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Summary report of XL CALPHAD—Rio de Janeiro, Brasil, 2011

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ABSTRACT

XL CALPHAD—Computer Coupling of Phase Diagrams and Thermochemistry conference was held in Rio de Janeiro, Brazil, May 22–27, 2011. The conference had an audience of 192 persons. There were 88 oral and 100 poster presentations.

Presentations were divided according to themes: ab initio; the CALPHAD method, and assessments; applications – energy; applications – steel, superalloys, oxides and experiments and databases. A total of 90 companies were represented among authors and audience.

In this summary, a brief description of the highlights of the conference is presented as well as the abstracts for the contributed papers.

1. Introduction

In its first edition in the Southern Hemisphere, XL CALPHAD—Computer Coupling of Phase Diagrams and Thermochemistry conference was held in Rio de Janeiro, Brazil, May 22–27, 2011. The conference had an attendance of 192 persons and a total of 88 oral and 100 poster presentations.

Presentations were divided according to themes: ab initio; the CALPHAD method, and assessments; applications – energy; applications – steel, superalloys, oxides and experiments and databases.

The ab initio sessions provided a broad overview of the relevant topics in the area, with featured papers by J.M. Sanchez, J. Neugebauer, T. Mohri, I. Abrikosov, P. Turchi, C. Colinet. In the CALPHAD method sessions lively discussions were initiated by the overview given by J. Agren in a session chaired by L. Kaufman. The situation concerning lattice stabilities and the current "inverted pyramid" analogy were discussed also in the featured presentations by L. Kaufman, B. Sundman and S. Fries. In the energy applications, featured presentations by P. Rogl, C. Gueneau and B. Sundman lead the sessions with a large number of applications related to nuclear materials, which harmonized with the view given by P. Turchi on the actnides and K. Ishida's overview on new Co based superalloys. The featured presentations by T. Matsumiya and M. Selleby focused on steels and advanced alloys while R. Schmid-Fetzer discussed databases for magnesium alloys. A significant presence of experimental contributions from well known researchers was also a highlight of this CALPHAD. Finally, B. Sundman, U. Kattner and S. Fries gave overviews of new developments in CALPHAD software, including a significant project on "open CALPHAD software".

The schedule was very busy but the attendance was consistently high even with the excellent weather in Rio de Janeiro and an interesting social program. Fig. 1 presents the official XL CALPHAD photograph. The poster sessions were held during four nights after dinner, with a drink service and there was extensive interaction and also lively discussions during these sessions.

During the CALPHAD banquet, the APDIC Industrial Award was presented to SANDVIK, as well as the CALPHAD best paper and best poster awards, and the APDIC best paper award. L. Kaufman was presented a plaque from the participants of the CALPHAD, in commemoration of his 80th birthday. A significant audience of "young calphadians" took active part in the conference (Fig. 2). Scholarships for students and academics were offered by PETROBRAS, CALPHAD Inc. and STT (Foundation of Computational Thermodynamics, Stockholm, Sweden).

2. Oral presentations

2.1. Ab initio

J.M. Sanchez

The cluster expansion method: first principles or phenomenology?

The cluster expansion (CE) method has been used extensively over the last 25 years to obtain effective cluster interactions (ECIs) that are expected to describe the energy of disordered alloys exhibiting short range order. Furthermore, these ECIs are extracted from the energies of a relatively small set of ordered compounds calculated using first-principles density functional theory (DFT). Thus, from its inception, the objective and/or promise of the CE has been to provide an important ingredient in the development of a first-principles thermodynamic theory of alloys. In this presentation, we will briefly review a rigorous mathematical formulation of the CE [1] that shows that the cluster basis developed by Sanchez, Ducastelle and Gratias [2] is a multidimensional discrete Fourier transform while the general formalism of Sanchez [3] corresponds to a multidimensional discrete wavelet transform. Weaknesses and strengths of the CE method, as well as its potential role in the quest for a first-principles thermodynamic theory of alloys, will be explored for several cases ranging from a simple pair potential model to energies obtained using DFT.

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Fig. 1. The XL CALPHAD group photo on the St. John Fortress, Rio de Janeiro.

Fig. 2. Young calphadians with L. Kaufman on the occasion of the XL CALPHAD.

References

[1] J.M. Sanchez, Phys. Rev. B 81 (2010) 224202.
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J. Neugebauer, B. Grabowski, A. Glensk, T. Hickel

Accuracy and limitations of ab initio approaches in predicting free energies for binaries and unstable phases

In order to extend and improve the algorithms and databases needed for the construction of phase diagrams, additional information on, e.g., the volume/pressure dependence of thermodynamic properties, the detailed balance of the various physical excitation mechanisms, and the free energy of unstable phases is crucial. Since an experimental approach to this information is partly not even feasible, the interest in ab initio based methods, in particular density functional theory (DFT), has been in the last few years re-intensified. Recently we have demonstrated that the presently available DFT exchange–correlation functionals are sufficient to predict the temperature dependence of free energies, heat capacities, thermal expansion coefficients and even defect properties of *unary* fcc metals with an accuracy that often rivals experimental data [1–3]. While these first results are very promising, many challenging questions remain. For example: how to compute free energies of instable phases that defy well established concepts based, e.g., on the quasiharmonic approximation (due to unphysical imaginary phonon modes) or molecular dynamics? Or: can these methods be extended to chemically more complex alloys and/or to compare several phases on an absolute energy scale? To address these questions, we carefully selected benchmark systems. We have chosen Mg–Si alloys as an example for a binary system and Ca for a system with an unstable phase and a phase transition. Extending our previous approach originally developed for unary systems we were able to compute all relevant free energy contributions such as configurational,