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Summary Report of CALPHAD L – Boston, USA, 2023

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Abstract

THE CALPHAD L 2023 conference was held in Boston, MA, USA from June 25th to 30th, 2023. We have 176 attendees from 23 countries. The activities in CALPHAD L 2023 included 84 oral presentations, 138 student posters, and two software workshops. The topics covered during the conference were gathered in nine categories.

Introduction

The CALPHAD L conference took place in Boston, MA USA, June 25–30, 2023. This is the first regular CALPHAD conference not affected by the COVID-19 since its outbreak. The conference attracted 176 participants and 15 accompanying persons, from 23 countries (conference photo Figure 1). Especially, we have 69 students attending. It is the 50th CALPHAD conference and was the 11th time the conference was held in USA, the previous times being 1973, 1975, 1982, 1985, 1988, 1994, 1997, 2000, 2007, 2012 (https://calphad.org/past-onferences).

Figure 1. The group photo of CALPHAD L

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Before the conference officially started, two scientific workshops were arranged in the afternoon of Sunday: (I) Diffusion Mobility Assessment Best Practices and Developing a CALPHAD Data Infrastructure and (II) Software Tools from Machine Learning to Phase Diagrams.

The conference followed the traditional layout of no parallel sessions with 84 oral presentations. Monday's four sessions were: CALPHAD: Past, Present, and Future to celebrate the 50th birthday of the CALPHAD conference; CALPHAD Modeling and Database Development (I); Atomistic Modeling and Prediction (I); CALPHAD Applications (I).

Tuesday continued with the following sessions: CHiMaD Sponsored session: Materials Genome and Materials Design (I); CHiMaD Sponsored session: Materials Genome and Materials Design (II); CALPHAD Applications (II); CALPHAD Applications (III).

Wednesday was the day of the excursion and therefore only two sessions were held in the morning: Experimental Equilibria and Phase Transformations; Atomistic Modeling and Prediction (II). In the afternoon there was the famous duck tour of Boston, aboard a W.W.II style amphibious landing DUKW vehicle that travels on land and across the Charles River. After that, the group photo was taken in front of the MIT great Dome (Figure 1). On the same evening, the Young Calphadian Night was organized by Wei Xiong and Richard Otis. One special activity was we celebrated the 80th birthday of Alexandra Navrotsky. On the young Calphadians stage, Charles Kuehmann, Raymundo Arroyave, and Rainer Schmid-Fetzer were summoned to give some advice to the younger audience.

Thursday continued with four oral sessions: Diffusion and Phase Transformations; CALPHAD Modeling and Database Development (II); Thermodynamic Software and Model Development; Thermodynamic Modeling, Database and Design Applications (I). The banquet was held in Odyssey Dinner Cruise from 7 to 10pm, which sailed around the Boston harbor. During the banquet many awards were announced:

- Gibbs Triangle Award: Dr. Rainer Schmid-Fetzer and Dr. Ursula Kattner
- 18 Larry Kaufman Scholarship awardees were presented by Dr. Zi-Kui Liu (Jeong-Min Cheon, Thomas Dumaire, Karoline Elerbrock Borowski, Lorenzo Fenocchio, Liangyan Hao, Manuel Löffler, Irene Moreno Flores, Amedeo Morsa, Vitória Silveira, Xingru Tan, Lucas Tosin Paese, Héléna Verbeeck, Jaemin Wang, Yanglin Wang, Nishant Tiwari, Srilekshmi Muraleedharan, Yindong Fang, Yu-ning Chiu)
- 16 NSF scholarship awardees were presented by Dr. Yu Zhong and Dr. Wei Xiong (Adetoye Adekoya, Thomas Avey, Michael Bustamante, Azhagu Devathai Dhanapal, Rushi Gong, Adam Krajewski, Samuel Krimmel, Luis Fernando Ladinos Pizano, Daozheng Li, Shuang Lin, Guangchen Liu, Michael Moodispaw, Alexander Richter, Hui Sun, Jize Zhang, Yifan Zhang)
- 11 STT scholarship, so called Hillert grants, was presented by Dr. Malin Selleby (Sang-Ho Oh, Joseph Moses, Loic Videau, Jia Qi, Chu-Liang Fu, Agustin Flores, Jia-Yi Fan, Tuan Minh Vu, Xue-Ting Wu, Yoongu Kang, Joonhyun Nam)
- The CALPHAD Best Poster Award went to Juliano Schorne-Pinto for the poster “Challenges in developing predictive thermodynamic models for complex molten salts” and Sofia Gambaro for the poster “High entropy alloys on graphite: wetting and reactivity evaluation by CALPHAD method”
- The FactSage Best Student Poster Award was awarded by Dr. Jean-Philippe Harvey to Sang-Ho Oh for the poster “Columnar grain formation in Nb_3Sn layer: a CALPHAD-coupled Monte Carlo study” and Chu-Liang Fu for the poster “A Cluster-Based Computational Thermodynamics Framework with Intrinsic Chemical Short-Range Order: Applications to Prototype Systems”
- The Best Paper Award for the best paper published in the Calphad Journal in 2022, according to a selection of the Calphad Editorial Board was granted to Gildas Guillemot, Oriane Senninger, Christopher A. Hareland, Peter W. Voorhees, Charles-André Gandin for their paper “Thermodynamic coupling in the computation of dendrite growth kinetics for multicomponent alloys”, Calphad, Vol. 77 (2022) 102429

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- The APDIC Best Paper Award, selected by APDIC among papers about phase diagrams and related topics published in 2021, was awarded Kostyantyn Korniyenko for the publication: Kostyantyn Korniyenko, Konstantin Meleshevich, Anatoliy Samelyuk, Viktor Sobolev, Lyudmila Kriklya, Phase Equilibria in the Al-Ti-Cr System During Solidification. J. Phase Equilib. Diffus. 43, 427–447 (2022). https://doi.org/10.1007/s11669-022-00983-4
- The APDIC industrial award 2023, was announced to be awarded to Usinas Siderúrgicas de Minas Gerais SA (USIMINAS), Brasil.
- Finally, Hans Seifert and Andre Schneider announced CALPHAD 2024 to be held in Mannheim, Germany May 26-31, 2024 and Joonho Lee announced CALPHAD 2025 to be held in Busan, South Korea May 25-30, 2025.

Friday offered two sessions: Thermodynamic Modeling, Database and Design Applications (II); Thermodynamic Modeling, Database and Design Applications (III). After that, the CALPHAD bell was transferred to the CALPHAD 2024 organizers: Hans Seifert and Andre Schneider. The conference ended with lunch.

Besides the regular presentation sessions every day, two poster sessions were arranged in the evening of Monday and Tuesday with 138 student posters in total.

All the abstracts (oral and poster) can be found in the book of abstracts in the supplementary document of this article.

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