



What's the usage of phase diagrams, thermodynamic calculations, and diffusion simulations in industrial laboratories nowadays? I can speak of my own experience in industry for about a decade—this is, however, strictly a personal view that is not based on any extensive survey. The good news is that phase diagrams and thermodynamic calculations are used on a literally daily basis. Diffusion calculations are used a bit less often, but are still a significant activity.

Binary phase diagram compilations/handbooks are the most widely used resources of phase diagrams. If we count the number of times people consult/look for phase diagrams, the binary phase diagrams account for more than half of all the activities. This is not to say that ternary and higher-order systems are not important—they are far more valuable than the binaries, but are often not available. I have seen many disappointed faces over the years when colleagues asked me for a ternary or multicomponent phase diagram and walked away empty handed. After all, since only about 5% of possible metallic ternaries are (even partially) determined experimentally, what can we expect?

Recently, thermodynamic calculations are becoming much more widely performed. They are very useful; however, to have higher impact, database improvement (both accuracy and elemental coverage) is the key. The usefulness of a database and its associated calculations quickly hits a plateau that is dictated by the accuracy of the database. Using CALPHAD calculations for trend analysis is very different from performing reliable quantitative predictions. The latter is far more valuable and useful. Even with tremendous efforts for Ni-base superalloy systems, the present databases are still not up to the challenge of predicting the upper solubility limit so as to avoid the detrimental intermetallic phases. Such prediction capability would make the databases much more valuable for superalloy design by cutting down the lengthy long-term exposure experiments now required to evaluate the propensity of the alloys to detrimental phase formation. The lack of reliable experimental data input is mostly responsible for some of the problems in the databases.

A *good* thermodynamic database is at the heart of computational design of materials. It provides multicomponent phase equilibrium data (phase formation, phase compositions, volume fractions, etc.); the driving force for precipitation modeling; the segregation, specific heat, and latent heat data for solidification modeling; and thermodynamic factors for constructing the diffusion coefficient matrices for multicomponent alloys. Thermodynamic databases are also linked to phase field and other models to predict microstructure evolution and certain properties in alloys.

Diffusion calculations are also widely used, but for the most part are limited to square root Dt (diffusion coefficient multiplied by time) calculations. Advanced calculations using commercial software are also gaining momentum with more availability of diffusivity databases. Lack of diffusivity databases often prevents us from performing more critical simulations in a timely fashion to impact projects that are usually moving at a fast pace.

It all boils down to the fact that we need more experimental data and better databases for wider applications and bigger impact. With flat or dwindling research support in the area, we need to take a hard look at the speed of experimentation and assessment. Experimentally, the diffusion triple/multiple approach is a good start. This highly efficient technique can provide crucial experimental data (phase diagrams) as input for quality CALPHAD assessments. At the same time, the CALPHAD community needs to develop faster, more efficient assessment techniques. Assessments of complex systems are currently too time-consuming, and the quality depends too much on the experience and patience of the individuals who are performing the assessments. We can learn a lot from the Human Genome Project—they have overcome many more challenges than what we are facing for CALPHAD assessments. It is also important to develop better and more efficient ways to measure thermodynamic quantities (heat of formation, activity, specific heat, etc.). As mentioned in previous editorials by other associate editors, only a few centers in the world are left that are still performing thermodynamic measurements. The funding situation probably will not get much better any time soon. With this constraint, it makes sense to look at alternative ways to speed up measurements of thermodynamic quantities without sacrificing the quality of the data. This argument probably sounds crazy to some people, but a lot of progress has been made to make crazy ideas work in other fields, why not in thermodynamics?

It is also imperative to develop automated software to quickly extract diffusion coefficients from binary diffusion profiles that have multiple phases—a situation one would encounter far more often than the ideal completely soluble systems. Along with high-efficiency diffusion multiples, this will accelerate the construction of diffusivity databases.

In the last few years, density functional theory (DFT) calculations have started to penetrate our laboratories. DFT is used to calculate: the heat of formation (at zero Kelvin), phonon dispersion (thus estimation of the specific heat), elastic modulus, electronic density of state, and other parameters when experimental data are not available. The accuracy of such calculations is surprisingly better than expected (perhaps our expectation of first-principles calculations is too low). More calculations are

being performed to take advantage of DFT. I anticipate that the amount of DFT calculations will match or even surpass that of the CALPHAD-type calculations in the near future. These two activities are not mutually exclusive. The DFT calculations can serve as an input to CALPHAD assessments. It seems important to perform a thorough benchmark study of the accuracy of DFT calculations in predicting the heat of formation and other properties. If adequate accuracy is attained, DFT may provide some critically needed best estimates of data for thermodynamic and kinetic databases.

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