

## Report to APDIC 2024

Activities of the phase diagram society in Japan

# Alloy Phase Diagram Society

(General incorporated association)



- Chair: H. Ohtani (Toyota Phys. Chem. Res. Inst.)
- Vice chair: I. Ohnuma and T. Abe (NIMS)
- Members: 14 companies and 42 from academia
- Annual meetings and seminars

The purpose of the association is to promote research on alloy phase diagrams in Japan.

1. To promote collaborations and cooperation among industry and academia.
2. To participate in and cooperate internationally with APDIC.

# Research group of Compt. Thermodynamics (placed in Japan institute of metals, JIMM)



- Chair: T. Abe (NIMS)
- 57 members from academia and 23 from industry

This group was established to discuss computational thermodynamics behind various phenomena through the construction of phase diagrams based on experiments and theories.

We will conduct theoretical studies of phase diagrams, establish new computational methods based on material informatics, propose methods for estimating phase diagrams, experiments, and machine learning, and study applications of industrial technologies based on phase diagrams. Seminars on the fundamentals of phase diagrams and thermodynamics will be held to educate researchers and engineers in academia and industry.

**Activities can be found at**

**<https://www.nims.go.jp/project/ext/comptd-jimm/>**



# Domestic Meetings (Phase diagram society)

The workshop on “Forescope and challenges in the phase diagrams”, March 4-6th 2023, (Nagoya on-site).

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## Day-1

### Invited talk

Tetsuo MOHRI, Hokkaido Univ.,  
“Future scope of phase diagram researchers”

### Session-1 : CALPHAD and Databases

Satoshi MINAMOTO, NIMS,  
“Thermodynamic database development and exit-strategies in the CALPHAD”

Toshihiro OHMORI, Tohoku Univ.,  
“CALPHAD from low temperatures”

Taichi ABE, NIMS,  
“How far can we go with CALPHAD?”

Welcome reception at Mercure hotel Nagoya

## Day-2

### Session-2 : Metastable phases

Hiroshi OHTANI Toyota PCRI, and Masanori ENOKI Shimane Univ., “Construction of theoretical phase diagrams based on first-principles calculations and utilization of metastable phases”

Masanori ENOKI Shimane Univ., and Hiroshi OHTANI Toyota PCRI, “Energy surface of metastable carbides of Fe-C”

Tatsuya TOKUNAGA, Kyusyu Inst. Tech.,  
“Metastable phase formation in supercooled liquid or amorphous phases”

### Session-3 : Hints for phase diagram usage for microstructure control

Toshiyuki KOYAMA, Nagoya Univ.,  
“CALPAHD method and phase-field method”

Nobuo NAKADA, Titech,  
“Affecting factors of Fe-C eutectoid transformation microstructure hidden in phase diagram”

Seiji MIURA, Hokkaido Univ.,  
“Effect of the control of factors on the microstructure of alloys”

Banket at Noritake Garden

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## Day-3

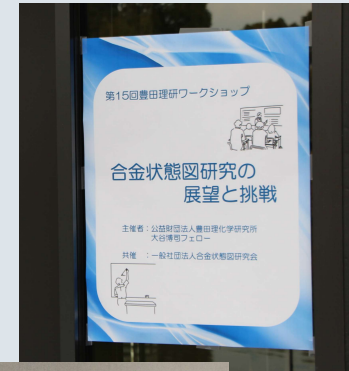
### Session : Applications of Gibbs energy and phase diagrams

Satoshi IKUBO, Kyusyu Univ.,  
“Device design application of microstructure control method”

Takeshi NAGASE, Univ. Hyogo, et al.  
“Development of Ti-based and high entropy casting alloys using thermodynamic calculation”

Ikuo OHNUMA, NIMS,  
“Experimental determination of phase diagrams and its application to practical processes”

### Session : General discussions and Wrap-up



# Annual Meeting (Res. Gr. Compt. TD. JIMM)

Nov. 21st 2023, (On-line).

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\*\*Experimental determination of the Mg-TM-Y systems and development of alloys  
Yuto HANDA, Chiba Univ.

Synthesis of Ti-Al powders using inhomogeneous reactions in the molten salt  
Terigele, Tohoku Univ.

The experimental measurements of the phase equilibria in the Al-Fe-O ternary system for evaluating the  $\text{Al}_2\text{O}_3$  precipitations in the molten steels.  
Yuxing LIU, Titech.

Inverse analysis of the diffusion profiles using the automated differentiation  
Kazuki SAKURAI, Nagoya Univ.

The phase equilibria and magnetic properties of  $\text{Taw}$  phase in the Mn-Al-X ternary system  
Kimika EDAGAWA, Tohoku Univ.

\*\*Thermodynamic assessment of the Sm-La-O ternary system for refining of Sm.  
Makoto YAMADA, Titech.

Machine learning-based segmentations of the secondary-dendrite arms simulated in the Phase-Field method  
Shinya FUJIWARA, Keio Univ.

Microstructural changes of the tool steels affected from the thermal histories  
Yuya FUKUTOMI, Daido Univ.

\*\*Experimental determination of phase equilibria in the Mn-Zn binary system  
Daisuke IMATOMI, Tohoku Univ.

CALPHAD-type thermodynamic assessment of the Fe-Pt system and Phase-Field simulations of the alloys  
Marino TANAKA, Keio Univ.

Evaluation of lattice distortion and phase stability of TiZrAl-based high-entropy alloys based on ab initio calculations  
Tetsuo YOSHINO, Univ. Tokyo

Effect of Ni addition on the activities in Fe-Zr melts at high temperatures  
Weirong YANG, Titech.

\*: Received Best presentation award

# Hosted and Co-organized Seminars

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Compt. Thermodynamics Seminar, Nov. 16-17<sup>th</sup>, 2023  
“Fundamental thermodynamics and CALPHAD techniques”  
M. Kajihara, (Titech) and T. Abe (NIMS)  
29 participants from industry  
This seminar will be annually organized.

## Summary: Activities in FY 2023

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- Annual Meetings of The Japan Institute of Metals (JIMM) x2
- Annual Meetings of The Iron and Steel Institute of Japan (ISIJ) x2
- Workshop of alloy phase diagram society x1
- Meetings of Res. Gr. Compt. Thermodynamics x1
- Seminars on fundamental thermodynamics and Calphad x1.