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Editorial

The position of editor of this journal offers the opportunity to observe the developing trends in our area of interest. What I see is the Calphad technique for calculating equilibrium phase diagrams reaching maturity and being used as a tool for solving practical problems. Since many materials are used in metastable states, we are seeing the early stages of including diffusion data into the calculations in order to choose processing paths to reach such metastable states. There is plenty of room for further development in this area. The bugaboo of all computational activity is the lack of reliability of input data. Obviously, direct experimental measurements should produce the most reliable data. However, time and money are two factors that mitigate against the use of this approach for every materials system that might be of interest. Thus, estimation procedures for generating usable values for thermodynamic functions are needed for calculating equilibrium diagrams and for generating diffusivity values for calculations aimed at defining processing paths. Kubashevski's fifth edition of *Metallurgical Thermodynamics* has a chapter devoted to estimation procedures and is the best encompassing treatment that I have found, but results are not guaranteed and are not a panacea. Theorists could be a big help by devoting some thought and effort toward this problem of estimation.

A second direction of development of computation has to do with the prediction of the physical properties of the phases that are predicted by a Calphad calculation. Of course these will be the structure-insensitive properties such as the elastic properties rather than structure-sensitive properties such as electrical resistivity. For instance, it is well known that the bulk modulus (reciprocal compressibility) is primarily an atomic property, so to a first approximation the bulk modulus of an intermediate phase will be the sum of the bulk moduli of the constituent elements weighted by the mole fractions of the constituent elements.

This can readily be shown by writing the bulk modulus in the form $-V(\delta^2 E/\delta V^2)_T$ where V is the volume, E is the internal energy, and T is the temperature. Then by plotting the cohesive energy curves (E vs. V) for an average of the uncombined elements and the combination in the form of the intermediate phase, one expects a small downward ΔE and a small contraction ΔV associated with the formation of the intermediate phase from the elements. One can then argue that the small displacement of the minimum between the two curves is unlikely to have much effect on the curvature, so the bulk modulus for the intermediate phase should be well approximated as the arithmetic average of the elemental bulk moduli. Then for a randomly oriented polycrystalline aggregate, one needs an estimate of only one other elastic parameter because the combination of any two elastic parameters will define any other elastic parameter that may be desired. For example, for metallic materials, experimental data have shown that Poisson's ratio in the vast majority of cases falls in the range 0.3-0.35. Combination of the bulk modulus and Poisson's ratio can then produce an expected range of values for Young's modulus, shear modulus, and so forth.

The foregoing two new directions of development are quite promising and are quite likely to produce worthwhile extensions of the Calphad calculations. However, the most exciting things that an editor sees are the papers that come in with new ideas. Some of these are, of course, blatantly wrong. For example, I once received a manuscript wherein the author thought that he had proven the validity of the inverse square law for electrostatic force. What he missed was that in LaGrangian mechanics, Hamiltonian mechanics, or quantum mechanics the form of the potential energy defines the form of the force since $F = -\delta V/\delta r$. Thus writing the Coulomb potential energy as $V = Ze^2/r$ guarantees that the force will be Ze^2/r^2. On the other hand, papers that come in with really new ideas are intriguing. As an example, Nirupam Chakrabarti has been cross-fertilizing with the life sciences by treating phases with a genetic algorithm. I don't know how far this will go, but it is definitely in a new direction. Initial results are encouraging, but it remains for the future to reveal its true value. In any case, if any of you have some "way out" ideas, I encourage you to submit them for consideration. History indicates that major developments seem to occur in quantum leaps.

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