

Editorial



I realize that I may be “preaching to the converted,” but there is little doubt that one of the major success stories in the field of phase equilibria in recent times is the advent and continuing progress in phase diagram modeling, or to use the more often used term, the *Calphad* technique. Since the early theories of Van Laar and the seminal work of Larry Kaufman in the 1960s, computational thermodynamics has always promised to set materials designers free from the laboratory, enabling hours of tedious experimentation to be replaced by a few keystrokes on a computer keyboard. There has been a steady shift in materials research, from experimentation to computation—it is far cheaper to buy a PC and some software than to buy a piece of sophisticated experimental apparatus. The modeling is becoming more complex; new exciting techniques, such as ab initio, phase field modeling and molecular dynamics, provide an ever-expanding tool box for the materials designer. But of course, experimentation is still a very important aspect to modeling. For those outside the field, this may come as a surprise, particularly in relation to *Calphad* modeling, where as we know, experimental observation is key to the derivation of parameters for the thermodynamic descriptions of the different phases.

In some ways, the success of computational thermodynamics has been at the expense of experimentation. This is particularly true with respect to experimental thermodynamics where there is a feeling that this is a field under considerable threat. For instance, high-temperature calorimetry is invaluable for successful *Calphad* modeling, but it is also very expensive when compared with the computational techniques it serves. It can take several weeks to produce a single set of data for the enthalpies of mixing of a series of liquid alloys, for example. Acquiring funding for this work, then, becomes increasingly difficult—where is the “wow-factor” for a funding body desperately trying to apportion their meager research budgets? With dwindling funding comes dwindling facilities. As many of our distinguished colleagues in the field of experimental thermodynamics retire from the “white-heat” of research, there are fewer ready to take their place. Equipment becomes idle and eventually discarded into the scrap bin.

We need to take a stand now, as a community, or we run the risk of losing this resource forever. It should be straightforward for those of us involved in experimental thermodynamics to create a global network of laboratories or researchers that have this valuable expertise: a sort of a “virtual laboratory” to enable the sharing of knowledge and experience. The first thing to address as the network is one of training. Finding funds for the exchange of postgraduate students, for example, should be relatively easy, particularly in Europe where there are many EU funding schemes for the mobility of young researchers. But we have to rely on our friends who are actively involved in modeling. We need to make sure that we have strong links with these research teams and persuade them to include us in their research programs. But maybe the biggest challenge is to persuade our colleagues in other fields of materials science that we are still relevant and that we make a valuable contribution to materials research. It is up to us; we have to take action now.

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