using Calphad Solidification Modeling and Graded Thermal Experiments

L. F. L. Pizano, W. Xiong
University of Pittsburgh, United States of America

11:20-11:40 O3.10

Molecular dynamics (MD) simulations of the nucleation of aluminum on TiB_2 interfaces with equivariant machine learning interatomic potentials (MLIAP)

D. Defrance, J-P. Harvey
Polytechnique Montréal, Canada

11:40-12:00 O3.11

CALPHAD assisted microstructural design to control precipitate and dispersoid evolution for improved strengthening in Al-Mg-Si-based alloys

S. K. Deb, A. Arora
Indian Institute of Technology Gandhinagar, India

Thursday

Diffusion, Microstructure, Properties

Chairs: Z.K. Liu & D. Larouche

8:20-8:40 O4.1

Thermodynamics and Diffusion Kinetics in Mn2Ti-type Hydrogen Storage Alloys

B.-J. Lee, J.-S. Lee, S.-H. Oh
Pohang University of Science and Technology, Korea (Republic of)

8:40-9:00 O4.2

Incorporation of molar volumes of diffusing elements in Onsager-type formulations of diffusion in alloys

A. R. khorasgani, S. Divinski, J. Kundin
Ruhr University Bochum, Germany

9:00-9:20 O4.3

The Thermodynamics of Planar Defects in Magnesium Alloys

P. Mathews, J. Janßen, A. Tehranchi, J. Neugebauer, T. Hickel
Federal Institute for Materials Research and Testing, Germany

9:20-9:40 O4.4

A predictive surface tension for liquid metallic solutions

Y. Kang, I.-H. Jung
Seoul National University, Korea (Republic of)

9:40-10:00 O4.5

Physics-based Thermal Conductivity Model Compatible with Multi-component CALPHAD Descriptions

Z. Liang, U. R. Kattner, M. J. Luebbe, F. Zhang, J. Martin, D. Kirsch, S. Chen
National Institute of Standards and Technology, United States of America

10:00-10:20 O4.6

Modelling Na–Mn–O cathodes and predicting cathode–electrolyte interface reactions for sodium-ion batteries

E. Povoden-Karadeniz, A. Khan, M. C. Poletti
Institute of Materials Science and Technology, Austria

CALPHAD for Oxides – 1

Chairs: E. Moosavi-Khoonsari & M. Perrut

10:40-11:00 O4.7

Systematics and thermodynamic modeling of the AEO-B2O3 (AE = Mg, Ca, Sr, Ba) binary systems

A. Pisch, N. Bouzid
Université Grenoble Alpes, France

11:00-11:20 O4.8

Revisiting RE-Ba-Cu-O Thermodynamics: From YBCO to Modern Gd- and Eu-Based Bulk Superconductors

D. Sedmidubský
University of Chemistry and Technology Prague, Czechia

11:20-11:40 O4.9

Thermodynamic Database Development for the Al2O3–CaO–MgO–SiO2–Fe2O3–FeO System and Its Application to Industrial Solid-Waste Utilization

F. Gao, Y. Liu, Hans J. Seifert, Y. Du
Central South University, China

11:40-12:00 O4.10

Thermodynamic Modelling of the CaO-MgO-SiO2 ternary system and its use in Ordinary Portland Cement Clinker Production

R. Bandak, W. R. Leal da Silva, A. Pisch
Université Grenoble Alpes, France

CALPHAD for nuclear applications

Chairs: S. Chen & P. Lafaye

13:30-13:50 O4.11

Software and Database Development for Design of Radiation-Resistant Alloys

N. Ury, B. Bocklund, N. Bertin, A. Perron
Lawrence Livermore National Laboratory, United States of America

13:50-14:10 O4.12

Enhancing Nuclear Reactor Safety: Thermodynamic Modelling of the Ag-Zr System in PWR Absorber Rods

C. Antion, M. Barrachin, P. Benigni, I. Crassous, A. Decreton, E. Fischer, S. Gyasi, A. Janghorban, M. Lomello, G. Mikaelian, I. Nuta, J. Rogez
University Grenoble Alpes, France

14:10-14:30 O4.13

Molten Salts Thermophysical Properties modelling: new insights into the effect of fission products accumulation in molten fuel salt systems

J. J. Soppo, O. T. Noordhuis, D. C. Alders, S. Couweleers, J. Vlieland, G. Pireddu, A. Salcedo, L. Ruszczynski, R. J. M. Konings, A. L. Smith
Delft University of Technology, Netherlands

14:30-14:50 O4.14

Thermodynamic Modeling of Phase Stability in Alloys under Irradiation

Y. Lu, C. Wang, X. Liu
Xiamen University, China

CALPHAD for Salts

Chairs: D. Lindberg & M. Saab

15:10-15:30 O4.15

Thermodynamic modeling and phase characterization in the Li2SO4-CoSO4-MnSO4-NiSO4 system for metal recovery from secondary resources

D. Lindberg, D. Sibarani, J. Biswas, G. Tewari, L. Klemettinen
Åbo Akademi University, Finland

15:30-15:50 O4.16

New thermodynamic model for salt-metal liquid solutions introducing charge defects within the CALPHAD approach

O. Kidari, P. Chartrand
Polytechnique Montréal, Canada

15:50-16:10 O4.17

Crystal Growth and Thermodynamic Assessment of the Thallium Alkaline-Earth Halides

E. van Loef, M. Inniss, M. Gillespie, K. Pestovich, L. Stand, L. S. Pandian, M. Zhuravleva
Radiation Monitoring Devices, Inc., United States of America

16:10-16:30 O4.18

Thermodynamic models for ternary deep eutectic systems

L. P. Zini, G. Teixeira, J.-P. Harvey, J. A. P. Coutinho, C. Robelin
Polytechnique Montréal, Canada

Friday

CALPHAD Applications to Metallic Systems

Chairs: U. Kattner & M. Selleby

8:00-8:20 O5.1
Understanding deformation-induced nanocrystallization in amorphous alloys: a multi-scale modeling study
S.-H. Oh, M. Wakeda
National Institute for Materials Science, Japan

8:20-8:40 O5.2
Liquidus projection of Cu-Se-Te ternary system
S.-W. Chen, C.-Y. Chung, Y.-C. Tsai, Y.-J. Chuang
National Tsing Hua University, Taiwan

8:40-9:00 O5.3
Phase-field modeling of austenitic fraction formation during tempering of 13Cr-4Ni martensitic stainless steels.
S. Valtierra, D. Paquet, V. Timoshevskii, D. Thibault, J-P. Harvey
Polytechnique Montréal, Canada

9:00-9:20 O5.4
Thermodynamic modelling of the Al–Ni–V system
B. Hallstedt, M. Noori
RWTH Aachen University, Germany

9:20-9:40 O5.5
Predictive thermodynamic modeling of the Suzuki effect in Co-Ni based alloys
A. Jacob, V. Razumovskiy, F. Moitzi, A. Robisson, E. Kozeschnik
TU Wien, Austria

9:40-10:00 O5.6
Optimizing Hardmetal Alloy Design Through CALPHAD and Experimental Investigation
T. Soria-Biurrun, S. Sridar, K. Frisk, L. Muñoz-Ortuño, F. Ibarreta-López, R. Martínez-Pampliega, J. M. Sánchez-Moreno
CEIT-BRTA, Spain

10:00-10:20 O5.7
Phase diagrams of Cu-Co-Sb ternary system
Yung-Chun Tsai, Ching-Yu Chuang, Cheng-Hsi Ho, Sinn-wen Chen
National Tsing Hua University, Taiwan

CALPHAD for Oxides – 2

Chairs: A. Pisch & D. Sedmidubský

10:40-11:00 O5.8
Gd3Sc2Al3O12 garnet scintillator: defect engineering
J. Ježek, J. Pejchal, D. Sedmidubský, P. Zemenová, V. Laguta, V. Babin, V. Jarý, A. Beitlerová, R. Kučerková, M. Nikl
Institute of Physics of the Czech Academy of Sciences, Czechia

11:00-11:20 O5.9
Thermodynamic Assessment of the Ba—Ti—O Ternary System
A. Albaalbaky, C. Gueneau, P. V. Borges Pinho
French Alternative Energies and Atomic Energy Comm., France

11:20-11:40 O5.10

Thermodynamic modeling of the CaO-Al2O3-P2O5-H2O system and applications to refractory materials design under H2-H2O conditions

G. Pei, I.-H. Jung
The University of Warwick, United Kingdom

11:40-12:00 O5.11

Development of a thermodynamic database for antimony oxide-containing metallurgical systems

A. Ahmadi Siahboumi, E. Moosavi-Khoonsari
École de technologie supérieure, Canada

Poster Presentations

Monday

Poster Session #1 - June 8, 19:30-21:00, Room 308/309AB

P1.1
Deep Alloy®: A New Frontier in Material Discovery
N. Adrián, Y. Fan, Y. Zhong
Worcester Polytechnic Institute, United States of America

P1.2
Thermodynamic model for sodium and potassium chromates, molybdates, and tungstates involved in high-temperature steel corrosion
S. Benalia, F. Tesfaye, D. Lindberg, L. Hupa, P. Chartrand, C. Robelin
Polytechnique Montréal, Canada

P1.3
Predicting thermal conductivity of graphite cathode blocks for aluminum electrolysis cells: A modeling approach
I. D. Bouzaine, P. Chartrand
Polytechnique Montréal, Canada

P1.4
Thermodynamic properties measurement of CaNdAl3O7 and CaNdAlO4
Y. Ma, S. Li, W. Wei, B. Yan, Z. Cao
University of Science and Technology Beijing, China

P1.5
Liquidus projection of the Cr-Nb-Ta system
V. M. Silveira, J. V. Luiz, K. E. Borowski, C. S. Barros, V. M. Chad, J. C. J. Gigolotti, C. A. Nunes, G. C. Coelho
University of São Paulo, Brazil

P1.6
Thermodynamic Modeling of the NaF-AlF_3-CaF_2-Al_2O_3-FeF_2-FeO-FeF_3-Fe_2O_3 System for Aluminum Production Using Inert Anodes : Experimental Study of the Fe-O-F Sub-System
C. V. da Silva Lima, P. Chartrand, C. Robelin
Polytechnique Montréal, Canada

P1.7
Thermodynamic and Microstructural Analysis of Lead-free Sn–Ag–Cu–Ga–Ni Solders
P. Danišovičová, I. Černičková, L. Ďuriška, R. Čička, T. Peričková
Slovak University Of Technology In Bratislava, Slovakia

P1.8
Integrating Machine Learning for Alloy Exploration
J. Foley, Y. Fan, Y. Zhong
Worcester Polytechnic Institute, United States of America

P1.9
Reconstruction of a Historical Silicon Arc-Furnace Thermodynamic Model Using SimuSage and FactFlow
K. Hack, G. Eriksson, K. Poëti, K. Oishi, J-P. Harvey
RWTH Aachen, Germany

P1.10

Microstructure Prediction of Ni–Cr–Al Alloys for Exhaust Valve Spindles Based on Thermodynamic Calculations

H.-S. Jang, J. G. Kim, Y.-y. Woo, E. Y. Yoon
Korea Institute of Materials Science, Korea (Republic of)

P1.11

Nickel Partitioning in Iron and Its Implications for Terrestrial Planet Cores

T. Kovačević, L.X. Benedict, P. Myint, S. Hamel, B. Buffett, B. Militzer
University of California Berkeley, United States of America

P1.12

Stacking Fault Energy in Fe–Mn Steels: Bridging the Gaps between DFT, Experiments and Thermodynamic Modelling

F. Larsson, Y. Mishchenko, Q. Chen, M. Selleby
KTH Royal Institute of Technology, Sweden

P1.13

Experimental Phase Equilibrium Study and Thermodynamic Optimization of the PbO-Na2O-SiO2 System

X. Ling, H. Abdeyazdan, M. Shevchenko, E. Jak, E. Moosavi-Khoonsari, M. Barati
University of Toronto, Canada

P1.14

Experimental Phase Equilibria and Thermodynamic Modeling of the Si3N4-MgO-SiO2 System

C. Luo, B. Yan, T. Deng
Wuhan University of Technology, China

P1.15

Investigation of Additions on β-AlFeSi and α-Hexagonal Phase Formation

V. Rioux-Frenette, P. Lafaye, K. Oishi, J.-P. Harvey
Polytechnique Montréal, Canada

P1.16

AI-Driven High-Throughput Design and Performance Iterative Optimization of High Entropy Alloy for Additive Manufacturing

Y. Hou, X. Li, Y. Song, Z. Bi
Research Institute of Advanced Materials CISRI (Shenzhen) Co., Ltd., China

P1.17

Integrated CALPHAD–DFT Study of the Al–Si Subsystem for Accurate Modeling of Si-Containing Steels

Y. Mishchenko, F. Larsson, A. Forslund, Q. Chen, M. Selleby
Royal Institute of Technology, Sweden

P1.18

Construction of Theoretical Phase Diagrams using NNP

H. Okabe, T. Suzuki, M. Enoki, H. Ohtani
JX Advanced Metals Corporation, Japan

P1.19

Microstructural modifications of a 6061 aluminum alloy by addition of iron and vanadium

A. Pomerleau, K. Oishi, M. Brochu, J.-P. Harvey
Polytechnique Montréal, Canada

P1.20

CALPHAD-Based Thermodynamic Framework for Disordered and Ordered Early-Stage Phases in Al alloys

E. Povoden-Karadeniz, E. Kozeschnik
Institute of Materials Science and Technology, Austria

P1.21

From Quantum-Informed Descriptors to Additive Manufacturing Process: A Scale-Bridging Workflow for TCP Phase Prediction

S. Rangaswamy, E. Kabliman
University of Bremen, Germany

P1.22

Advances in the experimental determination of the liquidus projection of the Al-Nb-Ta system

C.S. Barros, J.V. Luiz, C.A. Nunes, G.C. Coelho
University of São Paulo, Brazil

P1.23

Homogenization Kinetics of Refractory High-Entropy Alloys Predicted by Multicomponent Diffusion and DICTRA Simulations

B. Tak, D. Li, M. Ahn, W. Xiong
University of Pittsburgh, United States of America

P1.24

Revisit the Ab Initio Lattice Stability of Cr with R2SCAN Exchange Correlation Function

S. Yang, Y. Zhong
Worcester Polytechnic Institute, United States of America

P1.25

Improving Alloy Mechanical Property Prediction by Addressing Data Homogeneity through Noise Augmentation

Y. Zhang, D. Qiao
Xiamen University of Technology, China

P1.26

Thermodynamic modeling of the Ge-Al-Mg and Ag-Al-Mg systems

A. T. Phan and P. Chartrand
Polytechnique Montréal, Canada

P1.27

Thermodynamic Modeling of Titanium-based Ti-Al-Ca-O Liquid Alloy by Modified Quasichemical Model

G. Hils, M.-K. Paek
Clausthal University of Technology, Germany

Tuesday

Poster Session #2 - June 9, 19:30-21:00, Room 308/309AB

P2.1
Unexpected interfacial reactions in Co/GeTe and Ni/GeTe couples
C.-H. Ho, Y. Chen, S.-W. Chen
National Tsing Hua University, Taiwan

P2.2
Experimental Investigation of Phase Equilibria in Ni-Ce-Cr system
S. M. Dikonda, G. K, H. Tripathy, S. C, M. Vaidya
Indian Institute of Technology Hyderabad

P2.3
Diffusivities and atomic mobilities of fcc phase in Co-rich Co–Fe–Ti system: Experimental study and CALPHAD assessment
J. Sun, D. Ye, Z. Du
University of Science and Technology Beijing, China

P2.4
Thermodynamic modelling of battery cathode materials: early-stage results and perspectives
L. Fenocchio, B. Kaplan, R. L. Jurado, H. Mao, R. Naraghi, M. Selleby
Thermo-Calc Software AB, Sweden

P2.5
Thermodynamic modeling of the Hf-Nb-V system
T. G. Oliveira, A. A. A. P. Silva
Federal University of Itajuba, Brazil

P2.6
Study on microstructure and property of novel γ'-strengthened multi-component Co-based superalloys
F. Chen, Z. Du, D. Wei, J. Shi, C. Guo
University of Science and Technology Beijing, China

P2.7
Bayesian Active Learning of Zero-Phase-Fraction Lines
C. Hardcastle, B. Vela, R. Arróyave
Texas A&M University, United States of America

P2.8
A robotic calorimetry laboratory for phase diagrams on demand
K. Huang, J. Willwerth, A. Rauf, S. Tan, W. Sun
University of Michigan Ann Arbor, United States of America

P2.9
Thermodynamic investigations on the enthalpy of mixing of tributyl phosphate with nitric acid and gadolinium nitrate by micro reaction calorimetry
G. J. Rao, T. Prathibha, S. Balakrishnan, N. Ramanathan, C.V.S. B. Rao, R. Ganesan, V. Jayaraman
HOMI BHABHA NATIONAL INSTITUTE, India

P2.10

The top Calphad scientists according to their citation records

G. Kaptay
University of Miskolc, Hungary

P2.11

Assessment of the Thermodynamics and Thermophysical Properties of the Binary Ag-Pd System

Z. Liang, U. R. Kattner
National Institute of Standards and Technology, United States of America

P2.12

The experimental and theoretical study of the In-La-Ni system

A. Kroupa, R. Žižka, B. Smetana, O. Zobač
Institute of Physics of Materials, Czechia

P2.13

Comparison of model of hydrogen permeation through iron plates with analytical solutions & practical assessment

J.R. Leeman, N. Warnken
University of Birmingham, United Kingdom

P2.14

Modeling and experimental study of IMC formation at Sn/Cu interface

T. Peričková, R. Čička, P. Danišovičová, T. Tánczos
Slovak University of Technology in Bratislava, Slovakia

P2.15

Efficient Single-Phase Region Search via Gradient-Informed Gaussian Processes

C. Maguire, C. Kunselman, B. Vela, R. Arroyave
Texas A&M, United States of America

P2.16

Machine Learning–Accelerated Investigation of Phase Stability in TiVCrCoZr High-Entropy Alloys for Hydrogen Storage Applications

M. Palumbo, G. Pollini, E. M. Dematteis
University of Torino, Italy

P2.17

Thermodynamically Driven Microstructural Evolution and Property Regulation in the Process of Al-Mg-Si Alloys

P. Zhou, M. Yang, Y. Liu, Y. Du
Central South University, China

P2.18

Breaking the Charge Neutrality Boundary in Perovskite Using the PyCALPHAD Approach

A. Shenk, E. Cummings, S. J. Krimmel, R. Otis, Y. Zhong
Worcester Polytechnic Institute, United States of America

P2.19

Liquidus projection of the Co-Si-B system in the Co-rich region

E. K. S. Pellegrino, S. B. V. Boas, A. A. A. P. d. Silva, L. M. Ferreira, M. I. S. T. Faria, G. C. Coelho, C. A. Nunes
University of São Paulo, Brazil

P2.20

Topologically Constrained Machine Learning of Phase Diagrams Using Markov Random Fields

J. Teerman, B. Vela, C. Kunselman, R. Arróyave
Texas A&M University, United States of America

P2.21

Phase equilibria and thermodynamic activities for Li-ion battery electrolytes comprised of LiPF6 in ethylene carbonate and LiPF6 in dimethyl carbonate

M. Trabelsi, H. Al-Salih, Y. Abu-Lebdeh, J.Self
Polytechnique Montréal, Canada

P2.22

Phase diagrams and interfacial reactions of Ni-Bi-Sb ternary system

Y.-H. Lin, Y.-C. Tsai, C.-H. Ho, S.-w. Chen
National Tsing Hua University, Taiwan

P2.23

Physically-constrained prediction of the liquidus curve for multicomponent chemistries

J. Willwerth, S. Tan, A. Rauf, W. Sun
University of Michigan, United States of America

P2.24

Illuminating early-stage oxidation of ZrC using Small-Cell DFT MD

P. Wurzner, Q.-J. Hong, Y. Tang
Technische Universiteit Delft, Netherlands

P2.25

Intelligent Design and Development of Ultra-High-Strength Steels for Additive Manufacturing

X. Li, Y. Hou, Z. Bi
Research Institute of Advanced Materials, China

P2.26

Simulating natural gas substitution by hydrogen with process integration in DRI-MIDREX Process using a novel kinetic approach and equilibrium reactors

U. Mahue, C. Rincent, M. Dubé, G. Laforest, É. Bernier, M. Aghabaranejad, J-P. Harvey
Natural Resources Canada, CanmetENERGY in Varennes, Qc, J3X 1P7, Canada

CALPHAD 2026

Oral Presentation Abstracts

53rd International Conference on Computer Coupling of Phase Diagrams and Thermochemistry

June 7–12, 2026

Quebec Convention Centre, Quebec City, Québec, Canada

A Unified Thermodynamic Framework: From Equilibrium and Nonequilibrium to Zentropy, Cross Phenomena, and Artificial Intelligence

Zi-Kui Liu

Pennsylvania State University, Department of Materials Science and Engineering, University Park, PA, 16802, USA

e-mail: prof.zikui.liu@psu.edu

Thermodynamics is traditionally viewed as a theory of equilibrium because Gibbs formulated the combined law strictly for equilibrium systems[1]. This historical limitation motivated the emergence of irreversible thermodynamics as a distinct field. Subsequent advances, Kaufman's introduction of lattice stability enabling quantitative treatment of nonequilibrium phases[2], Hillert's integration of entropy production into the combined law[3], and Ågren's development of the modern theory of atomic mobility[4], collectively extended Gibbs's framework to describe real materials under evolving thermodynamic driving forces.

The present author further refined Hillert's nonequilibrium formalism by introducing partial internal energy[5], partial entropy[6], and partial volume[7] for each component directly into the first, second, and combined laws. This refinement yields an explicit expression for the chemical potential in terms of these partial quantities, resolving subtle interdependencies among entropy, volume, and composition in open systems[7]. Building on this foundation and Ågren's mobility theory, the author developed and later revised the theory of cross phenomena, deriving transport equations from the first law and addressing limitations inherent in phenomenological Onsager formulations[8].

In parallel, the author and collaborators established zentropy theory[9];, which unifies quantum mechanics with Gibbs statistical mechanics to predict entropy and Helmholtz energy from a full ensemble of symmetry-broken configurations. This framework enables quantitative free energy landscapes across stable, metastable, and unstable states. Together, these developments establish a unified thermodynamic framework spanning equilibrium, nonequilibrium, statistical, and quantum descriptions[10], and provide a thermodynamic bridge to modern artificial intelligence architectures exemplified by the zentropy-enhanced neural network (ZENN)[11], yielding physically grounded, interpretable, and predictions with internal containments in terms of structural containment via configuration partitioning and dynamic containment via zentropy-based regulation of driving forces and stability.

Biographical Note

Zi-Kui Liu is a professor in the Materials Science and Engineering department at The Pennsylvania State University.

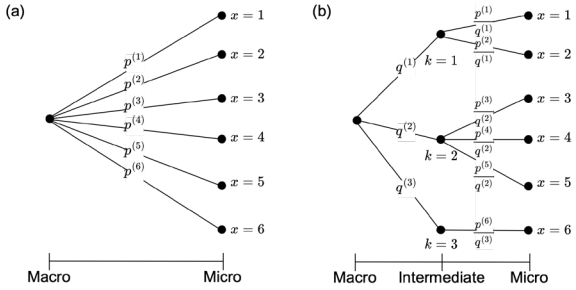


Figure 1: Probability tree diagrams illustrating (a) pure quantum-state configurations and (b) intermediate grouped configurations [12]

References

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Recursive entropy in thermodynamics: establishing the statistical-physics basis of the zentropy approach

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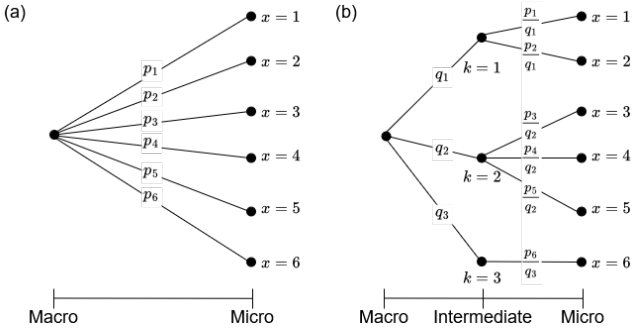
Accurate thermodynamic modeling increasingly draws on atomistic and multiscale inputs to capture finite-temperature disorder, but the underlying microstate space is combinatorially large. This work shows that the equation for entropy used in the zentropy approach, which is an exact multiscale approach to thermodynamics, is a statement of the recursive property of entropy. If configurations k occur with probabilities p_k and retain residual entropy S_k from degrees of freedom not fixed by k, then entropy may be written recursively,

$S = -k_B \sum_k p_k \ln\, p_k + \sum_k p_k\, S_k$,

decomposing the total entropy into configurational and intra-configurational contributions. This provides flexibility to define configurations at the coarse-graining level best suited to the problem. Building on this, we derive the Helmholtz energy and the partition function by maximizing entropy in the recursive form, as used in zentropy. The resulting framework is exact for a chosen level of description and enables principled coarse-graining, thereby reducing computational complexity while preserving thermodynamic consistency. These results position zentropy as a rigorous bridge between microscopic and macroscopic behavior, facilitating quantitative predictions and the study of emergent phenomena.

Figure 1. Probability tree diagrams illustrating the recursive property of entropy



$$S = -k_B \sum_x p_x \ln p_x$$

$$S = -k_B \sum_k p_k \ln p_k + \sum_k p_k S_k$$

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Biographical Note

Luke Myers is a third-year PhD student in Materials Science and Engineering at The Pennsylvania State University, advised by Prof. Zi-Kui Liu. His research uses thermodynamics, density functional theory, and machine learning for high-throughput materials discovery.

Thermodynamic Entropy as Information
A compression-based demonstration of the Shannon—Boltzmann equivalence in condensed matter

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Key words: entropy, thermodynamics, density functional theory, information theory

Entropy is the fundamental quantity linking information, disorder, and energy, yet its physical and informational interpretations have remained largely separate. While entropy connects the microscopic world of atomic configurations to the macroscopic laws of thermodynamics, its evaluation in real materials remains both computationally demanding and conceptually opaque. Traditional approaches decompose the total entropy into vibrational, configurational, electronic, and magnetic parts through coarse-graining, each requiring distinct models, approximations, and sampling schemes [1, 2].

Here we take a fundamentally different route: We demonstrate that Shannon's information entropy and the thermodynamic entropy of Boltzmann and Gibbs are quantitatively equivalent for real condensed-matter systems. By interpreting atomic configurations as information sources, we compute entropy directly from the compressibility of molecular-dynamics trajectories, without physical partitioning or empirical modeling. A custom lossy-compression algorithm measures the minimum number of bits required to describe a microstate at finite precision, and this bit count maps exactly to thermodynamic entropy through the Shannon–Boltzmann relation.

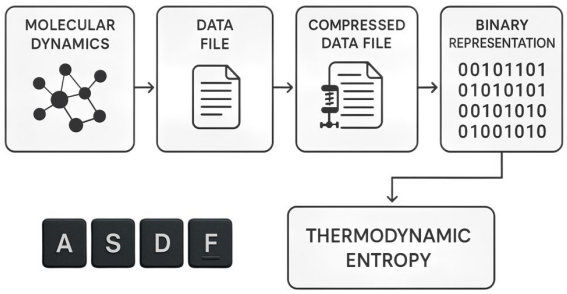

Figure 1. Overview of the *asdf* framework

The method as outlined in Figure 1 can be applied to any material system in any phase, establishing information as the fundamental quantity underlying thermodynamic disorder. This equivalence unifies information theory and statistical mechanics, providing a parameter-free, model-independent, generalized, and computationally efficient framework for determining entropies and free energies directly from atomic data.

Applied to metals, semiconductors, and refractory ceramics in both solid and liquid phases, this compression-based framework reproduces benchmark entropies from the SLUSCHI/mds [3] method and demonstrates that thermodynamic entropy is information, as seen in Figure 2.

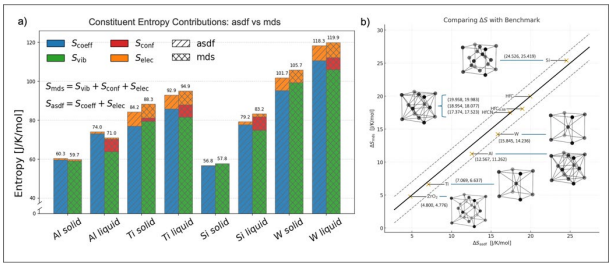

Figure 2. Comparing the accuracy of entropy, absolute (a) and ΔS (b), between benchmark *mds* and *asdf* for a wide range of materials

The diverse array of applications for *asdf* can be explored effortlessly now that *asdf* is deployed online. Integrating with the golden standard MD package SLUSCHI [3], *asdf* can compute the entropy for any vasp-generated MD trajectory here: https://faculty.engineering.asu.edu/hong/sluschi-api/

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Biographical Note

Dallin Fisher is a Ph.D. student and research assistant of Materials Science and Engineering at Arizona State University. Fisher received his Masters in MSE at ASU in 2024, and has researched computational material science since 2017, including at the Idaho National Laboratory and presenting research at CALPHAD (2025) and TMS.

CALPHAD Coupled Integrated Computational Materials Engineering (ICME) Framework for Microstructure Evolution and Property Optimization

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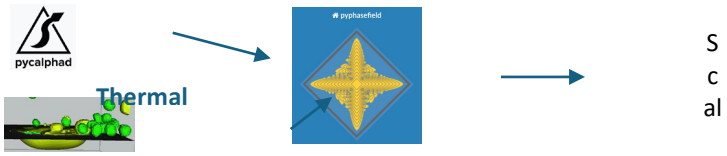
Multiscale integrated computational materials engineering (ICME) frameworks, coupled to CALPHAD, are essential in order to understand process-structure-property links to design novel materials with enhanced properties. Changes in processing condition and material lead to the development of different microstructures with different properties. In this work, CALPHAD databases are developed for the refractory high entropy alloy (HEA) Mo-Nb-Ta-V-W and Nb-Ti phase space. These databases are incorporated into an ICME framework (Figure 1) consisting of thermodynamic modeling (alloy specific information), computational fluid dynamics (thermal profiles) and phase field simulation to predict microstructure formation under additive manufacturing and cold hearth melting. The resulting microstructures can be used to optimize for mechanical properties and morphological uniformity.

The subset of HEAs consisting of refractory metals, including the Senkov alloy (MoNbTaVW), are known to have enhanced mechanical properties at elevated temperatures, important for applications in energy and aerospace. Additive manufacturing is a processing technique where part geometry can be easily tuned, leading to manufactured parts that are higher in strength and lighter, ideal for high temperature applications, without sacrificing performance. Microstructure formation is predicted, using the CALPHAD informed ICME framework, for MoNbTaVW as well as the subset of equiatomic binaries including W when processed under two additive manufacturing methods, selective laser melting (SLM) and directed energy deposition (DED). Analytic or machine learning based models can be used to assess yield strength [1] and ductility across the microstructure and the degree of tensile strength can be estimated from characterizing length scales in the dendritic morphology [2]. These predictions can be used to optimize the yield strength – ductility tradeoff, especially important for W-based materials that are known to have poor printability.

Electron beam cold hearth melting (EBCHM) is a manufacturing technique that produces high-purity ingots and is commonly used in titanium alloy production. A common issue with this technique is compositional uniformity in the ingots. It is unclear how processing parameters, such as electron beam intensity and crucible scan patterns impact spatial homogeneity. Using the CALPHAD informed ICME framework, the microstructure evolution of Nb-Ti under different processing conditions is explored. Morphological uniformity is assessed through prediction of critical length scales and calculation of the interfacial shape distribution, a map of the interface shapes as a function of principal curvatures. Insights into parameter optimization to achieve uniformity are presented. Prepared by LLNL under Contract DE-AC52-07NA27344.

Figure 1. Schematic of CALPHAD coupled ICME framework



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Biographical Note

Kate Elder is a Computational Materials Scientist at Lawrence Livermore National Laboratory and recently was a Fulbright Scholar at VTT Technical Research Centre of Finland. She holds a Ph.D. in Materials Science and Engineering from Northwestern University and B.Sc. and M.Sc. degrees in Physics from McGill University.

High-throughput calculation of eutectic compositions

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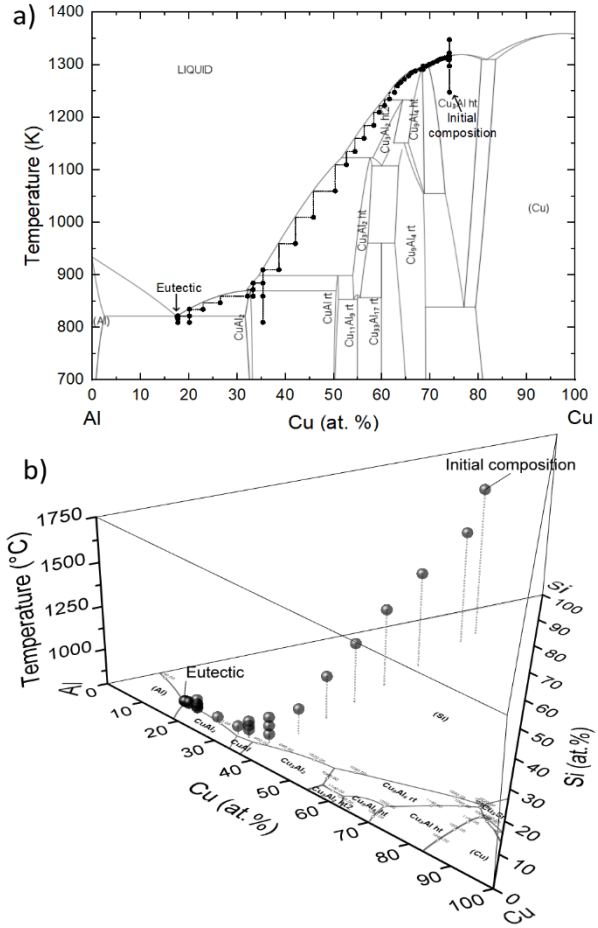
Eutectic alloys constitute an important class of materials, widely used as engineering materials and studied for new applications. Their fine microstructure, which combines the properties of different phases, can result in excellent mechanical performance [1], as aimed in the study of eutectic high-entropy alloys. In addition, their isothermal melting point, which is lower than that of the constituent solid phases, makes them attractive candidates for phase-change materials, casting alloys, solders, brazing alloys, and, when sufficiently deep, metallic glasses.

Figure 1. Method for calculating eutectic compositions with TC-Python® illustrated for a) Al-Cu and b) Al-Cu-Si, calculated using TCAL9. Each point indicates the sequence of single equilibria calculations



From a thermodynamic perspective, eutectic transformations occur at invariant points of the phase diagram. However, multiple phases can also solidify simultaneously at non-invariant isothermal melting points, forming eutectic-like microstructures. The CALPHAD approach is a powerful tool for identifying such alloys. Nevertheless, no study has yet been made for large-scale acquisition of eutectic compositions, due to the complexity of the calculation of high order systems (quaternary and higher) [2].

In this work, five commercial thermodynamic databases were screened in order to identify eutectic alloys and other isothermal melting compositions. Different computational strategies were suggested for the determination of eutectics, and a final approach was implemented for high-throughput screening. This TC-Python®-based method relies simply on single-equilibria calculations, with optimized temperature stepping, as illustrated in Figure 1. Considering 51 elements, more than 2500 eutectic compositions, over 900 congruent melting compositions, and more than 800 “non-invariant” eutectic compositions were identified in binary, ternary, quaternary, and quinary systems. Analysis of these results provides valuable insights into this important class of alloys.

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Biographical Note

Karoline is a Materials Science PhD student at ICMPE-CNRS, under supervision of Dr. J.-M. Joubert. She has a degree in Materials Engineering from the University of Sao Paulo, where she also pursued her Master’s degree in the same field, advised by Prof. G. C. Coelho and Prof. N. Chaia. She has experience with the CALPHAD method, experimental determination of phase diagrams and kinetics of alloys.

The Calfateria

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Constituting a multicomponent Calphad database is merging many published basic descriptions. This is the usual idea. Expert database managers will largely disagree on it as this view point will strongly underestimates the amount of work to setup a database of quality. Anyhow no one will disagree on the point that it is a very important part of the work.

The choice of a set of descriptions for the elements is obviously key but there is not always many options. When it comes to binary systems, many have been described many time and hopefully published. The limitations of a binary description will often appear only at the level of a ternary system. Thinking that excess ternary terms will fix all the problems is often a bad idea. Having the possibility to test other binary existing descriptions rather than just developing a new one that could just fall in the same pitfalls than some previous ones is a way to rationalize the work and save time.

Passing from an article with tables to a usable format can also require quite some time and even may be impossible in case of misprint. Expert database managers have many files ready to use available on their computers or they know who they could ask for a system they have never handled. It is of course not the case of everyone.

Imagine a place where all available binary descriptions would be accessible in a usable format. B. Hallstedt [1] published such a set. These files moreover often contain valuable comments related to the limitations of the descriptions or the differences between the different versions. Handling each of them and running comparisons can be quite tedious in some cases. Moreover the ability to compare to experimental data also demands extra work. Imagine that many of these tasks have been automated and their results are made available through a web site that will constitute **the Calfateria repository**.

The goal is to provide on line access to data related with open Calphad databases, in a first step largely based on the set recently released by B. Hallstedt [1]. Not only thermodynamic descriptions (TDB, DAT) will be made available but also experimental or theoretical data and command files allowing to produce figures comparing data and calculations. Currently mostly exp, TDB, TCM and OCM files are available. However, other format will also be considered when available, in particular, the XTDB format recently introduced [2]. More formats will be considered if such contributions are provided. For each description figures and the files used to produced them will be easily reachable. Calculated phase diagram, enthalpy and activity curves will be shown and compared with experimental data when included. The source of each file will clearly be available.

Including experimental data in this repository will save the time spent duplicating the extraction of data from figures or tables. Care will be taken to show data points corresponding to experiments rather than lines or formula resulting from their post-processing. Existing compilations reporting experimental phase diagram data without this possibility make difficult for their users to assess their uncertainty in the different area. If repositories do exist for experimental data, one for rough phase diagram data is missing.

Together with descriptions as well as rough data, critical point of view of human experts on the available descriptions and data will also be made available. This repository should become a tool of interest for database managers when extending or revising an existing database or when setting up new databases.

It is also expected that the availability of all these data will give the opportunity for the Calphad end users to understand the possible uncertainty of calculations in some area and thus to become more educated costumers of commercial databases

It is finally but not of least interest hoped that it will give to some people the wish to run experiments where they are missing or where unresolved disagreement remain.

Many people in the Calphad community have files in their computers that they wish to share. This repository will be the way to make it easily keeping the trace of the data, experimental or calculated. The repository will be hosted in a few mirror sites in order to try to avoid the possible disruption of the site availability.

The Calfateria is a cafeteria for Calphad people. They can come and just get what they need for their one use. It is also a place to interact strongly like in the coffee breaks so important for our community. The project will partly be based on donation. The speed of its developing and the priority of some systems will depend on the interest it will be able to attract. Waiting forward discussing with you !

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Development of Thermodynamic Databases Coupled to Alloy Design of Metallic Materials

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An accurate thermodynamic database is needed for successful computational alloy design, and it is often necessary to adapt the database. To be able to do this, databases in an open format are needed. A few such open databases are presented in this work, together with the strategies used for the development.

Development of thermodynamic databases in the 1980s and 1990s was mostly performed in open environments and collaborative projects, and mainly by academic researchers. The thermodynamic assessments were often discussed in groups, sometimes in the CALPHAD meetings, before finalizing them. These discussions made it possible to take different aspects and applications into account, and many of the assessments from these years are still used.

As CALPHAD progressed it has become clear how successful computational thermodynamics is as a tool for alloy design. Since alloy design usually requires a dedicated thermodynamic database, parallel database developments are ongoing. The dedicated databases are sometimes only minor adjustments to the original database, but in some cases application to a multicomponent alloy can give valuable basic information to be fed into the database.

Good descriptions for a specific application can be lost when new data is added; and the database is corrupted. This is a transparency issue and can cause problems for a user. With modern methods for data analysis this could be rapidly checked and repaired. However, most of the necessary information is not openly available: for example, experimental data, the thoughts of the assessor, optimization files, and the actual thermodynamic parameters.

Open format databases for specific applications, listed below, will be presented.

- High Nitrogen Steels
  - Simultaneous optimization of lower order systems [1]
- Hardmetals or Cemented Carbides [2]
  - Doping with Cr for grain refinement
  - C-windows for different compositions
- Development of a novel aluminium alloy for laser powder bed fusion
  - Database adjustment
- Database for Microalloyed Steel [3]
  - Carbonitride stabilities
- Oxide Reduction on Sintered Steel
  - Tailored experiments to validate the composition of the oxides, see Figure 1 [4]

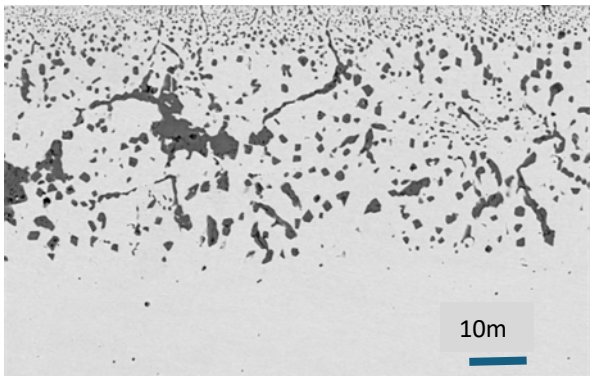

Figure 1. Internal oxidation of a Fe-6Cr-3Mn-0.1Si alloy at 900°C. The parameters for the experiment were determined by calculations. The main oxide (grey) is the spinel, and the smaller black oxides are Si-rich

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Biographical Note

Karin Frisk is PhD and Docent in Materials Science from KTH. She has long experience in database and alloy development of metallic materials. She is currently developing solutions for computational alloy development in Innomat AB.

Model Development and Design of High Strength, High Toughness Naval Steels: 10Ni-150

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The development of high-strength, high-toughness steels for structural applications has been a long-established endeavor in the field. Using these steels for naval applications, however, also introduce other performance indicators such as weldability and processability. To meet these demands, a carbide-strengthened martensitic steel is designed to contain Ni-enriched islands to optimize for transformation-induced plasticity (TRIP). Integrated Materials Design (ICMD) methods are applied to validate, calibrate and develop models that predict final microstructure, including martensitic start temperatures, precipitation strengthening capacity, austenite fractions and stability, as well as the processing parameters necessary to achieve the final material.

Validation and calibration has been executed through a series of high-resolution material characterization, including x-ray synchrotron and atom-probe tomography that confirm design feasibility. Mechanical tests further support the benefits of the design methodology by providing evidence of increased material toughness with limited strength trade-off.

In all, the 10Ni steel project exemplifies a success of material design with ICMD methodology in application- and real-material focused approach.

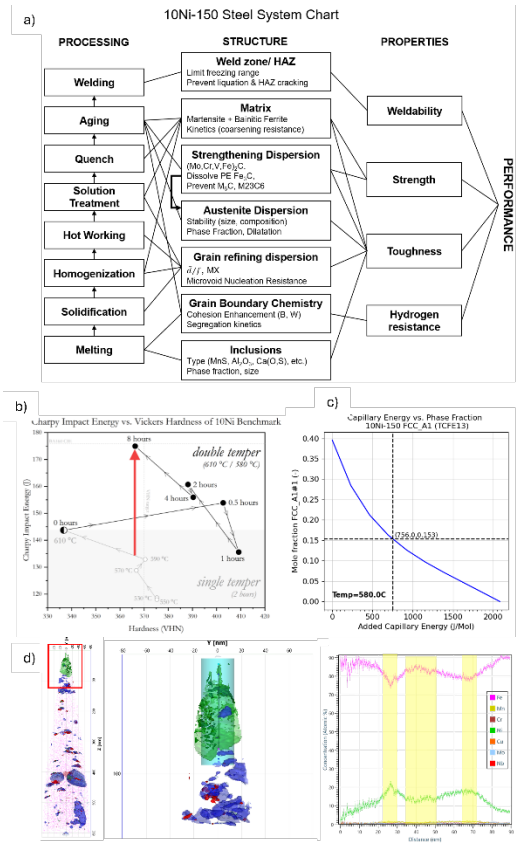

Figure 1. a) 10Ni-150 Steel Systems Chart, b) Hardness (VHN) vs. Charpy Impact Energy (J) of single- and double-tempered samples, c) Austenite Stability Parameter offset calibrated from the prototype alloy, d) atom-probe tomography of double-tempered sample with a captured austenite island

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Biographical Note

You Na Lee is a PhD candidate at the Massachusetts Institute of Technology, currently investigating the alloy design and micro-mechanics of naval hull steels under Professor C. Cem Tasan and Professor G. B. Olson. She got her Bachelor's in Material Science and Engineering from Korea University, South Korea.

CALPHAD-assisted design of high-performance titanium alloys and refractory materials for melting

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Titanium alloys have been widely applied in various fields such as aerospace, automobiles, shipbuilding and biomedical due to their high specific strength, resistance to high and low temperatures, corrosion resistance and biocompatibility. However, the high application cost of titanium alloys severely restricts their large-scale application. The cost of titanium alloy components can be divided into three parts: the cost of raw materials, the cost of melting, and the cost of processing.

Phase diagram thermodynamics plays a crucial role in material design and development. The CALPHAD method can be used for thermodynamic evaluation of multiphase materials. This study established a thermodynamic database for the Ti-Al-Fe-Cr-Mn system containing inexpensive alloying elements, which is used for the design of low-cost titanium alloys. For instance, the near-alpha titanium alloy Ti-6Al-4.5Cr-1.5Mn has an ultimate tensile strength of 1091.2 MPa and an elongation rate of 8.3%; the alpha plus beta titanium alloy Ti-3Al-8.5Cr-2Fe has an ultimate tensile strength of 985.9 MPa and an elongation rate of 19.6%.

A thermodynamic database for the BaO-ZrO_2-CaO-TiO_2-Y_2O_3 system was established, which is used to design special refractory materials required for the low-cost and efficient vacuum induction melting of titanium alloys. For instance, $BaZrO_3$, (Ba, Ca)ZrO_3, and $BaZrO_3$-Y_2O_3 dual-phase crucibles have all demonstrated excellent performance when used for melting alloys such as TiAl, TiFe, and TiNi.

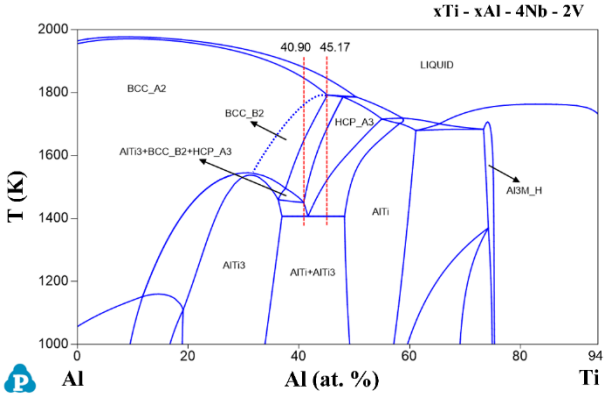

Figure 1. The pseudo-binary phase diagram of Ti-Al-Nb-V system

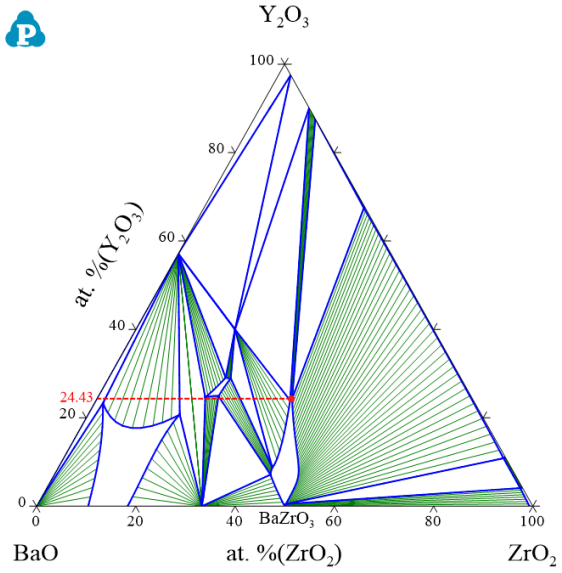

Figure 2. The calculated isothermal section of BaO-ZrO_2-Y_2O_3 system at 1750 ℃

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Biographical Note

My name is Haoyuan Zhu, a postgraduate student at Shanghai University, China. My research interests are the thermodynamic evaluation of Ti-based multi-element systems and design of high-performance titanium alloys. My tutor is Prof. Chonghe Li.

Constrained Target Function for Alloy Design

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The rapid development of advanced alloys increasingly relies on computational thermodynamics and kinetics to navigate complex, multi-dimensional composition–temperature spaces. CALPHAD-based simulation tools have become indispensable in accelerating alloy design by enabling predictive phase stability, microstructure evolution, and property evaluation prior to experimental validation.

Traditionally, high-throughput calculations (HTCs) have been employed to explore predefined compositional and temperature ranges. In this forward-screening approach, a large volume of simulations is generated, followed by post-processing and data analysis to identify alloy candidates that satisfy desired phase or property criteria. While effective, this brute-force methodology is computationally intensive and time-consuming, particularly for multicomponent alloy systems since the number of search points increases exponentially with the number of alloy components.

To address this limitation, we have developed a constrained target function within the Pandat software framework. Instead of performing exhaustive forward calculations, this new approach allows users to directly define:

- Compositional search space
- Temperature range
- Target property criteria

The constrained target function then intelligently identifies and outputs the compositions and temperatures that satisfy the specified targets. This inverse-design strategy transforms alloy development from passive screening to global, target-oriented optimization.

As a case study, we present an application of this approach to the development of secondary aluminum alloys, where the suppression of detrimental Fe-related intermetallic phases and stabilization of favorable phases are critical challenges. The constrained target function efficiently maps the compositional boundaries between phase-present and phase-free regions, significantly reducing computational cost while improving design precision.

Biographical Note

Dr. Shuanglin Chen graduated from the University of Wisconsin-Madison and joined CompuTherm in 1996. He is the lead developer of Pandat software and currently serves as Vice President of CompuTherm. Dr. Chen is a Fellow of ASM International.

Revisiting the Fe–Mo System: Structural Investigation and Thermodynamic Modeling of Frank-Kasper Phases

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The Fe–Mo system is of great industrial importance, particularly due to its role in the development of high-strength steels and superalloys. Although it has been extensively studied over the last century, significant discrepancies persist in the literature regarding its phase diagram and the stability ranges of its intermetallic phases. Previous Calphad assessments [1,2] reflected these contradictions, often leading to inconsistent sublattice models for the complex phases.

This work aims to solve these inconsistencies by investigating the atomic order of the Frank-Kasper phases to establish structural-based thermodynamic models. The μ y σ phases were characterized using laboratory X-ray diffraction (XRD). Given its highly complex crystal structure, the R phase was investigated using synchrotron radiation, allowing for a precise determination of site occupancies. Furthermore, the phase boundaries were validated through complementary techniques, as differential thermal analysis (DTA) and the characterization of equilibrated alloys by XRD and scanning electron microscopy (SEM/EDS).

The experimental study was complemented by a theoretical approach. Density functional theory (DFT) calculations were carried out to determine the ground-state of the Frank-Kasper phases in order to determine the energy of the end-members of the thermodynamic model.

A new thermodynamic assessment of the Fe–Mo system was performed based in the Calphad method (Figure 1). The selection of sublattice models was related to the site occupancy data obtained in this study, supplemented by data compiled from the literature [3,4]. The selection of sublattice models compatible with related isostructural phases enables their implementation into larger multi-component databases, ensuring both structural and model consistency.

The integration of site occupancy constraints led to a more robust and self-consistent description of the Frank-Kasper phases. The updated model successfully resolves previous contradictions in the Fe–Mo phase diagram, providing a reliable foundation for the development of multicomponent databases.

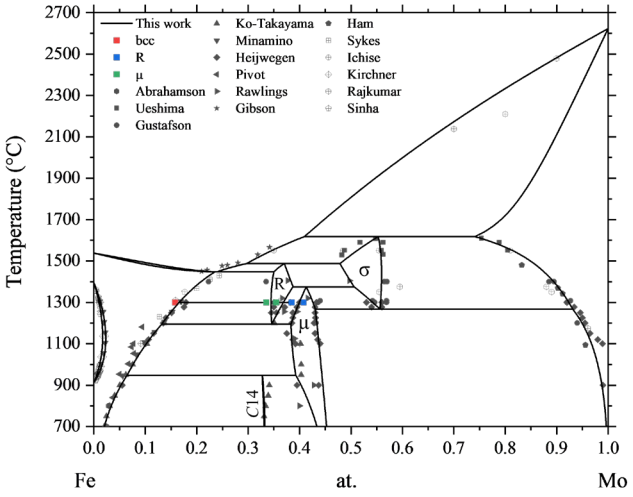

Figure 1. Thermodynamic assessment of the Fe–Mo system

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Biographical Note

Agustin Flores is a researcher at CEA Paris-Saclay, France. He obtained his Ph.D. in 2024, by the study and development of a thermodynamic database for Cobalt-free wear-resistant coatings. His current research focuses on the experimental measurement of thermodynamic properties and phase diagram determination, as well as its modeling by the Calphad method.

Optimization and Uncertainty Quantification of CALPHAD Model Parameters via the No-U-Turn Sampler

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Bo Jansson's implementation of gradient-free weighted nonlinear least squares in Themo-Calc's PARROT optimization module in 1984 marked one of the first software packages for algorithmic CALPHAD model parameter fitting. At this time, Jansson postulated that because any model predictions requiring equilibrium calculations are implicit functions of the model parameters, only derivative-free methods could be leveraged to fit CALPHAD models. Other developers of thermodynamic assessment packages followed suit, and to this day, gradient-free weighted nonlinear least squares is the most common method employed in CALPHAD optimization packages.

Optimization through this traditional approach generally requires significant manual intervention, to include dropping and re-adding data, fixing and unfixing parameters, and re-scaling parameters throughout the optimization process. To make the optimization process more automatic and transparent, thermodynamic assessment modules ESPEI and FactSage's CALPHAD Optimizer implemented black-box methods designed to solve the global optimization problem without the need for significant user intervention. However, while these packages certainly make solving the global CALPHAD model parameter optimization problem more automatic/approachable for non-experts and MCMC can provide organic uncertainty quantification (UQ) capability, as a result of their black-box nature, they unfortunately tend to exacerbate the problem of computational expense and scale poorly with increasing dimension.

Desiring an approach requiring little manual intervention which scaled more reasonably to high-dimensional problems, the current authors developed a generalized framework for gradient-based CALPHAD optimization utilizing Jansson derivatives with respect to model parameters within ESPEI [1]. When compared to Bayesian ensemble MCMC, a simple gradient-based routine could find a solution of comparable or superior optimality with a computational efficiency improvement as high as three orders of magnitude. Additionally, all parameters could be optimized simultaneously and an initial parameter scaling was the only required manual intervention.

However, similar to the traditional least squares approach, local gradient-based methods are not designed to solve the global optimization problem and they can struggle with non-smooth objective functions. Furthermore, since they are deterministic routines, they do not provide inherent UQ capability. The No-U-Turn Sampler (NUTS), an MCMC sampler with a gradient-informed Markov transition based on Hamiltonian dynamics and automated hyperparameter tuning procedures, could address the shortcomings of local deterministic routines while leveraging the computational efficiency advantages afforded by gradient knowledge. While NUTS is not inherently a global optimizer, it can provide an efficient mechanism for parameter space exploration which can be combined with a local deterministic routine to search for optimal solutions.

In this work, we combine the global exploration capability afforded by the gradient-informed sampler NUTS with local deterministic gradient-informed mode-finding refinement to efficiently optimize and quantify the uncertainty of parameters in the Cr-Fe binary and Cr-Fe-Ni ternary systems. Once quantified, we then propagate this uncertainty to thermodynamic observables through a first-order local expansion technique. We find that NUTS can discover solutions of similar optimality fifty times more efficiently than ensemble MCMC and demonstrate that our approach can be used to solve the global optimization problem for ternary models – the fundamental building blocks of multicomponent databases -- with minimal manual intervention. Prepared by LLNL under Contract DE-AC52-07NA27344.

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Biographical Note

Courtney Kunselman is currently pursuing a PhD in Materials Science and Engineering at Texas A&M University as a SECAF STEM PhD Fellow. Her previous degrees include a Bachelor's in Applied Mathematics from the United States Air Force Academy and a Master's in Materials Science and Engineering from Texas A&M University.

Efficient CALPHAD coupling of quasi-equilibrium thermodynamics using a hash-table-based extrapolation scheme

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The integration of CALPHAD thermodynamic models into phase-field simulations can be a computational bottleneck due to repeated Gibbs energy minimisations at each timestep and cell. As the number of components and phases increases, calculations performed using either in-house solvers [1] or through external software like Thermo-Calc [2] become computationally expensive. Precomputing and storing the data in look up tables is generally impractical as the number of variables also increases – requiring unrealistic computational storage.

To address this challenge, we focus on the interface between the simulation framework and thermodynamic calculations. Existing approaches either perform Gibbs energy minimisation directly during runtime, limiting computational efficiency, or employ numerical strategies such as extrapolation [3] or interpolation [4] to approximate equilibrium states, often at the cost of additional memory usage, computational overhead or reduced accuracy.

In this work, we propose a computational architecture that couples a high-performance hash table data structure with the thermodynamic extrapolation scheme of Eiken et al. [3]. A condition vector, composed of bulk compositions and phase fractions, is discretised through a chosen rounding precision (decimal places of mole fractions). Upon a thermodynamic query, the solver firstly checks the hash table for a previously calculated quasi-equilibrium state for that input vector. If successful, the thermodynamic values and phase compositions are obtained via extrapolating from the retrieved reference state, using the reference composition and driving force values [3].

The method was implemented in a multiphase-field CALPHAD framework. We compared four thermodynamic coupling schemes: a baseline run (quasi-equilibrium calculation at each timestep), hash table with 4.d.p. precision, thermodynamic extrapolation [3] and a combined hash-table extrapolation scheme. Benchmarking involved 10,000 timesteps on a 100x2 planar interface in a binary system consisting of two phases, where both phases are modelled using a two sublattice formalism. Fig. 1 shows performance measured as speed-up relative to the baseline, with accuracy assessed using the mean ΔG error and mean and maximum phase-composition errors.

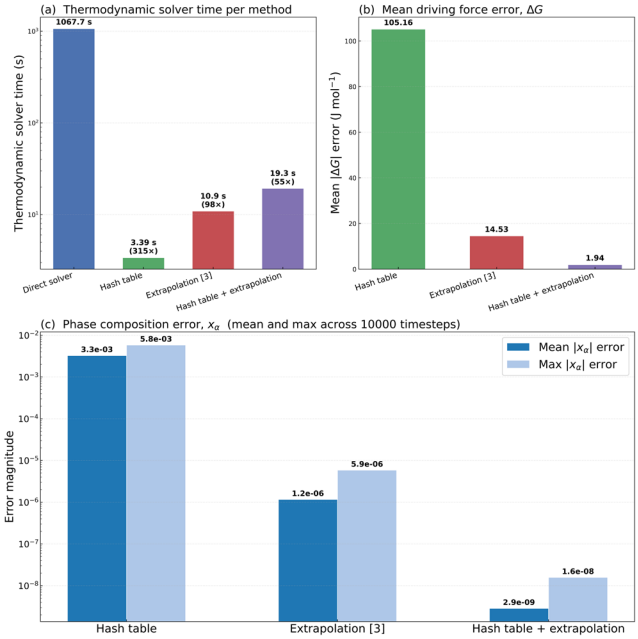

Figure 1. Comparison across all methods over 10,000 timesteps of: (a) the thermodynamic solver time, (b) the mean driving force error, (c) the mean and max phase composition error

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Biographical Note

Harry Craven is a 3rd Year PhD student studying under Dr Nils Warnken. His research focuses on computational approaches to diffusion, thermodynamics, phase-field methodology and corrosion.

Calphad assessment strategy and unexpected liquid miscibility gaps

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Usual Calphad strategy:

After choosing proper models for each phase the usual assessment strategy of interaction parameters is simplified if thermodynamic data for the liquid phase are available, such as the enthalpy of mixing. With $\Delta_{mix}H$(liquid) already fixed the excess entropy, $\Delta_{mix}S^E$(liquid), may be subsequentially described using the liquid+solid phase equilibrium data. The ambiguity that different combinations of $\Delta_{mix}H$(liquid) with $\Delta_{mix}S^E$(liquid) may result in essentially same phase equilibria is thus reduced. However, in the case of an unexpected liquid miscibility gap, especially in ternary systems, this approach may fail.

Example Sn-Bi-Cu system:

The liquid phase is completely miscible in all three binary edge systems of ternary Sn-Bi-Cu alloys. Therefore, ternary liquid demixing was not expected in the meticulous experimental study of $\Delta_{mix}H$(liquid) at 800°C along nine ternary composition sections by Flandorfer et al. [1]. In these drop-calorimetry experiments, where pure Cu is repeatedly dropped into a molten binary Bi-Sn alloy, there is no way to detect this unexpected effect because the microstructure of solidified samples was not studied. The ternary Redlich-Kister parameters, $L^{i,Flan}_{Bi,Cu,Sn}$, derived by fitting to just their ternary $\Delta_{mix}H$(liquid) data in kJ/mol are reported as follows [1]:

+5.808 (i=0), -67.614 (i=1), +51.555 (i=2) Eq. 1

Experimentally supported Sn-Bi-Cu liquidus projection:

The ternary liquidus projection was determined in recent and extensive experimental work by the present authors [2]. A large ternary miscibility gap was found, shown in the calculated projection from that work in Fig. 1. The present ternary Redlich-Kister parameters $L^{i}_{Bi,Cu,Sn}$ obtained from just these experimental phase equilibria are given in Eq. 2 in kJ/mol:

+52.0 (i=0), +84.0 (i=1), -52.0 (i=2) Eq. 2

The ternary $\Delta_{mix}H$(liquid) data are shown in Fig. 2 along the Bi/Sn = 9:1 section, also discussed in more detail in ref. [1]. It is stunning that both the calculations in the present work and the one from ref. [1] compare similarly well to the experimental data. Note that with the parameters from [1] the ternary miscibility gap is suppressed.

The intricacy behind this result will be explained in more detail in this presentation. The experimental activity data of Sn will also be addressed.

Figure 1. Liquidus projection of the Sn-Bi-Cu ternary system calculated with the present dataset

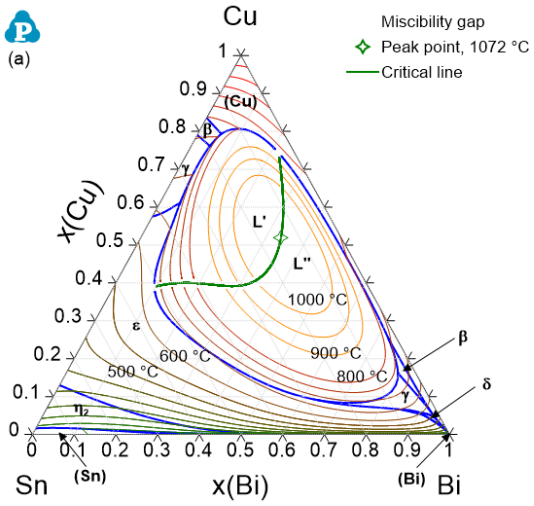
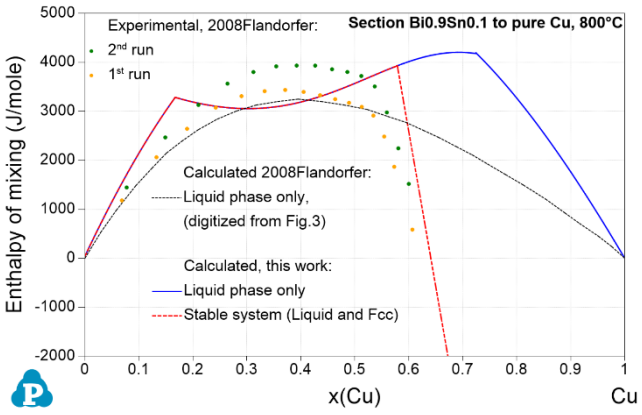


Figure 2. $\Delta_{mix}H$(liquid) at 800°C along section Bi/Sn = 9:1 compared with the experimental and calculated data



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Biographical Note

Rainer Schmid-Fetzer is professor emeritus. With background in metallurgy and physics he earned merits in thermodynamics, solidification, interface reactions and applications to alloy design. He is Fellow of ASM, awardee of both the Hume-Rothery Prize, IOM3, and William Hume-Rothery Award, TMS, and the Calphad Gibbs Triangle.

Comparison of different model equations for size- and shape-dependent integral and partial molar Gibbs energies of nano-phases to screen out the incorrect ones

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Equations for the integral molar Gibbs energy of nano-phases and the partial molar Gibbs energy of components dissolved in nano-phases have been derived here by extending the classical thermodynamics of Gibbs to nano-sizes in three different ways, found in the literature: according to Kelvin, the nano-effect is proportional to the curvature of the phase; according to Searcy (and later to Lee and Sim and recently to Wong and Wong), the nano-effect is proportional to dA/dV (where A and V are the surface area and the volume of the nano-phase respectively); according to the previous papers of the present author (and recently to Xue) the nano-effect is proportional to the specific surface area of the nano-phase defined as A/V. It has been shown in many experiments that for all possible shapes of all nano-phases their molar Gibbs energies are inversely proportional to their characteristic sizes, such as to the radius of a nano-sphere, to the side length of a nano-cube or to the thickness of a thin film. It is shown that the approaches due to Kelvin (curvature) and Searcy (dA/dV) lead to some controversial results vs experimental evidence, so they are excluded here. Moreover, they both contradict the nucleation theory of Gibbs, providing the same equations for the equilibrium size of a spherical nano-phase and for the critical size of the spherical nucleus, being the second reason to exclude these equations. Moreover, the model by Searcy contradicts the nucleation theory of Gibbs, providing the same equation for the equilibrium size of a cubic nano-phase and for the critical size of the cubic nucleus, being the third reason to exclude this equation. Moreover, the model by Searcy supposes that the surface area of a nano-phase and the amount of matter in it are proportional quantities, while they are independent state variables according to the thermodynamics of Gibbs. The surface area and the amount of matter in a phase are independent when the shape of the phase is changed or when the phase is divided into smaller pieces. It is also shown that the previous approach by the author (A/V) is free of such contradictions, so it is suggested for further use here. This approach will also be extended to the question of electrochemical synthesis diagrams.

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Biographical Note

George Kaptay was born in Hungary. He got his Master in metallurgical engineering from the Leningrad Polytechnic in 1984. He got his PhD from the same university in 1988. Since then his main affiliation is the University of Miskolc, Hungary. He was a founding director of BAY-NANO research institute of nanotechnology in 2006, and as a part-time senior researcher he is still with the BAY ZOLTAN Foundation for Applied Research, Hungary. His major interest is thermodynamics of bulk and interfaces of materials including nano-materials, electrochemical synthesis and modelling thermophysical phenomena. He published more than 200 papers and got more than 5,500 independent citations.

A Modified Scheil Approach for Nucleation-Dependent Solidification Pathways

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Microstructural control of near-eutectic alloys is of great importance for designing properties of cast alloys. Notably, the primary intermetallic phases need to be carefully controlled to achieve desired mechanical properties [1]. For alloys involving multiple components and phases, as-solidified microstructures are often predicted by Scheil-Gulliver solidification models. However, experimentally observed microstructures frequently diverge from these predictions especially at high cooling rates. Commonly observed experimental phenomena include the metastable-phase formation [2] and the primary-phase formation in eutectic regions generally described by a coupled zone [3].

Such deviations of as-solidified microstructures are caused by cooling-rate-dependent solidification pathways, a factor not captured by the Scheil-Gulliver model or variations thereof. Here, we present a model that incorporate the critical nucleation undercooling for each solid phase into the Scheil-Gulliver model.

We hypothesize that the non-equilibrium microstructure formation is primarily governed by a nucleation-competition mechanism. In contrast to growth competition, the nucleation-competition mechanism assumes that phase selection is dominated by the interfacial energetics associated with each solid phase, resulting in a distinct critical nucleation undercooling. The key advantage of the nucleation-competition mechanism is the compatibility with the Scheil-Gulliver approach for predicting solidification pathways and as-solidified microstructural constituents. Furthermore, the resulting model accounts for both stable/metastable phase selection and primary-phase formation within eutectic regions driven by asymmetric nucleation barriers.

In this presentation, we introduce the underlying principles and algorithm of the nucleation-implemented Scheil (NucleoScheil) model. The validity of model will be discussed against a hypereutectic Al-Fe alloy, where it successfully reproduces the experimentally observed microstructural constituents, revealing the key dependencies of solidification microstructure on nucleation kinetics (**Figure 1**). Furthermore, we demonstrate the direct applicability of the model to multicomponent systems using a hypereutectic Al-Fe-Si ternary alloy, which successfully predicts divorced eutectic microstructures and corresponding oscillatory solidification pathways along univariant lines.

This research was sponsored by the U.S. Department of Energy (DOE), Vehicle Technologies Office, Lightweight Materials Core Program (LMCP).

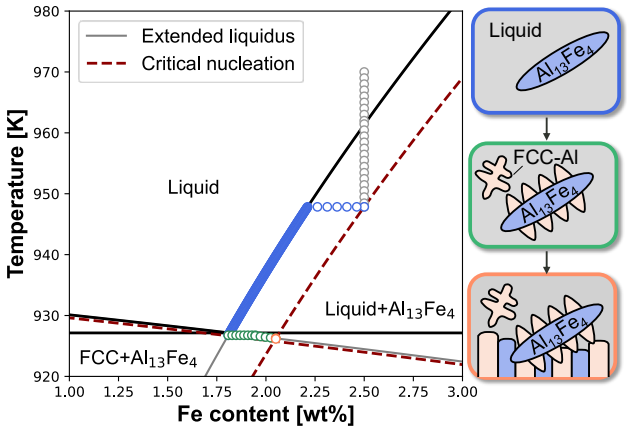

Figure 1. Prediction of solidification pathways and microstructural constituents for the Al-2.5Fe (wt%) alloy with the nucleation-implemented Scheil solidification model

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Biographical Note

Dr. Sun Yong Kwon is a R&D Staff in the Materials Sciences and Technology Division at Oak Ridge National Laboratory. He received his Ph. D. from the Department of Mining and Materials Engineering at McGill University in 2020. His research focuses on alloy design and microstructure evolution model guided by the CALPHAD approach.

Developing reliable Calphad descriptions: lessons from the Fe-Ni system

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Taking the Fe-Ni system as an example, this presentation provides insights into how appropriate models and high-quality data contribute to a reliable Calphad description.

Over the past decade, substantial effort has been invested in developing 3rd gen. Calphad models and descriptions. One notable advancement is the improved magnetic model for binary and higher-order systems [1], particularly in the treatment of magnetic moments and transition temperatures. This makes it possible to accurately describe the antiferromagnetic and ferromagnetic transition in Fe-Ni, which is essential for understanding the invar effect in Fe-Ni containing systems.

Experimental data are always crucial for developing Calphad descriptions. High-quality datasets provide the foundation for reliable Calphad assessments. This requires advanced experimental techniques, well-controlled experimental practice and thorough data analysis. Recent experimental work [2] has carefully determined the solubility of Ni in the bcc phase of Fe-Ni, which helped to improve the description of the bcc-fcc phase equilibria.

As the computational resources and capabilities have developed, the DFT calculated data have become more accessible, especially for metastable allotropes and end-members in the compound energy model where experiments are difficult or even impossible to perform. This enables to obtain a more reliable magnetic description of metastable fcc-Fe [3].

All these aspects contribute to a better Calphad description of Fe-Ni, resulting in a more reliable prediction of the T0 line.

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Biographical Note

Zhangting He is a researcher and project leader at Swerim, the Swedish Metals Research Institute, where she works on alloy development using the ICME approach based on the Calphad method. She earned her PhD degree from KTH Royal Institute of Technology and her thesis was focused on developing the third generation Calphad models and descriptions.

Using Universal Machine Learning Potential to Accelerate the Thermodynamic Database Development

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To development of CALPHAD-type thermodynamic database, large amount of input data ranging from thermochemical, phase equilibria measurement or sometime first-principles calculations data are necessary. Experimental procedure is time consuming and costly. To minimize the numbers of experimental data needed for the thermodynamic assessment, many first-principles calculations data are used to accelerate the assessment process [1]. However, first-principles calculations still required significantly computational resources, especially for the finite-temperature calculations, which involved the lattice vibrational contribution calculations. With the advancement in the materials discovery using machine learning, potential new material families are predicted. Timely and cost-effective development of the thermodynamic databases are become even more important. The same machine learning process can also generate the accurate interatomic potentials that can achieve the comparable accuracy with the first-principles calculation but significantly decrease the computational resources. It can be one of the paths that help accelerate the thermodynamic databases.

We demonstrated that using universal interatomic potential developed by machine learning can achieve the similar accuracy in constructing CALPHAD-type thermodynamic database. The thermodynamic database of the Al-Ni binary system is constructed using only the ground state and finite-temperature data obtained from machine learning potential [2]. The mixing energies between Al and Ni elements are obtained from the special quasi-random structures (SQS) [3] which represented the random mixing configurations between both elements in the specific lattice. The calculated free energies are used for the assessment of the thermodynamic database. The calculated phase diagram is similar to the phase diagram construct from only first-principles calculations data [4], but the computational resources required from the machine learning potential are several orders of magnitude lower than the first-principles calculations.

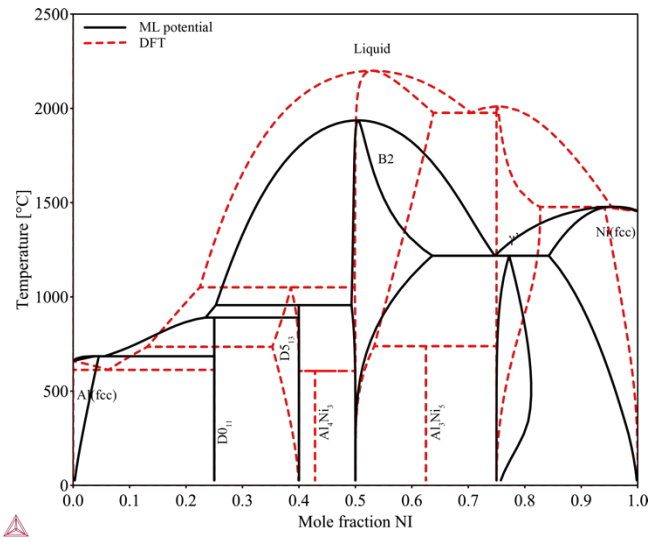

Figure 1. Calculated phase diagram from machine learning potential (solid) compared with calculated phase diagram from first-principles calculations data (dash)

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Biographical Note

Special researcher at Research Center for Structural Materials, National Institute for Materials Science, Japan. Epertise in computational thermodynamics focusing on 0K and finite-temperature first-principles calculations. Also experience in CALPHAD approach.

A hybrid methodology based on first-principles calculations and Calphad to predict the Ni-Co phase diagram incorporating configurational, vibrational and magnetic contributions

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Ni-Co alloys are extensively utilized in energy generation, aerospace and electrocatalalysis due to their outstanding mechanical behavior at high temperatures, superior corrosion and wear resistance. Moreover, Ni and Co are two important components of CoCrFeNiMn (Cantor alloy) and other fcc MultiPrincipal Element Alloys (MPEAs), which present exceptional mechanical properties. In particular, NiCoCr MPEAs provides the highest strength of all Cantor alloys at ambient temperature (> 1.1 GPa) [1] as a result of strain-induced fcc to hcp phase transformations and local stacking fault energy variations. Further improvements in the performance NiCo alloys and NiCoCr MPEAs, that can be achieved through changes in composition and heat treatments, require a precise knowledge of the phase diagram of the Ni-Co system. However, the current phase diagram, obtained from experiments and the assessment from the Calphad method [2], is based on a very limited experimental dataset.

A hybrid strategy is presented to determine the phase diagram of the Ni-Co system without experimental input through the combination of first-principles calculations, cluster expansion and Monte Carlo simulations with the Calphad methodology. To this end, the Gibbs free energies of the different phases in the convex hull were calculated from semi-grand canonical and canonical Monte Carlo simulations including the effect of the configurational, vibrational and magnetic entropic contributions. They were used to create the corresponding thermodynamic database (TDB) following the Calphad formalism to predict the phase diagram. The simulation results are in reasonable agreement with the accepted ferromagnetic-paramagnetic transition temperature but show significant differences with the accepted hcp/fcc two phase boundaries, particularly at low temperatures, providing more accurate information of the Ni-Co phase diagram. Moreover, they indicate that vibrational entropic play a key role in the Ni-Co phase diagram, while magnetic entropic only affects the Gibbs free energies at high temperatures. The efficiency and accuracy of this strategy to predict the Ni-Co phase diagram is anticipated to be further applied to NiCoCr-based MultiPrincipal Element Alloys.

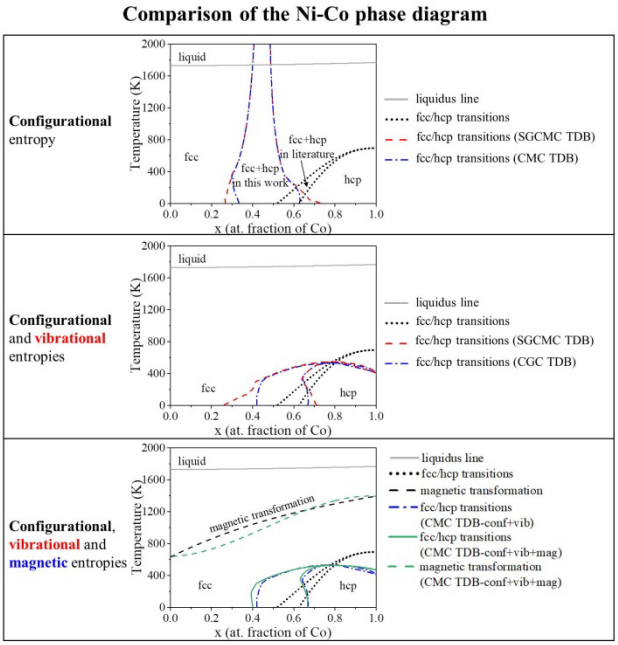

Figure 1. Graphical Abstract

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Acknowledgments

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Overestimation of Silica Melting at Ambient Pressure in DFT and High-Accuracy MLIPs: Tackling Unreachable Relaxation Timescales

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Accurate prediction of phase diagrams for network-forming materials like silica (SiO_2) at ambient pressure is crucial for understanding glass formation mechanisms and high-temperature materials behavior in ceramics and geophysics. However, achieving this remains a significant challenge due to the interplay between the accuracy of potential energy landscapes and severely limited simulation timescales imposed by the inherent sluggish dynamics near the glass transition.

Here, we investigate the melting properties of silica at ambient pressure using density functional theory (DFT) and a series of machine learning interatomic potentials (MLIPs) trained to varying levels of *ab initio* fidelity. Using both free-energy methods [1] and two-phase coexistence simulations [2], we observe a systematic trend: higher-accuracy MLIPs (closer to DFT-level precision) predict progressively higher melting points compared to the experimental value. Complementary analysis of the α-relaxation time, τ_α, reveals that more accurate potentials exhibit significantly larger τ_α at lower temperatures, indicating slower structural relaxation and stronger dynamical arrest. This enhanced kinetic sluggishness limits configurational phase space exploration within feasible MD timescales [3]. Therefore, the liquid free energy is artificially elevated due to missing configurational entropy, resulting in overestimated melting points for DFT and high accurate MLIP. In contrast, lower-fidelity potentials allows faster dynamics, enabling greater configurational sampling, lower liquid free energies, and melting points closer to experiment—but at the cost of misrepresenting the true underlying physics.

To address this, we estimate the temperature dependence of the configuration entropy of liquid silica based on frequency-dependent approach [3]. By explicitly including the missing configurational entropy in the liquid free energy calculations, DFT and high-fidelity MLIPs can provide accurate predictions of silica melting properties, reconciling the free energy landscape with observed thermodynamics.

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Biographical Note

Li-Fang Zhu works as a project leader in University of Stuttgart and as a guest scientist in Max-Planck-Institute for Sustainable Materials, with focus on developing efficient *ab initio* based methodologies for thermodynamic property study by integrating machine learning potentials.

Application of an uncertainty quantification method based on a heterogeneous ensemble of pretrained Universal machine learning interatomic potentials applied to steels with tramp elements

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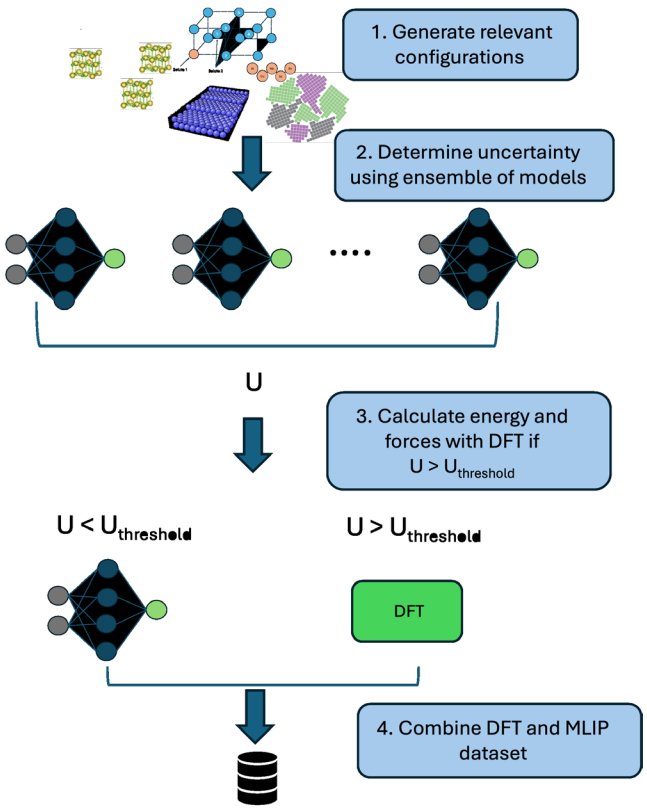
Recently, a framework for generating uncertainty metrics was developed using a heterogeneous ensemble of pretrained Universal Machine Learning Interatomic Potentials (uMLIPs) [1]. This approach leverages a selection of high-performing uMLIPs to achieve state-of-the-art accuracy while significantly reducing the need for expensive DFT calculations. Specifically, a predefined uncertainty threshold (U_t) is introduced: when the computed uncertainty metric (U) falls below this threshold, a suitable uMLIP is used to generate the corresponding energy and force labels, whereas DFT evaluations are reserved only for configurations where U exceeds U_t.

In this work, we apply this methodology to develop a specialized downstream potential for iron containing copper as a tramp element. Owing to its significantly lower computational cost, this derived child potential (see figure 1) is subsequently employed to carry out larger-scale simulations and systematically examine the energetics of Cu grain boundary segregation.

Figure 1. Schematic of the uncertainty-guided dataset generation process using a heterogeneous model ensemble. $U_{threshold}$ denotes the uncertainty limit beyond which DFT calculations are performed to provide ground-truth labels



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https://doi.org/10.1038/s41524-025-01905-x

Biographical Note

Naveen K. Mohandas is a PhD candidate at TU Delft, where he expects to complete his thesis in early 2027. He previously earned his MSc cum laude in Materials Science from the same institution. His research focuses on the development and application of machine-learned potentials, on which he has authored several papers.

Kai Liu earned his PhD from TU Delft in 2025. His research centers on interface-related atomistic modeling and the advancement of machine learning interatomic potentials (MLIPs).

Marcel Sluiter has served as a faculty member at TU Delft since 2005. His work primarily involves atomistic computer simulations focused on the thermodynamics and kinetics of materials.

Ab Initio Prediction of the Magnetic Thermodynamics of $LaCoO_3$ Perovskite Based on the Zentropy Theory

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Key words: ab initio, Thermodynamics, Zentropy, Perovskite

$LaCoO_3$ (LCO) is a correlated transition metal oxide that has garnered significant interest for applications in solid oxide fuel cells, catalysis, sensors, and spintronic devices. However, its magnetic and thermodynamic properties remain incompletely understood due to the presence of complex spin configurations.

Co^{3+} ions introduce complex magnetic behavior in $LaCoO_3$ by occupying octahedral sites surrounded by oxygen anions [1] (the slight rhombohedral distortion is typically neglected). This crystal field splits the d orbitals into a triply degenerate t_2g set (lower energy) and a doubly degenerate eg set (higher energy). For the $3d^6$ configuration of Co^{3+}, this splitting gives rise to three possible local spin states: low-spin (LS: t_2g^6 eg^0, S = 0), intermediate-spin (IS: t_2g^5 eg^1, S = 1), and high-spin (HS: t_2g^4 eg^2, S = 2). The IS state is expected to exhibit a strong Jahn–Teller distortion that lifts the degeneracy of the eg orbitals.

$LaCoO_3$ is nonmagnetic at low temperatures [2], with Co^{3+} ions remaining in the LS state below approximately 90 K. The material undergoes a nonmagnetic-to-paramagnetic transition near 90–100 K and an insulator-to-metal transition around 500 K. There is ongoing debate regarding the spin state of Co^{3+} ions above the onset of the first transition (~90 K). Some X-ray diffraction studies suggest the presence of IS Co^{3+}, while soft X-ray absorption and magnetic circular dichroism experiments point to a mixture of HS and LS states. Other X-ray absorption investigations support a continuous LS to IS transition around 90 K. All these interpretations are broadly consistent with the observed temperature-dependent magnetic susceptibility.

The higher-temperature insulator-to-metal transition (~500 K) is commonly attributed to a crossover from localized to delocalized eg electrons. Neutron diffraction data reveal anomalous thermal expansion associated with these magnetic transitions. Despite extensive research, consensus on the precise nature of the Co^{3+} spin state(s) in $LaCoO_3$ above 90 K remains elusive.

In this work, the magnetic thermodynamics and spin configurations of $LaCoO_3$ perovskite are systematically investigated by using Zentropy theory, a partition function-based framework for thermodynamic prediction, in conjunction with ab initio calculations. All relevant structural and spin configurations of $LaCoO_3$ are incorporated into the partition function to enable a comprehensive statistical description. Using this superposition approach, the entropy, heat capacity, thermal expansion, and charge disproportionation of $LaCoO_3$ are successfully predicted, explicitly accounting for magnetic transitions. The predicted results show excellent agreement with available experimental data.

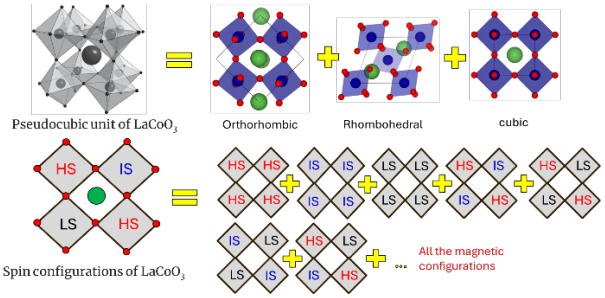

Figure 1. Statistical-mechanical calculations for $LaCoO_3$ considering multiple spin configurations and crystal structures

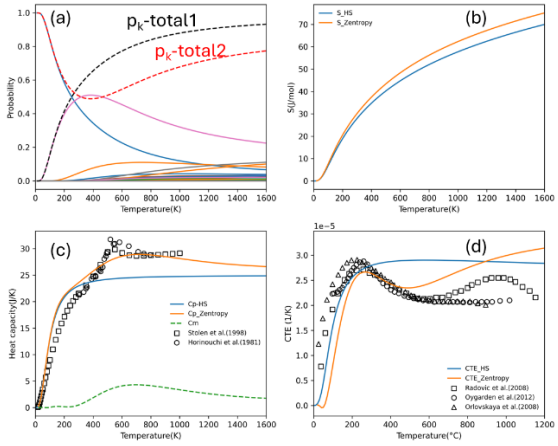

Figure 2. Thermodynamic properties of $LaCoO_3$ with the consideration of Zentropy theory

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Biographical Note

Yu Zhong is a Professor in the Mechanical and Materials Engineering Department at Worcester Polytechnic Institute (WPI). His research focus on CALPHAD, DFT, high-throughput calculations, and machine learning on the next generation materials design (ceramics and alloys).

Automated computation of ab initio bulk and defect phase diagrams

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Since the foundation of CALPHAD, zero-Kelvin ab initio energies have been integrated with sub-lattice or analytical models to address gaps in experimental data. However, extending this paradigm to full temperature- and composition-dependent Gibbs free energies has been hindered by the high cost of evaluating vibrational, electronic, magnetic, and anharmonic contributions across multicomponent spaces. Recent advances in machine learning (ML) interatomic potentials now make it possible to obtain density functional theory (DFT)-quality free energies at a fraction of the original expense. This development paves the way for the fully automated construction of bulk and defect phase diagrams.

In this study, we present a fully integrated workflow built on the Pyiron framework that automates every step, from high-throughput density-functional theory (DFT) and molecular-dynamics sampling via the ASSYST protocol, to machine learning (ML) potential training, validation, and thermodynamic integration. The resulting Gibbs energy models are then incorporated into a CALPHAD-compatible description of all relevant solid and liquid phases. This enables the rapid generation of binary and ternary bulk phase diagrams.

We extend the methodology beyond bulk equilibria to Metastable Defect Phase Diagrams (MDPDs), which incorporate the energetics of metastable and unstable bulk phases to predict the formation of planar defects (e.g., stacking faults and antiphase boundaries) in alloys such as Mg- and Fe-based systems. Coupling the ML-derived free energies with physics-informed AI (PIAI) constraints enables the workflow to deliver quantitative maps of defect stability as a function of composition and temperature. These maps provide a practical roadmap for defect-driven materials design.

We will demonstrate the effectiveness of our approach using selected binary and ternary systems. We will also discuss how we validated it against experimental solubility limits and defect observations. Finally, we will demonstrate the scalability of the workflow pipeline to higher-order alloy systems. Our work shows that digital high-throughput ab initio thermodynamic workflows can deliver bulk and defect phase diagrams with DFT accuracy at affordable computational and also human costs thanks to automation.

Biographical Note

Prof. Dr. Jörg Neugebauer is Director at the Max Planck Institute for Sustainable Materials (MPI-SusMat) and head of the department Computational Materials Design.

Bayesian Design of Experiments for Calphad Modeling

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Rapid exploration of materials design spaces relies on computational models and advanced experiments. Calphad models are often used to predict phase stability and thermophysical properties, however only about 25% of binary systems have thermodynamic Calphad assessments and fewer include phase-based thermophysical properties, primarily due to limited experimental data. Although high-throughput experimental techniques are advancing, there is still a need to efficiently design experiments for fundamental measurements of phase diagrams and properties. While optimal experimental design (OED) techniques are emerging in materials science, they often rely on physically inconsistent surrogate models. Here, we adopt a consistent Bayesian approach for OED that operates directly on Calphad-type models with quantified uncertainty. By propagating uncertainty in Gibbs energy parameters, we demonstrate that the expected information gain for experiments in the temperature-composition space of a phase diagram and correlates with actual information gain when new phase diagram data are incorporated via ESPEI.

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Biographical Note

Brandon Bocklund is a staff scientist Lawrence Livermore National Laboratory. He completed Ph.D. at the Pennsylvania State University in 2021. He is a co-lead for PyCalphad project (https://pycalphad.org) and the lead for the ESPEI project (https://espei.org) and the Materials Acceleration Platform at LLNL. His current research interests are in developing methods for maintaining Calphad databases, uncertainty quantification and propagation, first-principles density functional theory calculations, and building ICME tools for materials discovery and design.

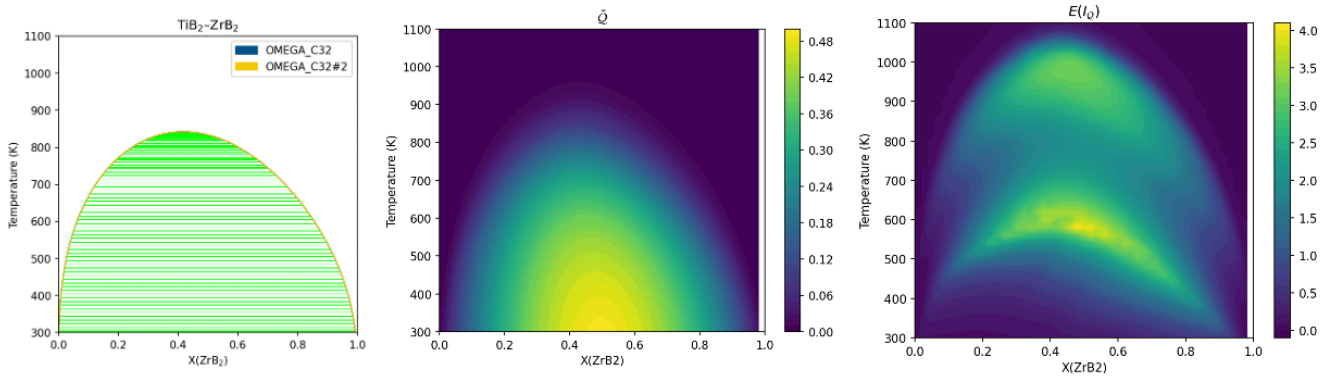

Figure 1. The (left) initial DFT-derived phase diagram for TiB2-ZrB2, (middle) the mean value of the push-forward prior for Q at all points in the experimental temperature-composition space, and (right) the expected information gain, E(I_Q), for each point in the experimental temperature-composition space that considers both the push-forward prior of Q and the distribution of experimental outcomes for an experiment that measures phase compositions of equilibrated TiB2-ZrB2 mixtures

Utilizing CALPHAD databases for alloy microstructure prediction via phase-field modeling

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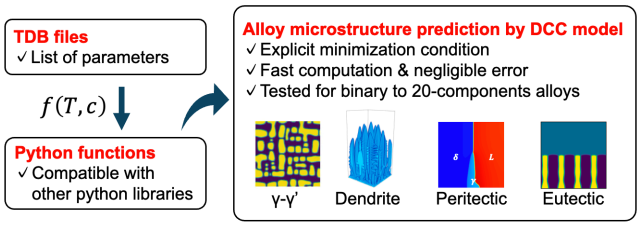
Over the past half century, the CALPHAD community has been able to construct thermodynamic databases covering thousands of combinations of elements. If these databases could be directly utilized for microstructure prediction, they would enable simulations across a vast range of practical multicomponent alloys. The phase-field method, widely used for microstructure prediction, is well suited for integration with CALPHAD databases because the method is founded on dissipation of free energy. For more than quarter century, significant efforts have been devoted to developing CALPHAD-coupled phase-field models. However, quantitative simulations that are computationally feasible have remained limited to systems with only three or four components.

CALPHAD-coupled phase-field modeling faces both theoretical and technical challenges. The theoretical difficulty arises from the need to satisfy two energy minimization conditions: the equal diffusion potential condition [1] and the internal equilibrium condition. The equal diffusion potential condition determines the partitioning of elements at interface, while the internal equilibrium condition specifies the site fractions of each sublattices. Because both conditions are expressed as implicit functions, they require iterative convergence procedures, and the computational cost increases exponentially with the number of components. For example, when CALPHAD software such as Pycalphad is used to solve the internal equilibrium condition during microstructure simulations of a 12-component Ni-based superalloy, the estimated computation time exceeds two years. The technical challenge stems from the difficulty of converting TDB file into a form that can be directly used in phase-field simulations. Since TDB files contain only thermodynamic parameters, CALPHAD software is required to compute free energies. Although such software offers APIs and functions for free-energy calculations, its slow calculation speed and limited compatibility with other numerical libraries make CALPHAD-coupled phase-field simulations difficult to implement efficiently.

To overcome these limitations, we first reformulated the two energy minimization conditions into explicit closed-form expressions, thus eliminating the need for iterative solvers. In addition, we developed a system that converts parameters in TDB files into Python functions suitable for direct use in phase-field simulations. Using this approach, we performed CALPHAD-coupled phase-field simulations across a wide range of alloy systems (Ni-, Fe-, Al-, and Ag-based), ranging from binary to 20-component alloys and various types of microstructural evolution, including dendritic solidification, peritectic and eutectic reactions, and solid-state transformations. In all cases, the two energy minimization conditions were satisfied with negligible error, and the computation time was sufficiently short.

Based on the explicit formulation, CALPHAD databases can now be directly coupled to the phase-field method. We refer to this model as Direct CALPHAD Coupling (DCC) model [2-4]. The DCC model enables microstructure prediction across a broad compositional range covered by existing thermodynamic databases.

Graphical Abstract



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Biographical Note

Takumi Morino is a doctoral student in Materials Science and Engineering at Yokohama National University, Japan. His research focuses on CALPHAD-coupled phase-field modeling for quantitative microstructure prediction in multicomponent alloys.

Toward Defect Phase Diagrams by Integrating Constraints into CALPHAD

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Extending CALPHAD to defect phases builds on the classical treatment of disturbances and generalized extensive variables for interfaces and constrained systems [1,2], and on recent advances in defect-phase thermodynamics [3]. We present an integrated workflow that couples atomistic simulations, experimental segregation measurements, and CALPHAD modeling to construct *defect phase diagrams* (DPDs). Using Mg–Ga Σ7 grain boundaries [4] as a model system, density-functional-theory calculations provide end-member energies and interaction parameters for T-type and A-type configurations. Experimental Ga-segregation data then refine these parameters, enabling quantitative prediction of grain-boundary phase transitions, including a T→A transformation near 0.5 at.% Ga for grain sizes on the order of 100 nm. Thus, we show that the standard CALPHAD methodology can be employed to describe defect phases.

A key feature of our approach is to represent defects through explicit constraints (ξ) that encode defect existence and stoichiometry. This formulation allows grain size to enter naturally via the amount of constraint per molar amount of atoms, thereby predicting how partitioning at defects evolves with grain refinement, and it provides a route to include defect–defect interactions within CALPHAD calculations.

Extending CALPHAD to defects dramatically expands the phase space: beyond all crystallographically distinct bulk phases, each bulk phase can host multiple, distinct defect phases. Capturing this structural complexity requires richer, machine-readable metadata (e.g., defect geometry, defect type, constraint definition, area density, and data provenance). To this end, we use the ThermML XML-specification [5] to store the Gibbs energy models together with defect-phase metadata, supporting automated research-data-management workflows that translate DFT and experimental datasets into CALPHAD-ready formats. Collectively, these developments advance defect thermodynamics toward the rigor and portability of CALPHAD.

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Biographical Note

Moritz to Baben is Managing Director at GTT-Technologies since 2017. He obtained his PhD at RWTH Aachen University in 2013 and joined GTT in 2016.

He is fascinated by the complexity in navigating chemical space. Working on defect phases, he learned that chemical space is only half of the story of materials science. Coordination space is the other half – and when he tried to combine them, his mind exploded.

Thermodynamic Modeling of Pure Elements with Quantitative Model Selection and Uncertainty Quantification using PyCalphad and ESPEI

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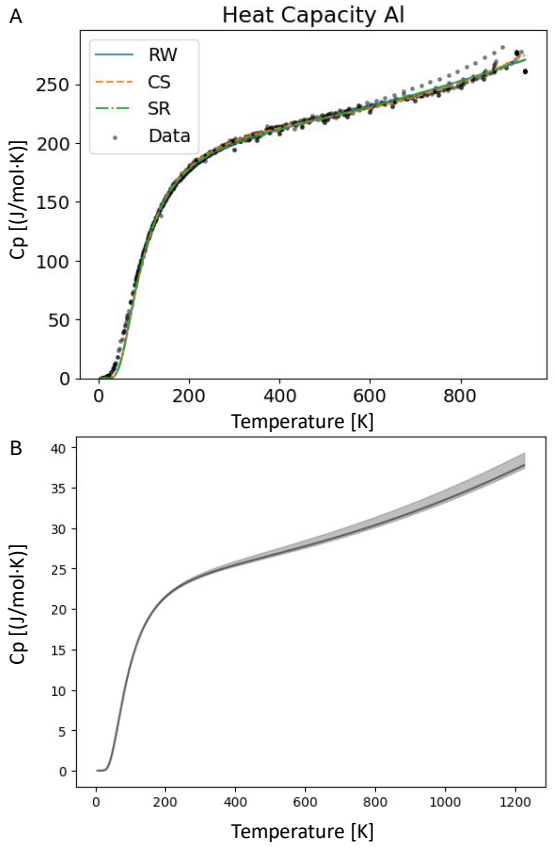
Thermodynamic modeling of pure elements is the foundational building block of CALPHAD. Recently, to describe Gibbs energy down to 0 K so that low temperature thermodynamic properties can be calculated rather than extrapolated from values above standard temperature, multiple physics-based models have been proposed, collectively known as "Third-Generation" models. To enable systematic and quantitative comparison of these models, the thermodynamic descriptions of pure elements and the computational tools needed to evaluate parameter sets and model fitness were implemented into the open-source software packages PyCalphad and ESPEI. Markov Chain Monte Carlo sampling in ESPEI enables rigorous uncertainty quantification of model parameters and their predictions, while Bayes factors allow direct comparison of model performance to support quantitative model selection. Through the remodeling of 41 pure elements, this work demonstrates efficient high throughput modeling of unary systems using multiple physics-based Gibbs energy forms and highlights their suitability for enabling future multicomponent CALPHAD assessments. These updated descriptions can be rapidly ingested into materials design workflows, allowing new results to be scaled to higher-order systems through integrated tools such as AMMap.

Biographical Note

Alexander Richter is a 5th year Ph.D. student in the Materials Science and Engineering department at The Pennsylvania State University. His current research focuses on material design of functionally graded materials via computational tools. He is developing python tools to improve unary descriptions of materials with PyCalphad and ESPEI as well as for alloy design in high dimension material space.

Figure 1. (A) This figure shows the heat capacity of three third generation models matched to experimental data for pure aluminum. Darker experimental datapoints indicate overlapping datapoints. (B) This figure shows the heat capacity of the segmented regression model distribution of parameters fit by the MCMC simulation for FCC Aluminum



A Cluster-Based Computational Thermodynamics Framework with Intrinsic Chemical Short-Range Order: New Developments and Implications for Precipitate Nucleation Kinetics

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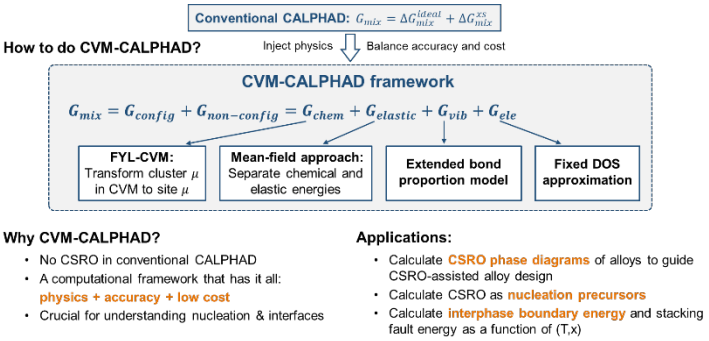
Incorporating chemical short-range order (CSRO) into CALPHAD has long remained a major challenge in computational thermodynamics. Conventional CALPHAD frameworks lack the ability to explicitly characterize CSRO, while cluster-based methods such as the cluster variation method (CVM) incur prohibitive computational cost when applied to multicomponent systems. In this talk, we present our newly developed CVM–CALPHAD framework, which achieves an effective balance between flexibility, accuracy, and computational efficiency. By applying the Fowler–Yang–Li (FYL) transform to the CVM formalism, the computational cost is significantly reduced without sacrificing thermodynamic rigor [1]. Furthermore, physics-based parameterization is employed to explicitly account for non-configurational free energy contributions, enabling resolution of vibrational, elastic, and electronic effects, as shown in Figure 1.

Recent applications of the CVM–CALPHAD framework will be demonstrated, including CSRO phase diagram calculations for the ternary Cu–Au–Ag system and thermodynamic modeling of the Ni–Cr system exhibiting both FCC and BCC phases. The role of CSRO as a precursor to precipitate nucleation will be discussed. In particular, we highlight the critical importance of incorporating CSRO to accurately evaluate coherent interphase boundary energies and to provide physically reliable input parameters for nucleation kinetics models in multicomponent alloys.

Figure 1. Summary of the CVM-CALPHAD framework



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Biographical Note

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Calphad models for the liquid phase

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The Temkin model [1] for molten salts using 2 sublattices was published 1945 and it inspired Hillert [2] to model Long Range Ordering (LRO) of carbon dissolved interstitially in steels and this evolved to the Compound Energy Formalism (CEF) [3] for crystalline solids. This formalism was then modified back to liquids in the Partially Ionic 2-Sublattice Liquid (I2SL) model [4] based on as-sessments of Fe-S, Fe-O and Ca-Fe-Si-O [5] in order to handle multiple valences. The I2SL model has been used in the development of large databases for metallic systems as well as the TAF-ID nuclear fuel database [6] and for molten salts [7].

The I2SL model uses ideal configurational entropy and at the same time the associated model [8] as well as the quasichemical MQM model [9] empha-sizing Short Range Ordering (SRO) for modeling in liquids were developed. In 2001 the Modified Quasichemical Model in the Quadruplet Approxi-mation (MQMQA) [10] extended the MQM model to a general liquid model including molten salts, nu-clear fuels [11] and other metallic and non-metallic liquids.

The introduction of a new unary database [12] will require modifications of software, databases and as-sessment methods and may initiate the develop-ment of new and more flexible model for liquids.

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Combinatorial Additive Manufacturing–Enabled Materials Discovery and Modeling of W–Re–Os Alloys

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Progress in refractory multi-principal element alloys is often limited by sparse high-temperature phase-equilibria data, uncertain lattice stabilities, and the slow, sequential nature of conventional characterization, challenges that hinder robust modeling in ternary and higher-order spaces. These constraints are well documented for high-entropy and compositionally complex alloys and motivate data-dense strategies that can better anchor thermodynamic and kinetic models.

Here we report a combinatorial additive manufacturing (AM) map spanning ~500 compositions in the tungsten–rhenium–osmium (W–Re–Os) ternary system, enabling rapid establishment of composition–microstructure–property relationships.[1] High-throughput screening identifies $W_{42}Re_{30}Os_{28}$ as a benchmark alloy that achieves ~1.8 GPa yield strength with ~9% compressive plasticity at room temperature and retains ~1.4 GPa yield strength with pronounced strain hardening at 1400 °C. Correlative microscopy reveals a hypoeutectic dual-phase architecture comprising a hexagonal close-packed (HCP) solid solution and a ReW-type body-centered tetragonal (BCT) intermetallic; deformation involves basal and non-basal slip, deformation twinning, and hetero-deformation–induced geometrically necessary dislocations (GNDs). These experimentally established features provide high-value constraints for modeling in this refractory space.

The dataset is expressly designed to inform modeling across scales. We outline how the measured phase coexistence, solvus/solidus bracketing, two-phase-field topology, and hypoeutectic morphology can (i) guide Calculation of Phase Diagrams (CALPHAD) parameter refinement for HCP and BCT phases; (ii) calibrate first-principles density functional theory (DFT) calculations of formation enthalpies, lattice stabilities, site preferences, and vibrational free energies; (iii) provide targets for molecular dynamics (MD) estimates of temperature-dependent elastic moduli and diffusion relevant to coarsening and strength retention; and (iv) seed phase-field and crystal plasticity finite-element (CPFE) simulations that rationalize microstructure selection and slip/twinning activity. By pairing high-throughput experimentation with modeling-ready outputs—without claiming a full assessment—this study accelerates reliable phase-stability and performance predictions in W–Re–Os and offers a generalizable template for other extreme-environment alloy systems.

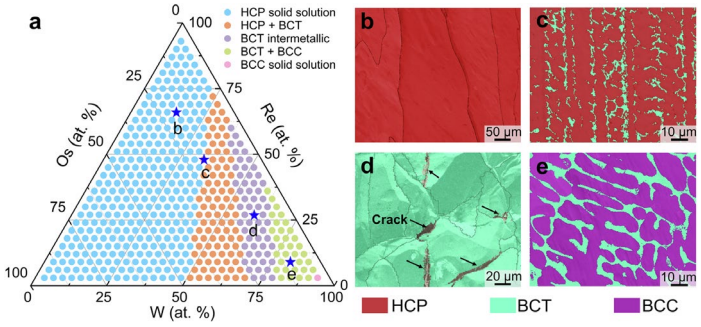

Fig a. Room-temperature phase mapping of W-Re-Os alloy system

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Biographical Note

Dr. Wei Chen is an Associate Professor at University of Buffalo, State University of New York.

Development of a high-throughput approach to assess oxidation resistance using chemically graded Ni-based superalloys

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In the context of the emergence of data-driven methods for material property predictions and corresponding capacities for accelerated alloy design, ONERA, SAFRAN and the Ministry of Armed Forces have been involved together in the ADAMANT (Accelerated Development of Alloys and Multilayer Systems for New Turbine Applications) chair. One of its main objectives is to develop high-throughput approaches to generate thermodynamic, metallurgical and mechanical data.

In this study, we focus on the problem of selective oxidation [1], which is known to be poorly predicted by machine learning (ML) algorithms. The oxidation of chemically graded samples could lead to a very high amount of data, helping to build more robust ML predictions.

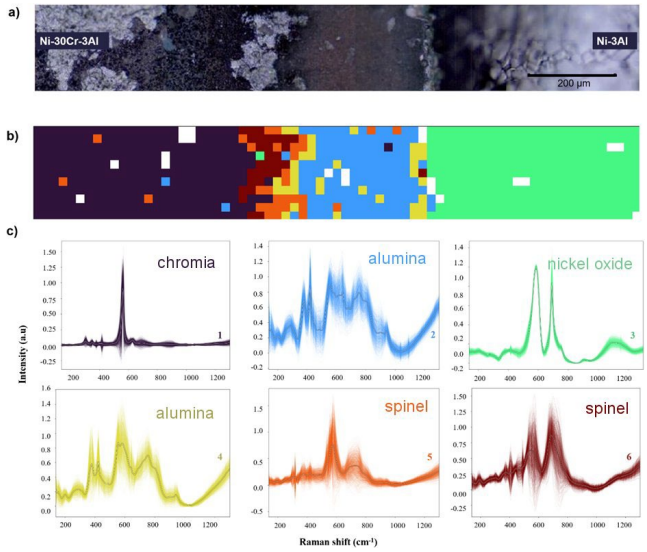
First, the feasibility was demonstrated on a Ni-Cr-Al model system, using a Ni-3Al-xCr chemically graded sample. It was shown that the expected transitions between three different types of high temperature oxidation behavior, forming respectively NiO, Al_2O_3 or Cr_2O_3 along the variation of chromium content [2]. Our non-destructive high-throughput characterization method combines Raman spectroscopy maps, SEM-EDS spectral maps and automated ML data processing in order to identify the nature and localization of the different oxides (cf Figure 1).

Knowledge regarding the transitions between the oxidation modes is also retrieved, with the detection of $Ni(Al,Cr)_2O_4$ spinel phases, that were confirmed by HRTEM characterization.

New experimental work has been performed using industrial Ni-based superalloys (CMSX-10 / AM1) for the diffusion couple. Despite the high number of chemical elements involved and the multiple oxides forming on the surface after high temperature oxidation, our method remains relevant [3]. The data processing method will be discussed, especially the unsupervised detection of the number of oxides, using both dimensionality reduction and clustering methods.

These results not only validate the high-throughput characterization approach, but also underline its potential to accelerate the evaluation process in unknown compositional spaces, even with a high number of chemical elements, leading to significant progress in both scientific understanding and innovative solutions for the design of oxidation resistant high temperature alloys.

Figure 1. Optical micrograph and processed Raman map of a Ni-30Cr-3Al / Ni-3Al diffusion couple after oxidation 20h at 1200°C (a, b) ; reconstructed spectra from clustering (c)



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Biographical Note

Mikael Perrut is a senior researcher at ONERA, the French aerospace lab. He is interested in the development of innovative experimental and numerical methods for the accelerated design of new materials (Ni-based superalloys, intermetallics, HEA) for aerospace applications using CALPHAD modeling, diffusion couples and multiples, machine learning techniques.

Evaluation of the Cu-Ti phase diagram and thermodynamic prediction of continuous and discontinuous precipitation

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Cu-Ti alloys exhibit excellent mechanical properties such as strength, stress relaxation, fatigue resistance, and bendability after undergoing a solution treatment followed by an aging heat treatment. Their high strength property is mainly due to the continuous precipitation (CP) during the aging treatment. However, a competing process called 'discontinuous precipitation (DP)' occurs, resulting in a deterioration of these superior properties. Therefore, it is important to understand the mechanism why and how DP occurs through over-aging treatment.

Since Kaufman and Bernstein [1] reported the calculated phase diagram for the Cu-Ti binary system, thermodynamic analyses using the CALPHAD method have been performed, defining many of the IMC phases as stoichiometric line compounds. In this study, the Gibbs energy of the Cu_pTi_q-IMC phases was described using a two sublattice compound model; $(Cu,Va)_p(Ti,Va)_q$ This model covers and reproduces the entire concentration range of the Gibbs energy curve, which exhibits a valley bottom near the stoichiometric composition. A thermodynamic evaluation of the Cu-Ti binary system was also performed, including the metastable miscibility gap in the fcc α-Cu phase. The mechanism of discontinuous precipitation in Cu-Ti binary alloys was then thermodynamically investigated.

Figure 1(a) shows the calculated phase diagram for the Cu-Ti system (at.%Ti ≤ 50), including the metastable miscibility gap of the fcc α-Cu phase. In accordance with the phase diagram and the Gibbs energy curves shown in Figure 1(b), the continuous and discontinuous precipitation processes can be explained as follows:

Firstly, a Cu-5at.%Ti alloy is solution treated at 900°C (①), followed by an aging treatment at 450°C within the miscibility gap (②), which results in the 'spinodal decomposition' into α+α' at the early stage of the aging treatment (③). The Cu_3Ti_2 phase, which has the largest driving energy for nucleation, then precipitates from the Ti-enriched α' phase (④), which could correspond to 'continuous precipitation'. 'Ti segregation' at the grain boundary (GB) can be predicted by a tangent line that is parallel to the common tangent for the (αCu)+Cu_3Ti_2 equilibrium (⑤). The cooperative growth of the (αCu) and β-Cu_4Ti phases could arise from the Ti-segregated GB, which has a large driving energy for 'discontinuous precipitation' (⑥). These microstructural evolutions are consistent with the experimental study reported by Semboshi *et al*. [2]

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Biographical Note

I. Ohnuma is a principal researcher in NIMS. His research interests focus on microstructure design and control of various practical materials using the CALPHAD method.

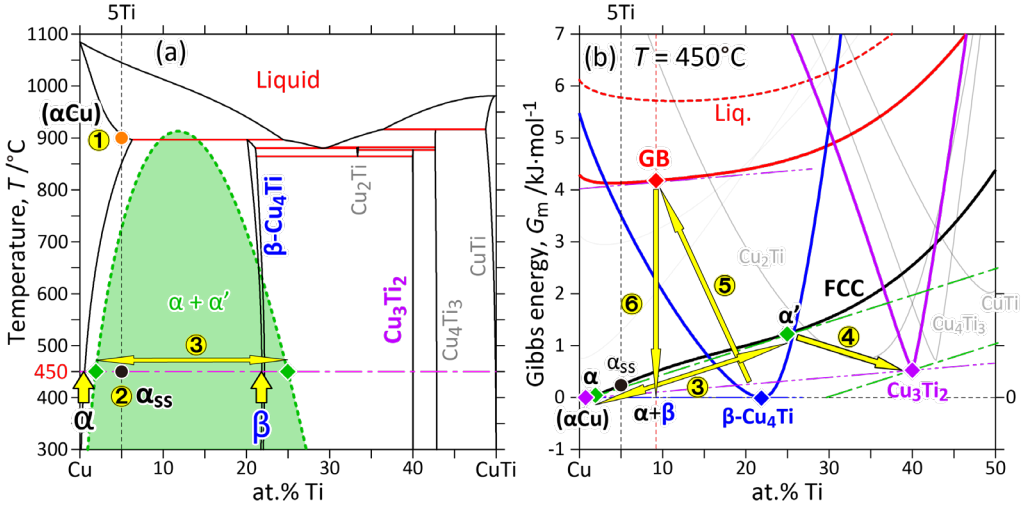

Fig.1 (a) Calculated phase diagram of the Cu-Ti system. (b) Thermodynamic prediction of continuous and discontinuous precipitation processes

Phase diagrams of Bi-Cu-Sn-Te quaternary system

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Key words: Phase diagram, Liquid miscibility gaps, CALPHAD-approach

The Sn-Bi-Cu-Te quaternary system is important as it encompasses many electronic solders and thermoelectric materials[1]. This study experimentally determines the liquidus projections of Sn-Bi-Cu, Sn-Bi-Te, Sn-Cu-Te, Bi-Cu-Te and Sn-Bi-Cu-Te. Alloys were prepared using pure constituent elements, melted and homogenized at high temperatures, and then quenched. The solidified alloys of different compositions were examined to determine their primary solidification phases[2]. A miscibility gap exists in the Cu-Te binary stable system. When alloys solidify while passing through this gap, unique microstructures are observed[3]. The miscibility gap of the Cu-Te system extends into the Sn-Cu-Te, Bi-Cu-Te, and Sn-Bi-Cu-Te systems. Additionally, miscibility gaps are found in the Sn-Bi-Cu and Sn-Cu-Te ternary systems, which are extended from the binary metastable systems. CALPHAD-type phase diagrams and thermodynamic modelling of the Sn-Bi-Cu-Te quaternary system and its sub-systems are assessed based on the experimental information determined in this study and those in the literatures[4]. Thermodynamic properties are calculated in this study, the calculated results agreed well with the experimental findings in the literatures. The liquidus projections, isoplethal sections and isothermal sections are then calculated using the models developed in this study and the results are in good agreement with experimental determinations.

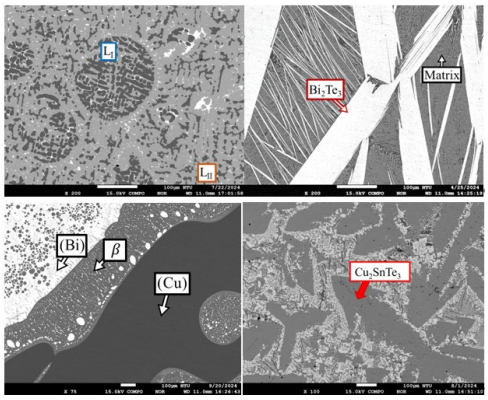

Figure 1: BEI micrograph of (a) Bi-Cu-Te; (b) Bi-Sn-Te; (c) Bi-Cu-Sn; (d) Cu-Sn-Te and (e) Bi-Cu-Sn-Te alloys

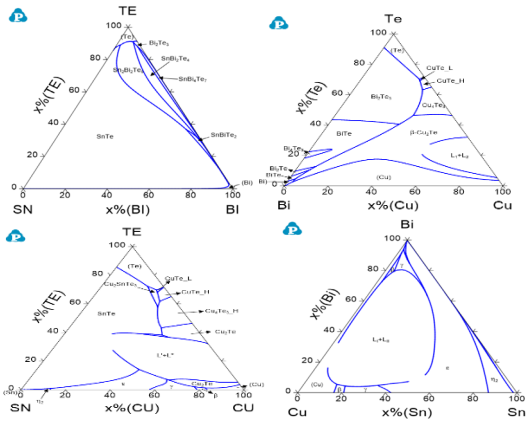

Figure 2: Liquidus projections of (a) Sn-Bi-Cu; (b) Sn-Bi-Te; (c) Sn-Cu-Te; (d) Bi-Cu-Te system

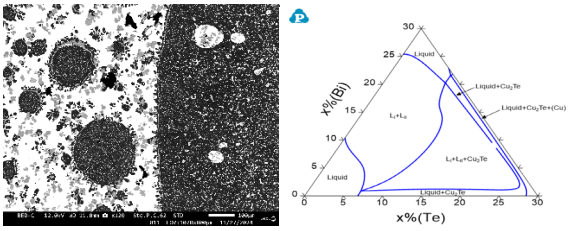

Figure 3: (a) BEI micrograph of Bi-Cu-Sn-Te quaternary system alloy, and (b) isothermal section of Bi-Cu-Sn-Te quaternary system at 900 °C, 70 at. %Cu

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Biographical Note

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Materials design of high-strength, ultra-pure copper alloys for the next-generation detectors to unravel the nature of dark matter

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The quest to directly detect dark matter and unravel the nature of neutrinos has driven the development of experimental techniques with unprecedented sensitivity, placing extreme demands on detector-material-induced radioactive backgrounds [1]. As a result, the choice of construction materials, particularly those in direct contact with the target medium, has become a critical limiting factor. Electroformed copper, thanks to its exceptional radiopurity, is the material of choice for low-background experiments [2]. However, its limited mechanical strength and ductility restrict its application in large-scale, high-pressure, or load-bearing components. Focusing on recent advances in the synthesis of high-strength, radiopure Cu-based alloys, specifically Cu-Cr and Cu-Cr-Ti, a materials design approach is suggested using computational thermodynamics [3]. It is demonstrated that besides the optimisation of thermal processing parameters and predictions of material properties, DICTRA and TC-PRISMA simulations can dictate the designing of the initial fabrication stage of electrodeposition, targeting at specific alloy compositions and mechanical performance [3,4]. This CALPHAD-based modelling enables rapid, predictive design of alloy compositions and thermal processing, allowing us to navigate the trade-offs between radiopurity, mechanical enhancement, and manufacturability in the most sustainable way. The physics impact of such materials breakthroughs will be illustrated through case studies of next-generation experiments.

This work motivated from fundamental science could also prove important to other applications, such as electronics, transport, metal purification for upcycling and clean energy technologies. More details here:

https://dematerializ.github.io/purealloys/

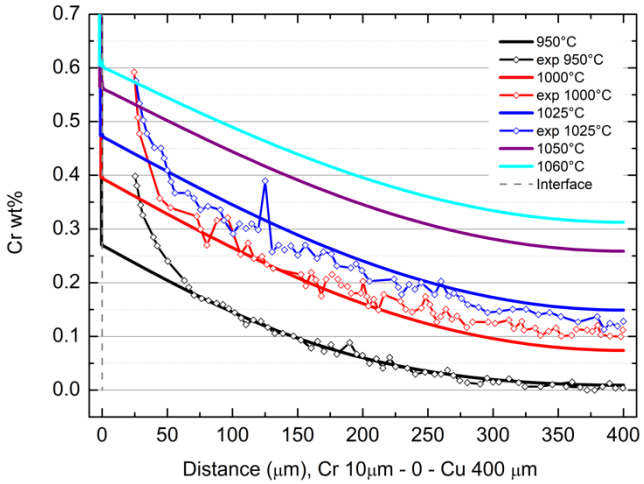

Figure 1. Cr concentration profiles of 400 μm Cu in contact with 10 μm Cr.

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Biographical Note

Dimitra Spathara is a materials scientist with research experience in structural and functional materials. She worked on high-temperature processing of Ni-based superalloys, in collabotation with Rolls-Royce plc. As a former UKRI Fellow and now a Marie-Curie Fellow explores further her interest in alloys development and manufacturing for a range of applications.

Thermodynamic and Kinetic Modelling of Oxide-Metal Reactions During Casting of Reactive Alloys

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The performance limits of ceramic moulds when casting reactive molten metals remain one of the critical bottlenecks constraining the progression of high-performance alloys toward their next phase of technological development. Oxide ceramics are widely used as mould materials for casting alloys owing to their exceptional thermal and chemical stability. Yet, when exposed to highly reactive molten metals such as titanium, interfacial reactions become effectively unavoidable [1]. These reactions accelerate mould degradation and release ceramic inclusions into the melt, fundamentally compromising microstructure control, dimensional fidelity and surface integrity. This limits alloys like Ti to processing windows that fall short of their full performance potential, restricting the production of defect-free, high-precision components required for next-generation aerospace and energy applications. Therefore, there is a constant rising demand for improved mould systems capable of withstanding temperatures approaching 2000 K while simultaneously resisting reduction and interfacial reactions.

Although many studies have examined oxide behaviour in contact with liquid metals, there is still limited understanding of how to design oxide systems with improved stability. Modelling efforts remain sparse, restricted by incomplete thermodynamic data, limited insight into metal–mould interfacial mechanisms, and reliance on oversimplified binary approximations that do not reflect real alloy complexity. To address these gaps, this study introduces a thermodynamic–kinetic framework for analysing metal–mould reactions under realistic multicomponent melt conditions. CALPHAD-based thermodynamic data was used to evaluate the interactions between molten alloys and mould oxides, explicitly capturing the competitive, composition-dependent reactions occurring among multiple dissolved species. These thermodynamic outputs provide inputs for an improved kinetic model based on the Frozen Gradient Approximation (FGA) [2], enabling the treatment of dissolution and growth as processes governed by evolving chemical potentials rather than fixed boundary conditions. This integrated approach predicts oxide behaviour in a dynamically changing liquid, capturing feedback between interfacial reactions, compositional shifts, and alloy redistribution as particle–melt interactions evolve.

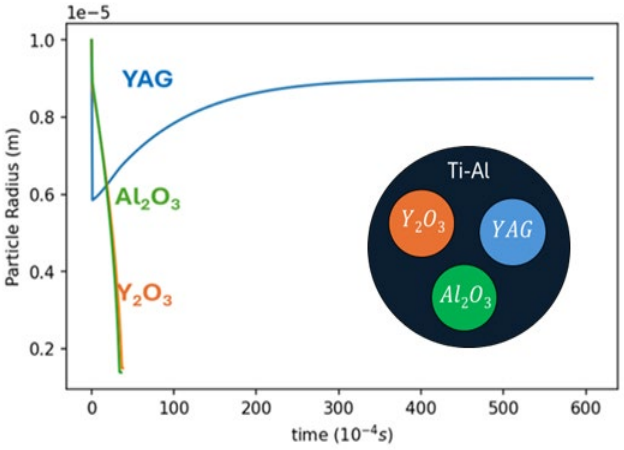

Figure 1. Numerical simulation showing the evolution of Al_2O_3, Y_2O_3 and YAG particles in Ti-Al melt

The results demonstrate that several strategies can be implemented to minimise reaction rates and enhance overall mould stability. In particular, careful optimisation of oxide formulation, compositional ratios, selective reaction pathways, and particle-size distribution significantly improves resistance to degradation under reactive molten-metal environments. Building on these insights, a new stability ranking of oxide systems has been developed, offering a more comprehensive basis for oxide selection and providing a revised perspective on designing mould materials for high-performance alloy casting.

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Biographical Note:

Dr. Joseph Moses is a postdoctoral researcher at the University of Birmingham. His research is primarily on modelling reactions between reactive molten alloys and oxide ceramics during investment casting.

Schaeffler diagram – a CALPHAD-view on an established application tool

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For the prediction of weld metal microstructures and of the weldability of stainless steels a constitutional diagram, the so-called Schaeffler diagram [1] was developed and applied. It is based on Cr and Ni equivalents and was further developed resulting in the WRC-1992 [2] constitution diagram. The phase fields are separated by straight lines and contain the phases ferrite and austenite and the microstructure constituent martensite. The Schaeffler diagram is also applied for the development of Cr-Ni steels (see for instance [3]) and this work focuses on this specific application.

In the framework of alloy design, chemical elements are usually classified according to their stabilizing effect on various phases such as ferrite or austenite. This is used in Schaeffler diagrams introducing so-called Cr- and Ni-equivalents.

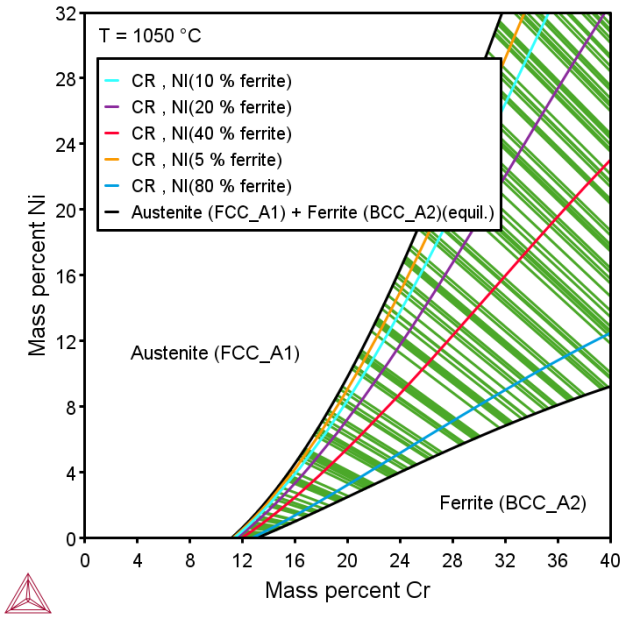
The chemical compositions of martensitic/ferritic 9-12Cr steels for high-temperature applications have to fulfill the condition that the alloy is located in the field “martensite” in the Schaeffler diagram. Some alloy compositions are fairly close to the boundary to the filed “martensite + ferrite” and these cases will be specifically discussed here. It is important to limit the volume fraction of ferrite in the martensitic matrix and thus such diagrams are useful for determining the limits for the occurrence of delta ferrite after the austenitization treatment (normalization). However, the predicting depends on factors like normalization temperature, contents of certain alloying elements, and micro-segregation state.

The ternary isothermal section at 1050 °C is the fundament of the discussed Schaeffler diagram. The austenite and 2-phase fields are separated by adding martensite in the Fe-rich part. It is shown based on isothermal sections calculated for various temperatures that the choice of the austenitization temperature determines the positioning of the phase boundaries between the austenite and ferrite fields.

The effects of the ferrite stabilizers Si, Mo, V, Al, Nb, Ti, and W and of the austenite stabilizers Co, Mn, C, Cu, and N on the respective solubility limits of ferrite and austenite relative to the effect of Cr and Ni are investigated with the result that the application of linear pre-factors for the ferrite and austenite stabilizing elements is limited to certain element contents.

During solidification of the alloys micro-segregation occurs and the resulting local heterogeneity of the chemical composition has to be considered as well. For this Scheil solidification calculations are performed followed by DICTRA simulations of the diffusional homogenization processes to better understand the status of alloys during the normalization procedure and their tendency to show delta ferrite or not.

Figure 1. The ternary isothermal section at 1050 °C is the fundament of the discussed Schaeffler diagram



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Deoxidation Equilibria in Liquid Alloys

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A thermodynamic database of oxygen in liquid alloys was developed to predict refining conditions and inclusion evolution in high-temperature pyrometallurgical processes, such as steelmaking, special steels, and various alloy production. The thermodynamic behavior of oxygen in alloy melts has been described based on the random mixing model. In general, metallic elements and oxygen exhibit significantly stronger attraction than typical metal-metal interactions. Thus, the array of atoms in liquid alloys is no longer considered a random-mixing configuration. The non-ideal configuration of atoms in the O-containing liquid solution can be described by Short-Range Ordering (SRO), which is accounted for by pair approximation using the Modified Quasichemical Model (MQM)[1]. By using an asymmetric interpolation method with the SRO, this model can minimize the number of model parameters. It means that integrating well-defined sub-binaries or -ternaries will provide better predictability and applicability of thermodynamic properties in multicomponent systems.

For an example, the aluminum deoxidation equilibria in normal Al-killed steels containing Al up to a few hundred ppm have been well described by Wagner's Internation Parameter Formalism(WIPF)[2] and associate model[3] shown as dashed line and dotted line, respectively, as shown in Fig. 1. However, these models formulated based on the dilute or ideal solution were not validated at high Al content region. On the other hand, the present calculation using the MQM shown by the solid line in Fig. 1 describes the Al-O relation in the Fe-Al melt over the entire Al concentration range from pure Fe to pure Al at 1600 °C.

Using the same modeling approach with critical experiments, the deoxidation equilibria in liquid alloys containing various deoxidizers like Al, C, Mn, Si, C, Cr, Ti, Ni, Ca, Mg, etc. were described using the MQM. A clear understanding of oxygen behavior in liquid alloys can be used to predict oxide inclusion stability, CO2 emissions, and future hydrogen steelmaking processes.

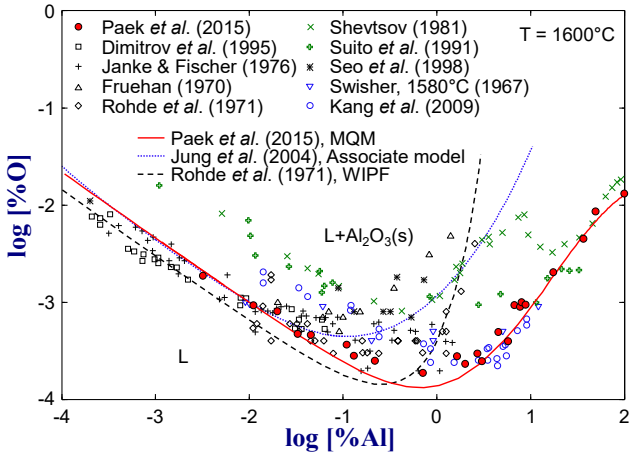

Figure 1. Al deoxidation equilibria in liquid iron at 1600 °C

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Biographical Note

Dr. Min-Kyu Paek was appointed as a professor of "Production of steel and non-ferrous metals and their process technology" at Clausthal University of Technology in 2025. He focuses on environmentally friendly alloy production processes such as steelmaking, special steel production as well as non-ferrous alloy production with byproduct recycling to reduce emissions.

Integration of thermodynamics with process development in ferroalloy production

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The development of thermodynamic solution models often happens in isolation to their future uses, however, there can be benefits to a more integrated approach where the model is compared to lab data (deportment studies) and discrepancies that arise are handled in a combined way – experimental and modelling. Results from the modelling can drive modifications to test work to better understand nuances in a multicomponent system, such as kinetics or side reactions that were not considered, and this can lead to a better understanding of reactions in the deportment study that might not have been recognized. This paper will describe both the modelling and experimental deportment work on real concentrate for FeNb production.

An assessment of hydrogen-induced NiTi martensite transition

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The NiTi alloy, well known for its distinctive shape memory behavior, is widely used in numerous application fields due to its functional and mechanical properties. In recent years, however, this alloy has also attracted increasing interest in the field of solid-state hydrogen storage. The absorption of hydrogen by metals, leading to the formation of metal hydrides, represents a promising and viable alternative to current hydrogen storage technologies, which are often characterized by high costs, safety concerns, and significant energy consumption.

Among the intermetallic systems investigated for hydrogen storage applications, titanium-based alloys have shown particularly interesting behavior in terms of hydrogen absorption capacity and process reversibility. In this context, the NiTi system represents a highly relevant case study, as it combines a well-defined intermetallic structure with complex phase behavior that is further influenced by the presence of hydrogen.

Nickel forms with titanium an intermetallic compound characterized by a body-centered cubic crystal structure, which is analogous to that of other systems widely investigated for hydrogen storage. The moderate solubility of the NiTi compound makes this system particularly interesting for the study of metal–hydrogen interactions and phase stabilization mechanisms in the presence of hydrogen. For this reason, a reliable thermodynamic description of the ternary NiTi–H system is essential to understand the behavior of these materials.

Within this framework, the main objective of the present work is the thermodynamic assessment of the NiTi–H system using the CALPHAD (CALculation of PHAse Diagrams) approach, with the aim of providing a consistent and reliable description of the system behavior in the presence of hydrogen. The experimental data used in this study were collected from the literature and critically assessed to ensure consistency and reliability. In addition, Density Functional Theory (DFT) calculations were employed to support the thermodynamic modeling, providing initial energetic values for hydrogen-containing end members.

Particular attention was devoted to the analysis of the martensitic phase transformation, which experimental evidence suggests may also occur in the presence of hydrogen. For this reason, both the austenitic B2 phase and the martensitic B19’ phase were modeled in the presence of hydrogen. Furthermore, a detailed analysis of the thermodynamic stability of both phases as a function of hydrogen content was carried out, in order to evaluate the effect of hydrogen on phase equilibria and on the stability fields of the considered structures.

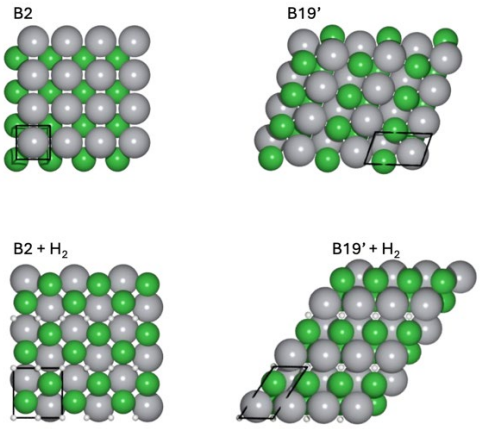

Figure 1. Crystal structure B2, B19' and B2, B19' with Hydrogen

The thermodynamic parameters of the modeled phases were subsequently optimized using the ESPEI module of the pycalphad library, based on the available experimental data and the calculated DFT energies. The optimization procedure resulted in a coherent description of the experimental data, demonstrating that the selected models are capable of reliably representing the thermodynamic behavior of the NiTi–H system.

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Biographical Note

Giorgia Pollini is a PhD candidate in Chemical and Materials Science at the University of Turin. Her research focuses on the design and investigation of the metal-hydrogen systems for hydrogen storage applications.

Investigation of the effects of tramp elements on the pearlitic transformation for a sustainable steelmaking industry

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Decarbonization of steelmaking will go through the increased use of Electric Arc Furnace (EAF), a route capable of incorporating up to 100% steel scrap. EAF routes can decrease CO_2 emissions by as much as 70% when compared with traditional blast-furnace operation [1]. However, steel scrap can vary in quantity and quality. The quality of the scrap influences the concentration of tramp elements (TE) present in the melt. TE, including copper, chromium, nickel, molybdenum, and tin, are of particular concern because they cannot be thermodynamically removed from the molten steel.

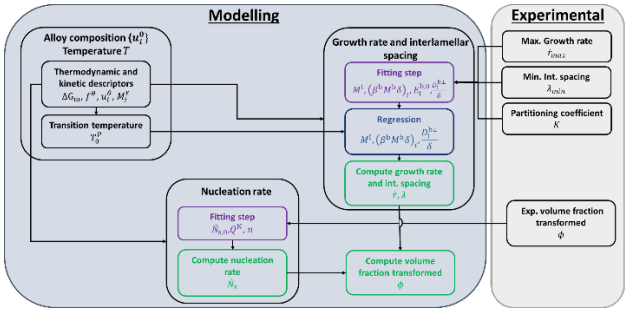
Bekaert, a leading Belgian company in advanced wire technology, aims to better understand how TE modify the metallurgy of pearlitic steels used in their production lines. Among the key steps in their processing route is the patenting heat treatment. During patenting, the wire is first heated to the austenitizing temperature to obtain fully homogeneous austenite. It is then submerged into a hot bath to promote the isothermal transformation of austenite into fine pearlite, a microstructure essential for wire applications, ensuring high strength and good ductility.

The present work focuses on improving the fundamental understanding of the effect of TE affect the isothermal austenite-to-pearlite transformation. A coupled numerical and experimental approach has been developed to build a predictive and reliable framework. Although the effects of elements such as Cr, Ni, and Mo on pearlite formation have been previously documented [2], [3], the influence of copper remains insufficiently characterized. A particular attention is paid to the effect of this element on transformation kinetics and pearlite microstructure.

A analytical mean-field model from literature [4], implemented within Thermo-Calc, is refined to include the specific effects of tramp elements. The model is a phenomenological steady-state formulation that accounts for ferrite–cementite interface creation, mixed diffusion, interface mobility, and solute drag. It contains parameters that must be calibrated using experimental measurements of pearlite growth rate, interlamellar spacing, and chemical distribution.

To quantify copper's influence and further assess the modelling tool parameters accounting for the effects of Cu, eutectoid steels with varying Cu contents are investigated using dilatometry, optical microscopy, scanning electron microscopy, and thermodynamic calculations based on the TCFE14 database. Experimental results show that copper delays pearlite formation across all temperatures studied, while thermodynamic analysis highlights how copper affects phase stability and how interactions with other alloying elements influence its solubility in both austenite and pearlite. A comparison between model prediction and experimental data is presented.

Figure 1. Modelling approach



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Thermodynamic Modelling of Protective Coating for Solid Oxide Electrolysis Cells

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Industries are increasingly shifting toward green hydrogen production to reduce carbon emissions.[1] Solid oxide electrolysis cells (SOECs) offer a promising route for efficient hydrogen generation via high-temperature water electrolysis (600-1000 °C), which lowers electrical energy demand and eliminates the need for costly metal catalysts. However, a major challenge limiting SOEC performance and durability is chromium volatilization from metallic interconnectors. At operating temperatures, chromium forms volatile species (CrO_3, $CrO_2(OH)_2$) that migrate and deposit on the oxygen electrode, leading to the formation of insulating phases such as Cr_2O_3, thereby degrading its performance.

Protective coatings for interconnectors represent an effective strategy to suppress chromium volatilization; however, suitable candidates must be thermally stable, have a compatible thermal expansion with the substrate and not degrade SOEC electronic conductivity. Spinel oxides (AB_2O_4) can be promising coating materials due to their structural flexibility, which allows accommodation of multiple cations in tetrahedral and octahedral sites, enabling tunable physical and chemical properties. While some ternary spinel systems have been investigated in terms of their dopant chemistry, crystal structure, and measured properties including electrical conductivity and thermal expansion[2], many doped compositions remain unexplored, and chromium solubility in these materials is still poorly understood. Furthermore, quaternary and higher-order spinel compositions have received little attention for SOEC applications, despite their strong potential for performance optimization through multi-element doping strategies.

Thermodynamic calculations were performed using Thermo-Calc[3] software coupled with the commercial TCOX14[4] oxide database, following its validation against experimental data. A Python-based screening tool using the TC Python API automates phase diagram and property calculations across composition-temperature space to determine: (1) single-phase spinel stability regions (Gibbs energy maps), (2) cation site occupancy (tetrahedral *vs.* octahedral) for polaron hopping conductivity, and (3) Cr solubility limits. A hierarchical methodology was implemented using industrially relevant cations {Ni, Fe, Co, Mn, Cu, Cr}. Binary oxides from this list serve as initial compositions, systematically doped with single elements at varying amounts to map spinel formation windows across temperature and composition space. Ternary spinels showing the broadest composition-temperature ranges are then selected as platforms for additional doping, initially with Cr to assess solubility and trapping capability, with other dopant elements to be explored. Subsequently, quaternary systems enable development of higher-order compositions through sequential doping.

As a representative example, in the $Ni_xFe_{3-x}O_4$ system, the widest composition–temperature stability range is obtained at x = 1 ($NiFe_2O_4$) between 600 and 1000 °C. Cation distribution analysis reveals that Ni^{2+} preferentially substitutes Fe^{2+} in octahedral sites, reducing Fe^{2+}/Fe^{3+} polaron hopping and thus decreasing electronic conductivity with increasing Ni content. Upon Cr doping ($NiFe_{2-x}Cr_xO_4$), Cr solubility exhibits strong temperature dependence: complete solid solubility is predicted above ~710 °C, while a miscibility gap limits Cr incorporation at lower temperatures. Under typical SOEC operating conditions (600-800 °C), Cr can be incorporated up to x ≈ 0.5-1 while maintaining a single-phase spinel, beyond which phase separation into Fe-rich and Cr-rich spinels occurs. Cr preferentially occupies octahedral sites, replacing Fe^{3+} and inducing partial Ni^{2+} migration to tetrahedral sites, degrading little the conductivity, as polaron hopping is already hindered.

This computational screening framework accelerates industrially relevant materials discovery by enabling rapid identification of optimized spinel coatings that mitigate chromium poisoning while meeting SOEC operational requirements.

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Modelling and probing solid solution-aqueous solution equilibria of aqueous nickel iron sulfate at 6 °C

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Transition metal aqueous sulfates have recently received attention due to their presence in hydrometallurgical recycling processes, for example those involving lithium-ion batteries. However, leachate solutions are often complex and require expensive and complicated treatment. Unfortunately, phase equilibria data is often lacking for ternary transition metal sulfates, precluding optimization of leachate separation and precipitation techniques. We report on measurements and modelling of solubility of ternary iron and nickel sulfate in aqueous solution.

Using custom glassware, solid-liquid equilibria was reached at a fixed temperature (6° C), and the solubility limits and solid composition were determined through material balance and chemical analysis. The collected data was compared to a thermodynamic model based on Pitzer equations for the ternary liquid aqueous electrolyte and the $(Fe,Ni)SO_4(H_2O)_7$ solid solution was taken as ideal. Previous binary solution thermodynamic modelling [1,2] in addition to ternary electrolyte Pitzer parameters [3] were used.

Although solubility constants of $NiSO_4(H_2O)_7$ and $FeSO_4(H_2O)_7$ system components in the $(Fe,Ni)SO_4(H_2O)_7$ solid solution been reported, they were found to incorrectly reproduce the reported biphasic gap of $(Fe,Ni)SO_4(H_2O)_7$ solid solutions. As such, revised solubility constants calculated from reported biphasic solid-solution composition ranges [4] were used. These allow description of the solid solution–aqueous solution equilibria and the tie lines which link aqueous solid compositions to their relevant solid solution composition at equilibrium. Our work shows promise for enhanced control of composition during chemical precipitation for leachates comprised of transition metal sulfates.

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Biographical Note

Julian Self is an Assistant Professor in the department of Chemical Engineering at Polytechnique Montreal. His research focuses include the physical chemistry of liquid electrolytes used in electrochemical devices and hydrometallurgical applications.

Unexpected Cracking in WAAM Cu-Ni Deposited on Steel Base Plates: Understanding the Role of Fe

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Copper-nickel (Cu-Ni) alloys are vital in the maritime industry due to their high corrosion and bio-fouling resistance in sea water. Conventionally, parts have been fabricated by casting and forging, but additive manufacturing (AM) offers a modern approach for producing complex components and improving supply chain resiliency. To reduce the fabrication costs of AM, steel is increasingly used as a base plate, a practice that introduces iron (Fe) contamination into the initial Cu-Ni layers. Literature reports that this is unlikely to result in cracking in the Cu parts with Wu et al. summarizing in a recent review that for Laser Powder Bed Fusion (LPBF) of Cu/Fe multi-material parts, cracking is only observed at the Cu/Fe interface or in the steel [1]. A CALPHAD-based model, Figure 1a, using the Thermo-Calc implemented Easton Crack Susceptibility Criterion model [2], supports the literature observations and it was concluded, initially, that Fe contamination in Cu alloys poses a low risk for solidification cracking.

In direct contrast to these expectations, this study observed significant inter-dendritic cracking in the first layer of a Cu-Ni alloy deposited on a steel plate using Wire Arc Additive Manufacturing (WAAM), Figure 1b. Cracking of this form is consistent with solidification cracking. Microstructural analysis revealed these cracks were confined to the high-Fe initial layer and propagated through Cu-rich inter-dendritic regions, Figure 1c. We propose this phenomenon is tied to the inherent micro-segregation of Cu-Ni during solidification. Fe partitions preferentially to the dendrite cores but Fe levels are still elevated in the Cu-rich inter-dendritic regions. EDS composition analysis shows 24 at% Fe in the dendrite cores and 9 at% in the inter-dendritic region within the first layer. While the observed cracks are consistent with those resulting from solidification cracking, we hypothesize that cracking is a result of Fe segregation affecting the properties of the inter-dendritic region, reducing the toughness and increasing the crack susceptibility post solidification.

This presentation will detail the metallurgical mechanism responsible for Fe-induced cracking in Cu-Ni alloys and the effect of other alloying elements such as Cr and Mn. We established a critical Fe concentration threshold to prevent cracking and introduce a CALPHAD-supported tool developed to predict and manage Fe dilution as a function of AM process parameters and steel base plate selection. This work provides critical guidance for successfully manufacturing Cu-Ni components on steel substrates and other multi-material AM parts.

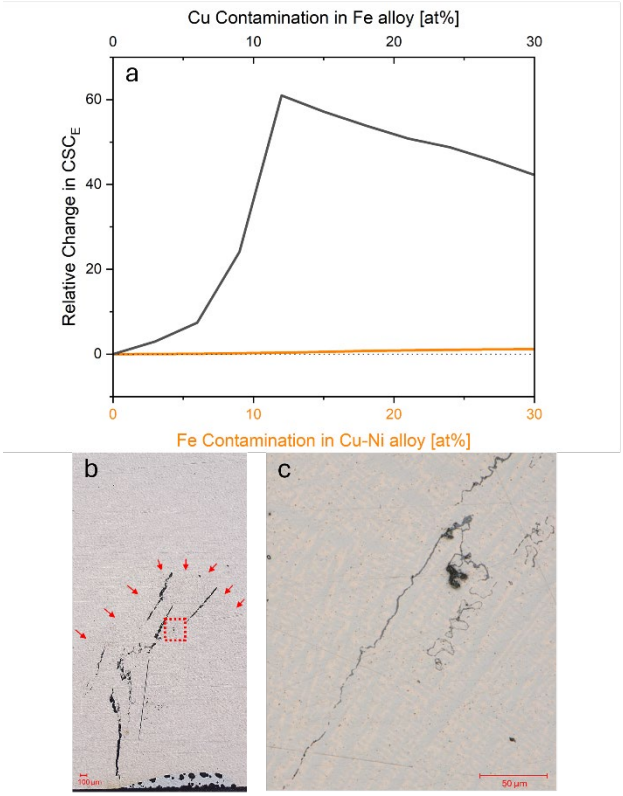

Figure 1. a) Relative change in the Easton calculated crack susceptibility vs the amount of Fe contamination in a Cu-Ni alloy and Cu contamination in a Fe alloy. b) Optical micrograph of the first and second layers of a WAAM Cu-Ni alloy. Red arrows point to the interface between the first and second layers. c) A higher magnification micrograph of the red boxed region in (b) showing a crack traveling through the inter-dendritic region.

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Blast Furnace Simulation Using a CASCADE Framework and ChemApp for Python

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Key words: CALPHAD, ChemApp, CASCADE modeling, blast furnace, direct reduction, rotary hearth furnace.

Thermochemical modeling and simulations play a central role in the quantitative understanding and optimization of metallurgical ironmaking processes. For blast furnace operation, predictive models that describe coupled multiphase flow, heat and mass transfer, and global process behavior across a wide range of operating conditions are required. In the present work, a CASCADE-based modeling framework, coupled with ChemApp for Python [1], is presented and applied to the blast furnace (BF).

The developed model is a steady-state, multi-effective equilibrium reaction zones simulation based on Gibbs energy minimization and mass- and energy-balance coupling.[2] The model incorporates detailed gas–solid reaction equilibria, phase transformations of iron oxides, and realistic process boundary conditions. Its primary objective is to predict detailed compositions of hot metal, slag, and gas (including minor elements such as S and P) under varying input boundary conditions. By employing chemical equilibrium calculations within a zoned framework, the model overcomes the difficulty of simulating counter-current reactors by normal steady-state simulation due to the mutually opposing time scales of material and inlet gas.

Fig. 1 shows a schematic overview of the BF CASCADE model, in which the furnace is discretized into horizontal levels from the charging to the tapping level, to enable sequential coupling of gas and condensed streams in a counter-current arrangement. At each level, ascending gas and descending condensed streams are processed through a local thermodynamic equilibrium module, after which the resulting outlet streams are passed to adjacent levels, forming the CASCADE structure. Heat losses to the furnace wall are explicitly accounted for at each level, contributing to the local energy balance. Special treatment is applied to the raceway and metal–slag zones to capture zone-specific reaction and phase behavior, enabling the model to identify and describe the presence of multiple characteristic zones within the BF.

In addition to equilibrium calculations, kinetic constraints are applied to key reactions—most notably the Boudouard and water–gas shift reactions—allowing deviations from equilibrium in temperature ranges where reaction kinetics dominate and cannot be described solely by equilibrium thermodynamics. Implementing kinetic constraints provides a more realistic representation of gas–solid reaction behavior and enhances the predictive capability of the model.

The level-by-level procedure is iterated until changes in temperature and phase composition at all levels fall below a prescribed convergence threshold, after which the simulation is terminated and results are evaluated. The simulations yield physically consistent temperature profiles, gas compositions, reduction degrees, and material throughput, with promising agreement with industrial reference data.

This simulation framework provides a transparent platform for sensitivity analysis, surrogate model development, and the integration of machine-learning techniques for process optimization and online simulation, with promising results. Beyond BF modeling, it has been tested on direct reduction shaft furnaces and rotary-type furnace processes, demonstrating its general applicability across ironmaking routes.

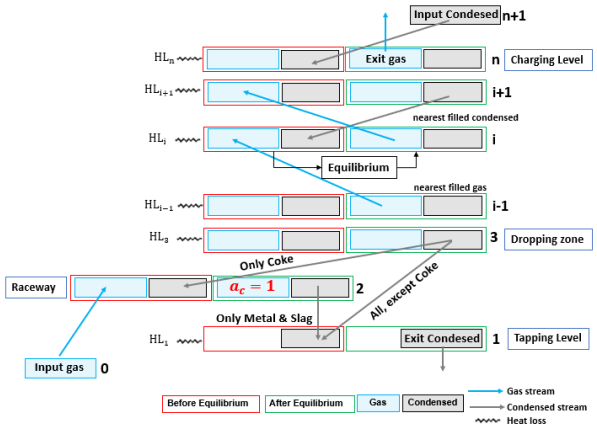

Fig 1. Axial CASCADE discretization of the blast furnace

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Biographical Note

Mr. Ahmed Mansy is a PhD researcher at Clausthal University of Technology specializing in CALPHAD-based thermochemical modeling of ironmaking processes. His research focuses on blast furnaces and related reactors using ChemApp and FactSage, with emphasis on sustainable metallurgy, process digitalization, and computational optimization, closely aligned with the CALPHAD community's mission.

Modelling of inorganic solid phases formed during pyrogasification of biomass

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The modeling of pyrogasification traditionally relies on either kinetic or thermodynamic equilibrium approaches. Both are mainly focus on the organic fraction of the feedstock, generally neglecting inorganic elements. However, these elements can have a significant impact on the process. They may exhibit catalytic or inhibitory effects on reactions, promote deposit formation, accelerate equipment corrosion, or act as a precursor of pollutant species in the syngas. The fate of inorganic compounds during pyrogasification remains poorly documented, and predictive models or correlations are still lacking. Kinetic models are inadequate here, as they depend on reaction-specific constants that are rarely available for complex inorganic systems, given the poor understanding of their reaction pathways. In this situation, thermodynamic equilibrium modeling offers a more appropriate alternative. However, the physical conditions in a bubbling fluidized bed reactor, such as finite residence time, do not allow the system to reach global thermodynamic equilibrium, which constitutes a fundamental limitation to the application of a simple equilibrium approach and reduces its predictive capability.

In this context, this study aims to develop a model that combines thermodynamic equilibrium calculations and mass transfer between gas and solid phases to simulate the local gas-solid interactions governing the fate of inorganic compounds during pyrogasification in a bubbling fluidized bed.

The model is based on a multiple local thermodynamic approach under non-stoichiometric conditions, describing the interactions between gas and solid phases. The gas phase is considered as a plug flow reactor, while the solid phase is modeled as a continuously stirred tank reactor. According to this hydrodynamic model, the gas phase is considered as a plug flow reactor, while the solid phase is modeled as a continuously stirred tank reactor. The amount of solid participating in the local equilibrium is treated as an adjustable parameter, defined at the start of the simulation. Moreover, the number of stages representing the number of local equilibria and the plug flow behavior is the second adjustable parameter. **Thermodynamic equilibrium calculations are performed using the FactSage software.** The amount of gas and its composition are governed by mass transfer models, calculated using appropriate mass transfer correlations and mass transfer is governed by the hydrodynamic behavior of the bubbling fluidized bed, based on the two-phase theory of fluidization proposed by Davidson and Harrison (1963) [1] and further applied by Yan et al. (1998) [2].

Model validation will be performed using experimental data from two sources: the fluidized bed pilot reactor at the ENGIE Crigen laboratory (France), and data from the literature [3]. Preliminary validation against the dataset of [3] yields the following comparisons:

A residual carbon content of 20.83 wt% is predicted by the model, versus 7.71 wt% reported for bottom ash in [3].

For the gas phase, [3] reports NH_3 (39,552 mg/L), H_2S (0.057 %v/v), and COS (0.003 %v/v). The model yields NH_3 (20,805 mg/L), H_2S (0.138 %v/v), and COS (0.0026 %v/v).

The observed discrepancies highlight the need for further calibration of the adjustable model parameters. Additional simulations are currently underway to improve the model's predictive accuracy.

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Biographical Note

David PINTO is a PhD candidate at M2P2 laboratories of Aix Marseille university and at laboratory of the R&D centre of ENGIE group in France (CRIGEN). Master's degree in "Process and bioprocess Engineering" from Aix Marseille university.

Machine learning-assisted crystal plasticity modeling of microcrack behavior in gradient-structured steels

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Gradient-structured metallic materials exhibit an exceptional combination of strength and ductility, making them highly promising for critical applications in aerospace, automotive manufacturing, and related fields. However, the initiation and propagation of microcracks remain critical factors governing fatigue life and service reliability, while the underlying micro-mechanisms in heterogeneous microstructures are still not fully understood.

In this study, a crystal plasticity finite element method (CPFEM) is employed to investigate microcrack behavior in gradient-structured high-strength steels. A user-defined material subroutine (Oxford-Umat) is utilized for the accurate implementation of the crystal plasticity constitutive model. Polycrystalline models with varying microcrack sizes and spatial distributions are constructed to systematically analyze the effects of microcrack geometry and their positions within the gradient structure under cyclic loading conditions.

The simulation results indicate that both the initial size and spatial location of microcracks within the gradient layer significantly influence crack initiation life and propagation paths, as well as strain localization behavior. These findings provide insights into the microstructure-dependent mechanisms governing crack evolution in gradient-structured steels.

To further enhance the predictive capability and computational efficiency, a machine learning-assisted framework is introduced to establish the relationship between stress states, microstructural descriptors (e.g., crystallographic orientation), and crack initiation behavior. Preliminary results demonstrate the potential of incorporating texture information into data-driven constitutive modeling, enabling efficient prediction of anisotropic mechanical response.

This work provides a microstructure-informed, data-driven pathway for understanding and predicting crack behavior in advanced steels, with potential integration into ICME frameworks compatible with CALPHAD-based materials design.

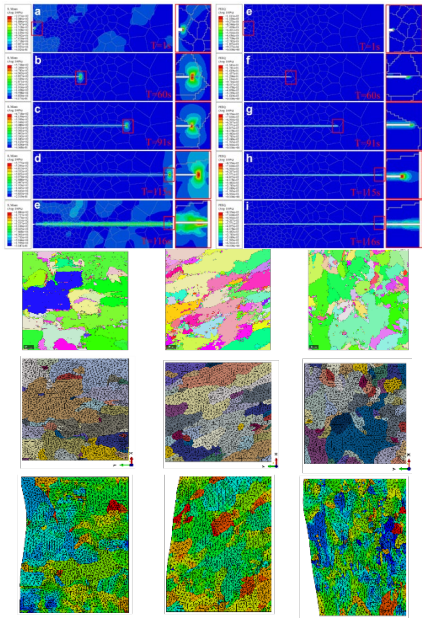

Figure 1. Mechanical simulation of materials using CPFEM

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Biographical Note

Xinxi Luo, a PhD student of the Central South University under supervisor Prof. Yong Du, is dedicated to the research on crystal plasticity finite element method for microstructure, properties and numerical simulation of steel materials.

Thermodynamic Modeling of Metal Hydrides: Workflows, Software, and Applications to Multicomponent Databases

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Metal hydrides are central to hydrogen storage, compression, and purification, yet predictive thermodynamic descriptions that transfer across structure families and multicomponent chemistries remain limited. In the hydrogen para-equilibrium regime, where hydrogen redistributes rapidly while the metal sublattice is compositionally frozen, robust Gibbs-energy models are essential to forecast hydrogen sorption properties.

We present two developed workflows, proven to enhance the thermodynamic modeling of multicomponent metal-hydrogen systems [1,2].

Because of the challenging para-equilibrium state, current programs and workflows are not suitable for the thermodynamic modeling of multicomponent metal hydrides. Additionally, the naturally complex site occupation behaviour of interstitial atoms demands a special treatment of the sublattice modeling in the compound-energy formalism (CEF) framework.

With our developed workflows we tackled these problems by creating open-source Python programs to model and optimize thermodynamic databases withing the CEF [2,3] and generate *ab initio* data to support and extend experimental findings [3].

By comparing, with unpublished data, the purely *ab initio* predicted sorption properties to 14 alloys of 8 relevant hydride structures, we show benefits and pitfalls of the developed workflow. Exchange-correlation functional dependencies, numerical accuracies, influences of chemical bonding types and isotope effects will be systematically revealed. Accuracies on the prediction of hydrogen capacities, equilibrium pressures and volume expansions will give a holistic picture of the accuracy of the workflow.

We show the application of these workflows on a multi-structure thermodynamic database that unifies first-principles energetics [1] and literature data [2]. The database spans multiple structure families (BCC/FCC, AB, AB_2 and AB_5) and covers more than ten technologically relevant elements.

For a long time, the bottleneck was not the physics but the missing machinery: without suitable programs and workflows, multicomponent para-equilibrium hydride thermodynamics remained out of reach. Now that the machinery exists and works, we can move from “can we?” to “how far?”, feeding it with advanced ab initio data and ML-driven potentials to explore composition-structure space faster and with sharper predictions.

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Biographical Note

Peter Hannappel is a materials scientist and PhD candidate at TU Dresden, working as a research fellow at Fraunhofer IFAM in Dresden. His research focuses on modeling and predicting the sorption properties of metal hydrides for hydrogen storage, compression, and purification, using tools like CALPHAD and DFT. He also explores integrating metal hydrides into PEM fuel cells to advance renewable energy technologies.

With international research stays in Italy and Korea, Peter has developed expertise in predictive modeling and programming, contributing to collaborative projects and impactful publications. His work reflects a commitment to driving the green energy transition through innovative hydrogen solutions.

PhaseForge: Automated CALPHAD-Compatible Phase Diagram Generation Using Universal Machine Learning Potentials

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The CALPHAD method has long served as the cornerstone for thermodynamic modeling and phase diagram prediction in materials science. However, traditional CALPHAD assessments face significant scalability challenges: fewer than 3% of possible ternary systems have been experimentally characterized, and expert-driven parameter optimization can require weeks to months per system. These limitations become particularly acute when exploring compositionally complex materials such as high-entropy alloys (HEAs), where vast chemical spaces remain thermodynamically uncharted.

We present *PhaseForge*, an open-source computational framework that bridges machine learning interatomic potentials (MLIPs) with CALPHAD-compatible thermodynamic modeling through integration with the Alloy Theoretic Automated Toolkit (ATAT). *PhaseForge* leverages our *MaterialsFramework* library to enable automated, high-throughput phase diagram generation across binary, ternary, and higher-order alloy systems with computational speedups exceeding three orders of magnitude compared to density functional theory (DFT) while maintaining DFT-level accuracy in phase stability predictions.

The framework supports multiple state-of-the-art universal MLIPs including eSEN, GRACE, MACE, SevenNet, and ORB, with comprehensive benchmarking revealing that certain models achieve accuracy approaching or matching DFT for formation energies and phase boundary predictions. *PhaseForge* automates structure sampling, vibrational free energy estimation via phonon calculations, and liquid phase modeling through molecular dynamics simulations. Critically, the workflow generates CALPHAD-style thermodynamic descriptions that can be integrated into existing databases and used with conventional CALPHAD software.

We demonstrate *PhaseForge*'s capabilities through case studies spanning binary systems (Cr-Mo, Cu-Au, Pt-W, Ni-Re, Cr-Ni) and multicomponent alloys including the quinary Co-Cr-Fe-Ni-V HEA system. Results show excellent agreement with experimental phase diagrams and traditional CALPHAD assessments, successfully predicting FCC, BCC, HCP, sigma phases, and intermetallic compounds with multi-sublattice structures. The framework accurately captures temperature-dependent phase boundaries, liquid phases, and miscibility gaps while enabling rapid exploration of composition-temperature space that would be prohibitively expensive with DFT.

PhaseForge also serves as a rigorous benchmarking platform for evaluating MLIP quality across diverse alloy chemistries and phase types. Its integration within CALPHAD workflows represents a paradigm shift toward high-throughput thermodynamic database development, enabling researchers to rapidly explore composition spaces previously inaccessible due to resource constraints. This presentation will discuss validation studies against experimental data and traditional assessments, current limitations, and future directions for MLIP-driven CALPHAD database expansion.

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Biographical Note

Doğuhan Sarıtürk is a Ph.D. candidate in Materials Science & Engineering at Texas A&M University, advised by Prof. Raymundo Arróyave. His research integrates MLIPs with CALPHAD-based thermodynamic modeling for accelerated alloy design. He is the lead developer and maintainer of several open-source software platforms, including *PhaseForge* for automated CALPHAD-compatible phase diagram generation and *MaterialsFramework*, for deploying and benchmarking universal MLIPs across diverse alloy systems. He holds an M.S. in Metallurgical and Materials Engineering from Middle East Technical University (METU).

Web-Based APIs for Automated Thermodynamic Property Generation: MAPP and SLUSCHI

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As thermodynamic modeling expands to increasingly complex materials systems, scalable and reproducible data generation has become a critical need for the CALPHAD community. In this work, we present web-based application programming interfaces (APIs) that expose advanced computational tools as accessible, programmatically controlled services. These include MAPP [1], a deep-learning–based property prediction framework for rapid screening across chemical space, and SLUSCHI, a first-principles molecular dynamics engine for entropy and high-temperature thermodynamic calculations.

Rather than requiring local installation and workflow engineering, users interact with these tools through RESTful APIs that enable remote job submission, monitoring, data retrieval, and integration into automated pipelines. The API layer standardizes input and output schemas, enforces reproducible workflows, and facilitates scalable thermodynamic data generation.

The API framework exposes a broad set of thermodynamic and structural analysis capabilities implemented in SLUSCHI, including entropy evaluation via single-trajectory molecular dynamics (MDS) [2] and information-entropy-based ASDF methods [3], atomic diffusivity calculations [4], bond valence sum (BVS) analysis, and automated space-group identification. By standardizing these high-temperature property calculations into reproducible API endpoints, the system enables consistent generation of thermodynamic and structural data for CALPHAD modeling and database development.

Representative case studies demonstrate how these APIs support automated thermodynamic assessment and CALPHAD-oriented data generation. The presentation will highlight practical workflows and their role in scalable thermodynamic database development.

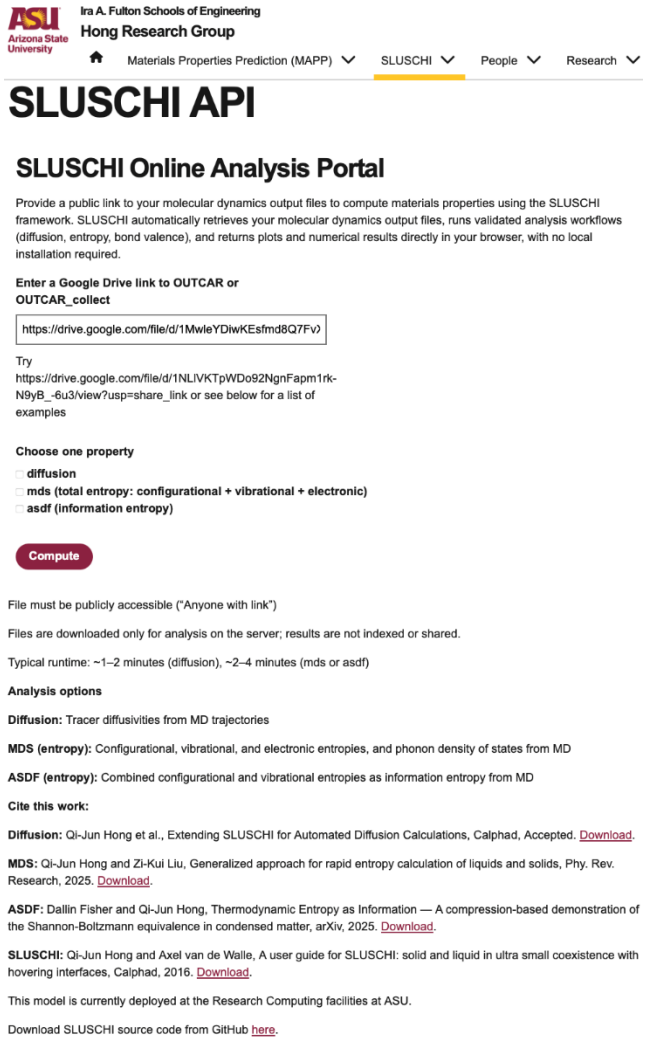

Figure 1. Web interface of the SLUSCHI API platform, enabling remote submission and management of first-principles molecular dynamics and entropy calculations for thermodynamic property generation

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Biographical Note

Qi-Jun Hong is an Assistant Professor of Materials Science and Engineering at Arizona State University. Hong received his Ph.D. in Chemistry from the Caltech in 2015. Before joining ASU, Hong was a Postdoc at Brown University and a Machine Learning Scientist at Amazon.com, Inc.

Building Interoperable CALPHAD Workflows: ThermML and Calphad Optimizer 3.0

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The rapid evolution of generative artificial intelligence (genAI) stimulates wide-ranging discussions across scientific and engineering communities regarding competitive advantage and intellectual differentiation. The computational thermodynamics and materials design domain rests upon decades of carefully assessed thermodynamic databases, physically grounded models, and rigorous scientific optimization workflows. However, traditional database formats (TDB, FactSage, ChemApp) rely on implicit conventions and positional syntax while lacking structured comments or metadata that machines can reliably parse. Thus, there is no reliable way to encode relationships between phases, species, parameters, and assessment metadata, limiting interoperability, automated validation, and AI integration. As genAI systems become increasingly capable of code and data synthesis, literature summarization, and data-driven hypothesis generation or tool-calling, the enduring value in CALPHAD tools shifts from algorithms to curated data, semantic structure, interoperability, and reproducible workflows.

This work demonstrates how the updated ThermML XML specification and updated Calphad Optimizer 3.0 software address these challenges [1, 2]. ThermML provides a semantically explicit database format where thermodynamic models are formally defined and annotated. We will demonstrate conversion of legacy FactSage (and TDB, through conversion with FactSage) databases to ThermML, showcasing how semantic annotation enables automated consistency checking, provenance tracking, and machine-readable documentation. ThermML preserves human access and long-term stability while allowing machine interpretability.

We present case studies demonstrating new Calphad Optimizer 3.0 workflows, including reproducible parameter assessments, and multi-format database export. Practical examples will illustrate how optimization histories can be audited, extended, and traced to human or generative data sources without loss of semantic fidelity. In a landscape where genAI may generate candidate models or suggest parameter updates, this provides necessary safeguards while enabling productive human-AI collaboration.

The CALPHAD community has historically advanced through published assessments, and incremental refinement of databases. This work is presented to invite discussion on pathways for community adoption and the evolving role of semantic infrastructure in the AI era.

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Biographical Note

Florian Tang is a Computational Material Scientist that has not worked with materials for a very long time, but rather spends his time at GTT Technologies developing tools to remove friction for the Calphad community. He previously learned the arts of assessments during his PhD with Bengt Hallstedt on modeling High Manganese Steels, but does not think he'll ever get back into working on actual data again.

FactFlow-Assisted Optimization of Aluminum Recycling Processing Balancing Economic Performance, Product Quality, and Environmental Impact

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Aluminum recycling from compositionally complex scrap requires simultaneous control of product specifications, metallurgical quality, process efficiency, economic performance, and environmental impact. This challenge is particularly important for mixed wrought scrap, where refining decisions affect impurity levels, alloy chemistry, phase constitution, reagent use, energy demand, off-gas generation, and the need for make-up additions to reach the target material. These factors collectively determine material quality, environmental impact, and overall process cost. Computational thermochemistry is essential for materials design and process optimization, offering insights into phase stability and chemical equilibria. However, current workflows often treat thermodynamic chemistry, process simulation, product-quality targets, Life Cycle Assessment (LCA), and economic considerations separately, making integrated evaluation difficult.

This study presents a FactFlow-based methodology for the evaluation and optimization of aluminum recycling routes. FactFlow is a thermodynamics-driven process-simulation interface coupled to the FactSage databases, enabling full multiphase equilibrium calculations at the unit-operation level together with stream-based mass and energy balances across the full flowsheet [1]. The framework can also be coupled to LCA inventory data to compare process scenarios using both metallurgical and sustainability criteria. In addition to conventional outputs such as phase assemblages, stream compositions, and enthalpy changes, process options can be ranked using user-defined performance indicators, including the Energy Processing Performance Index (EPPI, Γ) and CO2 Processing Performance Index (CPPI, ζ) [2].

A representative post-sorting aluminum recycling route is considered for mixed wrought scrap upgrading, including selective impurity removal and purification steps followed, where necessary, by final composition adjustment to meet product specifications and metallurgical targets [3]. The approach is designed to compare alternative refining strategies and identify favorable operating windows while accounting for trade-offs between product quality, process requirements, economic considerations, energy use, and CO2 impact. The analysis is carried out at the full-flowsheet level because the most effective purification step does not necessarily lead to the best overall recycling route once downstream processing requirements, make-up additions, and life-cycle-related effects are also considered.

The results demonstrate how thermodynamics-based flowsheet simulation can be used to screen aluminum recycling process concepts, reveal the main levers influencing metallurgical, environmental, and economic factors, and provide a rigorous basis for comparing alternative purification strategies under multiple criteria. More broadly, this work highlights the value of integrating thermodynamic process simulation, flowsheet-level analysis, LCA coupling, and user-defined performance indicators to support the design of more sustainable aluminum recycling routes.

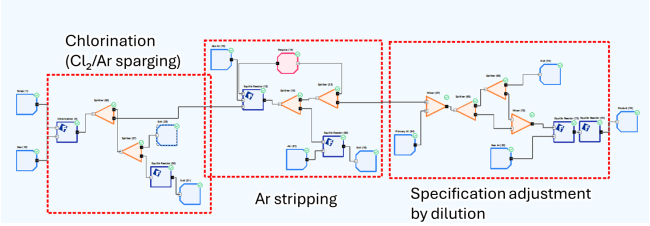

Figure 1. Example aluminum purification route modeled in FactFlow

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Development of a Modified Polyhedron Model for Improved Estimation of Thermodynamic Properties of Mixed Oxides

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The Polyhedron Model (PM) is based on the assumption that ionic compounds can be decomposed into invariant polyhedra consisting of a central cation surrounded by anions. The thermodynamic properties of a compound are then estimated by summing the contributions of these constituent polyhedra obtained through linear regression [1]. This approach is particularly advantageous for oxide systems where experimental data are limited or unavailable. The PM is valued for its simplicity and extrapolation capability, and previous modifications have incorporated effects such as cation site and magnetic order-disorder transitions [2]. However, the model still neglects important non-vibrational contributions, such as second-nearest-neighbor interactions, polyhedra distortion, and inter-polyhedra linkage [3].

To address these limitations, the present work introduces a next-generation framework, referred to as the Modified Polyhedron Model (MPM). The MPM integrates artificial neural networks (ANNs) with the classical PM to capture the contributions that are not explicitly considered in the original formulation. In this approach, the residuals obtained from the PM are used as inputs to the neural network, enabling the model to account for missing physical effects.

A dataset comprising 160 compounds within the Li–Na–K–Ca–Mg–Fe–Al–Ti–Si–O system was used, classified into 18 distinct polyhedra. Residual analysis confirms that the MPM consistently outperforms the PM. The MPM reduces the root mean square error (RMSE) by approximately 40% for enthalpy and 34% for entropy compared to the original PM, indicating a substantial enhancement in predictive accuracy. These improvements arise from the incorporation of previously neglected contributions through a nonlinear regression framework implemented via the ANNs. Comparisons with the Neumann–Kopp rule (NKR), the original PM, and experimental data further validate the improved performance of the MPM.

Overall, the MPM demonstrates strong potential as a predictive tool for thermodynamic properties of complex oxide systems; however, continued refinement is necessary. Future work should extend the MPM to predict heat capacity. Addressing discrepancies in Ti- and Mn-bearing systems is also required, which requires a broader dataset encompassing multiple oxidation states (Ti^{3+}, Ti^{4+}, Mn^{2+}, Mn^{4+}). Incorporating additional descriptors, such as molar volume—which is strongly correlated with entropy but currently not sufficiently represented—could further enhance the prediction accuracy. As a data-driven approach, the MPM would also benefit from an expanded training set covering a wider range of compounds and polyhedra configurations; however, this is currently limited by the scarcity of experimental data.

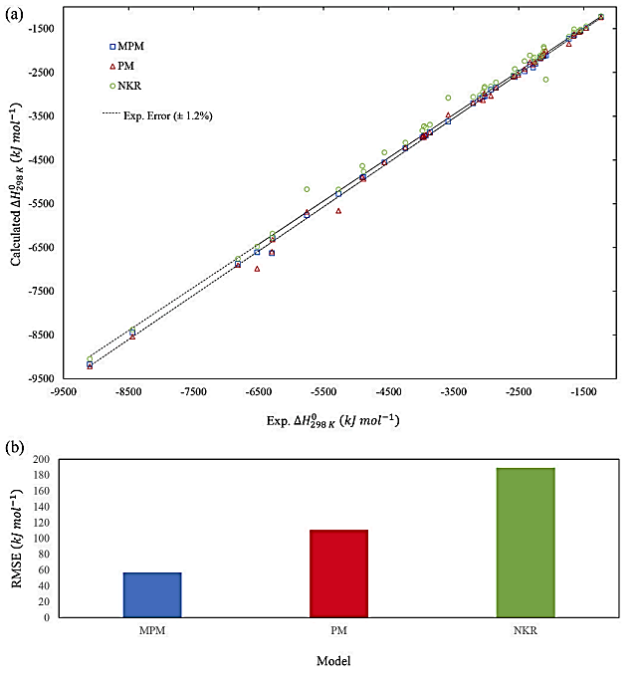

Figure 1. Comparison of enthalpy of formation calculations for mixed oxides from MPM and PM with experimental values: (a) scatter plot, (b) RMSE metric (values from NKR are also plotted)

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CALPHAD-driven discovery and rapid experimental validation of low-cost, high-strength, Al-alloys for additive manufacturing

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Keywords: Additive manufacturing, CALPHAD-based ICME modeling, Alloy design, Machine Learning

Aluminum (Al) alloys are widely used in structural components (e.g. chassis, body parts) for aerospace and automotive industries due to their high strength-to-density ratio. However, they experience a significant loss of strength at elevated temperatures (150-400°C), limiting their use in components such as intake fan blades, vacuum pumps, and combustion engine pistons. Enhancing strength and slowing coarsening behavior at elevated temperatures is required to bridge this gap. Exploiting rapid solidification in laser-based additive manufacturing (AM) is a pathway to achieving high strength. Rapid solidification promotes microstructural length-scale refinement and precipitation of metastable phases. An Al-alloy was developed to exploit these behaviors, forming coarsening resistant nanoscale $L1_2$ precipitates from a metastable ternary precursor. This benchmark alloy demonstrated high strength and coarsening resistance at elevated temperatures (up to 400°C) but requires high cost and criticality elements. To identify candidate substitute alloys which retains this performance while lowering cost, we used high-throughput calculation of phase diagram (CALPHAD)-based integrated computational materials engineering (ICME) techniques and Bayesian optimization to efficiently explore our alloy design space. Through this design pipeline, three candidate alloys were identified: (1) a coarsening resistant alloy replicating the ternary-to-$L1_2$ transformation, predicted to retain 95% of strength with 10% cost reduction; (2) a high room-temperature strength alloy that maximizes metastable phase fraction to achieve 60% strength enhancement and 20% lower cost; (3) an extreme low cost, room-temperature alloy which exploits metastable phase formation to . The three candidate alloys were validated using a rapid experimental workflow of preparing homogeneous samples via induction melting, and laser scanning to replicate the as-printed AM environment. This workflow verified the strength of the alloys and the microstructural features predicted by CALPHAD-based ICME techniques (ternary and $L1_2$ phases).

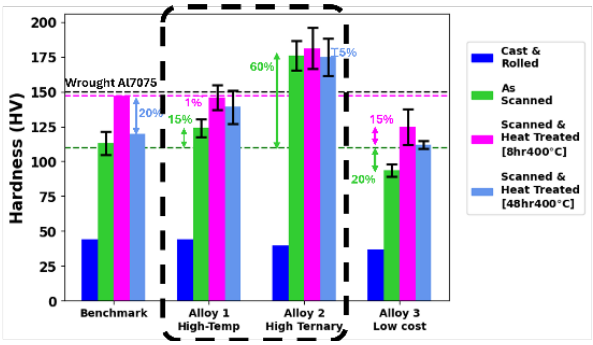

Figure 1. Hardness of custom alloy designs exploiting ternary and $L1_2$ features in as-cast, as-scanned and heat treated conditions compared to the benchmark alloy.[2] The high-temperature stable design exhibits 99% of the benchmark alloys strength in peak-aged (8 hours at 400°C) conditions, while the high-ternary achieved a 60% increase in hardness and retained this performance after prolonged heat treatment (48 hours at 400°C)

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Biographical Note

Benjamin Glaser is currently pursuing a PhD in Materials Science & Engineering at Carnegie Mellon University (CMU). His previous degrees include: Bachelor's in Materials Science & Engineering and Engineering & Public Policy, and Master's in Computational Materials Science from CMU. Benjamin is advised by Prof. S. Mohadeseh Taheri-Mousavi.

Thermodynamic modeling of the Al-rich Al-B system with LIBS/DSC *Liquidus* measurements

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The Al-rich Al-B system is relevant for industrial boron treatment of aluminum alloys; however, it remains inadequately described, with the *Liquidus* L/(L + AlB_2) phase boundary constrained by sparse and inconsistent data in earlier thermodynamic assessments [1,2]. Moreover, recent *Liquidus* measurements via liquid-phase laser-induced breakdown spectroscopy (LP-LIBS) reveal systematic deviations compared to thermodynamic predictions using commercial thermochemical packages. In this work, a revised CALPHAD description is presented, resolving these discrepancies through an integrated experimental-computational approach.

Numerically, Density functional theory (DFT) calculations were employed to determine the 0 K formation enthalpy of the AlB_2 compound, as well as to derive its heat capacity (C_p) via the self-consistent quasi-harmonic approach (QHA) by Jofré et al. [3]. For AlB_{12} (an intermediate phase between AlB_2 and pure B), the C_p was calculated using the modified Neumann-Kopp rule (modified NKR), informed by the DFT-based C_p of AlB_2. Experimentally, *Liquidus* data for the L/(L + AlB_2) phase boundary was obtained using LP-LIBS and differential scanning calorimetry (DSC). LP-LIBS has gained popularity as a reliable method for mapping the Al-rich *Liquidus* of binary systems, where the alloying element is present in low concentration and when cooling rates of 1 K/min are employed [4].

Finally, the numerical and experimental data were used for the Al-B thermodynamic modeling, employing the compound energy formalism (CEF) to describe the AlB_2 and AlB_{12} compounds and the modified quasichemical model (MQM) for the liquid phase. The resulting assessment provides a consistent and experimentally validated description of the L/(L + AlB_2) phase boundary, resolving prior ambiguities in the Al-rich Al-B system and establishing a reliable foundation for modeling multicomponent Al-B-TM (TM = Ti, V, Zr) systems.

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Comparative Assessment of Crack Susceptibility Criteria Using Calphad Solidification Modeling and Graded Thermal Experiments

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Solidification cracking is a major constraint in additive manufacturing and aluminum alloy casting, yet the predictive accuracy and comparative performance of existing crack susceptibility criteria (CSC) remain insufficiently understood. In this study, five widely used CSC models are systematically evaluated using solidification paths computed via Calphad under both Classic Scheil and Back-Diffusion Scheil assumptions. To strengthen predictive fidelity, key microstructural and solidification metrics, including secondary dendrite arm spacing (SDAS), stable phase formation, and local cooling rates, were experimentally measured at multiple locations within thermally graded samples produced using a newly developed wedge-shaped copper mold.

The predictive capability of each CSC model was assessed based on its ability to (i) capture the composition corresponding to peak cracking susceptibility and (ii) accurately identify crack-free composition windows. Three alloy systems of broad industrial significance, Al–Cu, Al–Si, and Al–Mg, were investigated. Results show that the Back-Diffusion Scheil approach, when coupled with experimental thermal–microstructural data, provides improved prediction of crack-free compositions and solidification phase evolution, particularly segregation behavior. Conversely, the Classic Scheil model more effectively predicts the location of peak CSC. Among all models assessed, the sRDG criterion demonstrates the best overall agreement with experimental observations across both crack-free regions and peak susceptibility compositions.

As shown in Fig. 1, this work introduces the wedge-shaped copper mold as a high-throughput experimental platform for generating controlled thermal gradients to systematically evaluate cracking susceptibility. The combined experimental–computational framework presented here offers a robust pathway toward more reliable prediction of hot tearing and supports accelerated alloy design for advanced manufacturing technologies.

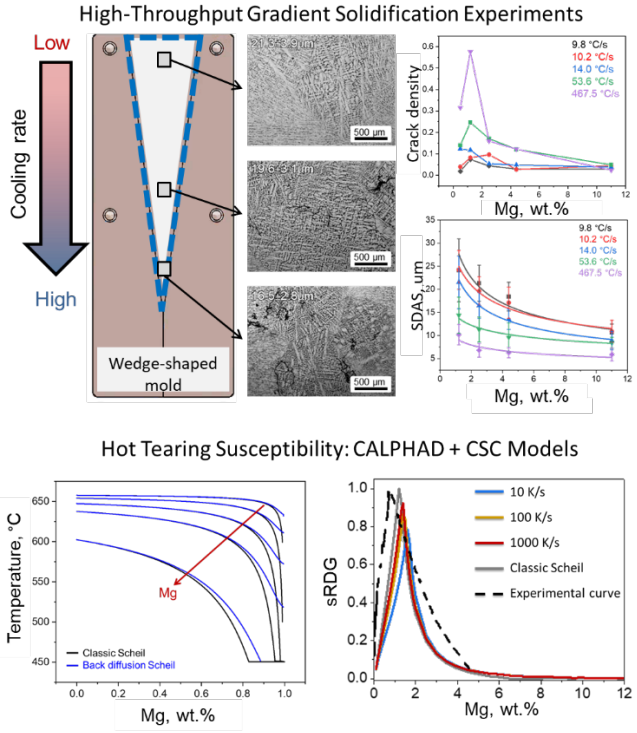

Figure 1. High-throughput experiment using the wedge-shaped mold cast to support Calphad-based CSC prediction

Biographical Note

Prof. Wei Xiong leads the Physical Metallurgy and Materials Design (PMMD) Laboratory at the University of Pittsburgh. His interests cover Calphad-based design, integrated computational materials engineering, high-throughput experiments, and advanced materials design and deployment. He received his PhD from KTH Royal Institute of Technology and conducted postdoctoral research at the University of Wisconsin-Madison and Northwestern University before starting his research group at Pitt in 2016.

Acknowledgements

Wei Xiong acknowledges funding from the National Science Foundation under the Faculty Early Career Development Award: CMMI 2047218.

Molecular dynamics (MD) simulations of the nucleation of aluminum on TiB_2 interfaces with equivariant machine learning interatomic potentials (MLIAP)

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Hot cracking is a common defect in cast aluminum alloys. Grain refinement, typically achieved through the addition of Ti and TiB_2, is an effective mitigation strategy, yet the nucleation mechanisms at the TiB_2 interface remain poorly understood. The presence of solute elements modifies the grain refinement efficiency of TiB_2, making experimental work covering all the relevant compositions very tedious.

Classical interatomic potentials cannot reliably predict energies and forces across the range of phases and compositions relevant to this problem. First-principles density functional theory (DFT) provides the necessary accuracy but remains limited to system sizes below those required to capture realistic nucleation events. Machine learning interatomic potentials (MLIAPs) bridge this gap, reproducing near-DFT accuracy at a fraction of the computational cost, enabling the large-scale molecular dynamics (MD) simulations necessary for this study.

In this work, structures within the Al-Ti-B-Si system are generated using the automated small symmetric structure training (ASSYST) package and the atomic simulation environment (ASE), covering ordered and disordered crystals, bulk solids, liquids, surfaces, and interfacial configurations. High-throughput DFT calculations, launched with the pyiron software, are performed using the r²SCAN meta-GGA functional to build a diverse reference dataset. Multiple Allegro equivariant MLIAPs are then trained on this dataset, and used to select additional training frames in an iterative active learning procedure. Preliminary large-scale MD results demonstrate the poisoning effects of Si on TiB_2.

CALPHAD assisted microstructural design to control precipitate and dispersoid evolution for improved strengthening in Al-Mg-Si-based alloys

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The mechanical behaviour and strengthening of Al-Mg-Si-based alloys strongly rely on the microstructural landscape with multiscale, multiphase precipitates. Over the years, studies on Al-Mg-Si-based alloys have mainly focused on incorporating elements that form additional nanoscale secondary precipitates alongside the primary β" precipitate to improve strength. These approaches, although effective for strengthening, lack high-temperature stability and fail to suppress recrystallization and grain growth during hot forming operations. A microstructural landscape that accommodates multiphase, multiscale precipitates, and provides similar or better strength with high-temperature stability, and grain control during any hot forming process is thus highly desirable. This study proposes a new CALPHAD guided design approach for Al-Mg-Si based alloy compositions that effectively integrates primary precipitates along with dispersoids for better strengthening and high temperature microstructural stability. A composition with tailored heat treatment schedules is designed and optimized in a way that results in a uniform and effective precipitation of thermally stable dispersoids along with high yield of primary β" precipitates. The designed composition is experimentally characterized to assess mechanical properties and to study microstructure with various predicted phase stability following simulation guided heat treatments. A comparative analysis with the popular commercial EN-AW 6082 alloy validates that the designed composition achieves a higher strength while retaining good ductility.

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Biographical Note

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Thermodynamics and Diffusion Kinetics in Mn_2Ti-type Hydrogen Storage Alloys

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C14 $Mn_{2-x}Ti$-type alloys are considered promising for hydrogen storage with their favorable hydrogenation kinetics. However, their thermodynamic properties during hydrogenation cannot be easily predicted since their thermodynamics has not been modeled. Further, although correlations between hydrogen diffusion and cell volume, alloy composition or lattice distortion have been mentioned, detailed mechanisms explaining how these factors influence hydrogen diffusion have not been clearly elucidated.

Here, we present a CALPHAD-type thermodynamic description of the C14 $Mn_{2-x}Ti$-H system [1]. Through a thermodynamic calculation on metastable phase equilibria, a possible range of compositional variation (range of x value in $Mn_{2-x}Ti$) could be proposed.

To investigate the diffusion mechanisms, we employed a molecular dynamics simulation, based on a newly developed machine learning interatomic potential [2]. Through a diffusion simulation, we could clarify that there is no correlation between cell volume and hydrogen diffusion. The effect of alloy composition (x value in $Mn_{2-x}Ti$) could also be clarified in term of lattice distortion and hydrogen trapping by anti-site Ti atoms.

The present work provides a basis for thermodynamic modeling of hydrogenation in multicomponent C14 alloys and a guide efficient design of hydrogen storage materials based on C14 alloys with comprehensive understanding on the hydrogen diffusion behavior.

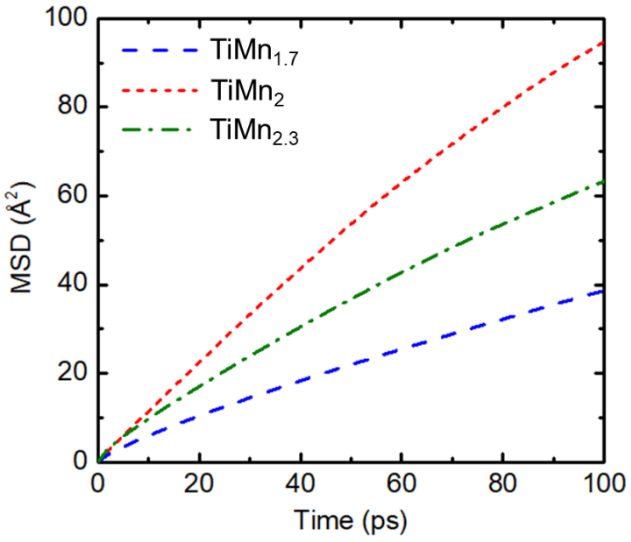

Figure 1. Mean squared displacement of hydrogen in $TiMn_{1.7}$, $TiMn_2$ and $TiMn_{2.3}$ at 500 K

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Biographical Note
Byeong-Joo Lee is a professor at the department of materials science and engineering, Pohang University of Science and Technology (POSTECH), Korea. He developed TCFE2000, a seed version of TCFE thermodynamic database series and the 2NN MEAM (second nearest neighbor MEAM) interatomic potential formalism.

Incorporation of molar volumes of diffusing elements in Onsager-type formulations of diffusion in alloys

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A precise modeling of diffusion phenomena, as a pivotal subject in material science, is a key for design and discovery of new alloys. Therefore, there has always been efforts to extend the diffusion models to account for all contributing factors based on accurate experimental data. One of the important factors that has been neglected in many models of diffusion are composition-dependent partial molar volumes of diffusing elements. In fact, in most of current models the molar volumes parameters are considered constant and equal values for all elements.

One promising way of modeling disunion is using a thermodynamically consistent framework based on the Onsager formalism coupled with CALPHAD-based thermodynamics and atomic mobility data. This approach is grounded in the phenomenological transport equations, where fluxes are related to chemical potential gradients through a matrix of Onsager mobility coefficients that satisfy reciprocity relations. A very practical application of this formulation is already used in Thermocalc software based on the pioneer works of Agren [1]. However most of those CALPHAD-based models neglect the effect of molar volume of elements.

The current methodology in this work, as depicted in figure 1, extend the current Onsager formulations incorporating the impact of variable partial molar volume of chemical elements. The resulting framework captures cross-diffusion effects, vacancy-mediated transport, and stress-free volume constraints in binary and multicomponent alloys. Numerical implementation demonstrates that accounting for partial molar volumes significantly affects predicted interdiffusion paths, especially in systems with large atomic size mismatch as FeGa.

Additionally, the diffusion models are coupled with phases field models of microstructure evolution in Ni-based superalloys. The stress arising due to change of molar volumes of elements as well as phases are considered in this way too. The proposed approach strengthens the predictive capability of diffusion simulations and provides a physically consistent basis for coupling thermodynamics, mobility databases, and phase-field modeling in advanced alloy design.

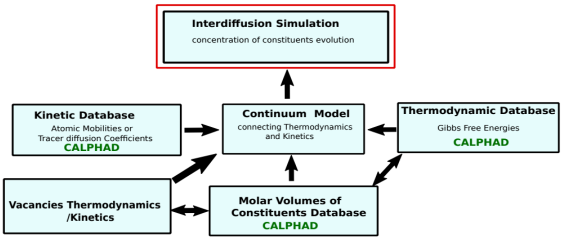

Figure 1. Schematic representation of the present CALPHAD-based methodology

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Dr. Ahmadreza Riyahi khorasgani is a Postdoc at Ruhr- University Bochum, Germany. His research interests focus on applying CALPHAD, phase field and continuum models for simulation of diffusion phenomena in complex alloys.

The Thermodynamics of Planar Defects in Magnesium Alloys

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The design of lattice defects is crucial for tailoring structural and functional materials properties. To this end, the knowledge-driven framework of defect phase diagrams (DPDs) offers a powerful approach to evaluate and understand chemical trends for bulk and defect phase stabilities as well as their competition. First, the insights from the ab-initio high-throughput segregation study to analyze grain boundary (GB) phase stabilities in Mg for elements across the periodic table are discussed. The preference of A and T type GB phases turns out to be dependent on the filling of electronic shells rather than atomic size. Selecting a few representative elements, binary DPDs for the GB are constructed to predict site-selective segregation trends, defect phase transformations and the relative stabilities in competition with bulk phases. The predictions show a very good agreement with the experimental datasets.

Extending DPDs to other planar defects in Mg, an integrated DPD is constructed to evaluate Ga-induced defect phase stabilities and assess their influence on deformation. The findings show that under equilibrium conditions, GB has a stronger influence on deformation compared to other planar defects. Following this, the temperature-dependent partial GB site occupations and chemical trends are explored using a sub-lattice based model and implication in the deformation behaviour are discussed. The findings from this model provide insights into the defect phase transformation process and solute-solute interactions. Finally, to facilitate the incorporation of defects into the CALPHAD methodology, a new approach to determine characteristic defect width using solute distribution probabilities and solute excess is presented.

A predictive surface tension for liquid metallic solutions

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Surface tension is a fundamental physical property that is essential for understanding surface and interfacial phenomena. Since Butler proposed a fundamental surface tension model in 1932, many surface tension models have been developed. However, they require empirical parameters and often fail for non-ideal solutions. In this study, a predictive surface tension model for binary liquid metallic solutions based on surface tension data of unary metals and thermodynamic property of binary bulk solution without any empirical model parameter was developed.

The present model calculates surface composition depending on bulk composition and temperature, determining the surface tension of the binary liquid solution as a linear summation of the surface energy of each surface component. We have tested the present model for 50 binary metallic systems where experimental data are available and confirmed the good reproducibility of all reliable surface tension experimental results. The model was further expanded to ternary and multicomponent system to calculate the surface tension of any multicomponent system.

The present model shall be used to calculate surface properties, such as surface energy, tension, and compositional segregation in metallic systems, essential for interfacial reactions and the thermodynamic stability of nano-metallic materials.

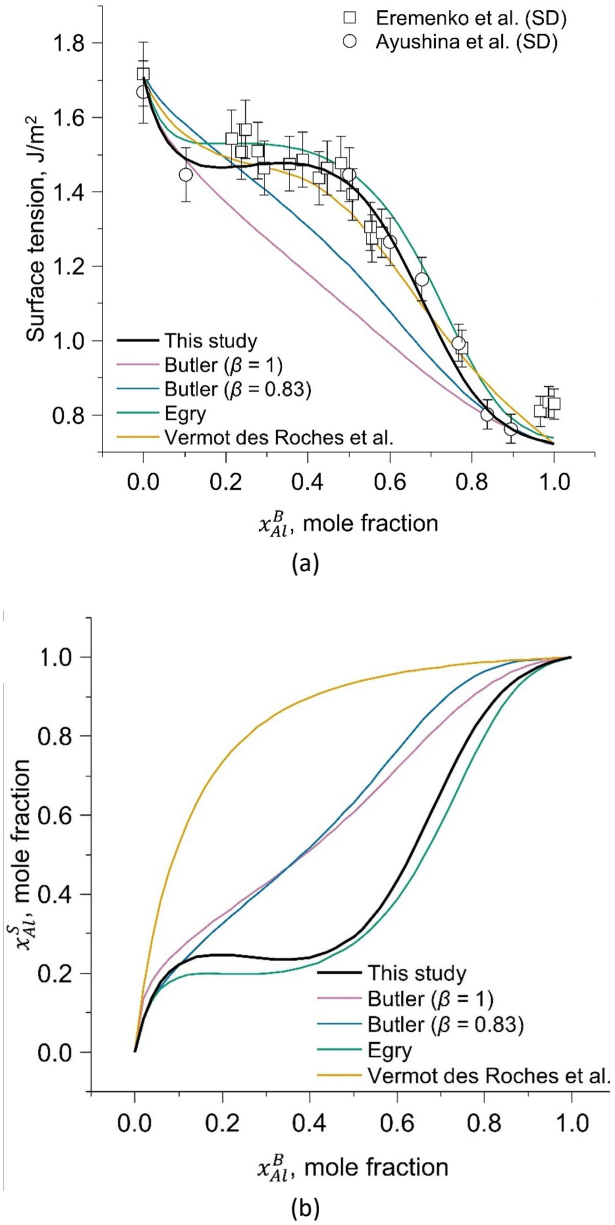

Figure 1. Comparison of experimental surface tension data and calculated results from various models for Al-Ni liquid solution at 1640 °C. (a) Surface tension and (b) surface segregation

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In-Ho Jung is a Professor at Seoul National University, South Korea, and the co-developer of FactSage software. His main research area is the thermodynamic and physical property database development and its application to materials design and process optimization.

Physics-based Thermal Conductivity Model Compatible with Multi-component CALPHAD Descriptions

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Thermal conductivity is a critical thermophysical property for materials used in semiconductor manufacturing applications such as wafer tables and packaging substrates [1, 2]. However, there is still a need for reliable thermal conductivity models for complex multicomponent alloys, creating a challenge for using digital twins to reliably simulate thermal behavior in semiconductor manufacturing. In this work, we developed a physics-based model that links thermal conductivity to phase constitution and composition data provided by CALPHAD.

This model has been validated in multiple unary (Ag, Al, Au, Cu, Mg, Pd, Si, SiC, Zn) and binary systems (Ag-Pd, Al-Cu, Al-Mg, Al-Si, Al-Zn) and predicts thermal conductivity across wide temperature and composition ranges by accounting for phase and composition effects. It is also readily applicable to multi-component systems. Specifically for Al-X binary systems, multiple measurements were conducted at NIST using thermoreflectance optical methods to provide reliable data for thermal conductivity modeling. The primary modeling effort was focused on describing solid solution phases since their cryogenic and elevated temperature behaviors change drastically compared with pure elements.

This approach facilitates future development of thermal conductivity model and database within the CALPHAD framework and enables improved design and qualification of advanced materials for thermal management.

This work was performed with funding from the CHIPS Metrology Program, part of CHIPS for America, National Institute of Standards and Technology, and U.S. Department of Commerce.

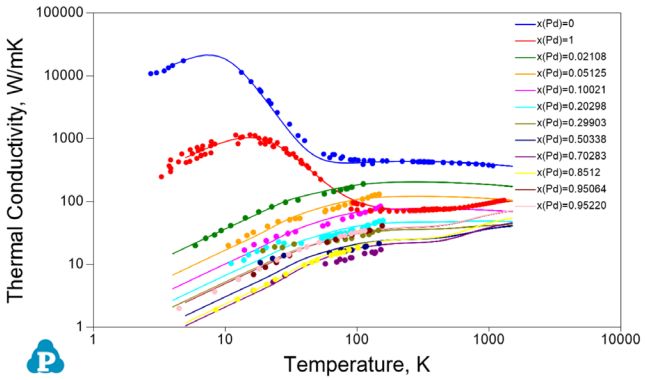

Figure 1. Comparison between experimental and calculated thermal conductivities in Ag-Pd binary system

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Biographical Note

Dr. Zhi Liang is a Material Scientist at the National Institute of Standards and Technology (NIST). His research focuses on the modeling of thermodynamic and thermophysical properties in semiconductor manufacturing applications sponsored by CHIPS Metrology Program at NIST.

Modelling Na–Mn–O cathodes and predicting cathode–electrolyte interface reactions for sodium-ion batteries

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Sodium-ion batteries represent a promising, sustainable, and lower-cost alternative to lithium-ion batteries. Computational materials engineering provides fundamental insights into the phase stability of cathode oxides as a function of temperature, composition, oxygen partial pressure (reflecting the thermodynamic redox stability of functional materials), and defect chemistry [1].

Optimisation of cathode materials involves identifying and describing realisable crystal structures [2] that differ in their charge-carrier transport properties and in their susceptibility to undesired phenomena, such as Jahn–Teller distortions associated with Mn valence states [3].

This work establishes a first comprehensive thermodynamic description of the Na–Mn–O system and therefore deepens the understanding of phase stability and phase transformations. As this ternary system forms the basis for more complex cathode materials, the insights obtained provide a foundation for improved materials design.

By comparing the thermodynamics of the cathode with that of advanced electrolyte systems [4], reaction trends at the cathode–electrolyte interface can be predicted using chemical potentials. This approach ultimately supports the optimisation of battery performance and durability.

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Erwin Povoden-Karadeniz is an Austrian materials scientist and Associate Professor of Computational Materials Engineering at the TU Wien (Vienna University of Technology). He studied earth sciences at the University of Graz and received his PhD in materials science from ETH Zurich in 2008. Since 2009 he has been affiliated with the Institute of Materials Science and Technology at TU Wien, where he leads the research group for Computational Materials Engineering. His research focuses on computer-assisted modelling and simulation of materials, particularly the thermodynamics and kinetics of phase transformations, diffusion processes, and microstructure evolution in sustainable multi-component materials.

Systematics and thermodynamic modeling of the AEO-B_2O_3 (AE = Mg, Ca, Sr, Ba) binary systems

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Alkaline Earth borates can be found in many applications, from glass science and earth science to single crystal growth. The binary systems are characterized by a complex short range order scheme in the liquid phase with a miscibility gap in the B_2O_3 rich section and a negative heat of mixing for Alkaline Earth rich compositions. Experimental information on phase diagrams is generally not very abundant. This is mainly due to experimental difficulties: volatilization of boron rich compositions, samples are generally hygroscopic and the liquid phase has a tendency to creep. In addition, melting temperatures can only be taken on heating due to the tendency for glass formation even at moderate cooling rates. Thermodynamic data is available for some compounds, but there is no systematic work in the literature to compare and evaluate the values as a function of the alkaline earth element involved.

This contribution aims to give a systematic overview over the AEO-B2O3 binary systems and its compound using theoretical calculations by DFT, key experiments and Calphad modeling of the binary systems.

DFT calculations were performed using VASP (version 6.3.2) and the SCAN / R2SCAN exchange correlation functional to determine the ground state properties of AE-borates at 0K as well as the temperature dependent properties using lattice dynamics (phonopy [1]). From these calculations, heats of formation at room temperature as well as heat capacities at constant volume were derived and compared to the available literature information.

Key experiments were performed on selected compositions to determine the phase equilibria with a focus on the CaO-B_2O_3 and SrO-B_2O_3 systems. For the first one, literature information from Carlson [2] is basically confirmed. For the second one, the observed equilibria in the SrO rich section of the diagram differ considerably from the available literature.

The thermodynamic modeling involves stoichiometric compounds and a complex liquid phase. The stoichiometric compounds are modeled with a multiple Einstein function to describe the heat capacity from 0K up to the melting point. The liquid phase was either described using the associate model [3], or with the modified quasi-chemical model (4] to take into account the short-range order and the change in the coordination of boron as a function of composition.

We will report on these new experimental and modeled data and a first result is reproduced in Fig. 1 for the CaO-B_2O_3 binary system. In addition, the observed systematics from MgO to BaO will be discussed for the solid compounds (structures, thermodynamic properties) and the evolution of the phase equilibria.

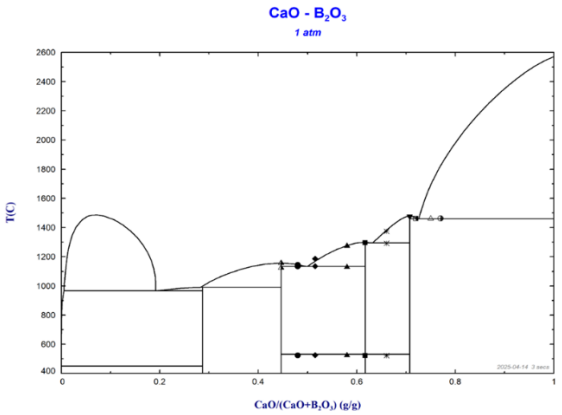

Figure 1. Calculated CaO-B_2O_3 binary phase diagram with new experimental data

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Revisiting RE-Ba-Cu-O Thermodynamics: From YBCO to Modern Gd- and Eu-Based Bulk Superconductors

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Nearly four decades after the discovery of high-temperature superconductivity in cuprates, RE-Ba-Cu-O (REBCO) systems remain at the forefront of applied superconducting materials. While $YBa_2Cu_3O_{7-\delta}$ (YBCO) established the structural and thermodynamic archetype of the RE-123 phase, modern single-domain bulk superconductors increasingly employ larger rare-earth elements such as Gd and Eu to enhance flux pinning and trapped-field performance.

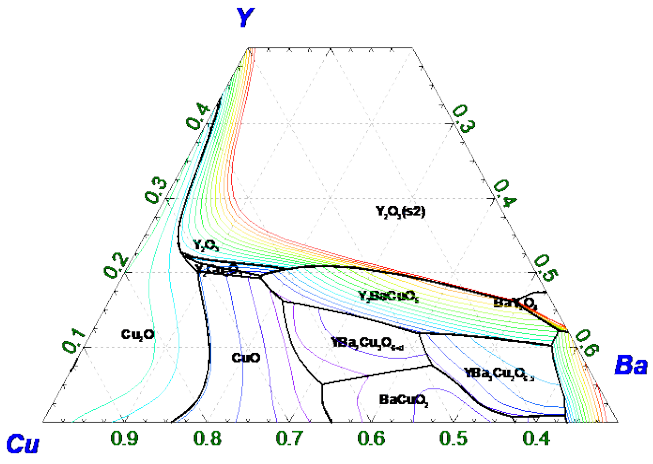
State-of-the-art bulk fabrication routes, including top-seeded melt growth (TSMG) and advanced seeded infiltration and growth techniques, rely critically on controlled solid–liquid equilibria [1]. The superconducting matrix phase $REBa_2Cu_3O_{7-\delta}$ (RE-123) forms peritectically from the RE_2BaCuO_5 (RE-211) phase and a complex oxide melt, while RE-211 inclusions act as intrinsic flux pinning centers [2]. Reliable thermodynamic descriptions of both the oxide melt and the oxygen non-stoichiometry of RE-123 are therefore essential for predictive process optimization. Applications of such materials include high-field trapped-flux magnets for compact MRI systems, magnetic levitation devices, and frictionless rotating machinery.

In this work, a thermodynamic assessment of the Gd-Ba-Cu-O and Eu-Ba-Cu-O systems is presented and systematically compared with the well-established Y-Ba-Cu-O reference system. The modeling strategy combines critically evaluated literature data of the relevant quasi-binary subsystems with new experimental thermodynamic data. The oxide liquid is described phenomenologically as a mixture of $REO_{1.5}$(l), BaO(l), and CuO_x(l), with CuO_x represented by the species Cu, CuO, and $CuO_{1.5}$, following earlier assessments of the Y–Ba–Cu–O system (see Fig.1) [3]. In contrast, the oxygen non-stoichiometry of the RE-123 phase is treated within the compound energy formalism, allowing a thermodynamically consistent description under variable oxygen content as a function of temperature and oxygen activity in the surrounding atmosphere. The variable oxygen content in the CuO_x chains is charge compensated by redox adjustments of copper in both the CuO_2 planes and the chain sites, reflecting the coupled $Cu^{+}/Cu^{2+}/Cu^{3+}$ equilibria.

The thermodynamic properties of the RE-123 phase incorporate literature data and new calorimetric measurements, including low-temperature heat capacity (PPMS) on oxygen-saturated samples and DSC/TGA experiments performed under controlled oxygen partial pressures. The enthalpy and entropy changes associated with oxygen incorporation/release are explicitly implemented, enabling a consistent description of oxygen non-stoichiometry under fixed oxygen activity.

Calculated phase equilibria are presented as quasi-ternary RE-Ba-Cu isoactivity (pO_2= 0.21, 1) and isothermal sections, as well as liquidus projections, with particular emphasis on the primary crystallization field of RE-123 and its peritectic reaction to RE-211. The comparative analysis elucidates systematic rare-earth effects on melt stability, peritectic temperatures, and processing windows relevant for single-domain bulk growth.

Figure 1. Liquidus projection of the Y-Ba-Cu-O phase diagram at fixed oxygen activity ()



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Thermodynamic Database Development for the Al_2O_3–CaO–MgO–SiO_2–Fe_2O_3–FeO System and Its Application to Industrial Solid-Waste Utilization

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In China, large quantities of bulk industrial solid wastes (e.g., steel slag, red mud, fly ash, and tailings) are generated every year, and their improper stockpiling and disposal can cause significant environmental and safety issues. Resource utilization (valorization) is therefore a key pathway to mitigate these hazards while enabling waste reduction and value creation. However, the large-scale deployment of solid-waste valorization is still constrained by an insufficient quantitative understanding of phase equilibria and phase-transformation pathways in the multicomponent oxide systems [1-2]. In this context, the Al_2O_3–CaO–MgO–SiO_2–Fe_2O_3–FeO system, as the major component of industrial solid wastes, plays a crucial role. Systematic phase equilibria and thermodynamic investigation of this system are of significant theoretical importance for advancing the utilization of solid waste resources.

In this work, the ionic two-sublattice model was applied to describe the short-range ordering behavior in the liquid phase of oxide systems, while the sublattice model based on compound energy formalism were used to capture ion occupation and crystalline characteristics in complex mineral phases. Thermodynamic database construction follows a rigorous bottom-up strategy. First, thermodynamic descriptions of binary subsystems reported in the literature were systematically reviewed, and three key binary systems were reassessed to remove artifacts include unrealistic high-temperature miscibility gaps and inconsistent pure component definitions in liquid models. Second, phase diagram and thermodynamic property measurements were conducted for key ternary subsystems. Together with selected experimental data from literature, eight ternary subsystems were assessed based on reliable thermodynamic descriptions of binary systems. Finally, thermodynamic descriptions of all subsystem (15 binary systems and 20 ternary systems) were integrated, and multicomponent interaction parameters were adjusted to establish the multicomponent aluminosilicate database. The reliability and accuracy of the resulting database were validated through extrapolated calculations across multicomponent composition spaces.

To demonstrate engineering relevance with solid waste utilization, the obtained database was applied to two representative high-temperature product systems incorporating waste-derived oxides: cement clinker and cordierite-based refractories. For the clinker compositions, thermodynamic calculations clarified how Fe_2O_3 and MgO regulate the firing window, liquid fraction, and mineral phase composition, providing quantitative guidance for composition design and process window control. In the case of cordierite refractories, the synergistic effect of CaO and Fe_2O_3 on liquid formation temperature and target-phase stability was quantified, providing a thermodynamic basis for solid waste blending.

Overall, a thermodynamic database for the Al_2O_3–CaO–MgO–SiO_2–Fe_2O_3–FeO system has been established in this work, providing a quantitative foundation for composition design, phase-stability assessment, and process contral in complex aluminosilicate solid-waste utilization.

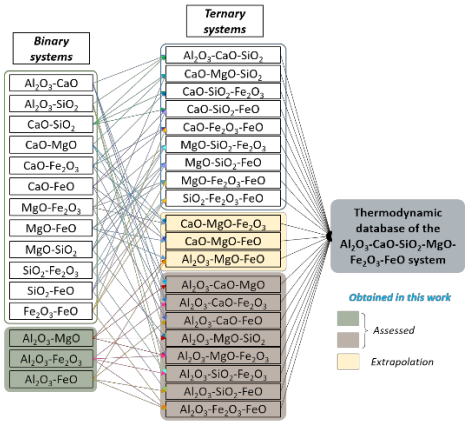

Figure 1. Construction of the thermodynamic database for the Al_2O_3-CaO-SiO_2-MgO-Fe_2O_3-FeO system

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Biographical Note

Fengyang Gao is a PhD student at Powder Metallurgy Research Institute in Central South University, China. His research focuses on the investigation of phase diagram and thermodynamic modelling in oxide systems.

Thermodynamic Modelling of the CaO-MgO-SiO_2 ternary system and its use in Ordinary Portland Cement Clinker Production

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Cement is the second most consumed material on Earth after water. Over 4 billion metric tons are produced each year mainly for its use in concrete. Cement production accounts for about 7 to 8% of global CO_2 emissions. Most of it is released in the high temperature manufacturing process of the clinker, the main component and major contributor to Ordinary Portland Cement (OPC) reactivity and strength on account of its mineralogy.

The chemical base system of any OPC cement is the CaO-SiO_2 binary system. Specifically, the two key compounds, Hatrurite Ca_3SiO_5 and Larnite Ca_2SiO_4. When considering the insertion of minor elements, they become Alite (Ca_3SiO_5 + minor) and Belite (β-Ca_2SiO_4 + minor).

The availability of high-purity natural limestone ($CaCO_3$), the main raw material for cement clinker production, is decreasing and, frequently, MgO (mainly as Dolomite $CaMg(CO_3)_2$) is present as a minor element. From a chemical outlook, this leads to MgO insertion in Ca_3SiO_5 and Ca_2SiO_4 with a considerable impact on their reactivity behavior in the final cement product.

Hence, thermodynamic simulations using the CALPHAD approach are an excellent alternative to the observed empirical formulas currently used as the standard to predict the mineralogical composition in OPC clinkers [1]. However, currently available thermodynamic databases do not consider the solubilities of MgO in the key Ca-silicates correctly. Such limitation calls for a new thermodynamic modeling of the MgO-CaO-SiO_2 ternary system focused on the CaO rich corner.

The proposed work combines new high temperature experiments and a coherent thermodynamic modelling to calculate the phase equilibria in the CaO-MgO-SiO_2 ternary system. For CaO-SiO_2, the most recent thermodynamic datasets [2,3] are used as a starting point. The experimental work focuses on the MgO-CaO rich section of the ternary diagram. Bulk samples are synthesized and characterized using X-ray fluorescence (XRF), X-ray diffraction (XRD), and scanning electron microscopy (SEM).

Our new modeling is compared to the available ones in the literature and commercial databases (FToxid, GTOX). To ensure compatibility with these two, the liquid phase is modeled either using the Associate Model (GTOX) or the Modified Quasichemical Model (FToxid). Finally, it is interesting to mention that the datasets in the commercial databases give different results in the CaO-MgO-rich region. In particular, FToxid v8.4 (Fig. 1) is not in agreement with the fact that Ca_3SiO_5, Ca_2SiO_4 and MgO are simultaneously observed in true cement clinker samples. The origin of these differences will be discussed.

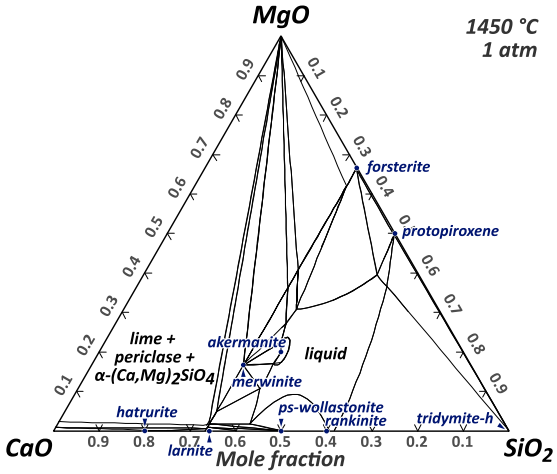

Figure 1. CaO-MgO-SiO_2 system at 1450°C (FToxid v8.4)

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Biographical Note

Ramón N. Bandak R. is a PhD candidate at Université Grenoble Alpes. His research focuses on thermodynamic modelling of high-temperature phases for mineralogical prediction of Ordinary Portland Cement Clinker. He has experience with experimental high-temperature oxides systems and simulations on FactSage in Cement Clinker production and Copper-Slag reduction using hydrogen to reduce waste and CO_2 emissions.

Software and Database Development for Design of Radiation-Resistant Alloys

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Plasma facing materials (PFM) in fusion reactors must be able to withstand high temperatures and high neutron fluxes over an extended period of time.[1] Refractory high entropy alloys (RHEAs) are promising candidates due to their high temperature strength and radiation resistance.[2] However, given the large design space of RHEAs and a lack of fundamental understanding of radiation-induced swelling, optimizing RHEAs for improved radiation resistance proves to be difficult. Several tools are being developed addressing this alloy design issue on multiple fronts: phase stability, defect and microstructure evolution, high-throughput screening, and black-box optimization.

For phase stability, the pycalphad and ESPEI software will be highlighted in our efforts to rapidly build medium- to large-scale thermodynamic databases. The ability to quickly develop large databases becomes beneficial not only to account for all the elements in the RHEA design space, but to also account for transmutation products, greatly increasing the complexity of the composition space. This allows for determining if any detrimental phases can form in a PFM during the lifetime of a fusion reactor.

Defect dynamics after a cascade can be modeled through kinetic Monte Carlo simulations. However, these simulations are limited by their short time scales to assess radiation damage after years of service. An in-house first-passage kinetic Monte Carlo (FPKMC)[3] library is being developed to address this issue by enabling simulations over large timescales while still preserving the underlying physics. For bulk-scale kinetic phenomena, diffusion and precipitation models (coupled with thermodynamics) are performed through the kawin software to design homogenization treatments as well as predicting phase formation and growth over time.

All the tools discussed so far pertain to predicting behavior of a single alloy composition. The Materials Acceleration Platform (MAP) and The Alloy Optimization Software (TAOS) allows for design of alloys by coupling the results of these tools as objectives or constraints. The MAP software enables high-throughput screening through high-performance computing, allowing hundreds of thousands of alloys with multiple design constraints to be evaluated. On the other hand, the TAOS software is intended to run on local machines, with a UI provided to increase accessibility even to non-experts. Recently, TAOS 2.0 has been commercially released providing support for bi-objective optimization, custom models and sensitivity analysis.

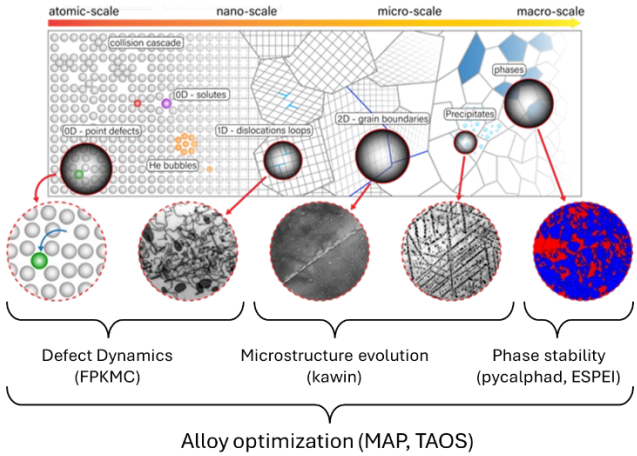

Figure 1. Multi-scale framework accounting for atomic-scale defect evolution all the way to macro-scale phase stability and how they can all be used to constrain an alloy design

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Biographical Note

Nicholas Ury is a staff scientist at the Lawrence Livermore National Laboratory. He received his Master's degree at Cal Poly Pomona. His work primarily focuses on developing software tools and thermodynamic databases and applying them towards alloy design.

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Enhancing Nuclear Reactor Safety: Thermodynamic Modelling of the Ag-Zr System in PWR Absorber Rods

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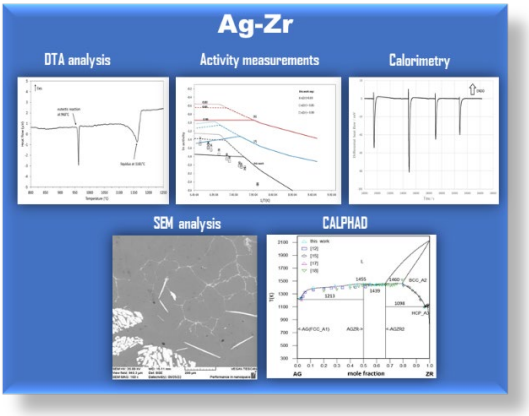
Absorber rods in PWRs use an Ag-In-Cd alloy (80% Ag, 15% In, 5% Cd) encased in stainless steel within Zircaloy-4 guide tubes to control core reactivity. In low-pressure accidents, the alloy melts between 743°C–831°C, but containment fails as rising temperatures and internal pressure (from helium and cadmium vapor) deform the cladding, enabling interaction with and dissolution of the Zircaloy-4 tube at 1000°C–1100°C. The resulting cadmium vaporization and Ag-In-Zr-(O-H) mixtures may migrate downward or partially vaporize, affecting aerosol mass in the coolant system and iodine chemistry—critical for short-to-mid-term environmental release risks.

After reviewing the existing literature on the Ag-Zr system, a thorough analysis of previous studies was conducted to identify gaps and inconsistencies. In parallel, a comprehensive experimental investigation was undertaken to refine the understanding of the Ag-Zr phase diagram.

Differential thermal analyses were performed across the entire composition range, providing critical data on phase transitions. Additionally, precise measurements of silver activity were carried out to better understand the thermodynamic behavior of the system. A calorimetric determination of the standard enthalpy of formation of AgZr was also conducted, offering new insights into the energetics of this intermetallic compound.

One of the long-standing debates in the field concerned the decomposition mechanisms of AgZr and AgZr2[1-4]. Through this study, it has been definitively established that AgZr undergoes congruent melting, while AgZr2 exhibits peritectic decomposition. These findings resolve previous ambiguities and provide a clearer picture of the phase behavior in the Ag-Zr system.

The newly developed CALPHAD model successfully reproduces the experimental phase diagram with a high degree of accuracy. In conclusion, this study not only presents a new and improved CALPHAD model for the Ag-Zr system but also sets the stage for future advancements. By addressing key experimental challenges and resolving long-standing debates, it contributes significantly to the broader field of materials science and thermodynamic modelling. The integration of innovative experimental techniques and rigorous data analysis ensures that this work will serve as a valuable reference for future nuclear material research.



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Biographical Note

Ioana NUTA, a chemical engineer, is a researcher at the SIMAP laboratory in Grenoble (France). She works in the field of materials science and researches gas phase thermodynamics using the Knudsen effusion method coupled with mass spectrometry. Her research focuses on the thermochemical properties of compounds mainly used in energy production and storage.

Molten Salts Thermophysical Properties modelling: new insights into the effect of fission products accumulation in molten fuel salt systems

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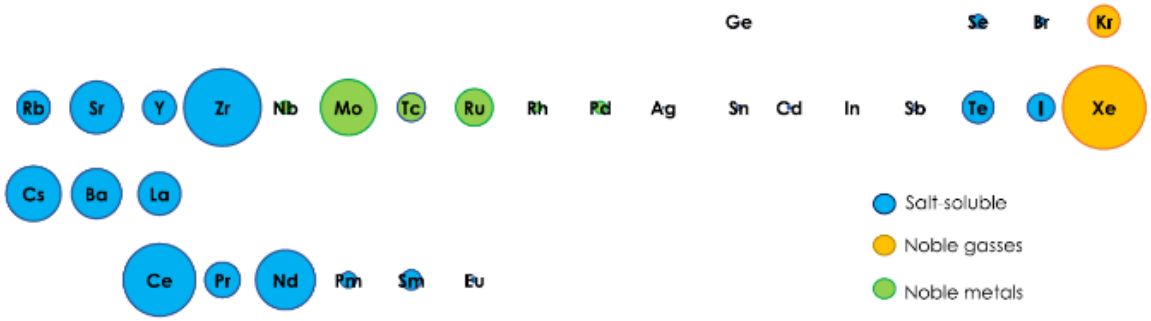
The Molten Salt Reactor (MSR) is one of the six selected reactor concepts of the Generation IV initiative for the next generation of nuclear reactors. In the MSR, molten salts serve as the reactor fuel, as coolant and/or moderator. During irradiation, the generated fission products (FPs) accumulate in the fuel salt, affecting its thermo-physical and thermochemical properties.

FPs can be divided in 3 categories as we can see on figure 1: (i) noble metals, which are insoluble elements in the salt, (ii) noble gases, (iii) and salt soluble FPs, which include e.g. alkaline, alkaline-earth, lanthanides, and are the main focus in this work [1]. The impact on molten salt density and viscosity of the latter fission products should be assessed to ensure the reactor safe operation.

An experimental set-up to measure density using the Archimedean principle has been developed at TU Delft and will be presented. Moreover, we will show density and viscosity models of fission products dissolved in selected molten fuel salt systems. The models are coupled to thermodynamic assessments of the same systems based on the CALPHAD methodology and quasi-chemical formalism for the liquid solutions [2]. These optimized coupled models, compatible with the JRCMSD [3], are used to predict higher order systems behavior, giving us more insights into irradiated fuel salt behavior. The focus is on key fission products of relevance for MSR designs, e.g. with a high fission yield, high volatility, and/or radiological impact.

Figure 1. Inventories of FPs in molten salt fuels [1]



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Acknowledgement

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Thermodynamic Modeling of Phase Stability in Alloys under Irradiation

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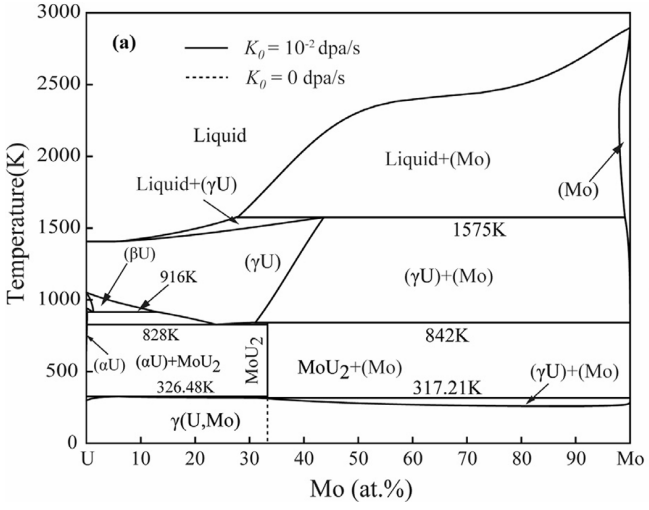
The phase stability of alloys undergoes significant alterations under irradiation, profoundly influencing the phase constitution and microstructural evolution of alloy materials utilized in the nuclear energy field[1]. Irradiation-induced defect accumulation and ballistic mixing are identified as the key factors driving changes in the thermodynamic free energy of alloys[2]. In this study, based on the CALPHAD method and a ballistic mixing energy model, a thermodynamic model was developed by integrating the Cahn-Hilliard equation. This approach accounts for local atomic mixing and defect proliferation to describe the dynamic equilibrium processes of atoms and defects. By calculating the free energy of various phases in uranium alloys under irradiation, the effects of dislocation density, displacement rate, and atomic replacement number on the total free energy were analyzed across different temperatures and irradiation doses. Furthermore, metastable phase diagrams under various irradiation conditions were calculated. The results indicate that irradiation exerts a substantial influence on the low-temperature region of the phase diagrams (As shown in Figure 1). A continuous solid-solution BCC phase emerges in this region, and the BCC phase region expands with increasing irradiation dose. Consequently, the phase relationships in the low-temperature section deviate significantly from those in the equilibrium phase diagram[3,4]. These findings are consistent with experimental reports regarding BCC phase stabilization and the phenomenon of low-temperature phase "inverse transformation" observed in alloys such as U-Mo.

Figure 1. Calculated steady-state dynamical phase diagram of U-Mo binary system under irradiation



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Biographical Note

Yong Lu is an Associate Professor in the College of Materials at Xiamen University, China. His research focuses on the thermodynamic assessments of metastable systems and phase field modeling. He has published over 40 articles in journals such as CALPHAD, Physical Review Letters, Acta Materialia, etc.

Thermodynamic modeling and phase characterization in the Li_2SO_4-$CoSO_4$-$MnSO_4$-$NiSO_4$ system for metal recovery from secondary resources

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The extraction of cobalt and nickel from secondary resources, such as battery waste has been studied previously by selective sulfation roasting of LCO black mass, NiMH battery scrap, followed by hydrometallurgical extraction of these metals [1,2]. One important aspect for optimizing such process routes is accurate knowledge of thermodynamic properties of the product phases, such as double lithium metal sulfates, such as $Li_2Co(SO_4)_2$, $Li_2Ni(SO_4)_2$ and $Li_2Mn(SO_4)_2$. This will enable predictions of optimal processing conditions, such as temperature or $P(SO_2)$ to produce the intermediate products for maximum yield in subsequent extraction processes.

In the present work, the double sulfates were synthesized and characterized to extract thermodynamic properties, such as heat capacity and standard entropy. Composition of the phases were measured using EPMA as well as LA-ICP-MS, and the phases were identified using XRD. Heat capacity was measured from 1.8 K to 300 K using Physical Property Measuring System (Quantum Design PPMS® DynaCool™) and standard entropy was derived from these measurements.

The thermodynamic measurements were used together with existing experimental literature data to optimize the thermodynamic properties for Li_2SO_4-rich solid solutions, $Li_2Me(SO_4)_2$ and binary Li_2SO_4-$MeSO_4$ liquids (Me=Co, Mn, Ni).

The resulting thermodynamic database was further used to predict the optimal conditions for formation of suitable phase for selective leaching in subsequent processing steps.

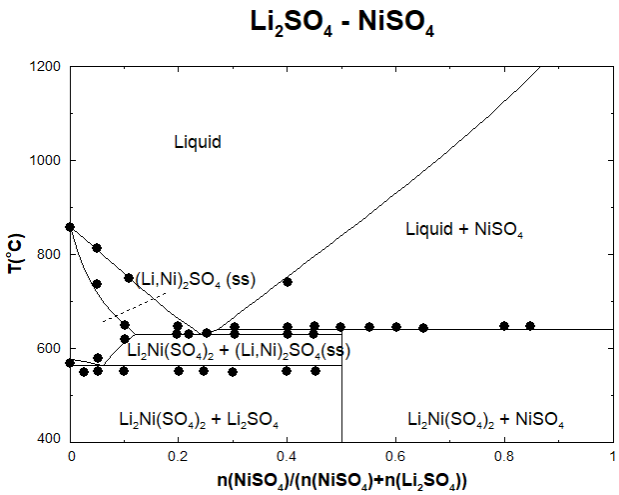

Fig 1. Optimized phase diagram of Li_2SO_4-$NiSO_4$ system

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The work has been done at Aalto University in the Batcircle 3 project, funded by Business Finland, and is presented by Professor Daniel Lindberg, who is professor in High-temperature chemistry and technology at Åbo Akademi University, as well as a visiting professor in Metallurgical Thermodynamics at Aalto University.

New Thermodynamic Model for Salt-Metal Liquid Solutions Introducing Charge Defects Within the CALPHAD Approach

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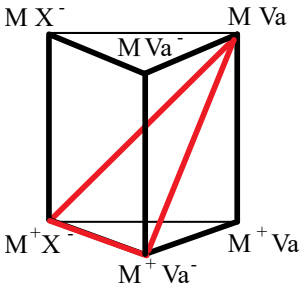
Metal halides are salts formed by the combination of a metal cation with a halogen anion (F^-, Cl^-, Br^-, or I^-). Depending on the type of metal, molten salt-metal solutions can exhibit metallic or non-metallic character. Molten salt-metal systems in which the metal imparts metallic character to the solutions include systems containing alkali metals (Li, Na, K, Rb, Cs) and alkaline earth metals (Be, Mg, Ca, Sr, Ba). These salt-metal systems are characterized by a distinct structure that varies depending on the composition [1].

Due to their importance, extensive experimental efforts were undertaken in the 1950s to characterize the properties of alkali metals (M) in their corresponding alkali halides (MX), the results of which were comprehensively compiled by Bredig [1]. The measured phase diagrams reveal notable similarities across the various MX-M systems, most notably the absence of intermediate compound formation and the presence of a liquid-phase miscibility gap. An exception to this behavior is observed in the RbBr-Rb and CsX-Cs systems, which do not exhibit a miscibility gap, but their measured phase diagrams show a tendency towards immiscibility. Despite the apparent simplicity of the phase diagrams, no existing model adequately captures the complex behavior of these systems. This is especially true in the metal-dilute region, where reproducing thermodynamic data is challenging due to the localization of electrons.

This work develops a new thermodynamic model for the liquid phase within the CALPHAD Approach, that capture both the ionic and metallic behavior in MX-M solutions, using the Modified Quasichemical Model in the Quadruplet Approximation (MQMQA) formalism [2, 3]. In the molten salt solution containing a small fraction of metal, the valence electron is treated as a separate entity forming an F-center-like region (Va^-). At higher metal concentrations, the valence electron is treated as an integral part of the alkali metal, capturing its delocalized behavior in the solution. The applicability of the proposed models is demonstrated by evaluating the NaF-Na, NaCl-Na, NaBr-Na, and NaI-Na, as well as KCl-K system. A critical evaluation of phase diagrams and thermodynamic data and a theorical assessment over the entire composition range is presented. All calculations and optimizations in this work are performed with the FactSage™ thermochemical software [4-6]. Despite the modeling challenges, this study has achieved a significant advancement, providing, for the first time, remarkable agreement between the computed results and experimental thermodynamic data. The developed liquid-phase model shows strong potential for application not only to alkali halide–alkali metal systems, but also to alkaline earth halide–alkaline earth metal systems.

Figure 1. 3D representation of the M^+, $M//X^-,Va^-$, Va liquid phase model, illustrating three reciprocal subsystems, along with the colored edges representing charge neutrality



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Biographical Note

Oumaima Kidari is a PhD candidate in Material Engineering at the Centre for Research in Computational Thermochemistry (CRCT), Polytechnique Montréal. Her research focuses on developing new thermodynamic models for both solid and liquid phases in salt-metal systems, with a focus on systems where metals impart metallic character to liquid solutions. Her work integrates this distinctive behavior into liquid-phase modeling and also accounts for the effects of defects (Frenkel, Schottky, F-centers) in solid solution modeling. Her efforts aim to advance the fundamental understanding of these challenging systems and improve modeling accuracy for applications in materials design and high-temperature processes.

Crystal Growth and Thermodynamic Assessment of the Thallium Alkaline-Earth Halides

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Thallium alkaline-earth halides with the composition $Tl_mAE_nX_{m+2n}$ (*AE* = Mg, Sr, Ca, Ba; *X* = Cl, Br, I) form a structurally rich and chemically complex family of compounds with unique optical and semiconductor properties [1]. Thallium-containing materials combine high density and effective atomic number, which makes them well suited for radiation detection applications such as homeland security and medical imaging. For example, the single crystal perovskite $TlCaCl_3$ shows excellent gamma-ray energy resolution [2] and can potentially be used for fast neutron detection utilizing neutron capture in ^{35}Cl [2,3]. Due to its high density and effective atomic number, $TlSr_2I_5$ doped with Eu^{2+} [4] is of interest for medical imaging applications, while $TlMnBr_3$ shows promise as a semiconductor detector.

However, in order to produce large and high quality crystals suitable for use in applications, a complete thermodynamic description and a good understanding of the behavior of the melt during crystal growth is required.

Consequently, we employed the Vertical Bridgman crystal growth technique in combination with first principle calculations and the CALPHAD method to determine the growth habit of the thallium alkaline-earth halides and elucidate the structure – property relationships.

Thermodynamic assessments were conducted using FactSage ™, supplemented by first-principles estimates for the heat of formation, standard entropy, and heat capacity of the components in the TlX – AEX_2 chemical space. Computational data was corroborated by performing differential scanning calorimetry (DSC), X-ray diffraction (XRD), and optical characterization measurements.

In this paper we present a few examples of the versatile and expansive family of thallium alkaline-earth halides and discuss their physical and chemical properties. For example, Figure 1 shows the phase diagram of the thallium alkaline-earth halide, $TlCaCl_3$, that was calculated using FactSage ™, based on empirical and first principles thermodynamic data.

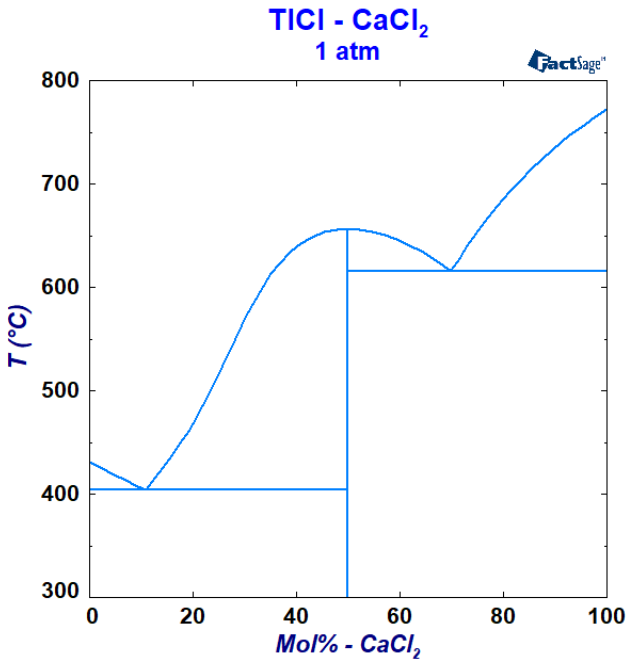

Figure 1. Phase diagram of TlCl – $CaCl_2$ calculated using FactSage

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Thermodynamic models for ternary deep eutectic systems

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Deep eutectic solvents (DESs) have gained significant interest over the past two decades as alternatives to organic solvents. Despite the various potential applications of DESs, such as electrochemistry and separation processes,[1] industrial utilization has not been reported to the best of our knowledge, and the lack of information on the thermodynamic behaviour of DESs is a limiting factor for their use beyond the laboratory scale.

Although phase diagrams of several binary systems have been measured, the phase behaviour of ternary systems remains largely unexplored.[2] The addition of a third compound may tune the physicochemical properties of DESs, and modelling phase equilibria of ternary systems would allow the selection of ternary compositions with values of the liquidus temperature within a specific range, thus avoiding a tedious and costly trial and error experimental approach.[3]

The Modified Quasichemical Model in the Quadruplet Approximation (MQMQA) has been widely applied by our group to describe the liquid phase of various inorganic systems.[4] However, it has not yet been applied to represent the behaviour of systems consisting of organic salts and molecular components.

The main goal of this work is to develop thermodynamic models for various ternary DESs and their binary subsystems using the CALPHAD approach for the first time. Up to now, three ternary systems of the type HBA/HBA/HBD, where HBA is a Hydrogen Bond Acceptor and HBD is a Hydrogen Bond Donor, have been investigated: (1) choline chloride (ChCl)/1-ethyl-3-methylimidazolium chloride ([C_2mim]Cl)/urea, (2) ChCl/$ZnCl_2$/urea, and (3) ChCl/[C_2mim]Cl/benzoic acid. The salts ChCl, [C_2mim]Cl and $ZnCl_2$ act as HBAs, while urea and benzoic acid are mainly HBDs.

All available experimental data from the literature were collected, and relevant binary and ternary phase diagrams (for which data were lacking) were measured by differential scanning calorimetry (DSC) and visual method (using a melting-point apparatus). The optimized model parameters for the binary subsystems along with suitable interpolation techniques were used to make predictions in the ternary system. To assess the validity of the developed thermodynamic models, our predictions of three isoplethal sections in system 1, of one in system 2, and of three in system 3 were compared to our in-house phase diagram data. Good agreement was achieved for systems 1 and 3. For system 2, owing to experimental challenges, agreement between the model and the scattered experimental data was less satisfactory.

The MQMQA does not explicitly consider hydrogen bonding, the intermolecular force governing the systems under study. It is suitable for mixtures consisting of cations and anions, which are governed by Coulombic forces. To overcome this limitation, we introduced HBD (undissociated) organic molecules on both the cationic and anionic sublattices. Also, charged, hydrogen-bonded species were added to the liquid model to correctly describe phase equilibria, thus increasing the number of end-members. These added species were based on density functional theory (DFT) calculations performed using the Gaussian software.

This work provides new phase equilibrium data and thermodynamic models for binary and ternary DESs. Our results show that the MQMQA is suitable for the rational design of DESs for targeted applications. Our future research will focus on HBA/HBD/HBD ternary systems.

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Biographical Note

Lucas P. Zini is a Ph.D. candidate in Chemical Engineering at Polytechnique Montréal (Canada) under the supervision of Christian Robelin and Jean-Philippe Harvey. In his work, he develops thermodynamic models for various ternary deep eutectic systems by combining experimental work with the CALPHAD approach.

Understanding deformation-induced nanocrystallization in amorphous alloys: a multi-scale modeling study

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Amorphous materials exhibit unique properties such as high strength and hardness, high elastic strain limit, excellent thermoplastic formability, and good resistance to wear and corrosion. Since the amorphous phase is a metastable state, transformation into a crystalline phase can naturally occur according to external conditions. In particular, dynamic precipitation of nanocrystalline particles during deformation has been reported in various amorphous materials, leading to further improvements in mechanical properties.

Extensive efforts have been made to clarify the primary mechanism of deformation-induced crystallization, and two hypotheses have been proposed (Fig. 1). One is that the instantaneous temperature increase during shear band formation leads to crystallization within the amorphous matrix [1]. A rise in temperature enables atomic diffusion, thereby enabling nucleation and growth of crystalline phases. Another hypothesis is that energetic instability due to deformation reduces the energy barrier for nucleation [2]. Deformation makes the system unstable, thereby raising its free energy. If the formation of crystalline nuclei leads to local stress relaxation, this can be regarded as a decrease in the nucleation energy barrier.

To control and utilize this phenomenon for the design of advanced materials, its underlying mechanisms should be clarified and well understood. However, nucleation is typically challenging to observe experimentally, and thermodynamic factors that significantly affect nucleation behavior (*e.g.*, chemical driving force, interfacial free energy) are difficult to address experimentally. Moreover, heat generation associated with shear band formation is also difficult to observe and control experimentally.

In the present work, deformation-induced crystallization behavior was investigated using a multi-scale modeling approach. CALPHAD calculations and atomistic simulations were employed to address the lack of fundamental information for the target alloy system. Based on the obtained materials properties, particularly those related to glass-forming ability, deformation-induced crystallization was reproduced and analyzed using a full-scale Monte Carlo Potts model.

According to the simulation results, the instantaneous temperature rise due to shear band formation is a necessary condition for deformation-induced crystallization, while a reduced nucleation energy barrier due to deformation can also have a meaningful influence once the temperature rise effect is sufficient. Based on the findings, alloying effects and key materials properties were further analyzed.

The comprehensive understanding obtained from the present work, together with the developed simulation framework can contribute to the effective development of novel amorphous alloys and amorphous-crystalline composites, by providing reliable guidelines and valuable insights.

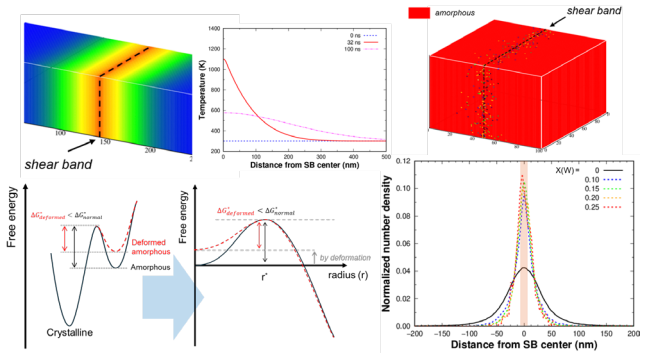

Figure 1. (Left) Schematic view of possible mechanisms for deformation-induced crystallization. (Right) Schematic view of MC Potts simulation results for deformation-induced crystallization.

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Biographical Note

Dr. Sang-Ho Oh is a postdoctoral researcher at the National Institute for Materials Science (NIMS) in Japan. His research focuses on materials thermodynamics, solid-state diffusion, and microstructure evolution. He employs a range of computational methods as well as multi-scale modeling approaches in his research.

Liquidus projection of Cu-Se-Te ternary system

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The Cu–Se–Te system is a ternary system of interest for thermoelectric applications. Compounds such as CuSe, Cu_2Se, CuTe, Cu_2Te, and solid solutions such as $Cu_2Se_xTe_{1-x}$ have shown promising thermoelectric performance. Despite its importance, available phase equilibria data for the Cu–Se–Te system remain limited, and its liquidus projection has not yet been reported.

This study experimentally determines the liquidus projection of the Cu–Se–Te ternary system, including ternary compounds, miscibility gaps, and invariant reactions. Various alloys were prepared from pure elements. Their primary solidification phases were determined using optical microscopy (OM), electron probe microanalysis (EPMA), and X-ray diffraction (XRD).

There are nine primary solidification phases in the Cu–Se–Te system: (Cu), Cu_4Te_3, CuTe, (Se,Te), $CuSe_2$, CuSe, $Cu_2(Se,Te)$, τ_1–$Cu_5Se_7Te_3$, and τ_2–$Cu_6Se_2Te_2$. The (Se,Te) and $Cu_2(Se,Te)$ phases are continuous solid solutions, whereas τ_1–$Cu_5Se_7Te_3$ and τ_2–$Cu_6Se_2Te_2$ are ternary compounds [1,2]. Since the univariant lines in a ternary liquidus projection delineate the boundaries between different primary solidification phases, the results of primary solidification phase were used to construct the liquidus projection.

Very interesting spherical-shaped microstructures were observed in some of the alloys, indicating the existence of liquid miscibility gaps [1,2]. When the alloys are at temperatures higher than the binodal curves of the miscibility gap, they are completely molten. Two liquid phases form when the alloys are within the gap, with the compositions of these phases varying at different temperatures. Efforts were also made in this study to determine the corresponding liquidus projections.

The Cu–Se–Te system contains two large liquid miscibility gaps. The liquid miscibility gap in the Cu corner extends from the Cu–Se side toward the Cu–Te side. This is reasonable, since the liquid miscibility gaps in both the Cu–Se and Cu–Te binary systems are large and located very close to the Cu corner. Excluding those present in the binary systems, there are nine invariant reactions in the Cu–Se–Te ternary system, including one intersection between a univariant line and the boundary of a liquid miscibility gap.

The liquidus projection is proposed, as shown in Figure 1, based on the experimental results of the primary solidification phases and the phase diagrams of the three constituent binary systems. The descending directions of the univariant lines, the types of invariant reactions, and the reaction temperatures are still under investigation.

The reaction temperatures of the invariant reactions were determined by differential thermal analysis (DTA) [3]. For thermal analysis, specimens weighing 15–20 mg were encapsulated in 1 × 3 mm quartz tubes. The thermal analysis experiments are currently in progress. With the determined reaction temperatures and mass balance requirements, the descending directions of the univariant lines can then be established.

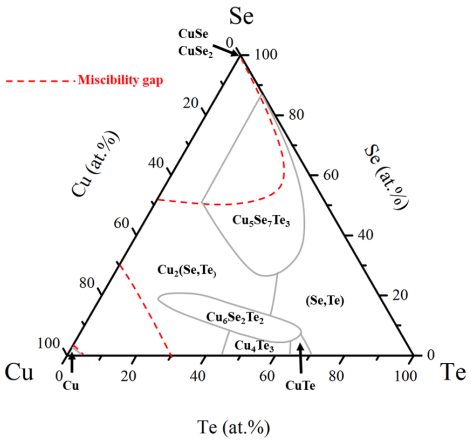

Figure 1. Cu-Se-Te liquidus projection

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Biographical Note

Professor Sinn-wen Chen is a Chair Professor. Ms. Chi-Yu Chung and Mr. Yung-Jen Chuang are master students. Mr. Yung-Chun Tsai is a Ph.D. student. All are in the Department of Chemical Engineering, National Tsing Hua University in Taiwan.

Phase-field modeling of austenitic fraction formation during tempering of 13Cr-4Ni martensitic stainless steels

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The amount of reformed austenite obtained after the tempering stage of martensitic stainless steels is a crucial step in optimizing the mechanical properties and fatigue life of alloys such as CA6NM and S41500. The tempering process is however challenging as the use of low temperatures results in prolonged heat-treatments and higher temperatures risk producing unstable austenite that retransforms to martensite upon cooling. Thus, searching for an optimal relation between temperature-time is an attractive task to obtain the highest possible amount of stable austenite.

We thus present a phase-field model capable of simulating the austenitic fraction formation. In this work, we limit the model to temperatures which are known to safely produce stable austenite after cooling and which are known to produce austenite through the diffusion of Ni. We also employ well-known CALPHAD free energies used to model Fe-Cr-Ni systems to parameterize the free energies used in the phase-field model.

The growth of austenite from the martensitic matrix is a Ni-diffusion controlled process where the stability of the reformed austenite is directly linked to the amount of Ni. Thus, as a first approach, we present a pseudobinary, phase field-model which predicts the amount of reformed austenite as a function of time at a given temperature. The model shows good agreement with respect to multiple experiments at different tempering conditions. We then present our findings to optimize the time and temperature conditions to obtain stable austenite during tempering.

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Thermodynamic modelling of the Al–Ni–V system

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Although the Al–Ni–V system consists of three very common and well-investigated elements, the ternary system itself has not been much in the focus of attention. In the course of constructing a database for multi-principal element alloys, this was one of the remaining un-assessed ternary systems. For a modelling point of view the system is of considerable interest as it contains B2, $L1_2$ and σ phase extending appreciably into the ternary. The Al-rich part of the system is comparatively simple, with no (known) ternary phases and limited extension of the binary compounds into the ternary. To support the modelling, we calculated energies of formation by DFT for all possible permutations of the σ phase within a full five sub-lattice model. This was then used to formulate a three sub-lattice model that was then used in the actual modelling. For the B2/bcc a two sub-lattice and for $L1_2$/fcc a four sub-lattice model were used. This enabled a reasonable description of the system with a rather small number of modelling parameters. Since the experimental information about this system is rather limited, the present modelling can be considered somewhat preliminary. Further work on this system is encouraged.

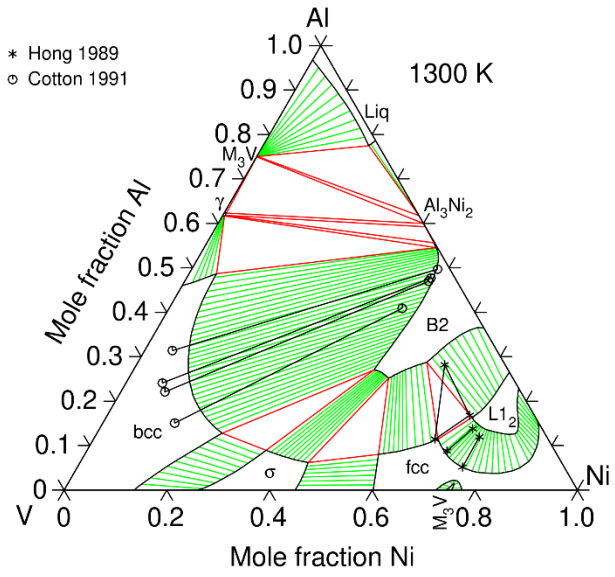

Figure 1. Calculated isothermal section at 1300 K of the Al–Ni–V system [1]

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Biographical Note

Bengt Hallstedt studied physical metallurgy and learned Calphad modelling at KTH, Stockholm during the 1980's and early 1990's. Since 2003 he is at RWTH Aachen University in Germany. He has done Calphad modelling for a large variety of materials, both metallic and ceramic.

Predictive thermodynamic modeling of the Suzuki effect in Co-Ni based alloys

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Solute segregation to planar defects, also called Suzuki effect, affects the stacking fault energy and alters mechanical properties. Although several studies have used theoretical or experimental work to quantify the effect for certain alloy composition, there has been no comprehensive study providing an overview of the Suzuki effect in a alloy across the composition and temperature spectrum.

In this study, we present a predictive model of the Suzuki effect in the Co-Ni binary system and its extension to ternary systems. This prediction is based on long-range diffusion simulations implemented in the MatCalc software.

For the present investigation, the authors revised the thermodynamic modeling of the Co-Ni system basing it on current DFT calculations of the enthalpy of mixing of the FCC and HCP phases as well as experimental work from the literature. The thermodynamic parameters obtained are then used to run long-range diffusion simulations and to investigate the effect of solute atoms on planar defects. The effect of Co in the Co-Ni FCC matrix system was evaluated for different compositions and temperatures. Increasing the temperature, result in a stronger segregation tendency of Co at the defect. According to the present study, the amount of segregation is primarily driven by the system thermodynamics, with diffusion having a limited impact.

The present contribution demonstrates how solute atoms influence planar defects, and it establishes trends across chemical composition and temperature. These insights are essential for understanding the effect of such defects on plastic deformation and, consequently, the mechanical properties of alloys.

This analysis is the first step toward developing a physical model to predict stacking fault energies (SFE) in metals and to assess the interfacial energies of planar defects in metallic alloys.

Biographical Note

Dr. Aurélie Jacob is since May 2025 Project leader at TU Wien in the department of Material Technology, Building Physics, and Building Ecology.

She obtained her PhD in 2015 at RWTH Aachen conducting her work at Forschungzentrum Jülich (DE) in the development of a thermodynamic database for high Cr ferritic steel. In 2016, she carried out her Post-Doc research at TU Wien in the development of thermodynamic databases used for thermokinetic precipitation simulations in complex, technologically important alloys.

Optimizing Hardmetal Alloy Design Through CALPHAD and Experimental Investigation

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The solidus and liquidus temperatures of the W-C-Co-Cr, W-C-40Fe-40Ni-20Co, and W-C-40Fe-40Ni-20Co-Cr alloys, together with their carbon content after sintering, were used to develop a CALPHAD (Calculation of Phase Diagrams)-type Gibbs energy database.

To assess the accuracy of the in-house developed database, experimental results from this study were combined with data reported in the literature. In addition, the database created here was compared with the commercial multicomponent steel database available in Thermo-Calc Software.

By integrating in-house experiments, literature data, and theoretical calculations, it was demonstrated that the errors in predicting solidus and liquidus temperatures were lower in the database developed in this work than in the commercial TCFE13 database. This indicates that phase-transformation predictions are more reliable with the newly constructed database and that experimental results can be reproduced with higher fidelity. Consequently, the database provides a strong foundation for applications in sintering design.

During the design exploration, the influence of chromium in the quinary W-C-Fe-Ni-Co system was examined, and the maximum Cr solubility required to prevent the formation of Cr-rich carbides was identified. Furthermore, both the carbon window (C-window) and chromium window (Cr-window) were established for these alloy systems.

The findings suggest that the in-house database developed in this study offers accurate predictions of the roofing effect when iron is used as a binder in cemented carbides. Overall, this work delivers valuable insights that will benefit the hardmetal industry.

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Biographical Note

Tomás Soria-Biurrun is a researcher in the Advanced Manufacturing Division at CEIT, part of the Basque Research and Technology Alliance (BRTA). His work focuses on the consolidation, characterization, and thermodynamic modeling (Thermo-Calc) of cemented carbides.

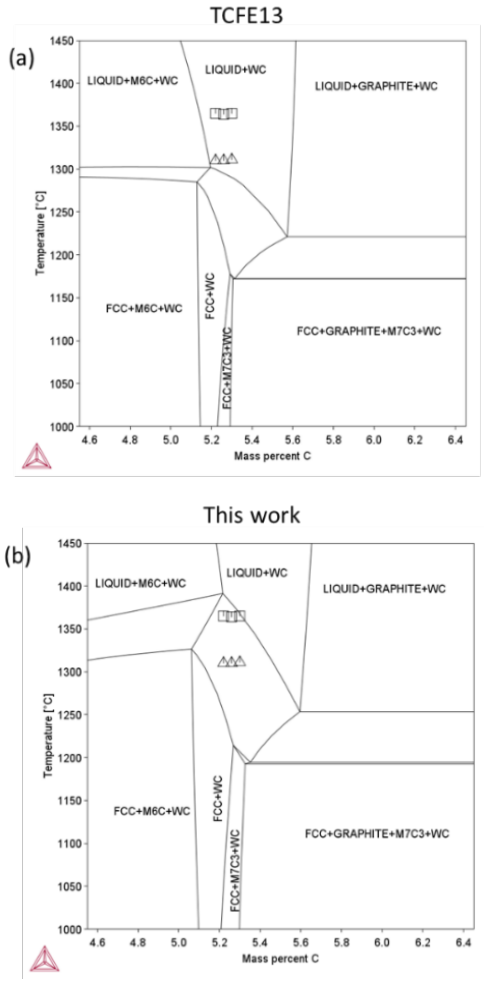

Figure 1. The calculated vertical section for WC-40Fe-40Ni-20Co-Cr using (a) the TCFE13 database and (b) the database developed in this work is shown together with the experimental data, where the triangles and squares correspond to the measured solidus and liquidus temperatures, respectively

Phase diagrams of Cu-Co-Sb ternary system

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The Cu-Co-Sb system has a variety of potential applications, among which thermoelectric materials are particularly important since they can enhance energy conversion efficiency. The thermoelectric properties of $CoSb_3$ have been extensively investigated, highlighting its significance in this system [1]. Meanwhile, Cu exhibits excellent electrical conductivity and is therefore widely employed in electronic components and circuits. To optimize and utilize these materials, comprehensive phase equilibrium information is crucial for understanding stability under various conditions. In this study, the phase equilibria of the Cu-Co-Sb system were systematically investigated through experimental measurements and binary phase diagram [2-4]. Equilibrated alloys were synthesized, and the equilibrium phases were carefully identified. No ternary compound is present in this material system. At 600°C, six tie-triangles have been determined, (Sb) + $CoSb_3$ + Liquid, $CoSb_2$ + $CoSb_3$ + Cu_3Sb, $CoSb_3$ + Cu_3Sb + Liquid, CoSb + $CoSb_2$ + Cu_3Sb, (Cu) + CoSb + Cu_3Sb and (Co) + (Cu) + CoSb. Interestingly, special phase transformation was observed, the β-Cu_3Sb will transform into ε-Cu_3Sb and η-Cu_2Sb since the alloy passes through the eutectoid reaction. At 800°C, four tie-triangles have been determined, $CoSb_2$ + $CoSb_3$ + Liquid, CoSb + $CoSb_2$ + Liquid, (Co) + CoSb + Liquid and (Co) + (Cu) + Liquid.

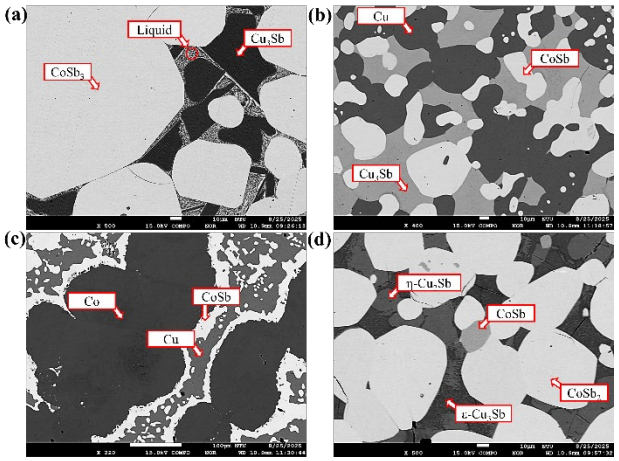

Figure 1. BEI micrographs of (a) alloy Cu-10at. %Co-50at. %Sb, (b) alloy Cu-10at. %Co-20at. %Sb, (c) alloy Cu-20at. %Co-20at. %Sb and (d) alloy Cu-20at. %Co-50at. %Sb equilibrated at 600 °C for 5 months

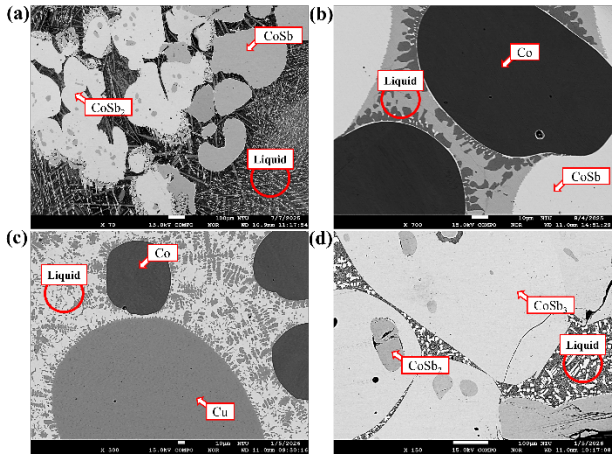

Figure 2. BEI micrographs of (a) alloy Cu-20at. %Co-60at. %Sb, (b) alloy Cu-60at. %Co-30at. %Sb, (c) alloy Cu-20at. %Co-10at. %Sb and (d) alloy Cu-25at. %Co-70at. %Sb equilibrated at 800 °C for 5 months

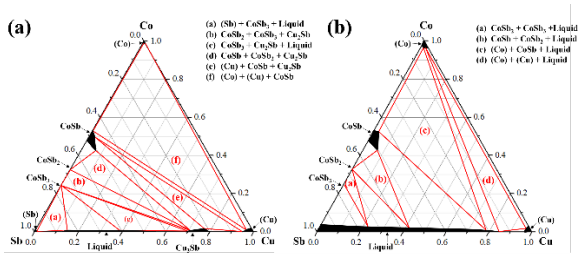

Figure 3. Cu-Co-Sb phase equilibria isothermal section : (a) at 600 °C and (b) at 800 °C

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Biographical Note

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$Gd_3Sc_2Al_3O_{12}$ garnet scintillator: defect engineering

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Multicomponent rare-earth garnets represent a new generation of fast oxide scintillators for medical imaging or high-energy physics. Among them, $Gd_3Ga_{2.7}Al_{2.3}O_{12}$ (GGAG:Ce) has emerged as a benchmark material, achieving light yield over 50,000 photons/MeV and excellent timing performance, able to compete with LuAG:Ce or LYSO:Ce. Its scintillation efficiency is attributed to Ga(3*d*), inducing a downward shift of the conduction band minimum (CBM). However, the presence of gallium requires crystal growth in expensive iridium crucibles, significantly increasing production costs.

Scandium-admixed garnets with general composition $(Gd,Sc)_3(Sc,Al)_5O_{12}$, particularly $Gd_3Sc_2Al_3O_{12}$ (GSAG), provide an attractive alternative. Sc incorporation produces a comparable CBM downshift while enabling growthin molybdenum crucibles under reducing atmosphere, offering substantial economic advantages. Despite this promising band-structure engineering, GSAG:Ce consistently exhibits lower light yield and slower scintillation kinetics than GGAG:Ce, indicating the presence of intrinsic limitations.

To investigate this difference, time-resolved photoluminescence and scintillation spectroscopy was combined with Thermally Stimulated Luminescence (TSL) and Electron Paramagnetic Resonance (EPR). EPR measurements performed on Gd-free analogues revealed that Sc^{3+} ions partially occupy dodecahedral positionsin the garnet lattice. These defects induces deep electron traps, forming a dominant bottleneck during the transport stage of the scintillation mechanism. The presence of these traps prolongs the overall 1/e decay time and limits the achievable light yield.

To further examine this behavior, the Density Functional Theory (DFT) calculations were performed using the VASP package. Several Sc-containing garnet configurations were structurally optimized, and their electronic densities of states were evaluated.

The calculations show that Sc(5d) states located at the dodecahedral site—unlike those at the octahedral site—are positioned below the CBM of the host matrix, confirming their role as electron traps and supporting the experimental findings.

The primary objective of the thermodynamic modelling using the FactSage software was to determine whether compositions with reduced scandium content in dodecahedral sites could be grown while maintaining phase stability of the garnet structure. The total energies of the optimized structures were used to derive enthalpies of formation relative to the corresponding oxides. Additional thermodynamic data were adopted from relevant pseudobinary systems. Solid solutions in both garnet and competing perovskite phases were modeled using the compound energy formalism (CEF), employing four end-members in the (Gd–Sc) and (Sc–Al) subsystems. The resulting phase diagram was assessed primarily near the $Gd_3Al_5O_{12}$ composition in the solid-state region, because of the lack of data in the rest of the ternary system.

The thermodynamic assessment was compared with experimentally determined single-crystal compositions and further validated using differential thermal analysis (DTA).

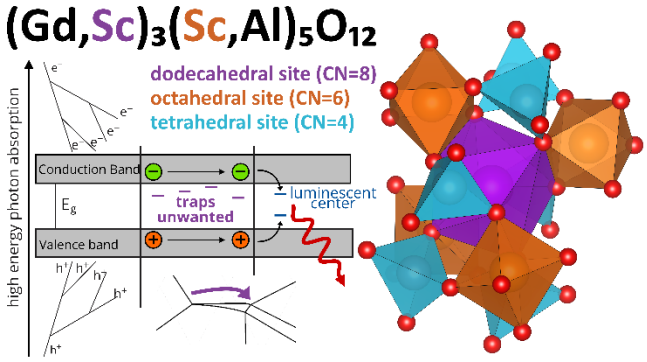

Figure 1. Graphical abstract of thermodynamic investigating of defects in Sc-containing garnets

Acknowledgement

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Biographical Note

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Thermodynamic Assessment of the Ba—Ti—O Ternary System

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Barium metatitanate ($BaTiO_3$) is a prototypical perovskite oxide that has attracted considerable attention since its discovery in the 1940s [1] due to its remarkable ferroelectric, piezoelectric, and dielectric properties [2, 3]. This ABO_3-type perovskite exhibits a rich sequence of structural phase transitions each accompanied by changes in spontaneous polarisation. These unique characteristics have established $BaTiO_3$ as a cornerstone material in modern electronics. Understanding the thermodynamic stability of $BaTiO_3$ and related compounds in the BaO—TiO_2 system is therefore essential for optimising processing conditions and tailoring material properties.

The BaO—TiO_2 pseudo-binary system exhibits a complex phase diagram featuring numerous intermediate compounds between the end-member oxides [4]. Beyond the technologically important $BaTiO_3$, several TiO_2-rich phases — including $Ba_6Ti_{17}O_{40}$, $Ba_4Ti_{13}O_{30}$, $BaTi_4O_9$, $Ba_2Ti_9O_{20}$, and $BaTi_5O_{11}$— play crucial roles in determining phase equilibria during sintering and high-temperature processing. These intermediate compounds exhibit distinct thermal stability behaviours: some appear only at elevated temperatures whilst others decompose upon heating. Accurate thermodynamic descriptions of these phases are indispensable for predicting microstructural evolution and optimising ceramic fabrication routes.

This work presents a comprehensive CALPHAD thermodynamic assessment of the ternary Ba—Ti—O system including the BaO—TiO_2 pseudo-binary line encompassing fifteen phases: the liquid phase, end-member oxides (BaO-halite and TiO_2-rutile), five $BaTiO_3$ polymorphs (rhombohedral, orthorhombic, tetragonal, cubic, and hexagonal), and seven intermediate compounds (Ba_2TiO_4, $BaTi_2O_5$, $Ba_6Ti_{17}O_{40}$, $Ba_4Ti_{13}O_{30}$, $BaTi_4O_9$, $Ba_2Ti_9O_{20}$, and $BaTi_5O_{11}$). The Gibbs energy of intermediate compounds is modelled using the Neumann-Kopp approximation as a baseline, supplemented by temperature-dependent correction functions of the form C = A + BT. A novel tie-line based methodology is employed to systematically determine these correction parameters. High-temperature phases (appearing above their formation temperature) require B < 0, whilst low-temperature phases (decomposing upon heating) require B > 0. The correction parameters are determined by two physical constraints: at the stability boundary (appearance or decomposition temperature), the compound is marginally stable and its Gibbs energy lies exactly on the tie-line between adjacent stable phases; within its stability range, the compound must be thermodynamically stable, meaning its Gibbs energy is sufficiently low to place it on the convex hull.

The assessed database has been rigorously validated through multiple approaches. Convex hull analysis at various temperatures confirms that all experimentally observed stable phases lie on the calculated stability envelope. The computed T-x phase diagram reproduces the experimental topology, including eutectic and peritectic invariant reactions, congruent melting points, and the temperature-dependent stability ranges of intermediate compounds. Furthermore, calculated thermodynamic properties —heat capacity (C_p) and enthalpy increment ($H_T - H_{298}$)— show excellent agreement with available calorimetric measurements for $BaTiO_3$, Ba_2TiO_4, and $BaTi_2O_5$.

Beyond equilibrium thermodynamics, ongoing work aims to model the ferroelectric polarisation of $BaTiO_3$ using Monte Carlo simulations. By coupling the CALPHAD-derived Gibbs energy landscape with a lattice-based statistical mechanics framework, the temperature dependence of spontaneous polarisation and the order-disorder characteristics of the ferroelectric transitions can be explored, bridging the gap between macroscopic thermodynamics and microscopic domain behaviour.

The resulting thermodynamic database, implemented in TDB format and validated using pycalphad, provides a robust foundation for phase equilibrium calculations and materials design across the full composition and temperature range of the BaO—TiO_2 system.

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Thermodynamic modeling of the $CaO-Al_2O_3-P_2O_5-H_2O$ system and applications to refractory materials design under H_2-H_2O conditions

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In order to mitigate the carbon footprint of the steel industry and work towards carbon neutrality, steel companies worldwide are developing low-carbon steelmaking technologies using H_2 gas. To keep pace with such technology development, it is crucial to design and evaluate the service performance of refractory materials under H_2-H_2O condition at high temperatures. For this purpose, the CALPHAD-type thermodynamic database of the $CaO-Al_2O_3-P_2O_5-H_2O$ system has been developed.

In this study, the developed thermodynamic database for the $CaO-Al_2O_3-P_2O_5-H_2O$ system was utilized to evaluate the service performance of alumina refractories with different kinds of binders under H_2-H_2O environment. Thermodynamic stability of refractories was calculated across a temperature range of 1000 ℃ to 1800 ℃. Potential degradation mechanisms resulting from solid phase formation and gaseous species evaporation for the refractory materials were proposed.

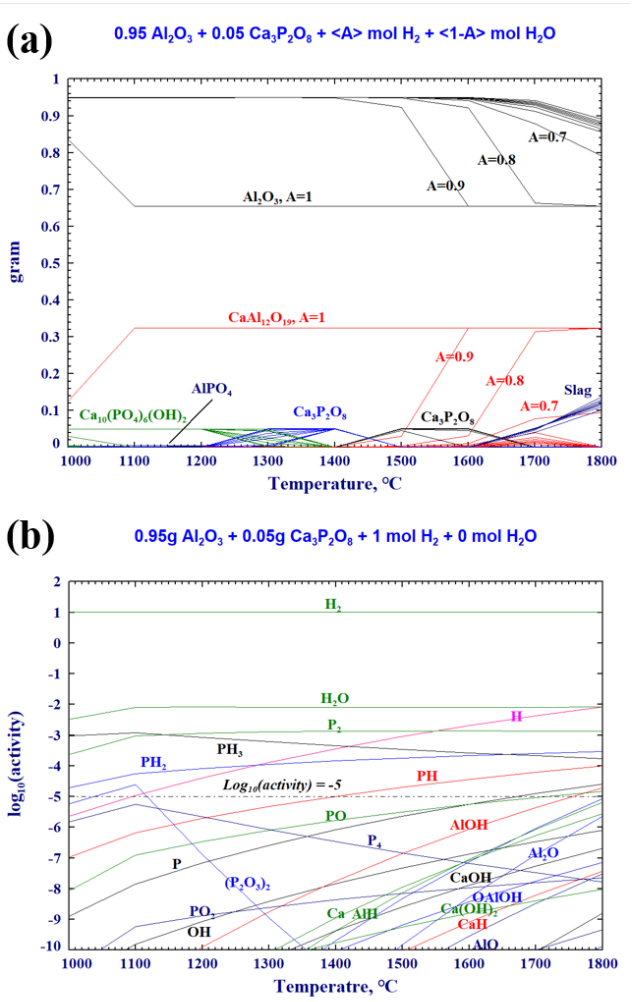

Figure 1. Solid phase distribution (a) and partial pressure of gas species (b) of 0.95 g of Al_2O_3 with 0.05 g of $Ca_3P_2O_8$ bonder material under various H_2/H_2O condition at 1atm across a temperature range of 1000 ℃ to 1800 ℃

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Biographical Note

Guishang Pei is an Assistant Professor at WMG, The University of Warwick. He is developing an accurate and extensive thermodynamic database of the $CaO-SiO_2-MgO-Al_2O_3-P_2O_5-Fe_2O_3-H_2O$ multicomponent systems, aiming to apply for designing and evaluating service performance of refractory materials under H_2-H_2O condition.

Development of a thermodynamic database for antimony oxide-containing metallurgical systems

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Antimony and its compounds, particularly antimony oxides (Sb_2O_3, Sb_2O_5), find extensive industrial applications such as semiconductors, batteries, catalysts, glasses, and flame retardants [1,2]. In addition, antimony has been listed as a critical and strategic metal by Quebec, Canada, the USA, and the European Union [2,3,4]. The current high supply risk of antimony has created a growing demand for higher production through optimizing current processes and developing sustainable recycling pathways. Wastes and residues generated during the processing of gold and copper ores contain significant antimony content [5], offering substantial potential for recovery, particularly in regions rich in these minerals, such as Canada [6].

Reliable knowledge of phase equilibria and thermodynamic properties is essential for designing efficient antimony recovery processes, yet such data are currently scarce or missing in the literature. Additionally, generating these data using purely empirical methods will be costly and time-consuming.

This research aims to establish a thermodynamic database for Sb_2O_3-containing systems using a combined modeling and experimental approach. The chemical system of interest was defined according to the chemical compositions of the potential resources for antimony recovery, and all the available literature data were collected and critically assessed. Preliminary models were developed and optimized according to the deviation between the predicted values and the available experimental data in the literature. This is followed by conducting key experiments using thermal analysis and equilibration-quenching techniques. The models were then refined based on the experimental data newly generated in this work. The thermodynamic optimization of the Sb_2O_3-X systems (X = Sb_2O_5, SiO_2, and FeO) is presented here, enabling accurate prediction of phase equilibria and thermodynamic properties across wide temperature and composition ranges relevant for metallurgical processing.

This work provides a foundation for extending the database to higher-order systems, facilitating future simulation and optimization of antimony recovery processes.

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CALPHAD 2026

Poster Presentation Abstracts

53rd International Conference on Computer Coupling of Phase Diagrams and Thermochemistry

June 7–12, 2026

Quebec Convention Centre, Quebec City, Québec, Canada

Deep Alloy®: A New Frontier in Material Discovery

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Traditional experimental approaches for discovering novel materials with targeted properties are inherently resource-intensive. They require substantial investments in raw materials, specialized equipment (such as furnaces, arc melters, and forging apparatus), and extensive labor for property characterization [1]. These limitations hinder rapid iteration and exploration of vast compositional spaces, particularly in complex multi-component alloys.

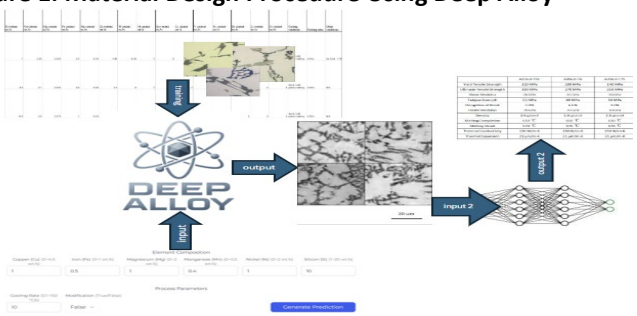
This poster presents a transformative machine learning (ML)-driven framework for accelerated alloy design and discovery. The approach dramatically reduces costs, development timelines, and required expertise by identifying promising candidates through computational simulation rather than physical experimentation [2]. By shifting the discovery bottleneck from empirical trial-and-error to predictive modeling, this strategy aligns well with CALPHAD methodologies that emphasize thermodynamic and kinetic modeling for phase stability and microstructure evolution.

Central to this methodology is Deep Alloy®, an innovative ML model trained to generate realistic metal alloy microstructures given input parameters such as elemental composition and cooling rate. The model employs a generative architecture to simulate solidification processes, capturing dendritic growth, phase fractions, and morphological features with high fidelity. By leveraging the direct, causal relationship between microstructure and macroscopic properties [3], Deep Alloy® integrates seamlessly with established property prediction models. Together, they enable a fully automated end-to-end materials discovery pipeline capable of screening thousands of compositions virtually.

To rigorously assess the model's robustness and accuracy compared to experimental methods, Deep Alloy® was trained on a comprehensive dataset of Aluminum-Silicon (Al-Si) alloys encompassing varied compositions and processing conditions. The model then generated 64 distinct microstructures for the industrially prevalent A356 alloy at seven different cooling rates (ranging from slow furnace cooling to rapid quenching). Average secondary dendrite arm spacing (SDAS) values were extracted from these outputs, producing an SDAS versus cooling rate (CR) curve. Direct comparison with well-established literature benchmarks [4] demonstrated excellent agreement, accurately reproducing the inverse SDAS-CR relationship and confirming the model's predictive fidelity across the tested range.

This ML-centric strategy, with its potential to incorporate CALPHAD-derived thermodynamic inputs for enhanced generality, offers substantial promise for revolutionizing materials discovery. It enables rapid, cost-effective exploration of vast compositional and processing spaces, accelerates innovation in alloy engineering, and paves the way for data-driven, high-throughput design of advanced structural and functional materials.

Figure 1. Material Design Procedure Using Deep Alloy®



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Biographical Note

Nicolás Adrián is an undergraduate student pursuing a degree in mechanical engineering. His research focuses on ML innovation in the Al-Si alloy system. In addition to materials engineering, he has a keen interest in manufacturing and product design. The ability to understand what makes these processes possible through a material perspective is something he really loves about his research.

Thermodynamic model for sodium and potassium chromates, molybdates, and tungstates involved in high-temperature steel corrosion

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This work aims to better understand high-temperature corrosion reactions (600-950°C), also known as «hot corrosion» [1], that occur during energy conversion processes in combustion environments rich in O-H-S-C-Cl species and alkaline salts. Multiple possible chemical reactions reported in the literature were investigated to develop a multicomponent thermodynamic model for predicting the formation of corrosive phases.

Steel and stainless steel components containing alloying elements such as Ni, Cr, Mo, W, and V are prone to hot corrosion under such conditions. Within the temperature range of 600 to 950°C, corrosive gases (CO_2, SO_2, O_2 and H_2O), fly ash, solid deposits, and molten salts may form, including (NaCl and KCl), (Na_2SO_4, K_2SO_4, $Na_2S_2O_7$, and $K_2S_2O_7$), (Na_2CO_3 and K_2CO_3), (Na_2CrO_4, K_2CrO_4, $Na_2Cr_2O_7$ and $K_2Cr_2O_7$), (Na_2MoO_4, K_2MoO_4, $Na_2Mo_2O_7$ and $K_2Mo_2O_7$) and (Na_2WO_4, K_2WO_4, $Na_2W_2O_7$ and $K_2W_2O_7$). Such species could initiate a series of reactions impacting equipment durability and performance.

The developed thermodynamic model considers all condensed phases involved in the system (NaCl + Na_2CO_3 + Na_2SO_4 + $Na_2S_2O_7$ + Na_2CrO_4 + $Na_2Cr_2O_7$ + Na_2MoO_4 + $Na_2Mo_2O_7$ + Na_2O + KCl + K_2CO_3 + K_2SO_4 + $K_2S_2O_7$ + K_2CrO_4 + $K_2Cr_2O_7$ + K_2MoO_4 + $K_2Mo_2O_7$ + K_2O) (diluted in Na_2O and K_2O). This model permits the evaluation of conditions that promote the formation of chromates, dichromates, molybdates, and dimolybdates, as well as those that inhibit their formation.

A critical evaluation of the crystallographic data and thermodynamic properties ($\Delta H^{\circ}_{298.15\,K}$, $S^{\circ}_{298.15\,K}$ and C_P) of the A_2MO_4 and $A_2M_2O_7$ compounds (A = Na or K; M = Cr, Mo, or W) was first carried out. The most reliable experimental data from the literature, along with our DSC-TGA measurements for A_2MO_4 salts were used to assess the thermodynamic properties of pure compounds and better identify possible solid solutions. Subsequently, chromates, dichromates, molybdates, and dimolybdates were incorporated into the existing thermodynamic model for the (NaCl + Na_2CO_3 + Na_2SO_4 + $Na_2S_2O_7$ + KCl + K_2CO_3 + K_2SO_4 + $K_2S_2O_7$) system. The CALPHAD approach was employed, and our model was implemented in the FactSage thermochemical software.

The liquid phase was modeled using the Modified Quasi-chemical Model in the Quadruplet Approximation (MQMQA) [2]. The Compound Energy Formalism (CEF) [3] was used for most solid solutions, while the MQMQA was employed for the high-temperature hexagonal hP22 solid solution.

Overall, 23 binary sub-systems, along with higher-order sub-systems were modeled using both the available data from the literature and the results of our DSC-TGA experiments. Additional experiments (SEM-EDS and DSC-TGA analyses) were carried out to characterize the non-stoichiometric phases of chrome-glaserite $K_3Na(CrO_4)_2$ and molybdenum-glaserite $K_3Na(MoO_4)_2$, and estimate the composition ranges of the hP14 solid solution in the binary sub-systems (Na_2CrO_4 + K_2CrO_4) and (Na_2MoO_4 + K_2MoO_4).

The thermodynamic behavior of the multicomponent system can be reliably described using the model parameters obtained for the binary common-ion, ternary common-cation and reciprocal ternary sub-systems. One can perform thermodynamic calculations to predict the conditions under which corrosion deposits form.

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Biographical Note

Sara Benalia is a Research Professional working on the thermodynamic modeling of inorganic salt systems. Her research focuses on phase equilibria and the thermodynamic modeling of high-temperature corrosion products. Her work combines computational thermodynamics with experimental validation of phase diagrams using DSC. She also studies the physical properties of inorganic molten salts, including density and ionic conductivity.

Predicting thermal conductivity of graphite cathode blocks for aluminum electrolysis cells: A modeling approach

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Graphite cathode blocks are now widely used in aluminum electrolysis cells, where they have replaced anthracite blocks due to their lower electrical resistivity and higher thermal conductivity. These cells operate at around 960°C, and they require a stable thermal profile in order to maintain the frozen cryolite ledge and extend the cathode service life, which is typically between 1500 and 3000 days [1]. Among the thermophysical properties of the cathode, thermal conductivity is a key property that directly controls this thermal stability, so a better understanding of it is necessary to improve the cathode performance and durability. Because graphite blocks are strongly anisotropic, their thermal conductivity, as a result, depends on crystallographic orientation. Moreover, the microstructure of these cathode blocks results from the manufacturing process they undergo, from the selection of raw materials (petroleum coke and pitch), forming, baking, and high-temperature heat treatment during graphitization. During this process, crystallite dimensions, pore structure, crystallite orientations, and lattice defects evolve, resulting in a complex anisotropic microstructure.

In this work, we propose a model to estimate the thermal conductivity of graphite as a function of temperature and microstructural parameters. Starting from an ideal single-crystal graphite case, thermal conductivities along the a-and c-axes are calculated using a lattice thermal conductivity formulation near the Debye temperature derived from the work of Morelli and Slack [2], with Debye temperatures and Grüneisen parameters defined for each axis, following graphite anisotropy. Corrections are then added to the ideal crystal conductivities to account for phonon scattering due to isotopic substitution, vacancies, crystallite dimensions, crystallite orientation, and porosity at both nano- and macro-scale.

The model predicts effective thermal conductivities parallel and perpendicular to the molding pressure direction. It is implemented in MATLAB [3] and validated against experimental data from the literature, first for pyrolytic graphite as the closest case to single-crystal graphite, and then applied to polycrystalline graphite, including industrial cathode blocks for aluminum electrolysis. Predictions show good agreement with available experimental data across a wide temperature range from room temperature up to 2000 K.

This model is intended to be integrated into the FactSage thermochemical software and databases [4] and provided to industrial partners for the optimization of cathode block design.

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This work was carried out as part of my PhD studies within the VLAB 4 project, funded through an Alliance Grant from the Natural Sciences and Engineering Research Council of Canada (NSERC), in collaboration with CRITM and the following companies: Rio Tinto, Alcoa, Hydro Aluminium, Elysis, and Constellium.

Thermodynamic properties measurement of $CaNdAl_3O_7$ and $CaNdAlO_4$

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In this work, the high-temperature drop solution calorimetry was employed to determine the high-temperature heat capacities (Cp) and enthalpies of formation of $CaNdAlO_4$ and $CaNdAl_3O_7$ at 298 K.

The temperature-dependent Cp relationships for $CaNdAlO_4$ and $CaNdAl_3O_7$ were derived as:

$Cp(CaNdAl_3O_7)=464.9-5.66T^{-2}-4054T^{-0.5}-200.4T^{-3}$ $(J\cdot mol^{-1}\cdot K^{-1})$ (673-1273K) ;

$Cp(CaNdAlO_4)=256.5-17720T^{-2}-1963T^{-0.5}-1.2T^{-3}$

$(J\cdot mol^{-1}\cdot K^{-1})$ (673-1273K) ;

The enthalpies of formation of $CaNdAl_3O_7$ and $CaNdAlO_4$ at 298K were derived as -4180.20 and -2455.16 $kJ\cdot mol^{-1}$.

Biographical Note

Zhanmin CAO received his PhD in metallurgical physical chemistry in 2001. His main research interests include phase diagram and thermodynamics properties calculation (CALPHAD) and measurement, and simulation of pyrometallurgical process.

Liquidus projection of the Cr-Nb-Ta system

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Phase equilibria data for the ternary Cr-Nb-Ta system are essential for the development of high-temperature structural materials, as these refractory metals are promising alloying elements in various multicomponent systems, for instance in Co- or Ni-based superalloys [1,2]. Moreover, among the numerous AB_2 Laves phases (with C14, C15 or C36 structures), $NbCr_2$ and $TaCr_2$ are particularly promising for high temperature applications due to their superior corrosion and oxidation resistance, low density, and high microstructural stability [3]. Thus, the present work aims to experimentally determine the liquidus projection for the Cr-Nb-Ta system based on the microstructural characterization of arc-melted as-cast alloys.

Nineteen as-cast alloys were produced from high-purity Cr, Nb and Ta elements (min. 99.7 wt.%). Ingots were arc-melted using a non-consumable tungsten electrode and a water-cooled copper crucible, under a high-purity argon atmosphere (min. 99.995 %). After melting, each alloy was sectioned using an Isomet precision cutter. One half was hot-mounted in epoxy resin, ground with SiC abrasive papers, and polished with colloidal silica suspension. The other half was mechanically ground for the X-ray diffraction (XRD) analysis. Microstructural characterization of the samples was carried out by means of scanning electron microscopy (SEM) in a SEM-FEG Tescan MIRA4 instrument. Chemical microanalysis via energy-dispersive spectroscopy (EDS) was performed using a EDAX detector. Phase identification was also performed by XRD using a PANalytical Empyrean diffractometer with Cu-Kα radiation. Qualitative and quantitative XRD phase analyses were performed by the Rietveld refinement.

Four primary solidification regions were experimentally identified: the BCC (Cr) phase field, the C15 Laves phase field confined to the vicinity of the Cr-Nb binary region, the C14 phase field, and the BCC (Nb,Ta) phase field, which dominates most of the ternary system, as expected from the stability of this phase in the binary subsystems. No evidence of ternary compounds was observed. Additionally, two type II ternary invariant reactions were proposed based on the experimental data: $L + C14 \leftrightarrow C15 + (Nb,Ta)$ (U_I), and $L + C14 \leftrightarrow C15 + (Cr)$ (U_{II}). These results provide a consistent experimental basis for the future assessment and optimization of thermodynamic descriptions of the Cr-Nb-Ta system.

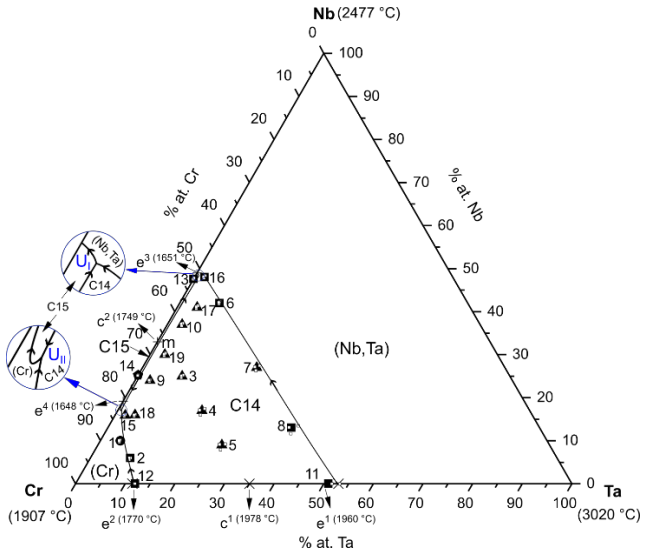

Figure 1. Liquidus projection of the Cr-Nb-Ta system proposed in this work

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Biographical Note

Gilberto Carvalho Coelho is a professor at University of São Paulo. He has experience in Materials and Metallurgical Engineering, with emphasis on the structure of metals and alloys, working mainly on phase diagrams, computational thermodynamics, intermetallics, superalloys, and structural materials for high-temperature applications.

Thermodynamic Modeling of the NaF-AlF_3-CaF_2-Al_2O_3-FeF_2-FeO-FeF_3-Fe_2O_3 System for Aluminum Production Using Inert Anodes : Experimental Study of the Fe-O-F Sub-System

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The development of inert anodes as an alternative to standard carbon anodes for aluminum electrolysis, particularly through CERMET materials containing iron, copper, and nickel compounds, requires a comprehensive understanding of complex phase equilibria involving various oxide and fluoride species that may dissolve in the cryolitic bath. Previous thermodynamic modeling using the CALPHAD approach by Renaud [1] established a foundation for Fe-containing species in the NaF-AlF_3-CaF_2-Al_2O_3 system, while subsequent work by Deschênes-Allard [2] addressed Cu-containing sub-systems and additional work in our research group was carried out for Ni-containing sub-systems.

The present work is an improvement upon this foundation, in part through a thorough thermodynamic modeling study of the Fe-O-F sub-system, coupled with experimental investigations to specifically address iron oxyfluoride stability at high temperature. By refining the thermodynamic description of oxyfluoride phases based on new experimental data, this work aims to extend the model's accuracy to broader melt composition range (in terms of cryolite ratio *CR*) and temperature range relevant to inert anode development and operation.

The Compound Energy Formalism (CEF) was used for solid solutions, whereas the Modified Quasichemical Model in the Quadruplet Approximation (MQMQA) was applied to the liquid phase. This model, which simultaneously considers short-range-ordering between first- and second-nearest-neighbors, is particularly suitable for molten salt systems consisting of multiple cations (Na^+, Al^{3+}_{IV}, Al^{3+}_{V}, Al^{6+}_{2}, Ca^{2+}, Fe^{2+}, Fe^{3+}_{IV}, Fe^{3+}_{V}) and anions (F^-, O^{2-}). Various coordination states are used for both Al^{3+} and Fe^{3+}, thus allowing a more accurate description of short-range- ordering in the melt.

Unary, binary, ternary and higher-order sub-systems were optimized using all available experimental data. Purely oxide-containing sub-systems have been extensively studied [3] and the relevant model parameters from the FToxid database (in FactSage) were integrated into the current model. The fluoride and oxy-fluoride sub-systems, initially modeled by Renaud [1], were re-evaluated. A rutile solution was added with the sublattice description $(Fe^{2+},Fe^{3+})_2(F^-,O^{2-})_4$ to account for FeOF stability at high temperatures, while the fluorinated spinel and rocksalt (primarily wüstite, $Fe_{1-x}O$) solid solutions were re-modeled as $(Fe^{2+},Fe^{3+})_1(Fe^{2+},Fe^{3+},Va^o)_2(O^{2-},F^-)_4$ and $(Fe^{2+},Fe^{3+},Va^o)(F^-,O^{2-},Va^o)$, respectively, to account for fluorine influence.

Experimental investigations were conducted using DSC, XRD, and SEM/EDS for selected compositions across the Fe-O-F ternary sub-system. The methodology and crucible design were adapted from Deschênes-Allard [2], with Inconel 600 (below 1350°C) or pure iron (above 1350°C) being used for the crucible external body. Inner liners were either pure iron (to maintain reducing conditions for Fe^{2+}-containing samples) or platinum (for inert conditions). Ten compositions were studied with estimated liquidus temperatures T_{liq} ranging from 863°C to 1529°C. Quenching experiments were performed by annealing above T_{liq} (up to 1450°C due to limitations of the experimental setup), followed by 24 hours at 920°C and air quenching. SEM/EDS analysis of quenched residues provided phase assemblage and composition data.

The Gibbs energies of the "end-members" of the fluorinated spinel were adjusted to best reproduce the available data from the literature and our in-house SEM/EDS results. Also, the thermodynamic description of the rutile solid solution was refined to better represent the FeOF-FeF_2 joint. Additionally, liquidus temperatures were refined for various compositions.

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This work, completed as part of C. V. da Silva Lima's PhD studies, is part of the VLAB 4 project, funded through an Alliance grant from the Natural Sciences and Engineering Research Council of Canada, in collaboration with CRITM and the following companies: Alcoa, Constellium, Elysis, Hydro Aluminium, and Rio Tinto.

Thermodynamic and Microstructural Analysis of Lead-free Sn–Ag–Cu–Ga–Ni Solders

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The development of modern solders and multicomponent alloys places increasing demands on precise control of thermodynamic and kinetic properties, particularly in systems where mechanical performance is highly sensitive to phase constitution and microstructural evolution. As the number of alloying elements increases and reliability requirements in electrotechnical applications become more strict, traditional experimental approaches become time-consuming and costly. Under these conditions, the CALPHAD method provides an efficient framework for alloy design by enabling the modeling of phase equilibria and thermodynamic properties based on assessed databases, thereby minimizing reliance on extensive experimental work [1].

By calculating liquidus projections, the CALPHAD approach enables identification of composition ranges with reduced stability of brittle intermetallic phases and lower solidification temperatures, which is beneficial for controlling phase formation during reflow and solidification. Software tools such as Thermo-Calc and DICTRA further extend these capabilities by allowing the calculation of both equilibrium and non-equilibrium states, including diffusion-controlled processes that govern solder solidification and microstructural evolution [2].
This research builds upon previous studies by Černičková [3], which showed that Ga additions reduce the melting temperature of lead-free solders, and Peričková [4] described like Ni additions suppress the growth of intermetallic compound layers in solder joints. The present study investigates whether the combined addition of Ga and Ni can simultaneously lower the melting temperature and limit intermetallic layer formation in SAC-based lead-free solder alloys.

Four SAC-based alloys with selected Ga and Ni additions were designed based on literature data and were studied using a combined computational–experimental approach. Thermodynamic calculations were performed using the CALPHAD method in Thermo-Calc with the TCSLD database to determine equilibrium phase fractions and melting behavior. Kinetic simulations of diffusion-controlled intermetallic growth in solder/substrate couples were carried out using DICTRA with the MOBSLD1 mobility database. The predictions were validated experimentally by differential scanning calorimetry (DSC) and by microstructural characterization using SEM/EDX and X-ray diffraction (XRD).

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Biographical Note

Patrícia Danišovičová is a PhD student in Advanced Materials and Material Design. Her research focuses on the impact of various additions into lead-free solders microstructure evolution and thermal behavior. She earned her Master's in Materials Engineering in 2024 with a thesis on The Influence of Different Solders on the Properties of Soldered Joints.

Integrating Machine Learning for Alloy Exploration

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Advances in materials science increasingly rely on computational tools to accelerate alloy design and reduce the cost and time associated with experimental trial and error. However, many existing tools are fragmented, difficult to use, or require specialized expertise, making it challenging to rapidly explore new material compositions and interpret results. This work presents DeepAlloy®, a web based machine learning platform designed to support materials scientists by providing fast, accessible, and intuitive insight into alloy microstructure, phase information, and material properties.

DeepAlloy® is built around a GAN based microstructure generator trained on metallography datasets and high-throughput CALPHAD results. The generator takes in data and produces a microstructure image using a convolutional up sampling architecture.[1] To support interpretation, DeepAlloy® includes an image analysis layer that extracts phase distribution and composition from generated microstructures.[3] These extracted measurements provide a bridge between visual outputs and data that can be compared across compositions. The platform also presents predicted phase information associated with each composition, allowing users to connect microstructure outputs with phase level interpretation within a single workflow.

Lastly, DeepAlloy® includes a component for predicting material properties, with an initial focus on mechanical strength. Composition inputs are passed to a supervised regression model trained on strength labeled materials data.[2] The model returns an estimated strength value, which is presented alongside the corresponding composition.

The components described above form the foundation of DeepAlloy®. This work focuses on integrating these tools into a unified web-based platform. The models are hosted within a Flask backend and communicate with each other in steps. The users then input alloy compositions which will be passed into the GAN model. Next, the generated Micrographs are created and then passed to the image analysis pipeline for feature extraction and phase composition, and these outputs are reused to estimate the properties. These steps happen in seconds and provide immediate feedback to the users.

The web architecture was built prioritizing usability and accessibility. By packaging microstructure generation, image analysis, phase information, and property estimation into an accessible platform. This lowers the barrier for applying machine learning techniques in materials research while enabling materials scientists to quickly explore candidate alloys, compare results, and reduce time and money spent on manual exploration.

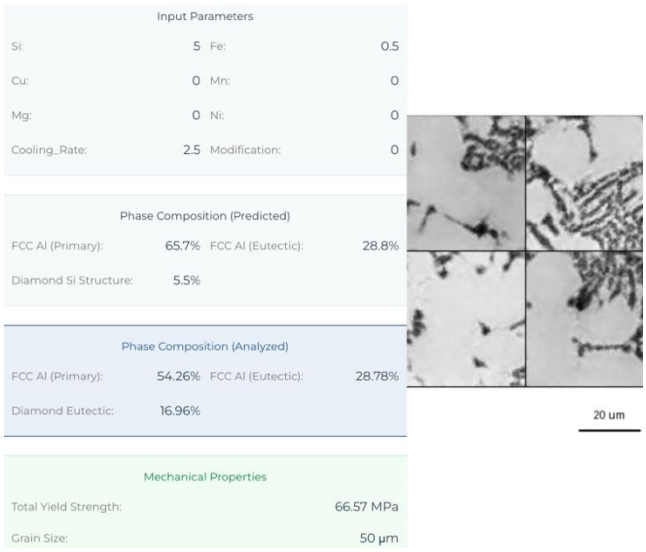

Figure 1. Example microstructure generated by ML model

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Biographical Note

Jake Foley is an undergraduate computer science student focused on applying machine learning and full stack development to materials science and computational thermodynamics. His work focuses on developing accessible, data driven tools on the web that support material scientists in the exploration and analysis of alloy design.

Reconstruction of a Historical Silicon Arc-Furnace Thermodynamic Model Using SimuSage and FactFlow

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Computational thermochemistry has long played an important role in the interpretation, design, and optimization of pyrometallurgical processes, particularly when direct observation of high-temperature reactors is limited and process behavior is governed by coupled multiphase equilibria, phase partitioning, gas formation, and enthalpy effects. Its value increases further when thermodynamic calculations are extended beyond isolated equilibrium states to staged reactor descriptions and complete process flowsheets, where local equilibria, internal circulation, and overall mass and energy balances can be examined together. In this context, thermodynamic process simulation refers to a staged representation of a reactor in which interconnected local-equilibrium zones are linked by co- or counter-current material and heat exchange, allowing reactor-scale behavior to be interpreted beyond a single isolated equilibrium calculation. A first version of such an approach was already integrated in the software ChemSage [1]. The early higher-level thermo-dynamic process simulation tool “SimuSage” was developed to connect multiple equilibrium calculations into practical flowsheet descriptions of industrial high-temperature processes [2].

The silicon arc furnace is a representative and historically important example of this challenge. Industrial silicon production in an electric arc furnace involves coupled gas-solid-liquid reactions, strong internal thermal gradients, and counter-current transport between ascending gaseous species and descending condensed phases. Historical thermodynamic studies showed that this process cannot be described adequately by either a simple stoichiometric reaction or a single equilibrium calculation, but instead requires several interacting local-equilibrium zones connected by internal heat and mass exchange [3]. The silicon arc-furnace case is therefore important not only as a successful thermodynamic model of an industrial process, but also as an early example of higher-level thermodynamic flowsheeting in metallurgy.

In the present work, this silicon arc-furnace model, originally implemented in the SimuSage, is reconstructed in FactFlow, a modern multi-stream, multi-unit thermo-dynamic process simulator embedded in FactSage [4]. The aim is to preserve the original process logic while transferring the case to a more transparent and flexible flowsheet environment for stream definition, staged reactor configuration, recycle handling, and systematic sensitivity analysis. The reconstructed model provides a direct basis for comparing the legacy and modern implementations of the same industrial case, while also examining the influence of carbon feed and imposed energy input. Particular attention is given to silicon yield, internal material circulation, intermediate phase formation, gas-phase chemistry, and the feasible operating window of the furnace, since historical studies showed that carbon feed and energy input strongly affect yield and operating feasibility. By revisiting this long-standing silicon arc-furnace model in a modern thermodynamic flowsheeting environment, the present study shows how legacy simulation knowledge can be preserved, clarified, and extended for more systematic analysis of pyrometallurgical processes and future process development.

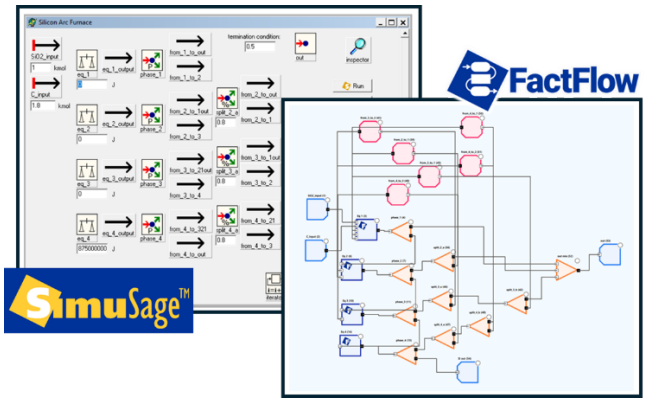

Figure 1. Historical SimuSage model and reconstructed FactFlow model of the silicon arc furnace

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Microstructure Prediction of Ni–Cr–Al Alloys for Exhaust Valve Spindles Based on Thermodynamic Calculations

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The exhaust valve spindle is a key component of marine engines, as it directly contacts high-temperature and high-pressure exhaust gases in the exhaust valve assembly and controls their discharge from the engine cylinder. Owing to these harsh operating conditions, the spindle material should possess superior resistance to high-temperature corrosion and wear. A Japanese Ni–Cr–Al–based alloy, DSA760, has been widely used for exhaust valve spindle applications. However, to reduce reliance on imported materials and promote localization, a new alloy with properties similar to DSA760 has been designed.

The newly designed alloy, referred to as Alloy760, was manufactured based on a Ni–Cr–Al system. During manufacturing, however, Alloy760 exhibited excessively high hardness, which led to severe cracking and poor processability. Microstructural observations revealed clear differences between Alloy760 and DSA760. DSA760 contained a large amount of α-Cr precipitates and showed a fine and dense lamellar microstructure, whereas Alloy760 exhibited a lower α-Cr fraction and a coarse lamellar morphology. These differences were identified as the main cause of the excessive hardness observed in Alloy760.

To reproduce a DSA760-like microstructure, thermodynamic calculations were performed to evaluate temperature-dependent phase fractions and coarsening rate coefficients of individual precipitates. For comparison, the same calculations were conducted for Chinese DSA760M and 3J40 alloys. The phase fraction analysis showed that DSA760 possesses the highest α-Cr fraction and the lowest γ-matrix fraction among the investigated alloys over a wide temperature range. In terms of coarsening rate, DSA760 exhibited a faster coarsening rate for α-Cr precipitates and a slower coarsening rate for the γ’ phase compared with the other alloys.

To modify the microstructure of Alloy760 toward that of DSA760, the effects of alloying element variations on coarsening rate coefficients were evaluated. The calculations indicated that Ti addition decreases the coarsening rate coefficient of the γ’ phase, while Mn removal increases that of α-Cr. These effects are expected to modify the microstructural evolution of Alloy760 toward that of DSA760. Experimental studies are planned to validate the thermodynamic predictions.

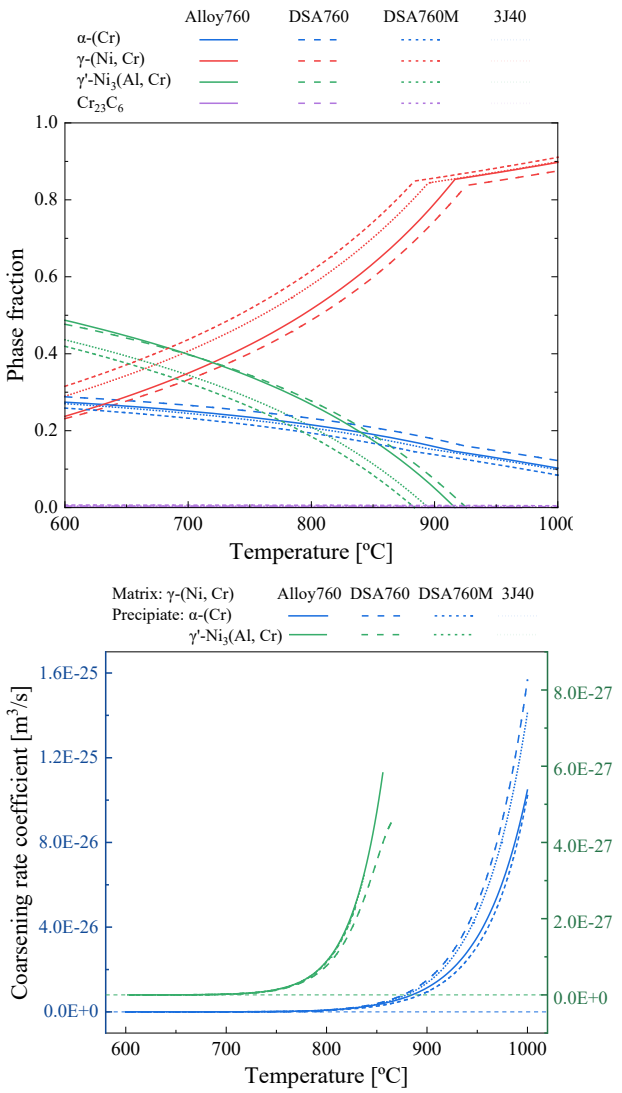

Figure 1. Phase fraction and coarsening rate coefficient

Biographical Note

Hyo-Sun Jang is a senior researcher at the Korea Institute of Materials Science. She received her Ph.D. degree at the Department of Materials Science and Engineering at POSTECH in 2021. Her research interests include molecular dynamics, first-principles calculations, computational thermodynamics, and machine learning in structural alloys.

Nickel Partitioning in Iron and Its Implications for Terrestrial Planet Cores

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Nickel is typically treated as a passive alloying component in planetary cores, assumed to mix nearly ideally with iron and exert little influence on equilibrium phase behavior in Fe-rich systems. Under this assumption, nickel would not be expected to partition between solid and liquid iron during core crystallization and is therefore often neglected in thermodynamic models of Fe-Ni mixtures. We test this assumption across various pressure-temperature-composition conditions relevant to terrestrial planets and show that this assumption breaks down.

In this work, we investigate the thermodynamic behavior of Fe-Ni mixtures using equations of state (EOS) for solid and liquid iron [1] and nickel [2] derived from density functional theory molecular dynamics (DFT-MD) simulations and constrained by high-pressure experimental data. These EOSs are combined within the Multicomponent, Multiphase Mixture (MM_Mix) framework [3] to construct mixture EOSs across a wide range of pressures and compositions. Phase coexistence is evaluated through Gibbs free energy minimization at fixed pressure and temperature.

Within an ideal mixing approximation referenced to pure endmembers, we assess the extent to which nickel partitions between solid and liquid iron as a function of pressure. Our results indicate that nickel does not behave as a strictly passive component under conditions relevant to planetary interiors. Instead, its partitioning behavior varies with pressure, reflecting differences in the underlying free energy landscapes of Fe and Ni in solid and liquid phases. These trends persist across a range of relevant compositions suggesting that they are governed by pressure-dependent chemical potential differences rather than concentration effects.

Although our initial analysis adopts an ideal mixing framework, we incorporate non-ideal contributions through a polynomial excess free energy model calibrated over a subset of the pressure range investigated. To further validate these trends, we include preliminary thermodynamic integration calculations at selected pressures, providing a first-principles benchmark for nickel partitioning behavior.

These results highlight the importance of accurately modeling mixture thermodynamics in dense metallic systems and demonstrate that even components traditionally treated as ideal can exhibit nontrivial behavior at extreme conditions. More broadly, this work illustrates how EOS-based mixture models can be used to rapidly evaluate phase coexistence and partitioning behavior in multicomponent systems, providing a bridge between first-principles simulations and CALPHAD-style thermodynamic descriptions at extreme pressure-temperature conditions.

Figure 1. Schematic of core crystallization from $t_0 \rightarrow t_{present}$

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Biographical Note

Tanja Kovačević is a Ph.D. candidate in Earth and Planetary Science at UC Berkeley and is an NSF Graduate Research Fellow. She works in the group of Burkhard Militzer. Her research focuses on first principles and thermodynamic approaches to understanding the behavior of materials at extreme conditions in planetary interiors.

Stacking Fault Energy in Fe–Mn Steels: Bridging the Gaps between DFT, Experiments and Thermodynamic Modelling

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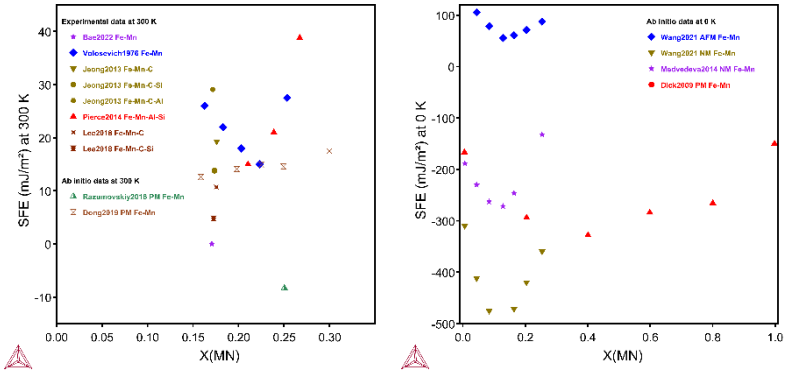
Stacking fault energy (SFE) is a key parameter governing the deformation behaviour of metastable face-centred cubic (fcc) alloys, particularly high-manganese Fe–Mn steels exhibiting twinning-induced plasticity (TWIP) and transformation-induced plasticity (TRIP). These steels demonstrate an exceptional combination of strength and ductility arising from deformation mechanisms such as dislocation glide, mechanical twinning, and strain-induced martensitic transformation, all of which are strongly correlated with the SFE [1].

Despite its importance, significant discrepancies persist between experimentally derived and ab initio calculated SFEs in metastable fcc alloys. Experimental approaches, commonly based on force-balance models and stacking fault width measurements, inherently yield positive SFE values due to underlying methodological assumptions [2]. In contrast, density functional theory (DFT) calculations frequently predict negative SFEs, reflecting the thermodynamic instability of the fcc phase relative to the hexagonal close-packed (hcp) phase in these systems [3]. This divergence complicates the interpretation of deformation mechanisms and limits alloy design.

The present work addresses this inconsistency through thermodynamic modelling of the Fe–Mn system, taken as a model alloy for TWIP/TRIP steels and as a basis for extension to the Fe–Mn–C–Si system. Using third-generation CALPHAD descriptions, the Gibbs energy difference between fcc austenite and hcp martensite is evaluated, enabling thermodynamic estimation of SFE. This approach links phase stability directly to deformation behaviour via the Olson–Cohen relation [4].

Attention is given to reassessing the experimental force-balance framework to determine whether negative SFEs can, in principle, be obtained from experimental data. In addition, thermodynamic SFE calculations are revisited with emphasis on the interfacial energy term, a major source of uncertainty in SFE predictions. The overall aim is to improve the thermodynamic description of SFE to facilitate more reliable predictions of deformation mechanisms in TRIP/TWIP steels using third-generation descriptions. Enhanced agreement between calculations and experiments will strengthen predictive capabilities and support the design of next-generation high-performance TWIP/TRIP steels for structural applications.

Figure 1. The discrepancy of various SFE values (from experimental and ab initio data) for Fe-Mn based alloys: (a) at 300 K, (b) at 0 K. AFM: antiferromagnetic, PM: paramagnetic, NM: nonmagnetic.



- 300 K. - 0 K.

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Biographical Note

Felicia Larsson is a PhD student at KTH Royal Institute of Technology, Sweden. Her work focuses on developing third-generation CALPHAD models and an improved model for stacking fault energies for TRIP/TWIP steels.

Experimental Phase Equilibrium Study and Thermodynamic Optimization of the PbO-Na_2O-SiO_2 System

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Lead-acid batteries represent the largest end-use application of lead worldwide, and the recycling of spent lead-acid batteries is therefore a major source of secondary lead production [1]. Pyrometallurgical processing is widely employed in secondary lead recycling due to its robustness and ability to handle complex battery-derived feed materials [2]. In the pyrometallurgical process of secondary lead recycling, a desulfurizing agent, such as Na_2CO_3 is added to minimize the emissions of sulphur into the atmosphere, while silica is introduced into the smelter as a fluxing material [3]. Subsequently, a significant amount of Na_2O and SiO_2 remain in the downstream reverberatory furnace and blast furnace slags. Presently, there is limited understanding of the thermodynamic behaviour of silicate-based lead slags rich in Na_2O, posing challenges in accurately determining the optimal conditions for targeted lead metal recovery and final slag composition. In this work, the equilibrium phase relations of the Na_2O-SiO_2 system in the SiO_2 primary phase field, as well as the PbO-Na_2O-SiO_2 system in the primary phase fields of Na_2SiO_3, $Na_6Si_8O_{19}$, $Na_2Si_2O_5$, $PbSiO_3$, and SiO_2 are studied via equilibration-quenching-microanalysis method. Samples with different compositions were prepared and held in platinum capsules or quartz capsules under air or vacuum. The samples were heated at temperatures ranging from 500 °C to 1550 °C until phases had reached equilibrium. The equilibrated samples were subsequently quenched in salt brine, and the phase compositions were measured by electron probe microanalysis (EPMA). The results were then compared to those of previous studies, and any discrepancies were resolved. Experimental data combined with available data in the literature were used in the development of thermodynamic models using CALPHAD approach. The Modifier Quasichemical Model (MQM) with two sublattices (Pb^{2+},Na^+, Si^{4+})(O^{2-}) was selected to describe the liquid phase while solids were modelled as stoichiometric phases.

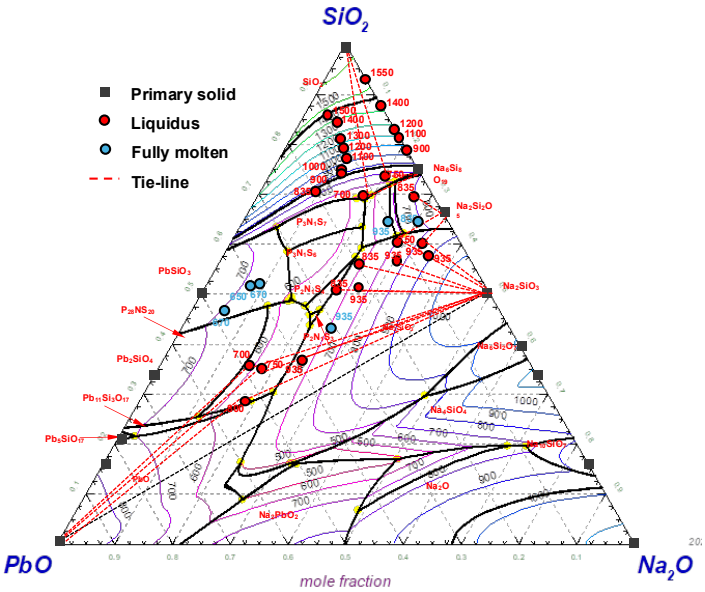

Figure 1. Predicted phase diagram compared to experimental results on PbO-Na_2O-SiO_2 system

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Biographical Note

Xi Ling is a PhD candidate in Materials Science and Engineering at the University of Toronto. Her research focuses on thermodynamics and phase equilibrium of sodium-containing lead slag systems, with an emphasis on CALPHAD-based modeling for lead-acid battery recycling. Her work combines high-temperature experiments, EPMA, and thermodynamic optimization to support more efficient and environmentally responsible metallurgical processes.

Experimental Phase Equilibria and Thermodynamic Modeling of the Si_3N_4-MgO-SiO_2 System

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The Si_3N_4-MgO-SiO_2 ternary system is fundamental to the liquid-phase sintering of Si_3N_4 ceramics, yet its complex phase relationships and liquid-phase behavior remain insufficiently understood. In this study, we present a systematic investigation of this system through integrated experimental investigations and CALPHAD-based thermodynamic modeling.

Equilibrium experiments were conducted at 1873 K using an equilibrium-quenching technique, with phase compositions characterized by XRD and EPMA. The liquid phase was described using the ionic two-sublattice model: $(Mg^{+2})_P(SiO_4^{-4}, SiO_2, SiN_{4/3}, O^{-2})_Q$. Our results show that the ternary phase equilibria are dominated by the liquid phase, featuring a miscibility gap extending from the MgO-SiO_2 binary system that results in MgO-rich (Liq#2) and SiO_2-rich (Liq#1) liquids.

Significant findings regarding Si_3N_4 solubility were obtained: solubility is notably higher in Liq#2 than in Liq#1. Within the Si_2N_2O-Liq#2 region, solubility increases with MgO content due to the role of Mg^{+2} as a network modifier. However, in the Si_3N_4-Liq#2 region, elevated MgO does not enhance solubility as SiO_2 species are depleted. Additionally, thermodynamic analysis of crucible reactions reveals that Si_3N_4 oxidation under low oxygen partial pressure produces Si and SiO. These results provide a self-consistent thermodynamic description and critical guidance for the science-based design of nitride ceramic processing conditions.

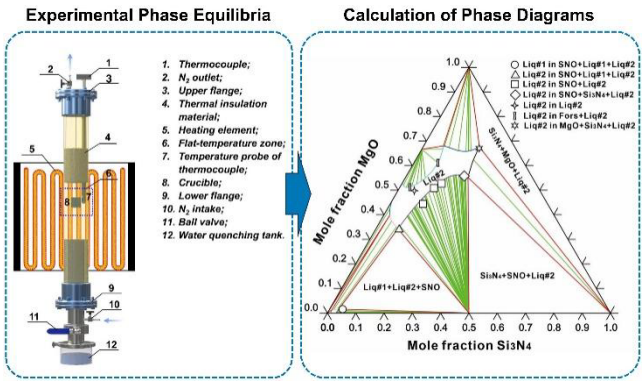

Figure 1. Integrated experimental and thermodynamic modeling approach for the Si_3N_4-MgO-SiO_2 system

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Biographical Note

Tengfei Deng:

Professor at the State Key Laboratory of Silicate Materials for Architectures, Wuhan University of Technology. Mainly engaged in basic research on the high-temperature thermodynamics and kinetics of oxide and nitride ceramic systems, with a focus on the optimization of sintering performance for architectural ceramics, development of high-performance heating ceramic technology, and industrial applications. Published over 40 papers in top ceramic journals and holds multiple patents, including an authorized U.S. patent.

Baijun Yan:

Professor at the University of Science and Technology Beijing. Mainly engaged in research on the thermodynamic properties of metallurgical melts containing transition metals and the physical chemistry of new functional materials. Focuses on the efficient utilization of vanadium-titanium resources and the determination of thermodynamic and kinetic parameters for oxide preparation through gas-solid reactions. Published over 30 SCI/EI papers.

Chunxi Luo:

PhD student at the State Key Laboratory of Silicate Materials for Architectures, Wuhan University of Technology. Mainly engaged in the experimental investigation and thermodynamic modeling of advanced ceramic systems. Focuses on the liquid-phase sintering mechanism of silicon nitride-based materials, phase equilibrium relationships, and the application of the CALPHAD approach in material design.

Investigation of Additions on β-AlFeSi and α-Hexagonal Phase Formation

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The presence of β-AlFeSi intermetallic phases in aluminum alloys is well known to inducedetrimental mechanical effects, including reduced ductility and increased susceptibility to crack initiation and propagation. These phases, typically forming as platelet-like morphologies during solidification, act as stress concentrators and significantly degrade the structural integrity of recycled aluminum systems where iron is an unavoidable impurity. Understanding and controlling the formation of such phases is therefore of critical importance for improving alloy performance.

In this study, in situ synthesis of Al–Fe–Si alloys was conducted using differential scanning calorimetry (DSC). Controlled additions of vanadium, manganese, and chromium were progressively introduced to investigate their impact on phase equilibria and solubility within the τ5 (β-AlFeSi) and τ6 (α-hexagonal) phases.

The experimentally determined equilibria will be directly integrated into FactSage thermodynamic databases, enhancing their predictive accuracy and enabling more reliable determination of the Cr, V, and Mn concentrations required to tailor phase stability in Al–Fe–Si alloys.

AI-Driven High-Throughput Design and Performance Iterative Optimization of High Entropy Alloy for Additive Manufacturing

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Additive manufacturing technology serves as a core enabling technology for the integrated fabrication of high-performance metallic components in aerospace, energy and petrochemical, high-end equipment, and other industries. However, existing commercial alloys generally face common bottlenecks, including poor compatibility with additive manufacturing processes, high hot cracking susceptibility, strength-ductility trade-off, and low research and development efficiency arising from the traditional trial-and-error approach.

In this study, an integrated intelligent material R&D system is established, which is driven primarily by artificial intelligence and integrates an autonomous iterative optimization engine, high-throughput thermodynamic calculation, high-throughput additive manufacturing, and fully automatic high-efficiency characterization.

Based on this system, closed-loop iterative optimization is performed to improve the strength-ductility matching of the FeCoCrNi quaternary high-entropy alloy. After four rounds of experimental verification, the tensile strength of the alloy is increased from the initial 985 MPa to 1265 MPa while maintaining its elongation. Multiple optimal compositions with both high strength and high ductility are obtained, and a remarkable breakthrough is achieved on the Pareto front of comprehensive properties. This fully validates the reliability and iterative optimization capability of the system, and significantly shortens the R&D cycle of additively manufactured alloys.

This work provides theoretical support and a technical framework for the intelligent design of other additively manufactured alloys.

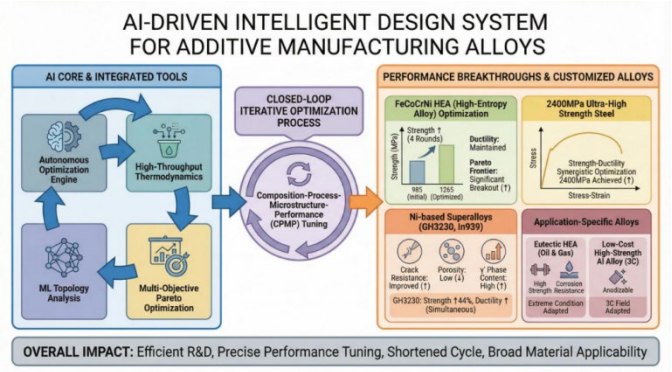

Figure 1. Graphical Abstract

Biographical Note

Hou Yaqing, Doctor of Materials Science and Engineering, Professor-level Senior Engineer, and Postgraduate Supervisor. She has long been engaged in intelligent materials R&D technologies, including intelligent materials design, Highthrough CALPHAD design of materials, laser in-situ alloying of heterogeneous powders, etc.she serves as Secretary-General of the Technical Committee for Materials Industry Blockchain, Member of the Technical Committee for Virtual Simulation of Heat Treatment in China, and Young Editorial Board Member of Metallurgical Automation.

As the technical principal, she invented the technology of in-situ alloying of heterogeneous powders, and led the development of the high-throughput additive manufacturing system for bulk samples (HTSLM) and the AI Materials Data Factory system, which have been applied in ultra-high strength steels, superalloys and other fields. As the project leader, she applied multi-scale computation and materials blockchain technology to lead the development of a full-process cross-scale cloud computing and data aggregation platform for additive manufacturing, which has been used in the intelligent design and development of four aerospace superalloys.

She has published more than 30 academic papers, obtained 9 authorized invention patents and more than 20 authorized software copyrights. She took the lead in compiling and reviewing 1 group standard for material blockchain, and participated in the compilation of 2 group standards.

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Integrated CALPHAD–DFT Study of the Al–Si Subsystem for Accurate Modeling of Si-Containing Steels

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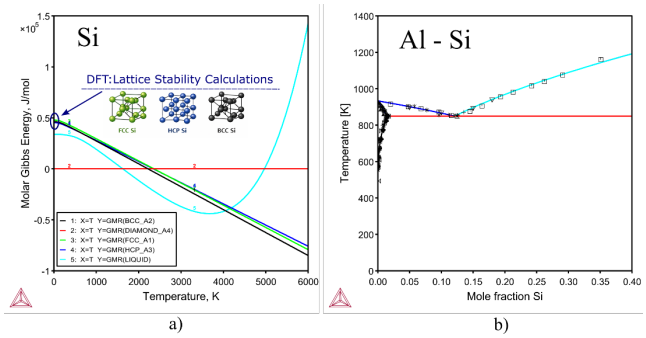
Transformation-Induced Plasticity (TRIP) and Twinning-Induced Plasticity (TWIP) steels have attracted significant industrial interest due to their exceptional combination of strength and ductility [1]. The mechanical behaviour of these steels is largely governed by their stacking fault energy (SFE), which depends on thermodynamic interactions among key alloying elements such as Mn, Al, Si, and C [2]. Accurate prediction of SFE, and consequently the dominant deformation mechanism, requires a reliable thermodynamic description of all relevant subsystems.

In this study, the Al–Si binary subsystem was reassessed using the CALPHAD approach supported by first-principles calculations. Third-generation thermodynamic descriptions for pure Al and for the liquid and diamond phases of Si were combined as a starting point [3], [4]. However, the metastable and mechanically unstable Si phases (FCC, HCP, and BCC) were not described in the previous assessment by Bajenova [4]. In order to consistently combine the Al and Si descriptions and determine a new set of binary interaction parameters, Density Functional Theory (DFT) calculations were performed to evaluate the energy differences between the unstable Si phases and the stable diamond structure. The obtained energies were used to recalculate the lattice stabilities of the FCC, HCP, and BCC phases of Si. The molar Gibbs energy curves for the diamond, FCC, HCP, BCC and liquid phases of Si, incorporating the DFT-derived lattice stabilities, are presented in **Figure 1(a)**.

Additionally, the elastic constants of these phases were computed using DFT. Application of mechanical stability criteria based on the calculated elastic constants showed that FCC and BCC Si are mechanically unstable, whereas HCP Si is metastable.

Using the DFT-derived lattice stabilities for pure Si, a new set of binary interaction parameters for the FCC and Liquid phases in the Al-Si binary system was then determined by fitting to available experimental data using the Parrot optimization module of Thermo-Calc software. The results of the optimization are demonstrated in **Figure 1(b)**, where the experimental data employed in the assessment are plotted together with a calculated section of the Al–Si phase diagram obtained using the newly determined binary interaction parameters.

Figure 1. (a) Molar Gibbs energy curves of pure Si for the diamond, FCC, HCP, BCC and liquid phases, incorporating lattice stabilities derived from DFT calculations. (b) Calculated section of the Al–Si binary phase diagram obtained using the optimized set of binary interaction parameters determined in this study, with experimental data points used in the assessment overlaid for comparison.



a) b)

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Biographical Note

Yulia Mishchenko is a postdoctoral researcher in the Department of Materials Science and Engineering at KTH -Royal Institute of Technology, where she works on third-generation thermodynamic modeling.

Construction of Theoretical Phase Diagrams using NNP

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Introduction

In recent years, first-principles methods have enabled highly accurate calculations of electronic states and energies across various material systems. Furthermore, a wide range of applications such as molecular dynamics (MD) simulations and crystal structure searches have become feasible by executing these calculations in parallel. Nevertheless, first-principles calculations remain computationally demanding; for example, first-principles MD simulations are typically limited to picosecond timescales and systems comprising only a few hundred atoms. To accelerate such computationally intensive applications, the use of neural network potentials (NNPs) has attracted considerable attention.[1] NNPs represent the local atomic environment as structural descriptors and model the relationship between these descriptors and the system's energy using neural networks (NNs). Once constructed, NNPs enable rapid energy evaluations for given structures. Our research group has previously reported a methodology for constructing theoretical phase diagrams based on DFT calculations.[2] In this study, we aim to accelerate this approach by applying NNPs to compute the energies of various structures in the Al–Cu binary system and subsequently derive theoretical phase diagrams from the resulting free energies.

Computational Methods

First-principles molecular dynamics (MD) simulations were performed using the VASP code for multiple FCC/BCC ordered structures, liquid phases, and intermetallic compounds in the Al–Cu binary system. The atomic snapshots obtained from the MD trajectories were used as training data to construct a neural network potential (NNP) using DeePMD-kit.[3] The developed NNP was then utilized to compute the finite-temperature free energies of liquid phases, solid solutions, and intermetallic compounds. These free energies were incorporated into a thermodynamic model based on the CALPHAD approach to calculate theoretical phase diagrams.

Result

Figure 1(a) shows the Al–Cu binary phase diagram constructed using the present computational approach, while Figure 1(b) depicts the theoretical phase diagram based on first-principles calculations. Overall, the two diagrams exhibit reasonably good agreement. However, discrepancies remain; for example, the BCC phase observed in the low-Al concentration and high-temperature region of (b) does not appear in (a). On the other hand, the free-energy difference between the two methods is at most approximately 3–4 kJ/mol, indicating that our NNP reproduces DFT thermodynamic quantities within a few kJ/mol. We are also carrying out MD–Monte Carlo (MC) simulations using the NNP to access time and length scales that are difficult to reach with DFT calculations. The corresponding results will be included in the presentation.

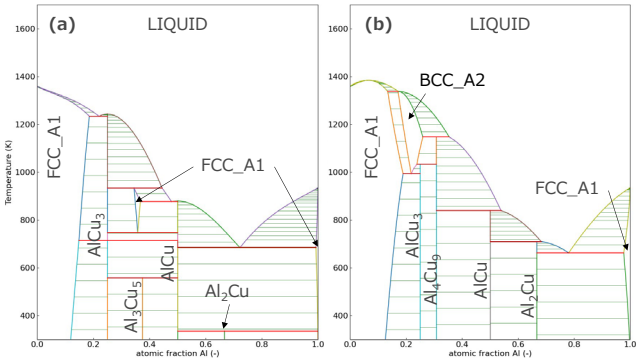

Figure 1. (a) Theoretical Al–Cu phase diagram constructed with the NNP, and (b) the first-principles-based theoretical Al–Cu phase diagram.

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Hirokazu Okabe is engaged in the development of an integrated computational approach for copper alloy design using neural network potentials (NNPs).

Microstructural modifications of a 6061 aluminum alloy by addition of iron and vanadium

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Traditionally, wrought aluminum alloys are rarely produced from recycled materials due to their low impurity tolerances. However, the higher demand for wrought alloys makes these materials ideal candidates to increase recycling activities. To explore contamination limits, this work reports effect of some tramp elements, Fe and V, on the microstructure of 6061 alloy. A commercial 6061 alloy is artificially contaminated with various concentrations of Fe and V by adding pure powder. The microstructures of contaminated alloys are observed by optic and electronic microscopy and phases are identified using energy dispersive spectroscopy and electron backscatter diffraction. Also, computational thermodynamic simulations performed with FactSage software are compared to the phase assemblage of the samples. It is shown, in the presence of 1 wt.% of Fe (well above typical contamination levels), that vanadium modifies the morphology of the AlFeSi- and Al(Fe,Mn)Si phases formed upon casting. At 1 wt.% of V in 6061 alloy, Al20V2Mg intermetallic is primarily formed with a polygonal shape, which is different from the 0.5 wt.% of V predicted by FactSage. Furthermore, the Scheil solidification simulation describes only the phase assemblage of 6061 alloy without manganese correction of iron-rich phases and without vanadium interaction. The transformation of iron-rich phases may stem from modifications of thermodynamic equilibrium of the liquid and the solid solutions containing vanadium by substitution of some Fe or Al atoms. Factsage's database does not include solution models with iron substitution by Mn or V in Al(Fe,Mn,V)Si phase which limits the describability of their energetic impact. Understanding the interaction of tramp elements supports the development of creative strategies to open recycling to larger variety of feedstock. More research is needed to include the substitution of Fe and Al by Mn and V in solutions to reliably simulate a contaminated 6061 with iron correction.

CALPHAD-Based Thermodynamic Framework for Disordered and Ordered Early-Stage Phases in Al alloys

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Early-stage phases in Al–Mg–Si and Al–Mg–Zn-(Cu) alloys control microstructural evolution during heat treatment and guide the formation of hardening particles that determine mechanical performance. Predictive models of the competitive evolution of disordered clusters and ordered GP-zones are not yet available.

We present the first CALPHAD-based approach to capture the formation, stability, and mutual interactions of disordered clusters and ordered GP-zones across varying Mg, Si, and Zn contents. In our modelling, disordered clusters represent small, unstructured aggregates of atoms, which, however, are large enough for the CALPHAD framework to be applied, at least in a rough approximation. These are represented by a solid solution model. The presentation will illustrate the challenges of modelling small disordered clusters and the strategies to address them. Ordered phases are modelled with a four-sublattice Compound Energy Formalism, allowing atoms in the face-centered cubic alloy lattice to occupy distinct sites upon ordering [1].

We combine first-principles formation enthalpies with differential scanning calorimetry-derived dissolution temperatures to parametrise the models. The framework captures demixing of clusters, chemical ordering, and low-temperature metastable behavior. It predicts phase fractions, precipitation kinetics, and processing sensitivity, providing a tool to optimise alloy composition and heat treatment for improved hardening response.

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Biographical Note

Erwin Povoden-Karadeniz is an Austrian materials scientist and Associate Professor of Computational Materials Engineering at the TU Wien (Vienna University of Technology). He studied earth sciences at the University of Graz and received his PhD in materials science from ETH Zurich in 2008. Since 2009 he has been affiliated with the Institute of Materials Science and Technology at TU Wien, where he leads the research group for Computational Materials Engineering. His research focuses on computer-assisted modelling and simulation of materials, particularly the thermodynamics and kinetics of phase transformations, diffusion processes, and microstructure evolution in sustainable multi-component materials.

From Quantum-Informed Descriptors to Additive Manufacturing Process: A Scale-Bridging Workflow for TCP Phase Prediction

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Topologically close-packed (TCP) intermetallic phases such as σ in steels and μ in Ni-based alloys are recurring degradation mechanisms that can strongly reduce long-term mechanical performance and corrosion resistance. In sustainable alloy and process design, reliable TCP-risk prediction requires linking physics across scales: chemical disorder and phase stability originate at the electronic-structure level, thermodynamic driving forces are governed by Gibbs-energy descriptions, and additive manufacturing (AM) outcomes depend on non-equilibrium solidification followed by solid-state precipitation kinetics under complex thermal histories.

Within the AIM project (AI-guided Computational Materials Design for Sustainable Manufacturing and Materials Innovation)[4], we develop a scale-bridging workflow that links electronic-structure-informed stability descriptors to high-throughput CALPHAD thermodynamics and precipitation kinetics, and then to interpretable surrogate models. At the quantum-informed level, chemically disordered TCP-related states are treated using EMTO-CPA to derive stability-relevant quantities (e.g., energetic and occupancy/disorder descriptors). At the CALPHAD scale, equilibrium calculations, Scheil-Gulliver solidification, and precipitation-kinetics simulations are executed using assessed thermodynamic and mobility databases. For AM-relevant conditions, a two-step strategy is employed: Scheil-Gulliver simulations capture segregation during rapid solidification, and the resulting segregation-informed states are propagated into subsequent kinetic precipitation simulations. The workflow is designed to support methodological transfer across TCP families, leveraging concepts established for σ-phase risk in steels toward μ-phase assessment in Ni-based systems.

This contribution focuses on the benchmarking and validation of the physics-based pipeline for a representative Ni-based benchmark system. The resulting benchmark dataset and evaluation criteria provide a transparent basis for assessing predictive reliability and for enabling accelerated TCP screening under AM-relevant processing scenarios.

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Biographical Note

Sachin Rangaswamy is a first-year PhD student at the Leibniz Institute for Materials Engineering (IWT) and the University of Bremen. In the AIM project, he has planned to develop scale/bridging workflow that couples quantum-informed descriptors with CALPHAD thermodynamics and precipitation kinetics to assess TCP phase risk under additive-manufacturing-relevant thermal histories. He earned an M.Sc. in Materials Science and Simulation from Ruhr-Universität Bochum (ICAMS) in 2025 and a B.Sc. in Physics, Chemistry, and Mathematics in 2022 from Christ University (Bengaluru, India).

Advances in the experimental determination of the liquidus projection of the Al-Nb-Ta system

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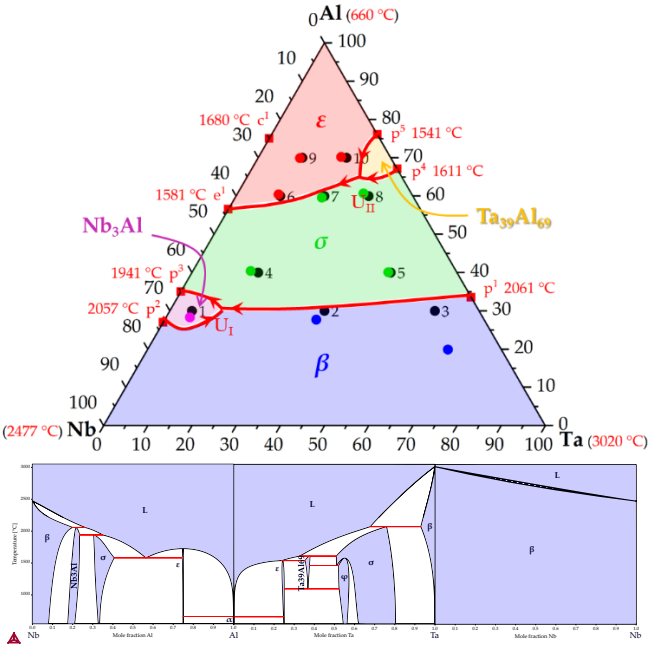
High Entropy Alloys (HEAs) containing Al and refractory metals are promising structural materials for aeronautical applications, serving as complementary materials to Ni-based superalloys due to their high-temperature performance, low specific mass, and therefore, interesting specific properties [1-2]. The development of such alloys depends, among other aspects, on the development of thermodynamic databases, which in turn rely on the experimental study of low-order systems – such as binary and ternary systems – and their extrapolation to higher-order systems. A subclass of HEAs of particular interest is related to those containing Al and high-melting-point metals. In this scope, our research group has been studying binary and ternary systems of the Al-Cr-Nb-Ta-Ti-V-Zr multicomponent system [3-4]. Among those, the Al-Nb-Ta ternary system is one for which limited information is available in the literature. The objective of the present work is to experimentally investigate the liquidus projection of the Al-Nb-Ta system through microstructural characterization of arc-melted samples.

The alloy compositions were designed based on the nature of the invariant transformations of the boundary binary systems, as well as the similarity between the crystal structures of certain phases. The samples were prepared from high purity elements Al (min. 99.96 wt %), Nb (min. 99.8 wt %) and Ta (min. 99.8 wt %). The starting materials were arc-melted under argon atmosphere (min. 99.995 %) with non-consumable tungsten electrode in a water-cooled cooper crucible. The as-cast samples were submitted to the usual metallographic preparation (cutting, mounting, grinding and polishing). Micrographs were obtained in a TESCAN-MIRA4 scanning electron microscope (SEM-FEG) in the backscattered electrons mode. The chemical compositions of the phases were obtained by energy dispersive X-ray spectroscopy (EDS) using EDAX Octane Elect EDS/EDX detector. X-Ray Diffractometry (XRD) characterization was performed in a Panalytical Empyrean diffractometer using Cu-Kα radiation. The XRD data collected were analyzed and refined using the Rietveld method, implemented through the FullProf Suite software. Complementary analyses via electron back scattered diffraction (EBSD), using the EDAX Hikari Super EBSD detector, were performed on some samples for the identification of fine phases.

The characterization results of the as-cast samples showed no signs of ternary phases and only primary solidification fields from binary phases were observed. The primary solidification fields of β-BCC, σ-Me_2Al, and ε-$MeAl_3$ phases are dominant, while the $Ta_{39}Al_{69}$ and Nb_3Al primary solidification fields are confined to regions close to their respective binaries, as can be seen in Figure 1. Two class II (U_I and U_{II}) ternary invariant transformations were proposed.

Figure 1. Liquidus projection of Al-Nb-Ta system and boundary binary systems



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Biographical Note

Caio Simão de Barros is a PhD student in Materials Engineering at University of São Paulo (USP), Brazil, under supervision of professor G.C. Coelho. He has experience with experimental determination of phase diagram.

Homogenization Kinetics of Refractory High-Entropy Alloys Predicted by Multicomponent Diffusion and DICTRA Simulations

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Contemporary nuclear reactors (Gen IV) offer several advantages in terms of safety, operational efficiency, and sustainability. They are prone to operation in environments with high temperatures, extreme radiation, and severe corrosion. The fuel pin cladding materials, which serve as a boundary between irradiated fuel and the core environment, play a key role in advancing the development of advanced nuclear reactors. Zircaloys have significant market dominance as the fuel-cladding tube material in the nuclear reactor production industry. However, Zircaloys are vulnerable to failure by hydrogen embrittlement, especially at elevated temperatures [1]. Nowadays, refractory high-entropy alloys with a single-phase body-centered cubic (BCC) structure are considered a promising candidate for fuel cladding materials due to their outstanding performance in terms of high-temperature stability, resistance to void swelling, and low susceptibility to irradiation-induced segregation [2].

In this work, single-phase (BCC) refractory Zr-Nb-Ti-Mo-V-Ta-Al alloys were designed and produced by arc melting. Hot Isostatic Pressing (HIP) was then applied to the samples to reduce porosity and improve specimen homogeneity. However, the performed microstructural analysis showed that the HIP process was insufficient to achieve a fully homogenized microstructure. It is known that refractory elements (Nb, Mo, Zr, V) tend to form segregations due to their large atomic sizes, high melting points, and relatively slow diffusion during manufacturing [3].

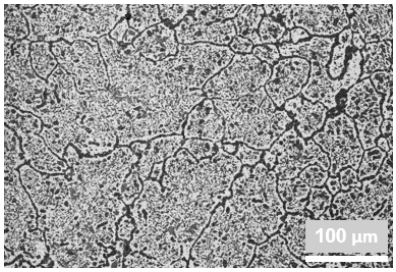

Figure 1. Microstructure after 2 hours HIP at 1200°C

In this study, a homogenization heat treatment was applied after HIP to eliminate the observed microstructural segregation. Estimating the required time accurately is becoming crucial to achieve a homogeneous microstructure without sacrificing mechanical properties during the homogenization post-process. To establish the relationship between process-structure-property, CALPHAD-based modeling approaches were used to identify the correct time information using the Einstein relation and DICTRA homogenization simulation.

For the Einstein relation-based calculations, the full multicomponent interdiffusion matrix was obtained from the CALPHAD mobility database. Eigenvalue decomposition was performed to identify characteristic diffusion modes, and the smallest eigenvalue, corresponding to the slowest compositional decay mode, was used to estimate homogenization time scales. Lastly, the diffusion length was estimated from the characteristic segregation spacing measured by SEM (Scanning Electron Microscopy). Accordingly, the required information was gathered to apply the Einstein diffusion calculation model for the homogenization duration design.

On the other hand, to determine the required time range for the homogenization process, DICTRA homogenization simulations were performed for the same specimens. Scheil-Gulliver simulations were conducted to construct conservative microsegregation profiles of the as-solidified alloys. Thermodynamic calculations verified that the segregated compositions remained within the single-phase BCC stability domain at homogenization temperatures. These profiles were subsequently implemented as initial conditions in single-phase DICTRA simulations to model diffusion-controlled homogenization kinetics [3].

Finally, the outputs of each model were analyzed within a complementary framework to assess the advantages of the Einstein relation and the DICTRA homogenization simulation fed by the Scheil-Gulliver model in the design of the homogenization process.

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Biographical Note

Batuhan Tak is a first-year PhD student and Graduate Research Assistant at the Mechanical Engineering and Materials Science department, University of Pittsburgh.

Revisit the Ab Initio Lattice Stability of Cr with R2SCAN Exchange Correlation Function

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Key words: ab initio, lattice stability, R2SCAN, Cr

Ab initio electronic-structure calculations and the CALPHAD method are two main ways to study lattice stability in metals and alloys. These approaches generally agree well, but significant discrepancies (up to a factor of three or more) appear for elements like Cr, Mo, Ru, W, and Os — a known challenge in materials science [1-2].

Many BCC phases of elements stable in FCC or HCP, and FCC phases of BCC-stable elements, are mechanically unstable at 0 K. These show negative elastic constants and imaginary phonon modes across the Brillouin zone, making entropy and enthalpy hard to define physically.

Such unstable phases can sometimes be stabilized under extreme conditions, like high temperature (e.g., anharmonic effects stabilizing FCC-W at ~3500 K or FCC-Mo at ~10,000 K via ab initio molecular dynamics) or high pressure [3] (e.g., FCC-W stable above ~12 Mbar). However, lattice stability data for CALPHAD integration usually prefers ambient conditions.

Spin polarization (magnetism) also strongly influences lattice stability [4]. For elements like Fe, Co, and Zr, magnetism stabilizes BCC structures. Proper magnetic configurations (e.g., antiferromagnetic FCC-Fe vs. ferromagnetic BCC-Fe) yield energy differences close to CALPHAD/SGTE values, unlike non-magnetic calculations that show larger errors.

While magnetism in Fe, Co, Ni, and Zr has been extensively studied, less attention has been given to other transition metals like Cr, Mo, V, and W. In PBE calculations, antiferromagnetic states often converge to nonmagnetic ones due to weak exchange-correlation effects (e.g., in Cr, where AFM vs. NM differences are tiny and debated).

This work revisits pure Cr lattice stability using ab initio methods. It employs both PBE and R2SCAN functionals to calculate total energies and phonon spectra for FCC, BCC, and HCP phases under different magnetic configurations. It then evaluates high-temperature stability via the quasi-harmonic approximation (QHA), including phononic and electronic contributions, and analyzes the origins of past discrepancies between ab initio predictions and CALPHAD results.

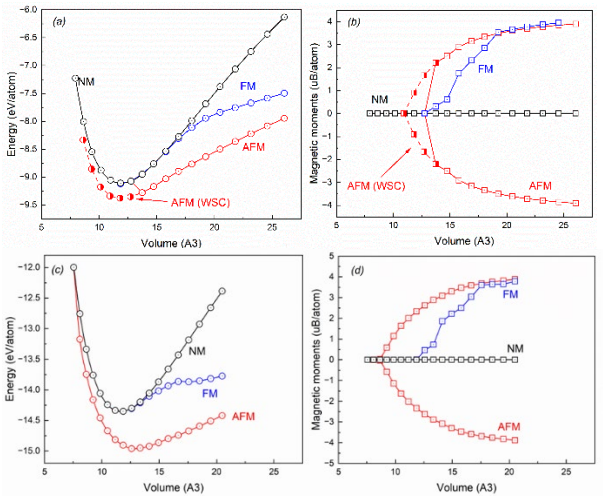

Figure 1. Total energy, Magnetic moments vs. Volume curve of FCC-Cr. (a)-(b): PBE; (c)-(d): R2SCAN

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Biographical Note

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Improving Alloy Mechanical Property Prediction by Addressing Data Homogeneity through Noise Augmentation

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Machine learning(ML) models for predicting mechanical properties in age-hardenable alloys often struggle with experimental datasets characterized by limited diversity with severe homogeneity, wherein aging time varies while composition and temperature remain fixed.

Here, a noise augmentation strategy was proposed that introduces small perturbations bounded by experimental uncertainties to simulate realistic process fluctuations in the input features. Using two experimental alloy datasets (age-hardenable Mg-Al-Zn and Al alloys), multiple ML regression models (Extreme Gradient Boosting, Random Forest, Support Vector Regression, Gradient Boosting Regression, and Adaptive Boosting) were trained and evaluated with and without data augmentation. The noise-augmented models achieved higher accuracy and produced feature importance rankings that aligned more closely with physical expectations as confirmed by SHAP (SHapley Additive exPlanations) analysis. This demonstrates that the strategy can significantly reduce experimental trial-and-error costs by an estimated 20%-40% while maintaining high predictive accuracy, thereby effectively accelerating the alloy optimization process.

This data-centric augmentation approach provides a practical solution to data homogeneity issues, enhancing the generalization and interpretability of ML models for materials design. The efficiency of the noise augmentation strategy is heavily contingent upon precise a priori knowledge of the experimental error margins. In practical implementation, a lack of comprehensive insight into the fluctuations inherent in specific experimental apparatus or processing parameters may lead to ill-defined noise amplitudes, potentially compromising the physical consistency of the augmented dataset. By increasing the diversity of data, this approach can reduce the complexity and cost of experimental designs, accelerating the alloy optimization process in industrial applications.

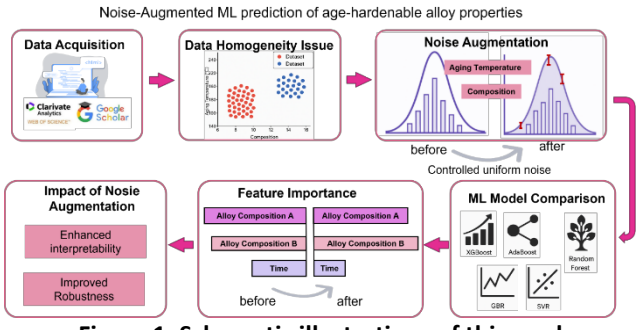

Figure 1. Schematic illustrations of this work

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Biographical Note

Dr. Yuhui Zhang received her Ph.D. degree in Materials Science and Engineering from, Central South University, where she completed her undergraduate through doctoral studies. She also conducted research at the Helmholtz-Zentrum Geesthacht (MagIC-HZG), Germany. She is currently an assistant professor at Xiamen University of Technology.

Her recent research focuses on thermodynamics and kinetics of magnesium alloys, experimental and computational investigations of age-hardening and precipitation behavior, as well as AI-assisted materials design and performance prediction.

Thermodynamic modeling of the Ge-Al-Mg and Ag-Al-Mg systems

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Germanium (Ge) and silver (Ag) are minor alloying elements in aluminum- and magnesium-based alloys. In this study, reliable thermodynamic descriptions of the Ge-Al-Mg and Ag-Al-Mg systems are developed using the CALculation of PHAse Diagrams (CALPHAD) approach, based on a critical assessment of available phase diagram and thermodynamic data from the literature. The Mg-Ge, Al-Ge, and Al-Ag binary systems are reassessed using the Modified Quasichemical Model (MQM) to account for short-range ordering in the liquid phase, while the solid solutions are described using the Compound Energy Formalism. The liquid phases of the corresponding ternary systems are likewise successfully modeled within the MQM framework. The calculated Ge-Al-Mg phase diagram shows good agreement with experimental data reported in the literature. In addition, a comprehensive thermodynamic description of the Ag-Al-Mg system is presented, including the two ternary solid phases: AlAgMg and τ-$(Al,Ag)_{49}Mg_{32}$. The resulting thermodynamic descriptions provide a robust foundation for predicting the thermodynamic behavior of complex Al- and Mg-based multicomponent alloy systems.

Thermodynamic Modeling of Titanium-based Ti-Al-Ca-O Liquid Alloy by Modified Quasichemical Model

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High-temperature solution thermodynamics of titanium-based Ti-Al-O liquid alloy are essential to various pyrometallurgical processes for the extraction, recycling, or casting of titanium metal and its alloys. This applies in particular to unconventional processes such as aluminothermic reduction of titanium oxide or melting and casting of titanium in alumina-based refractories.

The present work first compiles and assesses measured literature data on the thermodynamic equilibrium between Ti-Al-O liquid alloy and solid alumina. The liquid alloy is then modeled in FactSage™ 8.4 using the Modified Quasichemical Model (MQM) in the pair approximation to account for its strong short-range ordering. Model parameters for binary subsystems Al-Ti, Al-O and Ti-O are accepted from a recent modeling of iron-based Fe-Al-Ti-O liquid alloy [1]. Introduction of a single ternary parameter $g^{001}_{\mathrm{TiO(Al)}}$ of constant value for the Ti-Al-O liquid alloy improves the agreement with measured data significantly, compared to both a commercial database and a prior Ti-Al-O modeling [2].

Expansion by calcium in the quaternary Ti-Al-Ca-O liquid alloy is crucial for unconventional processes such as calcium deoxidation and melting and casting in calcia-based refractories. For this purpose, relevant measured literature data are compiled and assessed, and the liquid phase of the binary subsystems Ca-Ti and Ca-O is re-modeled using the Modified Quasichemical Model. Combining with the aforementioned Ti-Al-O modeling results yields improved agreement with measurements compared to the state of the art.

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Biographical Note

Dr.-Ing. Gereon Hils graduated in process metallurgy from Clausthal University of Technology, Germany in 2009. Since then, he has been working in academic research at Universities of Clausthal and RWTH Aachen in Germany, focusing on ferrous and non-ferrous pyrometallurgy by means of lab-scale experiments and application of computational thermodynamics. He received his doctorate from Clausthal University of Technology in 2025 on production of high-grade manganese ferroalloys.

Unexpected interfacial reactions in Co/GeTe and Ni/GeTe couples

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Thermoelectric devices have a wide range of applications in enhancing energy efficiency and serving as a renewable energy source [1]. These devices function by converting temperature differences into electrical energy, enabling the harnessing of waste heat to power various systems. Thermoelectric devices are typically composed of arrays of P-N legs and feature multiple joints. The properties of these joints are crucial to the performance and reliability of thermoelectric devices. A barrier layer, a thin layer of material that prevents direct contact between thermoelectric substrates and joining materials, plays a vital role in enhancing device performance [2]. Germanium telluride (GeTe) is a vital thermoelectric material [3], and this study examines the interfacial reactions in Co/GeTe and Ni/GeTe systems, where cobalt (Co) and nickel (Ni) were electroplated onto a GeTe substrate. After a 24-hour reaction at 500 °C, the Co/ GeTe interface produced CoTe、Co_5Ge_3、CoGe and CoGeTe phases. Surprisingly, similar phases were also detected on the outer side of the Co layer, away from the GeTe substrate. For the Ni/GeTe interface, phases including Ni_3Te_2, Ni_3Ge, Ni_5Ge_3, NiGe, $Ni_{5.45}GeTe_2$, and Ni_3GeTe_2 were detected, along with NiTe, Ni_2Ge, and Ni_3Ge on the outer Ni layer. To investigate the source of the reactants, solid-gas reactions at 500 °C were performed, yielding results consistent with those in the Co/ GeTe and Ni/GeTe systems. Phase stability diagram has various applications [4]. For example, famous Pourbaix diagram is also one type of stability diagram. As a preliminary step, we have undertaken Calphad-type modelling of the Co-Ge-Te and Ni-Ge-Te systems. The phase stability diagrams were then calculated to provide a better understanding of the reaction results.

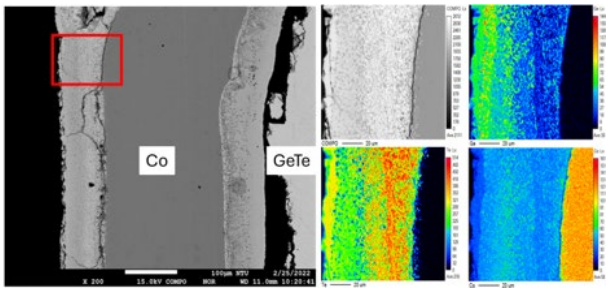

Figure 1: BEI micrograph and elemental mapping micrograph of the Co/GeTe couple reacted at 500 ˚C for 14 days

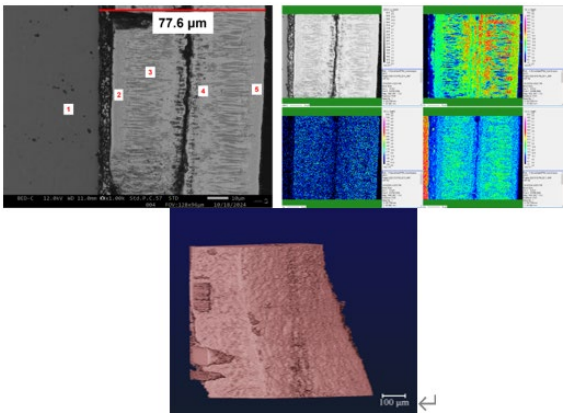

Figure 2: (a)BEI micrograph, elemental mapping micrograph and (b) projection X-ray micrograph of the Co/GeTe solid-gas reaction couple reacted at 500 ˚C for 10 days

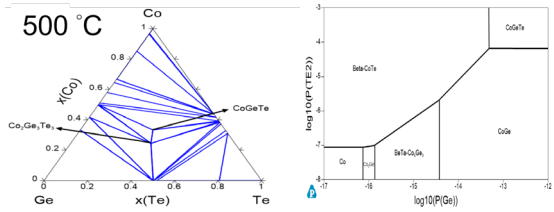

Figure 3: (a)Isothermal section of Co-Ge-Te ternary system at 500 ˚C; (b) Phase stability diagram of Co-Ge-Te ternary system at 500 ˚C

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Biographical Note

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Experimental Investigation of Phase Equilibria in Ni-Ce-Cr system

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Rare earths, a group of 17 elements that includes lanthanides along with Sc and Y are vital to modern engineering applications due to their exceptional magnetic, optical, chemical and structural properties [1], [2], [3]. They are studied actively for their potential to enhance high temperature properties by improving tensile strength, creep, oxidation , wear resistance etc. Even in small additions, they can significantly alter alloy behaviour by stabilizing phases and enhancing properties[3]. Despite the promising potential of rare earth elements, their widespread utilization in structural alloys remains limited, primarily due to the lack of comprehensive and reliable phase equilibria data. Systematic phase equilibrium studies involving rare earth elements in combination with technologically important metals such as Fe, Cr, Ni, Nb, and Ta is still scarce.

Among the rare earth elements, cerium is the most abundant and has attracted considerable attention due to its promising high-temperature characteristics relevant to both structural and functional materials. Ni and Cr, on the other hand, are well-established alloying elements known for their excellent high-temperature strength, corrosion and oxidation resistance with widespread usage in superalloys. The Ce–Cr–Ni system is therefore of particular interest, especially in the context of nuclear reactor environments, where rare earth elements such as Ce are generated as fission products during nuclear reactions. These elements can interact with Ni–Cr–Fe-based cladding materials, leading to the formation of intermetallic compounds that are potentially detrimental to reactor integrity and performance [4]. Consequently, a thorough understanding of phase equilibria in the Ce–Cr–Ni system is essential for predicting material behaviour under reactor operating conditions and for improving the design and reliability of cladding alloys.

An extensive survey of the existing literature revealed that there are currently no experimental phase equilibrium investigations reported for the Ni–Cr–Ce system. To address this significant data gap, the present study focuses on the experimental investigation of several alloys within this ternary system, with emphasis on their microstructures, phase constitution, and phase compositions. The alloys were synthesized using the vacuum arc melting technique to ensure compositional homogeneity, followed by long-term heat treatments to approach equilibrium conditions. The resulting microstructures were systematically characterized using XRD, SEM, EDS, and EPMA, while thermal behavior and phase transformation characteristics were examined using DSC.

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Biographical Note

I am Swathi Mallika Dikonda, a PhD student from the Department of Material Science and Metallurgical Engineering at the Indian Institute of Technology, Hyderabad, India. My research focuses on the thermodynamic assessment of rare earth-containing alloys, integrating both experimental investigations and computational techniques. I also explore the high-temperature oxidation behavior of materials, contributing to understanding the alloy performance in extreme environments.

Diffusivities and atomic mobilities of fcc phase in Co-rich Co–Fe–Ti system: Experimental study and CALPHAD assessment

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The development of aerospace and energy industries has put forward higher and higher requirements on the heat-resistant materials, and superalloys are the most reliable and economical solution to meet these challenges. The novel Co-based superalloys with the γ′-phase precipitation strengthening [1] exhibit enhanced high-temperature strength in comparison with conventional Co-based high-temperature alloys, and greater potential than Ni-based superalloys [2]. The alloying elements have a significant effect on microstructure and phase stability in Co-based superalloy [3].

Diffusion kinetics is a critical factor during the design of superalloys, and it will influence the prediction of elemental segregation, γ/γ′ phase transformation, microstructural evolution, and interdiffusion behavior [4]. However, there is currently no atomic mobility description available for fcc phase in Co-rich Co–Fe–Ti system.

Two groups of ternary diffusion couples A1–A6 and B1–B5 of fcc phase in Co-rich Co–Fe–Ti alloys were prepared and annealed at 1473 K for 18 h (hours) and 1373 K for 48 h. The interdiffusion coefficients of Co–Fe–Ti system were determined by means of the experimental concentration profiles using the Whittle-Green method in combination with electron probe microanalysis (EPMA). The results indicated that Ti diffuses faster than Fe in the fcc alloys. Subsequently, the atomic mobility parameters were assessed using CALPHAD method. The reliability of the obtained parameters was verified by comparing the simulated and experimental results for the interdiffusion coefficients, concentration profiles, and diffusion paths.

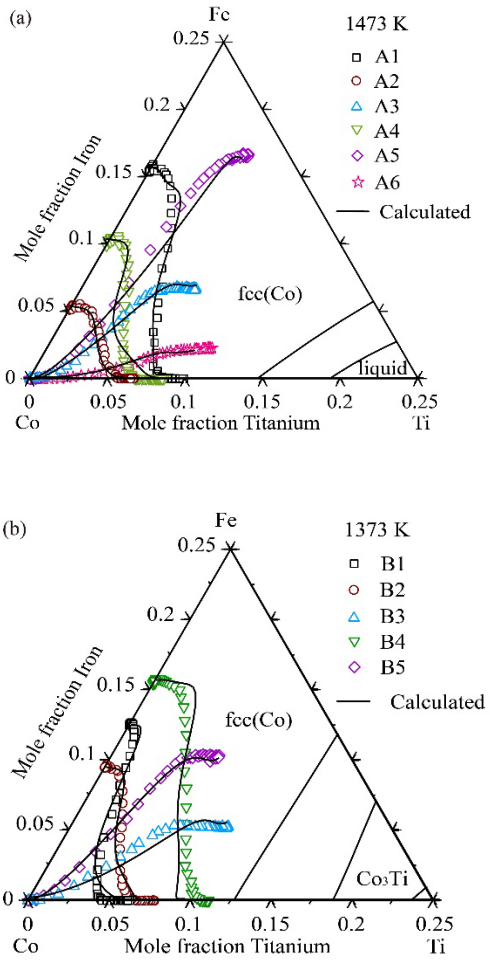

Figure 1. Simulated diffusion paths in comparison with experimental data: (a) 1473 K; (b) 1373 K

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Biographical Note

Jiaxing Sun, a PhD student from University of Science and Technology Beijing, is mainly engaged in experimental phase diagram determination and thermodynamic research of Co-based superalloys.

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Thermodynamic modelling of battery cathode materials: early-stage results and perspectives

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The growing global demand for high-performance batteries for electric vehicles, grid-scale energy storage systems, and portable electronics requires materials with increasing energy density and reduced reliance on critical raw materials. At present, the battery industry accounts for the largest share of global cobalt consumption, raising significant economic and sustainability concerns. Despite this, much of current battery research focuses on novel cell configurations and synthesis routes rather than on fundamental materials design.

Within this context, the ACCESS project (Addressing Critical Raw Materials Challenges in Energy Storage Systems – funded by Wallenberg Initiative Materials Science for Sustainability, WISE) aims to provide the battery industry with Integrated Computational Materials Engineering (ICME) tools for the accelerated design of innovative battery materials. By coupling CALPHAD and Density Functional Theory (DFT), the project seeks to enable faster and more accurate predictions of battery material behavior, thereby reducing dependence on costly and time-intensive experimental studies.

Among the battery components, cathodes are particularly well suited for this approach due to their high potential compositional flexibility. Moreover, thermodynamics plays a central role in governing their stability and performance, although this is still not fully exploited in current research and development efforts. In particular, Ni–Mn–Co layered oxides (NMCs) represent a highly relevant class of materials characterized by significant crystallographic complexity, including layered structures and order–disorder phenomena. This intrinsic structural complexity, together with the scarcity of data on the key phases in the subsystems of main dopant elements, makes their thermodynamic modeling especially challenging.

In this contribution, we present early-stage results on the thermodynamic modeling of NMCs, with particular emphasis on model development and preliminary validation with relevant experimental cases.

Starting from the sublattice model proposed in [1–2] and later improved in [3] through the introduction of metal–oxygen associates, we developed a new, more physically consistent description that explicitly includes charged species. Although more complex, this formulation aims to better capture the thermodynamic and electrochemical behavior of these layered NMC-based systems. The main improvements and preliminary results obtained with the charged-species model are presented and compared with those of the associate-based description. Moreover, the limitations and open challenges associated with the proposed approach are discussed, highlighting both its potential advantages and the inherent difficulties in establishing a predictive thermodynamic framework for such complex cathode materials.

In summary, this work lays the foundation for the future development of a dedicated thermodynamic database for battery materials, supporting the systematic design and optimization of next-generation energy storage systems.

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Biographical Note

L. Fenocchio completed his PhD in Materials Chemistry at University of Genova (Italy) in 2025 with a thesis on thermodynamic modelling and experimental characterization of High-Entropy Alloys (HEAs). His main research interests included HEAs, 3rd Generation CALPHAD modelling and determination/critical evaluation of phase diagrams. More recently, L.F. has joined Thermo-Calc Software AB as a database developer within the framework of a WISE-funded postdoctoral project (ACCESS) in collaboration with KTH Royal Institute of Technology.

Thermodynamic modeling of the Hf-Nb-V system

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Multi-principal element alloys (MPEAs) and high-entropy alloys (HEAs) gained the scientifc community attention due the interesting mechanical properties, thermal stability, and corrosion resistance, making them promising candidates for advanced engineering applications [1,2]. The refractory elements Hf, Nb, and V are particularly attractive for these alloy systems due to their high melting points, strength retention at elevated temperatures, and good oxidation resistance.

Investigating the phase equilibria and thermodynamic behavior of the Hf-Nb-V ternary system is the base for design and optimization of refractory HEAs. However, despite its importance, a comprehensive thermodynamic assessment of this system has not been previously reported in the literature. The CALPHAD (CALculation of PHAse Diagrams) method provides a framework for developing thermodynamic databases that enable the prediction of phase stability, composition ranges, and transformation temperatures [3], thereby accelerating alloy development and reducing experimental costs.

In the present study, a comprehensive thermodynamic modeling of the Hf-Nb-V ternary system using the CALPHAD method is introduced for the first time. Thermodynamic descriptions for the binary systems were derived from the established literature to ensure consistency with well-established data. The optimization of ternary parameters was based on experimental data from isothermal sections and our results for the liquidus projection, which were incorporated into the thermodynamic model to improve its accuracy.

The resultant thermodynamic parameters align with experimental observations, demonstrating the reliability of the developed database. This work presents the Laves C14 and Laves C15 solubilities in the isothermal sections at 1100 (Figure 1) and 1300 °C, and the tie triangles of C14-A3-A2 equilibria and C14-C15-A2 equilibria. For the liquidus projection, the primary solidification fields for the A2 and C14 phases were successfully calculated, providing information for processing route design.

In conclusion, this investigation provides a thorough thermodynamic characterization of the Hf-Nb-V system, offering an resource for the development of thermodynamic databases relevant to multi-principal element alloys (MPEAs) and high-entropy alloys (HEAs), and contributing to the advancement of computational materials design in refractory alloy systems.

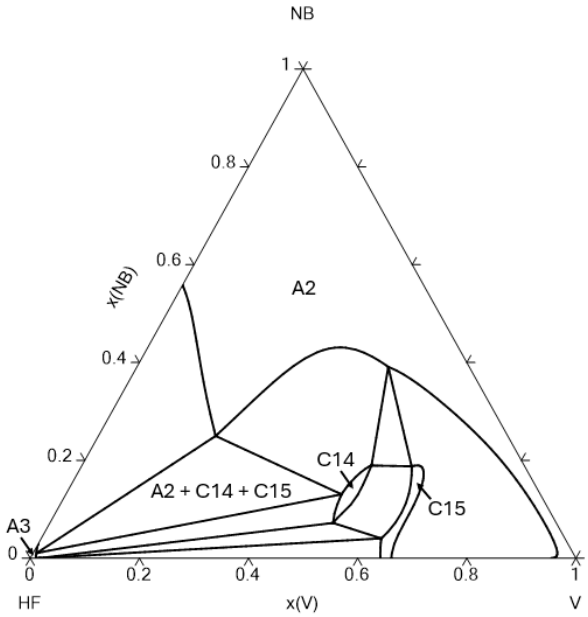

Figure 1. Isothermal section calculated for the Hf-Nb-V system with optimized parameters at 1100 °C

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Biographical Note

Thiago Gonçalves de Oliveira is a PhD student at the Federal University of Itajubá (UNIFEI), Brazil, and an academic professor at the University Center of Itajubá (FEPI). He holds a Master's degree in Materials Engineering. His research interests include computational thermodynamics, phase equilibrium calculations, and the CALPHAD method. His current doctoral research focuses on the development of thermodynamic databases for multicomponent systems, specifically the Cr-Hf-Nb-V system. His previous research experience encompasses polymer evaluation for 3D-printed orthoses and multicomponent alloys for biomedical applications.

Study on microstructure and property of novel γ'-strengthened multi-component Co-based superalloys

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The development of Co-based superalloys has been historically constrained due to the lack of suitable strengthening phases. As such, this has been changed since the $L1_2$-Co_3(Al, W) phase was discovered by Sato et al. [1]. The Co-based alloys also have excellent comprehensive properties, such as corrosion and oxidation resistance Alloying elements are essential for improving alloy properties. They directly influence the microstructure of superalloys, and the microstructure characteristics of the γ' phase are sensitive to both the content and type of alloying elements.

The complexity of interactions between elements is challenging during the alloy design process. Consequently, the "trial and error" method for designing alloys is inefficient. It is crucial to find a method to improve experimental efficiency and save experimental costs in the research and development of Co-based superalloys. CALPHAD (CALculation of PHAse Diagrams) method is efficient for designing multi-component alloys based on the Gibbs energy database [2].

Four novel Co-based superalloys were designed based on the thermodynamic database using CALPHAD method. A preliminary evaluation was conducted on the compression mechanical properties, density, and transition temperature of alloys. After aging at 1000 °C for 720 h, the alloys exhibited a stable γ/γ' two-phase microstructure, and no harmful secondary phase, such as the topologically close-packed phase (TCP), was observed in the alloys. The novel Co-based superalloy Co30.0Ni9.0Al3.0W1.0Ta4.0Ti9.0Cr (at.%) possesses a higher γ' solvus temperature (1117 ± 2 °C) and a lower density (8.55 ± 0.03 g/cm³). Furthermore, the yield strength exhibits a positive temperature dependence from room temperature to 600 °C in the compression process. The yield strength of the alloy is 797 ± 3 MPa at 600 °C, which is appreciably higher than that of the commercial Mar-M-509 superalloy.

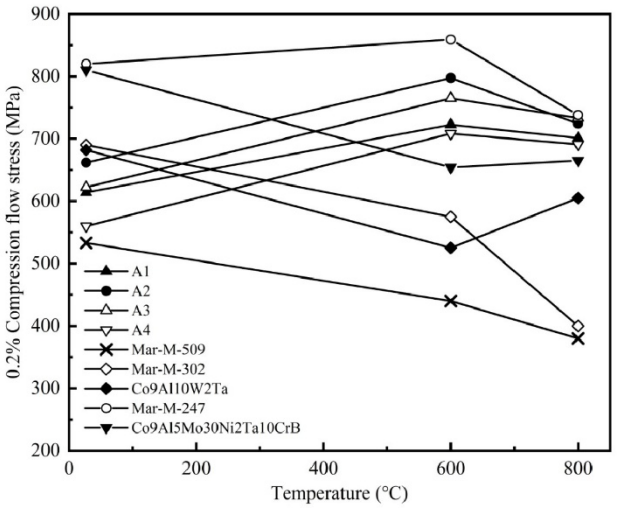

Figure 1. Compressive yield strength of alloys A1, A2, A3, and A4 plotted versus temperature including reference alloys Co9Al10W2Ta, Mar-M-509, Mar-M-302, Mar-M-247 and Co9Al5Mo30Ni2Ta10CrB [3, 4]

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Biographical Note

Feikuo Chen, PhD student from University of Science and Technology Beijing, is mainly engaged in experimental phase diagram determination and composition design of Co-based superalloys.

Bayesian Active Learning of Zero-Phase-Fraction Lines

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New strategies are increasingly appearing in the literature to accelerate phase diagram construction, with active-learning approaches showing particular promise in reducing the number of expensive queries required to resolve phase boundaries [1,2]. For example, in our previous work we used Bayesian search-schemes equipped with informative priors regarding solid-solution stability to identify single phase FCC and BCC regions in a ternary phase diagram using a limited number of queries. This improved learning efficiency; however, the acquisition policy was based on Shannon entropy, a statistical metric associated with the Bayesian surrogate model used, rather than a directly thermodynamic quantity.

Following Morral's insight [3] that phase diagrams can be thought of as a set of zero phase fraction lines (i.e. loci in thermodynamic space where a phase first appears/dissappears) we introduce a Bayesian active-learning framework with a ZPF-targeted acquisition policy. This acquisition function preferentially queries conditions predicted to lie on or near ZPF lines, concentrating data collection in the most information-rich regions for phase diagram construction. An example of these predictions is shown in Figure 1.

The surrogate model is a multi-task Gaussian process regression (MT-GPR) framework that jointly predicts (i) phase fractions and (ii) phase-existence indicators for each candidate phase. Phase existence is represented via a latent GP transformed through a logistic sigmoid, yielding probabilistic phase-presence predictions. This joint formulation enables task-to-task information transfer and straightforward incorporation of physics-based priors. The proposed acquisition function combines predicted phase fraction and phase-existence probability to prioritize ZPF-proximal queries.

In this work, CALPHAD phase fractions computed in Thermo-Calc are used as in-silico ground truth. In practical closed-loop campaigns, the framework can assimilate experimental observations while using CALPHAD-informed nonzero priors as a first approximation, enabling iterative bias correction and faster convergence to experimentally validated phase boundaries.

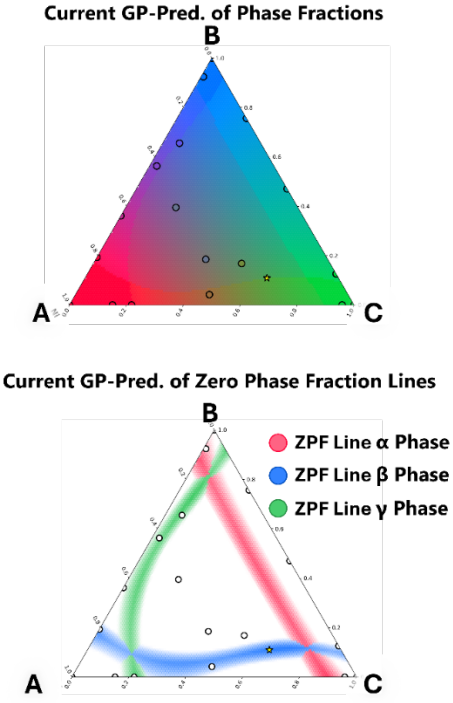

Figure 1. Examples of GP Phase Fraction and ZPF predictions in an exemplar ternary alloy system

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Biographical Note

Christofer Hardcastle is a PhD candidate in Materials Science and Engineering at Texas A&M University. His research focuses on computational methods for materials discovery, including Bayesian optimization and constraint satisfaction modeling. Applications include discovering refractory high entropy alloys that can withstand extreme environments and be 3D-printed using laser powder bed fusion additive manufacturing.

A robotic calorimetry laboratory for phase diagrams on demand

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Recent developments in autonomous materials synthesis labs have ushered in a new era of materials discovery. While these laboratories can generate large quantities of data, there still exists the need for synthesis guiding tools – namely, the phase diagram. Experimental phase diagram assessment requires extensive tedious measurement and is often hindered by practical considerations, while computing phase diagrams purely computationally can be extremely costly for complex systems. Here, we present a strategy for using computation to assess the energies of solids, and selective differential scanning calorimetry (DSC) experiments to increase the accuracy of the computed liquidus. We conclude with a vision for a unified computational and robotic experimental platform that consolidates materials synthesis and processing, robotic calorimetry, ab initio thermodynamics, CALPHAD thermodynamic modeling, and artificial intelligence/machine learning (AI/ML), to generate phase diagrams on demand.

Thermodynamic investigations on the enthalpy of mixing of tributyl phosphate with nitric acid and gadolinium nitrate by micro reaction calorimetry

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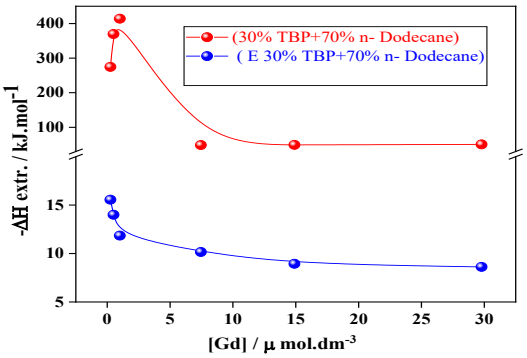
Thermodynamic investigations of solvent extraction systems are crucial for optimizing metal ion separations, as they provide the fundamental data necessary to precisely identify and select the most appropriate extracting ligands, diluents, and operational parameters required for efficient and selective extraction. Spent fuel reprocessing plants are built with inherent safety with respect to criticality owing to its high fissile plutonium content. The criticality issues are avoided by having proper storage & handling containers or by controlled addition of neutron poisons. Gadolinium is a preferred neutron poison and specifications of recycled nuclear fuel limit its concentration [1]. Hence distribution of Gd between organic / aqueous phases is important and separation of Gd later needs to be explored. This work probes the interaction of tri-butyl phosphate (TBP) solution with aqueous gadolinium nitrate and dilute nitric acid. This attempt is to explore and quantify such interactions on the basis of calorimetry.

An isothermal micro reaction calorimeter from M/s. Thermal Hazard Technology (UK) was used to measure the enthalpy of complexation and extraction (ΔH_{extr}) of Gd^{+3} by 30% TBP in n-dodecane solvent. Heat effects as a function of Gd concentration was also measured. Experiments were carried out with i) fresh TBP (30%) and ii) TBP (30%) equilibrated with 4N nitric acid. In both the cases, [Gd^{+3}] of 0.1 and 2.9 M were injected into the extractant (TBP) at a dosing volume of 2.5, 5 and 10 µL. The enthalpy of extraction was plotted as a function of [Gd^{+3}] in Figure 1 in both the cases. To understand the interaction of 30% TBP with nitric acid, separate measurements were carried out without Gd^{+3} ion. Extraction behavior of TBP due to pre-equilibration & after equilibration were also studied.

Upon addition of nitric acid / metal ion into TBP, the quantity of heat increases proportionally with nitric acid concentration or TBP concentration (100%). A similar behaviour is observed at low concentrations of [Gd^{+3}] i.e upto 1 µmol.dm^{-3}. At higher concentrations of [Gd^{+3}], the quantity of heat released is nearly constant, implying that the complexation is complete wherein the ligand sites are fully occupied. When equilibrated TBP (30%) was used, the complexation is less exothermic. The exothermicity of complexation decreased as a function of [Gd^{+3}]. Such a decreasing trend is also reported in the case of Eu^{+3} complexation by TODGA [2]. A nearly constant value of the enthalpy of complexation indicates that the TBP had reached its maximum capacity of extraction.

This work is a first attempt in quantifying the heat effects of interaction / complexation of TBP, HNO_3 and $Gd(NO_3)_3$. These results highlight that the presence of HNO_3 and metal ion (Gd^{+3}) concentration are the dominant factors that influence the overall exothermicity and efficiency of the extraction.

Figure 1. Enthalpy changes during the extraction of Gd (III) by 30% TBP and equilibrated 30% TBP at 298 K



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Biographical Note

Mr. Gude Jogeswara Rao is a Research Scholar at the Homi Bhabha National Institute (HBNI), Department of Atomic Energy, India. His research interests include microreaction calorimetry, measurement of thermophysical properties of nuclear fuels, calorimetry and synthesis of nuclear fuel materials.

The top Calphad scientists according to their citation records

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In recent years the top 100,000 (or top 2 % per field) scientist are evaluated by Elsevier based on the citations their works obtained. In the latest edition published in 2025 the career results of 1960-2024 and the single year results of 2024 are summarized (https://elsevier.digitalcommonsdata.com/datasets/btchxktzyw/7). Among them there are 9187 people with their basic field "Materials". The top Calphad people are listed below with their ranking within the best 9187 materials scientists of the world. This poster is printed for young Calphad people so they know the names they should be proud of.

50. Alexandra Navrotsky (Arizona State Uni, USA),
86. Mats Hillert (KTH, SWE),
95. Zi Kiu Liu (Pennsylvania State Uni, USA),
113. Gregory B. Olson (MIT, USA),
168. Byeong-Joo Lee (Pohang Uni, KOR),
188. Kiyohito Ishida (Tohoku Uni, JAP),
245. Arthur Daniel Pelton (Poly Montréal, CAN),
247. Bo Sundman (KTH, SWE),
354. Ingo Steinbach (Ruhr-Universitat Bochum, DEU),
363. E.J. Mittemeijer (Uni Stuttgart, DEU),
369. John Agren (KTH, SWE),
397. Hiroaki Okamoto (Asahi Uni, JAP),
515. Günter Gottstein (Hohschule Aachen, DEU),
533. George Kaptay (Uni Miskolc, HUN),
616. Alan Thomas Dinsdale (Hampton Thermod, GBR),
662. In-Ho Jung (Seoul National Uni, KOR),
687. Ryousuke Kainuma (Tohoku Uni, JAP),
1079. Yong Du (Central South Uni, CHN),
1123. P.F. Rogl (Uni Wien, AUT),
1175. Fritz Aldinger (Max Planck Inst, DEU),
1199. Armando Ferněndez-Guillermet (Bariloc, ARG),
1200. Rainer Schmid-Fetzer (Uni Clausthal, DEU),
1250. Ernst Kozeschnik (Uni Wien, AUT),
1386. Y. Austing Chang (UW-Madison Coll Eng, USA),
1391. Raymundo Arróyave (Coll Eng, USA),
1435. Geoffrey K. Sigworth (GKS-Eng, USA),
1532. Bengt Hallstedt, Hochschule Aachen, DEU),
1598. Philip G. Nash (Illionis Inst, USA),
1641. Jean-Marc Joubert (Paris ICMPE, FRA),
1711. Sigmund Jarle Andersen (SINTEF, NOR),
1732. Larry Kaufman (Calphad Inc, USA),
1734. Marcel H.F. Sluiter (Uni Gent, BEL),
1792. Christopher W. Bale (Poly Montréal, CAN),
1822. Thaddeus B. Massalski (Carnegie Mel Uni, USA),
2066. Nigel Saunders (Thermotech, GBR),
2082. Guy Makov (Ben-Gurion Uni, ISR),
2208. Gerhard Inden (Max Planck, DEU),
2335. Gunnar E. Eriksson (Hohschule Aachen, DEU),
2620. Hans Jürgen Seifert (Karsruher Inst, DEU),
2633. Uwe Glatzel (Uni Bayreuth, DEU),
2863. Britta Nestler (Hohschule Karlsruhe, DEU),
2913. Olga B. Fabrichnaya (Bergakad Freiberg, DEU),
3211. Frank Stein (Max Planck, DEU),
3745. André L.V. Costa E Silva (Fluminense, BRA),
3760. Patrice Chartrand (Poly Montreal, CAN),
3894. Ole Jakob Kleppa (James Franck Inst, USA),
3902. Ferdinand Sommer (Max Planck, DEU),
3924. Yoshio Waseda (Tohoku Uni, JAP),
4154. Bruno Predel (Uni Stuttgart, DEU),
4206. Klaus Hilpert (Jülich, DEU),
4240. Ibrahim Ansara (CNRS, FRA),
4428. Victor T. Witusiewicz (ACCESS, DEU),
4448. Toshihiro Tanaka (Uni Osaka, JAP),
4492. Günter E. Petzow (Max Planck, DEU),
4609. Charles B. Alcock (Uni Toronto, CAN),
4612. Alfred Peter Miodownik (Termotech, GBR),
4624. Dirk Holland-Moritz (DLR, DEU),
4727. Herbert Ipser (Uni Wien, AUT),
5411. Tetsuo Mohri (Hokkaido Uni, JAP),
5491. Ikuo Ohnuma (Nat Isnt Mater Sci, JAP),
5646. Malin Selleby (KTH, SWE),
5666. Joonho Lee (Korea Uni, KOR),
5676. Susan V. Meschel (Illionis Inst, USA),
5844. Ales Kroupa (Brno, CZE),
5992. Krzysztof Fitzner (AGH Krakow, POL),
6529. Gueorgui Penev Vassilev (Plovdiv Uni, BGR).

Biographical Note

George Kaptay is a metallurgical engineer (Leningrad Polytechnic, 1984). He is a Hungarian Calphadian whose hobby is scientometrics.

Assessment of the Thermodynamics and Thermophysical Properties of the Binary Ag-Pd System

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Knowledge of phases and thermophysical properties of candidate materials is essential for the development new materials for semiconductor manufacturing applications such as wafer tables and packaging substrates. New Calphad models, so called 3rd generation descriptions of the temperature dependence, have been developed to describe thermodynamics [1] and thermal expansion [2] in multicomponent systems. However, there is still a need for reliable thermal conductivity models. To test the proposed models [3] a test system needed to be identified that is simple but with large solubility ranges of its phases and well described by experimental data. The elements forming this system must be free of extra physical contributions that affect thermodynamics and thermophysical properties, such as magnetism. It was found that the Ag-Pd system fulfills all of the above criteria.

The proposed thermal conductivity model is based on 3rd generation descriptions of heat capacity and molar volume. However, existing thermodynamic assessments of the Ag-Pd system as well as the molar volume of the pure elements are based on 2nd generation temperature dependence descriptions and are not compatible with the 3rd generation description for the thermal conductivity. New assessments of the thermodynamic and molar volume of the pure elements and the binary system were therefore necessary to obtain compatible description of the heat capacity and molar volume.

The 3rd generation description of the molar volume is based on the heat capacity and the bulk modulus. Consequently, for the full description of Ag, Pd and the binary Ag-Pd system all these properties have been assessed and the obtained model description reproduce the experimental data well.

This work was performed with funding from the CHIPS Metrology Program, part of CHIPS for America, National Institute of Standards and Technology, U.S. Department of Commerce.

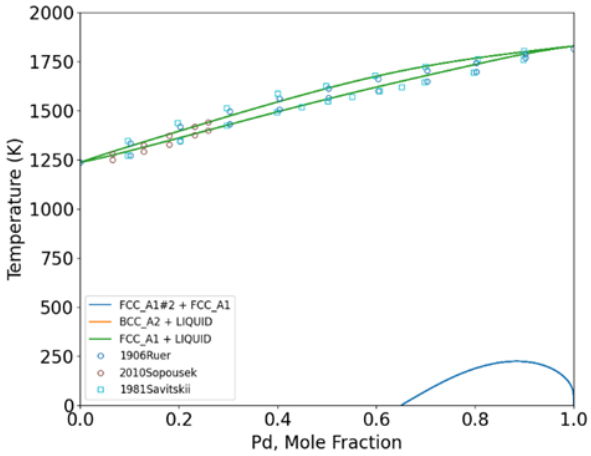

Figure 1. Comparison between experimental and calculated phase diagram of the binary Ag-Pd system

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Biographical Note

Ursula R. Kattner is a physical scientist at NIST. Her work focuses on computational thermodynamics and phase diagram evaluations. She has worked on a variety of alloy and metal-hydride systems and is currently working on the development of Calphad databases for superalloys and advanced wafer table materials.

The experimental and theoretical study of the In-La-Ni system

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Hydrogen storage in powdered hydrides represents a sustainable alternative to energy storage, overcoming safety risks and transport inefficiencies. This study is part of a larger project focused on **La-Ni-based alloy systems**, which are highly promising due to their rapid sorption kinetics at ambient temperatures. The addition of a third element can optimize the thermodynamic and kinetic sorption and desorption properties.

Experimental phase equilibria of the **In-La-Ni ternary system** were investigated at 400, 500, and 600 °C across the whole concentration range. Samples were synthesized via arc-melting and characterized using **SEM-EDX, XRD, and DSC** to determine microstructure, chemical composition, crystallographic structures, and phase transition temperatures. Results revealed a complex system with fourteen stoichiometric ternary phases identified at 400 °C.

These findings provide the foundational data for thermodynamic modeling using the **CALPHAD method**. Furthermore, hydrogen reactivity and sorption/desorption kinetics were evaluated, utilizing **pressure-composition-temperature (p-c-T) curves** to define two-phase fields. These results establish a critical baseline for extending the thermodynamic description to the quaternary **La-Ni-In-H system** for advanced energy storage applications.

The theoretical modelling was carried out using assessments of the relevant binary system, as reported in the literature [1-3]. Currently, there is no known theoretical assessment of the ternary system. Also, there is quite a significant lack of experimental data.

Only one paper [4] in the literature was found that addressed phase equilibria in this system, describing the isothermal section of the phase diagram at 397°C and 597°C. No studies on thermodynamic data or liquidus surfaces are available.

There is only partial agreement between the work of Nichiporuk et al. [4] and our own experimental results. The main disagreement concerns the solubility of Indium in the $LaNi_5$ phase at 400°C. Also, some differences were identified in observed ternary phases.

The preliminary assessment published here is based primarily on our own experimental data, as we have consistent results across three different temperatures. Nevertheless, the study [4] was also taken into account. Given the disagreement in the mentioned studies, special attention was given to the region near the $LaNi_5$ region. As no experimental data are available for the liquidus surface, the calculated liquidus surface is a prediction only.

This work was carried out as part of the project No. CZ.02.01.01/00/22_008/0004631 MATUR OP JAK financed by the EU and CR.

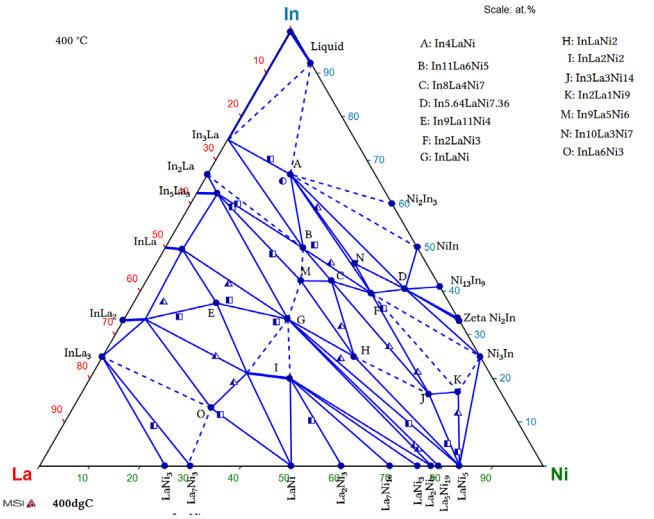

Figure 1. The In-La-Ni experimental phase diagram at 400°C

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Biographical Note

Dr. Ales Kroupa is the senior scientist at the Structure of Phases and Thermodynamics at the Institute of Physics of Materials, CAS, in Brno. He specialised in the thermodynamics of alloys, theoretical and experimental assessments of phase diagrams of complex systems, and database development.

Comparison of model of hydrogen permeation through iron plates with analytical solutions & practical assessment

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Understanding the kinetic behaviour of hydrogen is increasingly pertinent for metal systems as hydrogen's role in the energy economy expands. Obtaining diffusivities for hydrogen in these systems, often complex, under application-specific environmental conditions is critical to produce models of hydrogen's movement, the anticipation of hydrogen embrittlement (HE), and for the selection of materials robust to hydrogen environments.

In the present work, the thermodynamic formulation of diffusion is used to predict the shape of permeation transients and the instantaneous diffusivities of hydrogen through Iron plates generated by ISO17081, an electrochemical method of diffusivity assessment proposed by Devanathan and Stachurski in 1962[1]. The plates are modelled as cold-rolled, allowing the modelling of hydrogen traps via strain-dislocation-density relations available in literature [2]. The model predictions are compared to transients produced by the McNabb-Foster equation, an analytical solution for hydrogen-traps effects on hydrogen flux, and to practical assessments under the model conditions [3]. The agreement is assessed using ANOVA.

In the present model, instantaneous diffusivities are calculated from temperature-dependent mobility and the local molar fraction of hydrogen (the kinetic coefficient) and the chemical potential of *hydrogen-only*, without explicit inclusion of cross-effects- possible because, by Liu[4], this kinetic coefficient and the chemical-potential of hydrogen are already a function of diffusion-affecting state variables and of the other molar quantities in the system.

By comparing the present model, which unlike the McNabb-Foster equation does not depend on a prior assessment of the lattice diffusivity of the specific material or under specific conditions, to McNabb-Foster predictions and to practical data, we can demonstrate the descriptive power of models in which kinetics derive largely from CALPHAD thermodynamic assessments. Through this, the authors hope to move towards models of the diffusion of hydrogen in more complex metal systems, without the need for time-consuming diffusivity assessments highly specific to individual industrial applications.

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Biographical Note

Jack Leeman is a 3rd Year PhD student at the University of Birmingham in computational modelling of metallurgical systems. Previously, he worked in the AM industry, developing cemented carbide compositions for production via blown-powder-DED.

Modeling and experimental study of IMC formation at Sn/Cu interface

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As electronic devices continue to miniaturize, the integrity of solder joints has become largely dependent on the microstructural characteristics of the joint's interface. While the initial formation of intermetallic compounds (IMCs) is essential for a strong metallurgical bond, their continuous growth during a product's lifecycle is a major reliability concern [1]. Because IMCs are inherently brittle and have higher electrical resistivity than bulk solder, their excessive growth is detrimental to the mechanical properties, such as fatigue, and shear strength and often leads to premature joint failure [2, 3]. Analyzing solder/substrate interactions offers critical insight into interfacial evolution from a metallurgical perspective. Phase-field modeling has proven to be an effective tool for simulating these soldering reactions, allowing for a detailed description of complex intermetallic compound (IMC) evolution [1-4]. This study investigates the growth kinetics and morphology of Cu_6Sn_5 and Cu_3Sn phases within the Sn/Cu system. A multi-phase field model was developed and coupled with the TCLSD thermodynamic database to simulate the growth of IMCs at the Sn/Cu interface. Simulations were performed in one and two dimensions. The experimental part of the work involved the preparation of Sn/Cu joints subjected to isothermal aging at different temperatures (150°C, 155°C and 180°C) and times (50, 100, 250, 500, and 1000h). A representative BEI micrograph and linescan of a joint aged at 155°C for 500h is presented in Fig. 1. The microstructure and chemical composition of the Sn/Cu interface were analyzed using scanning electron microscopy (SEM) and energy-dispersive spectroscopy (EDX). The thickness of the IMCs was measured using a convolutional neural network that was specifically trained for this system. Results showed that the total IMC thickness follows a parabolic law, confirming that the process is diffusion-controlled across the temperature range. Thermal analysis was performed using differential scanning calorimetry (DSC) at 250°C to observe the growth of IMC formation. DICTRA simulations were used to compute concentration profiles across the Sn/Cu interface. From these profiles, the individual thicknesses of phases were estimated and compared directly against experimental data obtained from DSC and SEM. This comparison allowed for calibration of the phase-field kinetic parameters, ensuring the model accurately captures the diffusion-controlled growth seen in the experiments.

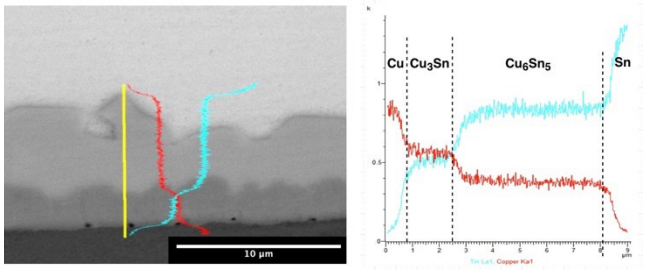

Fig. 1 BEI micrograph and the linescan Sn/Cu joint aged at 155°C for 500h

Acknowledgement

This work was supported by Programme to support excellent teams of young researchers at STU under project 1366.

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Biographical Note

Tereza Peričková is a PhD student in Advanced Materials and Material Design. Her research focuses on the Development and analysis of lead-free solder systems, specifically investigating microstructural evolution through a combination of experimental techniques and computational modeling. She specializes in experimental techniques like scanning electron microscopy, X-ray diffraction, and differential scanning calorimetry to study interfacial reactions and employs multiphase-field modeling to simulate phase growth in solder systems.

Efficient Single-Phase Region Search via Gradient-Informed Gaussian Processes

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Key words: Phase Stability, Gradient-Enhanced Gaussian Processor, Driving Force

Identifying single-phase regions in multicomponent alloy systems is a recurring bottleneck in workflows for inverse materials design, as these regions can be narrow and highly nonlinear. Current search techniques inefficiently employ dense grids of equilibrium calculations over high-dimensional composition spaces. CALPHAD-based thermodynamic models provide a physically grounded route to predicting phase stability, but their practical utility for identifying initial feasible regions for the problem of inverse materials design depends on the ability to efficiently locate and characterize composition subdomains where a target phase is uniquely stable under prescribed temperature–pressure conditions.

In this work, we develop an active-learning workflow for efficient single-phase region search that couples CALPHAD equilibrium calculations with gradient-informed Gaussian process (GP) modeling. Phase stability is encoded through a scalar metric based on the residual driving force concept [1]. Specifically, the overall system composition defining the stable hyperplane and vertex composition of the target phase are set equal, resulting in compositions in the target single-phase region exhibiting zero driving force, while positive values indicate the presence of other stable phases. The search objective is therefore constructed to drive this residual toward zero, effectively turning the single-phase region search into a global minimization problem. An example of this minimization is shown in Figure 1.

To conduct this global optimization, we train a gradient-informed Gaussian Process (GP), where gradients of the residual driving force objective are obtained via the recently formalized Jansson derivative method [1]. The resulting gradient-enhanced GP improves local fidelity near stability transitions and yields more informative uncertainty estimates in sparsely sampled regions. We then apply an uncertainty-aware acquisition strategy to adaptively select new compositions, balancing exploitation of predicted low driving force with exploration of uncertain regions to avoid premature convergence.

This exploration–exploitation mechanism mitigates a key failure mode of purely local, gradient-based optimizers (e.g., steepest descent and related methods), which can become trapped in local minima of nonconvex stability landscapes and thereby miss disconnected or narrow single-phase regions. By maintaining a global probabilistic model of the objective and explicitly allocating evaluations to reduce uncertainty, the proposed approach is less sensitive to initialization and more robust to multimodality, enabling efficient discovery of small regions of single-phase stability in high-dimensional composition spaces.

The novelty of this work is two fold: i) We are using the residual driving force as a thermodynamically relevant search objective within a Bayesian scheme for single-phase alloys and ii) we are using GPs informed by the gradient of residual driving force itself, thus leveraging yet more thermodynamic information in the search scheme.

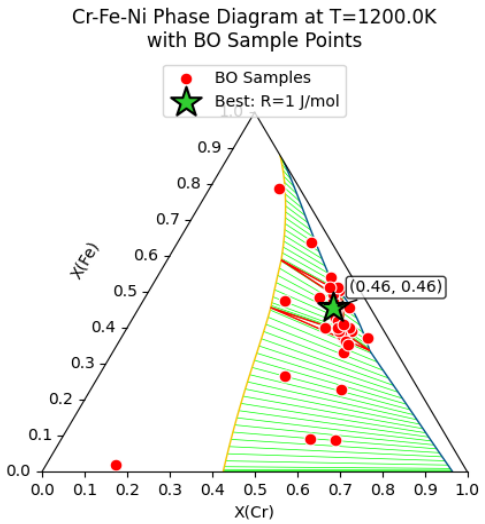

Figure 1: Example of gradient-informed minimization of the residual driving force of the σ-phase in the Fr-Cr-Ni ternary

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Biographical Note

Cayden Maguire is currently pursuing a B.S in Computer Science at Texas A&M University. His research involves Bayesian active learning for constraint satisfaction in the context of alloy design.

Machine Learning–Accelerated Investigation of Phase Stability in TiVCrCoZr High-Entropy Alloys for Hydrogen Storage Applications

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The growing interest in sustainable development has driven the scientific community to investigate alternative solutions for energy production and storage, with hydrogen emerging as a key energy carrier for future low-carbon technologies. Among solid-state hydrogen storage materials, high-entropy alloys (HEAs) have attracted increasing attention due to their exceptional mechanical stability, tunable functional properties, and vast compositional flexibility, which enable targeted design of material performance [1].

This work investigates the stability of the five-element high-entropy alloy TiVCrCoZr through a combined computational and machine-learning framework. The primary objective is to compare the formation energies of body-centered cubic (BCC) and face-centered cubic (FCC) phases to identify the most thermodynamically stable structure, a critical requirement for hydrogen storage and other energy-related applications demanding high material stability. First-principles calculations were performed using the Vienna Ab Initio Simulation Package (VASP) based on Density Functional Theory (DFT), providing reliable reference formation energies for different structural configurations.

To accelerate the exploration of alloy stability, a Random Forest regression model was initially employed to predict formation energies from atomic descriptors, evaluating the capability of conventional machine learning approaches. Building on these results, Crystal Graph Convolutional Neural Networks (CGCNN) were implemented as a more advanced deep learning method capable of representing crystal structures as atom-bond graphs. By adapting CGCNN to high-entropy alloy systems, the model effectively captured structural and chemical interactions and predicted formation energies with accuracy comparable to DFT while significantly reducing computational cost.

In parallel, recent advances in deep-learning surrogate modeling combined with CALPHAD calculations demonstrate how temperature-dependent phase behavior in refractory multi-principal element alloys can be rapidly predicted across large compositional spaces [2]. These surrogate models preserve thermodynamic fidelity while achieving orders-of-magnitude speedups compared with traditional CALPHAD workflows, enabling efficient screening of millions of candidate alloys and supporting discovery of stable BCC phases over wide temperature ranges. Such approaches highlight the importance of integrating physics-based thermodynamic calculations with data-driven models to map phase stability, predict phase fractions, and guide experimental synthesis strategies.

The comparison between traditional machine learning and graph-based deep learning underscores the superior generalization capability of advanced neural network architectures for complex alloy systems. More broadly, the combined use of DFT simulations, CALPHAD-informed datasets, and AI-driven modeling provides a scalable pathway for accelerating materials discovery while reducing the costs and computational resources associated with conventional experimental and simulation-based approaches.

Overall, this study demonstrates how the synergy between computational materials science and artificial intelligence can deepen understanding of HEA phase stability and enable rapid, data-guided design of next-generation materials for hydrogen storage and energy applications. The methodology presented here offers a flexible framework that can be extended to temperature-dependent phase prediction and high-throughput exploration of complex alloy systems, ultimately supporting faster development of technologically relevant materials.

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Biographical Note

Mauro Palumbo is an Associate Professor at the University of Turin, Italy. He teaches courses in materials science, metallurgy, and computational methods in materials science. His research focuses on phase transformations in metallic materials and on materials for energy storage.

Thermodynamically Driven Microstructural Evolution and Property Regulation in the Process of Al-Mg-Si Alloys

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Key words: Al alloys, Thermomechanical processing, Dispersoids, Dislocation, Thermodynamic prediction.

Inevitable Mn/Cr/Fe dispersoids in Al–Mg–Si alloys often exacerbate microstructural inhomogeneity and deformation resistance during processing. Their coarsening and high solid solubility during aging alter matrix solute distribution, interfering with strengthening phase precipitation and weakening alloy performance [1,2]. While conventional processing relies on solution–aging for nano-phase strengthening, the role of dislocations in regulating strength and toughness is often neglected. However, introducing dislocations at specific stages can mitigate the negative effects of coarsen dispersoids by modulating solute distribution and dislocation–dispersoid interactions [3].

Guided by thermodynamic predictions of solute behavior and dispersoid stability, this study maps these results onto thermomechanical processing (TMP) to achieve staged dislocation–dispersoid regulation. We compared two processing sequences: Cold Rolling–Pre-aging–Artificial Aging (CR–PA–AA) and Pre-aging–Cold Rolling–Artificial Aging (PA–CR–AA). Microstructural characterization and mechanical testing were employed to elucidate the impacts on precipitation, dislocation storage, and synergistic mechanisms.

Results indicate that both pathways significantly accelerated aging kinetics, achieving peak hardness within 1 h at 180 °C (158 HV for CR–PA–AA; 163 HV for PA–CR–AA), thereby enhancing process efficiency. Thermodynamic Scheil solidification path analysis revealed distinct dominant mechanisms. In CR–PA–AA, pre-cold rolling defects enhanced local diffusion and nucleation, promoting precipitation around dispersoids to eliminate dispersoid-free zones (DFZs) and improve homogeneity. Conversely, in PA–CR–AA, pre-existing dispersoids and coarsened phases strongly pinned dislocations during subsequent rolling. This inhibited dynamic recovery and drove dislocation evolution from disordered tangles to ordered cellular networks, yielding higher peak dislocation densities (~1.98×10^{15} m^{-2}).

Ultimately, the deformation–aging sequence fundamentally alters dislocation–solute coupling and storage modes. The PA–CR–AA route achieved superior strength–ductility synergy (UTS ~487 MPa, elongation ~11.67%), transitioning fracture behavior from cleavage-dominated brittleness to dimple-induced fracture. Consequently, precisely designing processing sequences based on thermodynamic predictions of structural evolution offers a robust theoretical framework for optimizing ultra-high strength 6xxx series aluminum alloys.

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Biographical Note

Pengfei Zhou is a Ph.D. candidate at the Institute of Powder Metallurgy, Central South University. His research focuses on the design of aluminum alloys by coupling machine learning with thermodynamics and kinetics.

Breaking the Charge Neutrality Boundary in Perovskite Using the *PyCALPHAD* Approach

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In mixed ionic-electronic conductors the formation of Space Charge Layers (SCLs) greatly impacts the concentrations of point defects and charge carriers near grain boundaries [1]. This phenomenon increases resistance and greatly reduces material performance. Variations in defect concentrations in the bulk and surface of crystals are often attributed to space charge phenomena. Despite their importance, the thermodynamics of SCLs remain underexplored and are addressed in this work.

Prior investigations of the SCL predict defect chemistry in the Fe-O binary system, allowing for calculation of the volumetric Gibbs free energy of non-charge-neutral systems [2]. The approach in this research expands this method to a perovskite system. The perovskite $(La,Sr)_{1-y}MnO_{3\pm\gamma}$ (LSM) is chosen as a case study due to its importance in Solid Oxide Fuel Cells (SOFCs). Hydrogen fuel cells, including SOFCs and Solid Oxide Electrolysis Cells (SOECs), can store and generate electricity in remote or isolated applications.

Commonly, thermodynamic equilibrium of a material system is considered only in charge-neutral conditions. The present framework utilizes PyCALPHAD, a free and open-source program, to modify the charge balance required for equilibrium. This software applies a Compound Energy Formalism (CEF) and sublattice model to compute the molar Gibbs energy of a material system. For LSM, $(\mathrm{La}^{3+},\mathrm{Mn}^{3+},\mathrm{Sr}^{2+},\mathrm{Va})_1(\mathrm{Mn}^{2+},\mathrm{Mn}^{3+},\mathrm{Mn}^{4+},\mathrm{Va})_1(\mathrm{O}^{2-},\mathrm{Va})_3$sub lattice model is used. Molar Gibbs free energy is computed for a range of feasible overall charge balances which are observed in the SCL [3]. This is accomplished by imposing a constraint for equilibrium where the ratios of charged endmembers must be equal to some constrained ratio of electrons. This method requires additional sampling of the composition space, which is addressed in this work. Gibbs energy is then minimized with respect to the extra constraint for equilibrium.

An expression for conductivity of LSM is applied which considers the concentration of the Mn^{4+} charge carrier and the mobility of this ion [3]. Quantitative Brouwer diagrams are constructed which depict defect chemistry as a function of oxygen gas partial pressure.

The Poisson-Boltzmann distribution is applied to calculate concentrations of charged defects relative to surface voltage. This procedure involves calculating defect chemistry for various charge-constrained conditions and solving the Poisson-Boltzmann distribution for this range of charges. This allows for conductivity to be calculated as a function of distance into the space charge layer.

This research provides a framework with which defect chemistry and conductivity of perovskites can be calculated. This allows for space charge phenomena and properties of functional oxides to be predicted, ultimately providing an improved understanding of the defect chemistry and thermodynamics of space charge layers in functional ceramics.

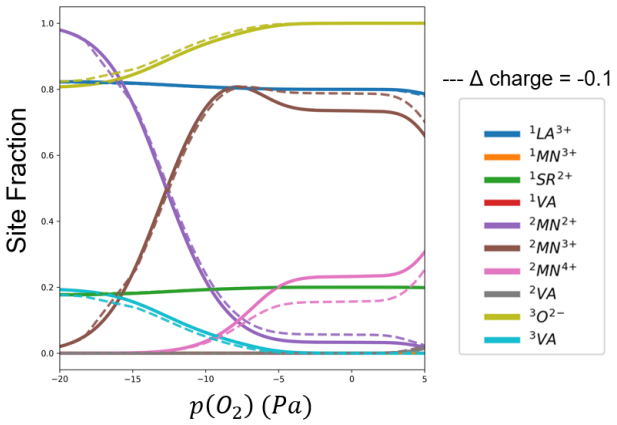

Figure 1. Quantitative Brouwer Diagram of LSM-20 perovskite as a function of oxygen gas partial pressure

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Biographical Note

Adam Shenk is a second year PhD student at Worcester Polytechnic Institute. His research focuses on computational thermodynamics, CALPHAD, high-throughput alloy screening, and laboratory experiments including arc melting and TGA-DSC.

Liquidus projection of the Co-Si-B system in the Co-rich region

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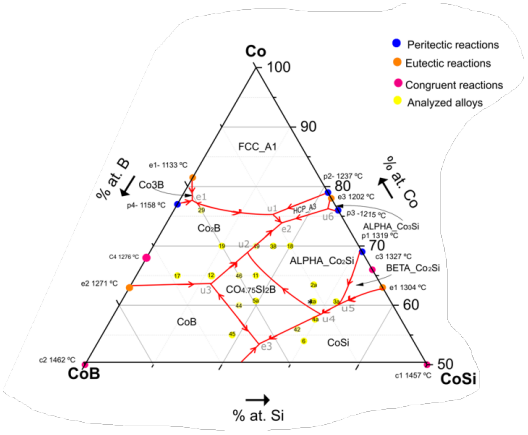
Metal-based alloys with Silicon and Boron are studied for their interesting magnetic properties. These alloys are typically obtained by adding approximately 20% of metalloids (Si, B, Al, C, and P) to cobalt- or iron-based alloys. The combination of these elements in different compositions can result in a wide variety of magnetic properties. Therefore, the study of phase diagrams is essential for defining the compositions suitable for their respective applications and, especially, for creating thermodynamic databases. Notable examples include the Co-Si-B, Fe-Si-B, and Ni-Si-B systems, with the latter two having more available information in terms of phase diagrams. However, there is no record in the literature on the liquidus projection of the Co-Si-B system in the cobalt-rich region (Co-50at.%B-50at.%Si), which is the main objective of this investigation.

The alloys used in this work were prepared from Co (min. 99.97%), Si (min. 99.9999%), and B (min. 99.5%). The samples were melted in an arc furnace using a water-cooled copper crucible, non-consumable tungsten electrode, and high-purity argon atmosphere. Based on the interpretation of the as-cast microstructures, associated with uncertainties in composition extrapolations, all samples were characterized by Energy Dispersive Spectroscopy (EDS), Electron Backscatter Diffraction (EBSD), and X-ray Diffraction (XRD). This approach allowed verifying the primary phase and constructing the liquidus projection of the Co-Si-B system. The results have shown the primary precipitation of the following phases: Co_2Si,CoSi,CoB,Co_2B and $Co_{4.75}Si_2B$. The ternary $Co_{4.75}Si_2B$-phase is formed from the liquid through a peritectic-type reaction L+Co_2Si=$Co_{4.75}Si_2B$.

Figure 1. Liquidus projection of Co-Si-B system proposed in this work



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Biographical Note

Ester Kelly Starick Pellegrino is a Master's student in Materials Engineering at University of São Paulo (USP), Brazil, under supervision of professor Carlos Angelo Nunes. The author has experience with experimental determination of phase diagram.

Topologically Constrained Machine Learning of Phase Diagrams Using Markov Random Fields

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Phase diagrams are governed by thermodynamic and topological constraints, yet most machine-learning surrogates for phase mapping are trained primarily for local predictive accuracy (e.g., phase class or phase fraction at sampled points) [1] rather than global topological admissibility. Recent active-learning workflows have demonstrated substantial gains in sample efficiency for phase-diagram construction, particularly through uncertainty-driven querying, but they can still return boundary geometries or neighborhood relations that are not physically admissible when data are sparse or imbalanced [2].

Here, we present a topology-constrained phase-field classifier via a Markov random field (MRF) prior over a thermodynamic state space. The key idea is to represent phase labels as nodes in a neighborhood graph and nforce physically admissible local transitions through prescribed pairwise jump probabilities in the MRF [3]. In its simplest form, the model discourages direct contact between incompatible single-phase fields (A|B) and promotes physically admissible transitions through multiphase regions i.e. (A|(A+B)|B). The imposed A|(A+B)|B adjacency prior reflects convex free-energy topology i.e. equilibrium phase boundaries arise from common-tangent coexistence, so single-phase domains are separated by multiphase regions rather than direct single-phase contact. This converts qualitative phase-diagram knowledge into quantitative regularization during inference. We implement both hard constraints (zero-probability forbidden edges) and soft penalties (energy-based discouragement) to balance strict physical plausibility against robustness to noisy labels.

The phase classification with MRF show improved topological accuracy, reducing spurious islands, nonphysical phase field adjacencies, and fragmented phase fields. Relative to unconstrained baselines, the proposed method yields phase maps that are more interpretable to CALPHAD practitioners and more consistent with classical connectivity logic around phase boundaries, while preserving the data-efficiency advantages of uncertainty-guided acquisition reported in recent literature.

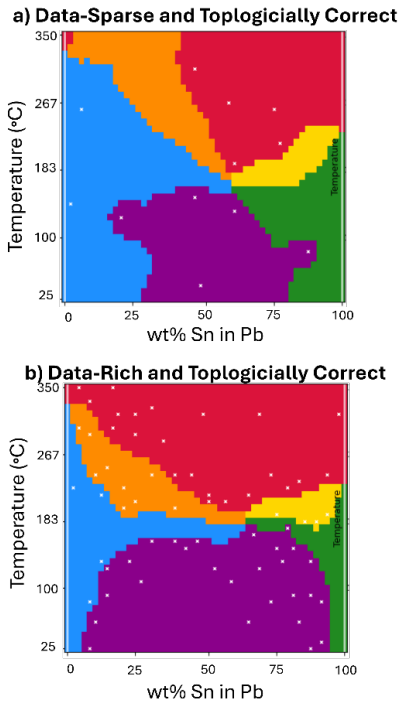

Figure 1: a) Data-Sparse MRF classifier predictions correct topology of Pn-Sn despite missing some 2 phase observations. b) Data-rich MRF classifier has correct topology and has local classification accuracy

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Biographical Note

John Teerman is a freshman undergraduate researcher at Texas A&M working with Dr. Raymundo Arroyave on physics informed machine learning models for phase diagram construction.

Phase equilibria and thermodynamic activities for Li-ion battery electrolytes comprised of $LiPF_6$ in ethylene carbonate and $LiPF_6$ in dimethyl carbonate

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Lithium-ion batteries (LIBs) dominate modern energy storage technologies and are widely used in portable electronics and electric vehicles[1]. Despite their high energy density and low self-discharge rate[2], several challenges remain, many of which are related to the electrolyte solution.

LIB electrolytes typically consist of ternary or higher-order non-aqueous liquid mixtures composed of lithium salts dissolved in organic carbonate solvents[3]. Under low-temperature conditions and/or at high salt concentrations, these electrolytes exhibit reduced ionic conductivity and increased internal resistance due to phase instability, leading to significant performance degradation.

Understanding electrolyte behavior under such conditions requires accurate thermodynamic data, including species activities and phase equilibria over a wide concentration range.

However, these data are generally unavailable, particularly at high salt concentrations where solid solvates may form or coexist with the liquid phase. This raises the question of the practical determination of solution energetics from liquid-solid phase equilibria in non-aqueous binary and ternary electrolyte systems in which solid solvates can form.

We investigate the binary electrolytes solutions $LiPF_6$ in EC (ethylene carbonate) and $LiPF_6$ in DMC (dimethyl carbonate) through the determination of thermodynamic activities of individual species up to 3 molal. Using literature liquid temperatures and enthalpies of fusion of solid solvates obtained by DSC (differential scanning calorimetry), species activities were derived through thermodynamic relationships. Conversely, the calculated activities, together with thermodynamic quantities such as latent heats of fusion, enabled the calculation of phase diagrams for the investigated electrolyte system. The calculation of binary non-aqueous phase diagrams will allow the treatment of the ternary system $LiPF_6$ in EC and DMC mixtures.

Figure 1. DSC curves for $LiPF_6EC_4$ and $LiPF_6DMC_3$ solid solvates. The curve corresponding to 3.39 m has been vertically offset by 1 W/g for clarity

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Biographical Note

Maissa Trabelsi is a PhD student in materials engineering at Polytechnique Montreal. Her research focuses on the thermodynamics of lithium-ion battery liquid electrolytes including the phase equilibria and solution energetics. Her work targets the understanding of electrolyte behavior at high salt concentrations and low temperature conditions for advanced energy storage technologies.

Phase diagrams and interfacial reactions of Ni-Bi-Sb ternary system

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Ni-Bi-Sb ternary system is an important material system with potential applications in many fields. (Bi,Sb) alloys exhibit excellent thermoelectric properties, which can be further enhanced by Ni addition [1,2]. Bi-Ni and Ni-Sb intermetallic compounds show catalytic activity for hydrogen evolution reaction [3,4]. Bi and Sb are often added to Sn-based lead-free solders, while Ni is a commonly used barrier layer in electronic devices [5]. This study aims to determine the Bi-Ni-Sb phase diagrams, including the isothermal section at 500 °C ,300 °C and the liquidus projection. The invariant reactions associated with the liquidus projection will also be identified. These results could then be used for CALPHAD-type modeling. Furthermore, in the electronics industry, there is a continuous effort to develop suitable high-temperature solders, but no breakthrough has been achieved so far. Bi and Sb form a continuous solid solution, with melting temperatures ranging from 271.4 °C to 630.6 °C, which is a very suitable range for high-temperature solders. The (Bi,Sb) alloys serve as a promising base candidate for high-temperature solder development. Since nickel is commonly used as a barrier layer, this study also investigates the interfacial reactions between (Bi,Sb) and Ni. Knowledge of the Bi-Ni-Sb phase diagram will be used to analyze the reaction mechanisms.

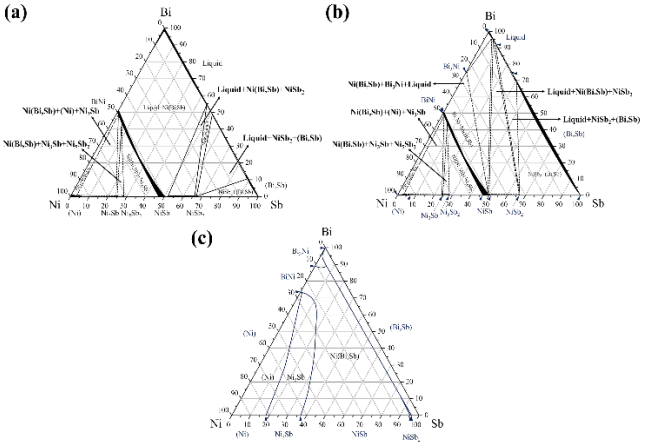

Figure 1. Ni-Bi-Sb ternary system：(a) phase equilibria isothermal section at 600 °C, (b) phase equilibria isothermal section at 800 °C and (c) liquidus projection

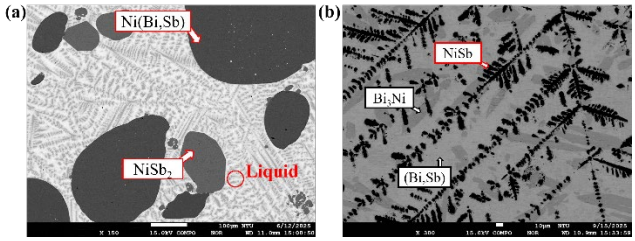

Figure 2. BEI micrographs (a) alloy Ni-30%Bi-50%Sb equilibrated at 500 °C for 5 months and (b) as-quenched alloy Ni-78.2%Bi-7.3%Sb

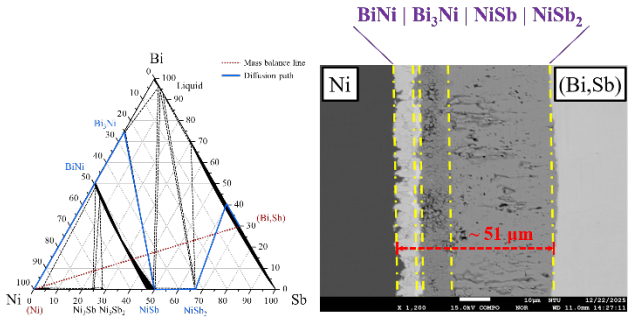

Figure 3. The diffusion path and BEI micrograph of Ni/(Bi,Sb) interfacial reaction at 300 °C for 10 days

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Biographical Note

Mr. Yung-Chun Tsai is a PhD student in the Department of Chemical Engineering at National Tsing Hua University in Prof Sinn-wen Chen’s group.

Physically-constrained prediction of the liquidus curve for multicomponent chemistries

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Accurately predicting the liquidus curve in high-component space remains a challenge for present implementations of the CALPHAD method. Here, we present a framework for creating a self-consistent, DFT-referenced binary solution database of 70 elements, with applied boundary conditions to improve extrapolative ability in multicomponent space. In this framework, we utilize random forest models with features derived from elemental and DFT-calculated properties to predict Redlich-Kister coefficients. We discuss how data science techniques can be utilized to improve model performance by pruning spurious training data. Finally, we demonstrate how accurate predictions can be made with only a few experimental measurements.

Biographical Note

Joshua Willwerth is a third-year PhD student at the University of Michigan. His research focuses on applying CALPHAD methods to predict phase diagrams using phase energies calculated via density functional theory (DFT). He is also interested in the data science of high-throughput experimentation to experimentally verify CALPHAD-predicted results.

Josh is passionate about science education and community engagement. During both his undergraduate and graduate studies, he has served on the boards of materials science student organizations and has participated in outreach events that bring materials science education to public schools across Michigan.

Illuminating early-stage oxidation of ZrC using Small-Cell DFT MD

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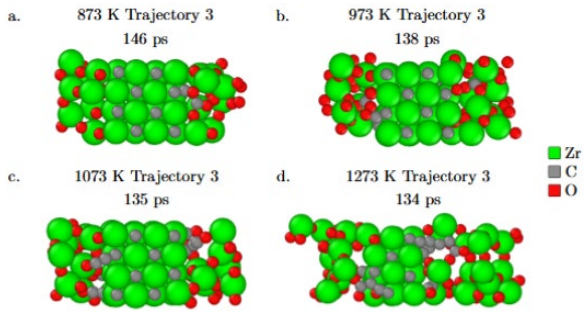
Zirconium carbide (ZrC) is a candidate material for thermal protection systems and next-generation nuclear fuel cladding, but its deployment is limited by poor oxidation resistance in the intermediate temperature range (873–1273 K). Macroscopic oxidation experiments report widely scattered activation energies and conflicting kinetic models across this range, suggesting that bulk measurements alone cannot isolate the intrinsic rate-limiting processes. We present a DFT-based small-cell statistical framework that resolves these processes at the atomistic level while retaining ab initio accuracy.

Building on the small-cell methodology of Hong and van de Walle [1], we implement a dynamic gas-exchange algorithm within ab initio molecular dynamics (AIMD) that maintains a constant oxygen impingement flux by replenishing consumed O2 and removing gaseous products (CO, CO2) as they form. Similar to SLUSCHI [1], our SGUSCCHI (Solid-Gas in Ultra Small Coexistence with Hovering Interfaces) methodology employs molecular dynamics simulations across an ensemble of small cells to statistically determine key oxidation properties, such as activation energies. This scheme sustains reactive conditions over simulation timescales of ~130 ps per trajectory at effective partial pressures of ~150 bar pure O2. 16 trajectories (four per isotherm at 873, 973, 1073, and 1273 K) provide a statistical ensemble from which we extract temperature-dependent reaction rates, carbon product ratios between gas-phase and solid-phase products, and the Shannon entropy of Zr–O coordination environments as a structural order parameter for the developing oxide network.

Figure 1. Snapshots of selected MD trajectories



The simulations reveal three regimes governed by a kinetic crossover between two competing processes: the oxidative removal of interfacial carbon as CO/CO2, and the thermally driven consolidation of the Zr–O coordination network. At 873 K, both rates are sluggish and oxidation proceeds stochastically, producing large trajectory-to-trajectory variance consistent with nucleation-limited growth. At 973 K, carbon oxidation accelerates ahead of network consolidation, yielding peak configurational entropy (~1.71 nats), maximum CO evolution, and minimum solid-phase carbon retention, signatures of a maximally disordered, non-protective oxide. Above 1073 K, network consolidation outpaces gas generation, sealing the interface and redirecting mobilised carbon into solid-phase retention. An Arrhenius analysis of the reaction-controlled window yields an intrinsic activation energy of 13.3 kJ/mol, in close agreement with an experimental value of 14.2 kJ/mol for the linear oxidation stage [2].

These results demonstrate that the macroscopic active-to-passive transition in ZrC originates from a nanoscale competition between carbon gasification and oxide network ordering, and that small-cell DFT with dynamic gas exchange can quantify the intrinsic interfacial kinetics and model the mechanism adequately. The identified crossover framework offers a physically grounded basis for developing kinetic descriptions of oxidation within thermodynamic databases, and for computationally screening dopant strategies for ZrC that shift the crossover toward improved oxidation resistance.

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Intelligent Design and Development of Ultra-High-Strength Steels for Additive Manufacturing

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Ultra-high strength maraging steels of the 18Ni350 grade and its derivatives are key candidates for critical structural components in the high-end manufacturing field, but their strength-ductility trade-off restricts large-scale use in 3C electronics and load-bearing applications. This study implements a full-process intelligent R&D framework of computation-driven design, high-throughput preparation, rapid validation, mechanism elucidation, and iterative optimization to optimize simultaneously the composition, process, microstructure, and performance, and ultimately develop a novel maraging steel system that combines ultimate strength with excellent ductility.

2. Methods

This work includes two core high-throughput modules: (1) thermodynamic calculation and composition screening; (2) additive manufacturing and characterization.

2.1 Thermodynamic Calculation & Screening

A thermodynamic model assessed C, W, Mo, Si, Ta, and Al effects on precipitation of key strengthening phases ($Ni_3(Ti,Al)$, Ni_3Mo, and Fe_2Mo Laves phase). From a 38,016-composition thermodynamic database, candidates were pre-screened using nano-precipitate regulation, and a heat-treatment window suppressing coarse brittle phases was identified to guide process design.

2.2 Additive Manufacturing & Characterization

A multivariate Selective Laser Melting (SLM) matrix of 14 compositions, 12 laser parameter sets, and paired heat treatments was built for rapid composition-process-microstructure-performance mapping. SLM was optimized for relative density by tuning laser power and scan speed. High-throughput hardness screening preceded room-temperature tensile validation of target alloys, with synchronous microstructure and precipitate characterization clarifying the mechanism.

3. Results

3.1 Thermodynamic Calculation & Preliminary Screening

Screening of 38,016 compositions yielded 14 candidate alloys with excellent nano-precipitation regulation potential. 450-550 ºC was identified as the optimal precipitation window, suppressing coarse brittle secondary phases and grounding the heat-treatment design.

3.2 SLM Process Optimization & Hardness Screening

Optimal SLM parameters (185 W, 1000 mm/s) gave specimens with 99.73% relative density. Across 336 hardness measurements, 33 alloy-process combinations exceeded 650 HV (12 exceeded 700 HV), defining targets for tensile testing.

3.3 Tensile Property Verification

The optimized alloy reached ~2450 MPa ultimate tensile strength (UTS) with 4.5% elongation; selected specimens reached 2535 MPa UTS and 3.5±0.5% elongation. For 3C-electronic applications, an alloy with ~2350 MPa UTS and >5% elongation was also developed.

4. Discussion

Our approach replaces the slow, poorly coupled trial-and-error route: thermodynamic screening of >30,000 compositions rapidly identified high-potential candidates, and the SLM-based multi-variable matrix yielded a quantitative composition-process-microstructure-performance mapping, enabling collaborative multi-element and process optimization.

Strength-ductility balance depends on the size, density, and distribution of nano-strengthening phases. The 450-550 ºC window promotes precipitation of high-density $Ni_3(Ti,Al)$ and Ni_3Mo nano-phases while suppressing coarse brittle Fe_2Mo Laves phases – the core mechanism for the excellent strength-ductility matching of alloys. The 3C-specific alloy confirms the route's adaptability for lab-to-engineering translation.

5. Conclusion

A full-process intelligent R&D paradigm, from computation-driven design to iterative optimization, was established for 18Ni350-series ultra-high strength maraging steels. Combining high-throughput thermodynamic calculation with SLM experiments permitted to develop multiple alloys spanning ultimate strength, engineering, and 3C requirements.

This approach offers a replicable path for ultra-high strength-ductility metals with significant engineering and industrialization potential.

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Simulating natural gas substitution by hydrogen with process integration in DRI-MIDREX Process using a novel kinetic approach and equilibrium reactors

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The DRI-MIDREX process for steelmaking is responsible for approximately 45 million tonnes of anthropogenic CO_2 emissions globally in 2024, driven by its reliance on natural gas as a reducing agent, which is carbon-intensive although less than blast furnaces [1]. Green hydrogen is a candidate reducing agent with an even lower carbon intensity, but it does not behave identically in this process. This work presents a robust thermodynamics and experiment-based model of the shaft furnace and of the entire MIDREX process, which is then used to optimize GHG reductions for the partial replacement of natural gas by hydrogen.

In the model, the shaft furnace unit is formulated as a series of counter-current equilibrium reactors, with gas bypass parameters used to regulate reduction reactions at each stage. These bypass parameters were optimized through black box optimization and modelled using an adapted shrinking core model for the pellets, providing a numerical fit to align the reduction behavior with experimental results. The rest of the process, containing simpler unit operations such as natural gas reforming, is simultaneously modelled through equilibrium reactors.

As such, it is possible to study the complete simulated impact of varying process parameters such as the H_2 to natural gas ratio, recirculation ratio (top gas to top gas fuel) or other process parameters, and to monitor the associated CO_2 emissions, DRI metallization degree, furnace heat balance, as well as the DRI carbon content.

The process simulation model was validated with known MIDREX process datasets found in the literature, while furnace results were validated with multiple experiments varying bustle gas compositions, particularly the H_2 to CO ratio, in a lab scale reduction furnace.

The main strength of this model, compared to other typical models found in the literature, is the added flexibility granted by the use of known and validated thermodynamics database as a basis for the furnace model. This allows quick computing of the entire process, a stepping stone towards digital twin applications. It also allows changing pellet composition and impurities such as SiO2 without rebuilding the model, giving it more flexibility than most other computational methods.

Results show that, realistically, a 30% replacement of natural gas by H_2 is achievable without requiring important retrofits of the process and that, with modifications to the operating conditions, important GHG reductions can be attained. This model represents a novel way of simulating kinetics of gas-solid interface reactions and its applications to a pyrometallurgical process, using rather simple equilibrium reactors each with a carefully calibrated gas bypass, instead of costly Computational Fluid Dynamics simulations [2].

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