Editorial

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Adjusting materials chemistry and processing conditions have been a common practice of materials scientists/engineers in the design of new materials with desired properties and the improvement of the properties of existing materials. Traditional approaches relying on pure experimentation and trial-and-error are no longer viable due to limited resources. With the recent advancement of computational materials engineering and modern information technology, materials design processes can be greatly accelerated with the aid of modeling tools. Integrated Computational Materials Engineering (ICME), which integrates materials information obtained from computational tools with engineering product performance analysis, has recently been highlighted as a methodology that can unlock great potential for significant benefits in cost-effective, efficient materials and process design.

What is the role of *Journal of Phase Equilibria and Diffusion (JPED)* in ICME? As illustrated by its name, the nature of JPED is to publish papers related to phase diagrams and diffusion. Phase diagrams are road maps for materials scientists in the selection of alloy chemistry which satisfy the specific phase stability and materials performance requirement. Traditionally, most of the published phase diagrams were experimentally determined ones, but more and more papers published in *JPED* today are entitled ''Thermodynamic Assessment'', ''Thermodynamic Modeling'', and ''Thermodynamic Evaluation'' of a system. Attributed to the CALPHAD approach developed a few decades ago, we can now tackle very complicated multi-component, multi-phase equilibria which are very difficult to be determined solely by experimental approach. This is critically important since most, if not all, of the commercial alloys are multi-component in nature. The essence of the CALPHAD approach is to develop a self-consistent thermodynamic database, so that the thermodynamics of a multi-component system can be represented by those of the constituent binaries and ternaries. In recent years, this approach has been used beyond its original scope for phase diagram calculation. For example, it is used to construct mobility database which can be combined with thermodynamic database for the simulation of diffusion controlled processes.

At the same time, commercial software packages are being developed to bridge phase diagram calculation with property optimization in the framework of the CALPHAD approach. In such an attempt, thermodynamic calculation, kinetic simulation, and materials property prediction are integrated in the same workspace. Thermodynamic calculation provides chemical driving force for the nucleation and growth of precipitates, while the instant update of phase equilibrium information, such as phase stability, phase fraction, and phase composition, are direct input for the simulation of particle evolution. The microstructure features obtained from kinetic simulation, such as volume fraction of precipitates, precipitate size and size distribution can then be used in the microstructural and property models to predict the performance of a material. There is no doubt that an integrated computational tool coupling a robust calculation engine, reliable thermodynamic databases, and mobility databases will play an essential role in ICME.

Now the question is how to develop reliable thermodynamic and mobility databases. It is not difficult to understand that the quality of a multi-component database depends on the excellence of the descriptions of the constituent lower order systems, which, on the other hand, were developed using available experimental data. Certainly, the developers of the multi-component databases have put great efforts in developing self-consistent databases, those who published experimental phase diagrams, thermodynamic assessments of lower order systems, and mobility data have also made significant contributions. With all that being said, I think JPED has done a good job in publishing these data and assessments. All the authors and editors deserve some credit for it.

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