Editorial

JPEDAV 29:389
DOI: 10.1007/s11669-008-9417-6
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This summer I attended the 2008 Calphad conference in Finland. While listening to the meeting presentations I was reminded of what my centenarian father had once said. It was that "one test is worth a thousand computer predictions." His saying is a variation of the well known phrase "one test is worth a thousand expert opinions" and it was his reply to my claim that some day people would design heat treatments on a computer.

Today it is universally recognized that both computer software and databases must be validated by comparing the results with experimental tests before they can be used with confidence. However, the question often remains as to what type of tests and how many tests must be performed before they are adequately "validated." Consider a computer program designed to predict the heat treating time and temperature required to solutionize an alloy. A few trials comparing computer predictions with experimental tests on alloys with different initial microstructures receiving a variety of heat treatment schedules would give a quantitative account of the program's accuracy. This would allow for temperature and solutionizing times to be selected that would take into account expected variations in alloy compositions and heat treatments as well as uncertainty in the computer predictions. However, to obtain greater accuracy in the predictions or to validate the program for a wider range of alloys, one would have to probe deeper into the program predictions.

It was apparent from the Calphad talks that over the last decade important advances have been made in the ability to predict thermodynamic and kinetic properties using first principle calculation programs like VASP (Vienna Ab-initio Simulation Package). In some cases the agreement reported at the meeting between predicted and experimental values were impressive, even within experimental error. However, validation of the solutionizing program would have to go beyond fundamental thermodynamic and kinetic properties like heats of formation and atomic mobilities. Critical parameters in the kinetic equations for solutionizing would have to be predicted correctly. For example, an accurate description of the solvus temperature and its composition variation with temperature would be critical for making accurate solutionizing predictions. As a result, it may be necessary to design special databases which sacrifice the accuracy of less important phase boundaries in favor of phase boundaries concentrations that appear in the models. Also, mutual diffusivities are critical properties in solutionizing models. Today these are calculated from mobility and thermodynamic databases. At present the methods of validating multicomponent diffusivities are debated. A question asked is "can an n-component diffusivity be validated with a single diffusion couple or does it require more?"

There was talk at the Calphad meeting of universities that had closed their experimental laboratories and were now working exclusively with computers. Perhaps that is not a problem when universities team with experimentalists at other institutions, but students may not learn the lessons of hands-on research that teach which experimental data to trust and which to question. It is possible that the day will come when computer predictions are sufficiently accurate that experiments are no longer needed. However for now, one test may still be worth more than a thousand computer simulations which have not been validated.

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