Editorial

Over the last few years we have witnessed significant interdisciplinary activity, mostly between the condensed matter physics and the materials science and engineering communities, directed at the computation of phase diagrams. As it is often the case with new joint endeavors, there is at present a great deal of enthusiasm in testing each other's techniques, which is, by and large, fueled by the initial fascination with the capabilities of the other side. The process, however exciting, inevitably leads to some degree of confusion. Old ideas are rediscovered, new terminology for well-known phenomena created, and most threatening for the tree population of the world, a great many unnecessary papers are submitted to scientific journals resulting, among other things, in additional work for editors everywhere. However, unless you are a tree, it can be easily argued that the long-term benefits of these cross-disciplinary activities far outweigh their shortcomings. In any event, this level of activity has convinced me that the phase equilibrium community, including the group involved in the computation of phase diagrams, is alive and doing well.

There are, to be sure, some serious difficulties afflicting the discipline. Leading among these is the apparent lack of interest of young scientists in experimental and systematic studies of equilibrium phase diagrams. This particular problem needs to be addressed by the professional societies, the industrial and academic communities, and ultimately, our funding agencies. Perhaps the subject should be addressed editorially in our *Journal*, but, if so, it will be done some other time. Right now I am quite pleased with the flurry of activity in the computational side of the business.

Although I am strongly biased, I would opine that the ability to compute a phase diagram, embodying precious information that unlocks the potential usefulness of most materials systems, is almost irresistible to any materials engineer, no matter how amateurish he or she may be. After all, we're introduced to the ubiquitous phase diagrams very early in our careers, never being truly able to break away from the relationship. For scientists, the realization of abstract concepts into a map of macroscopic properties, a process that is bridged by an almost unimaginable number of computations, is, likewise, a most rewarding experience. Thus, I would say the key lies in the fact that the number of scientists and engineers taking up the challenge must grow at a pace closely matching that at which theoretical and computational capabilities become available. We must, however, further stimulate the interest of young scientists and engineers in order to ensure the flux of new talent so crucial to the future well-being of the discipline.

This brings me to the point of this editorial. Those of us involved in the computation of phase diagrams have the responsibility to educate, not only the younger generation, but also the community at large as to what it really means to "compute" a phase diagram. In particular we should be able to articulate clearly what can and, more importantly, cannot be done at the present time. To the uninitiated, a cursory look at the phase diagram literature over the last few years may lead to the erroneous conclusion that phase diagram computation is, if not trivial, a fairly closed scientific problem. He or she may not be able to do it, but so and so certainly can; and in fact, a relatively modest expenditure will bring the capability to "compute" a phase diagram to his or her desk-top. In my opinion, this not only misrepresents the current state of affairs, but it also tends to turn away from the discipline our brightest candidates. The fact remains that, despite the significant advances of the last few years, each and every one of the techniques employed in phase diagram computations are limited in application and scope. More importantly, the limitations are, in all cases, serious and will require new approaches, new concepts, new algorithms and especially new talent. When it comes to the computation of phase diagrams, the situation is apparently not much different now than it was in 1929 when P.A.M. Dirac expressed his rather optimistic and superbly confident views regarding his celebrated equation: "The underlying physical laws for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known . . . and the difficulty is only that the application of these laws are much too complicated to be soluble."

As the field matures and computational materials science and engineering begins to gain acceptance as a predictive tool, we should keep reminding ourselves that closing the gap between expectations and reality will require our best effort and talent. For those involved, the rewards will be, in all likelihood, significant. Let us make sure to carry both messages to the younger generation.

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