JPEDAV (2008) 29:475–476
DOI: 10.1007/s11669-008-9420-y
1547-7037 ©ASM International

Editorial

Integrating Methods for Phase Equilibria and Phase Property Data Determination

The advances in computer technology have enabled the use of increasingly sophisticated computational methods in materials science. These computational methods cover the entire length scale of materials from atomistic to macroscopic. With this progress a new discipline, Integrated Computational Materials Engineering (ICME), has begun to emerge. ICME holds the promise of integrating computational tools for accelerated materials development, improving the optimization process in engineering design, and easing the transition between design and manufacturing. Data are one of the fundamental components of ICME. For development of new materials in the ICME framework, phase property data such as thermodynamic properties, diffusion mobilities, molar volume, etc. are required. These data must have a high degree of accuracy and must cover a wide array of materials and compositions for reliable predictions and simulations. Most of these data have been obtained by experimental measurements, but they are also increasingly generated by computational methods.

The Calphad (**Cal**culation of **pha**se **d**iagrams) method describes the Gibbs energy of each phase as function of composition, temperature and, if needed, pressure and is traditionally used to calculate equilibrium phases by minimizing the Gibbs energy of the system. The parameters of these functions are traditionally obtained from experimental data. The approach used by the Calphad method can also be used to describe other phase properties such as diffusion mobilities and molar volume. The Calphad method, as implemented in a number of software tools, enables the development of thermodynamic and physical property databases and the extrapolation of these property data from binary and ternary systems to higher-order systems. For reliable extrapolation of the higher-order systems, the assessed functions must reproduce the experimental data well, and the models used for the phase descriptions must be physically reasonable. However, the data in the experimental database may be insufficient for accurate determination of all parameters. Furthermore, data from different sources may contradict one another or data for the metastable extension of homogeneity ranges may be missing. In these cases, data from first principles methods are particularly valuable.

Although the Calphad method is very powerful in predicting properties of higher-order systems, it cannot predict properties of phases or order-disorder phenomena of phases that do not occur in the constituent subsystems. Density Functional Theory (DFT) methods can be used to overcome some of these problems. DFT makes it possible to predict which intermediate phases are likely to be stable in a specific system and to obtain properties of metastable end-member phases that are needed for modeling homogeneity ranges. However, DFT calculations require input of the crystal structure. For the metastable end-member phases the crystal structure is the same as for the stable phase. For the prediction of new phases, it is common practice to test crystal structures which are the “usual suspects” for the given element combination. In recent years more systematic approaches have been introduced for selecting the crystal structures for testing. Data mining techniques rely on databases with a sufficiently large number of known crystal structures while other techniques use cluster expansions or a Monte Carlo approach.

For DFT calculations, the Wyckoff sites of a crystal structure must be occupied by one kind of atom, allowing only predictions for perfectly ordered crystals. However, disordered solution phases and order-disorder transformations are important features in many key systems for commercial alloys, e.g., Ni-Al or Ti-Al, and it is necessary to correctly describe the energetics for reliable predictions of higher-order systems. Unfortunately, the stable phase diagrams of the constituent subsystems may not have sufficient information to properly model these phase transformations. Valuable information for the Calphad modeling of the order-disorder phase transformations can be obtained from Monte Carlo (MC) simulations or from the Cluster Variation Method (CVM). Atomistic simulations can also provide property data that are either very difficult or impossible to measure experimentally.

The significant progress in computational methods for obtaining phase properties and phase diagrams may lead to the conclusion that experimental measurements are no longer needed. This is absolutely wrong. Experimental measurements are as valuable as ever; they are not only valuable input to the calculations, but are also crucial for verifying the predictions from the computational methods. Furthermore, data from experiments are needed to refine and improve the computational tools. In return, the computational methods allow the design of critical experiments for the determination of a system, thus reducing the number of experiments that are required for a full description of the system. The synergism between experiments and the various computational methods, and within the computational methods themselves is fundamental for fast and efficient progress in the design of new materials. The systematic investigation of fundamental properties will enable the construction of databases that are not limited to a specific class of materials and will ultimately enable the use ICME for development of entirely new materials and processes.

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