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Editorial

A Second Opportunity for Old ''Friends''?

Today's omnipresence of nanotechnology, either for its dazzling advances and outstanding promise in all possible paths of humanity, or for its uncertainties and potential threat often colored in scenarios akin to Mary Shelley's central character, compels the scientific community to rethink what, up to now, has been accepted as *commonplace knowledge*.

The manipulation of matter at scales of less than one billionth of a meter presents a major challenge, as, at near-atomic level, the bulk optical, electrical, magnetic, and other macrocharacteristics of a material lose their meaning. The multiphysics interplay becomes critical, and computations based on first principles, such as molecular dynamics simulation, are often restricted to a few hundred atoms due to limitations related to computer power and software development. Other shortcomings are often linked to the numerical tool itself; for instance, the molecular dynamic simulation yields results less than satisfactory when applied to high-temperature conditions and/or multicomponent situations. Therefore, most likely as an intermediate solution and as a transition in knowledge and resources, it is suggested that often mesoscopic scale methodologies with moderate modeling are an acceptable, if not fully adequate, approach. A case in point is the situation that I presented in one of the keynote lectures at the 13th International Heat Transfer Conference (2006) dealing with a transient heat conduction process in thin (nanoscale) films, where my ''trusted'' Fourier Law that served me well for more than 20 years is no longer valid; however, a ballistic-diffusive model incorporating the required physics and combined with a meshless particle-based simulation technique yielded surprisingly good results. Similarly, the materials community seems to be finding innovative ways to compromise with new situations.

Understanding the phase equilibrium of nanometer-sized particles, which is markedly different from that of the corresponding materials, is a requirement for the establishment of phase diagrams of nanometer-sized alloy systems. These diagrams are an essential concept in metallurgy-they are equilibrated at a constant temperature and display the crystalline phases with their respective compositions, therefore providing the required information to facilitate the use of these particles in industrial applications, such as nanoelectronics. Several thermodynamic models have been proposed to examine the effect of the particle size on the phase stability of pure metals, especially on the solid-liquid phase transformation; however, these models have limited applicability because they primarily address single components. Moreover, nanophase equilibrium is metastable in nature and its measurement presents major challenges; however recent advances in transmission-electron microscopy lend promise to this methodology.

For bulk materials, the CALPHAD (CALculation PHase Diagram) method with its extensive database of thermodynamics and physical properties has reached its maturity and has been widely used in the calculation of phase stability of not only pure metals but also alloys. Recently published work indicates the CALPHAD method can be extended from bulk to nanometer-sized systems if the finite size effect is taken into consideration. This is a fascinating finding, although it is doubtful whether the method can be applied to predict submesoscopic phase stability, because of the potential dominance of the atomic interaction energy. It can be argued that appropriate correction measures may be modeled to extend the method's applicability-an exercise that may prove itself to be of limited value, if at all viable! In any case it is a *comforting* thought that the CALPHAD method with appropriate adjustments can be used beyond its expected applicability range. Is this the right step, although small, toward the goal of continuous nanophase diagrams along with combinatorial synthesis and screening? I do not know, but, for sure, time will tell!

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