



In his editorial in the February issue of this journal, Jack Smith referred to the remarkable growth and development of computer programs and thermodynamic databases that have occurred over the last 30 years in the phase equilibria calculation field. These developments, comprehensively recorded by Nigel Saunders and Peter Miodownik in their 1998 book [1998Sau], have resulted in powerful thermodynamics software and databases becoming readily available to potential users from various groups, such as FACTSAGE, MTDATA, Pandat, SGTE, Thermo-Calc, and Thermotech.

Despite these advances, it would appear that the teaching of thermodynamics and phase equilibria in Materials Science and Engineering degree courses is receiving less attention and emphasis than was previously the case. While the importance of thermodynamics as core material in such courses is widely recognized, the amount of time spent allocated to students to study the topic is apparently decreasing. This change in emphasis can be attributed to several factors, including the competing interests of academics, the ever-widening types of materials receiving attention. In his classic 1967 textbook [1967Cot], Sir Alan Cottrell said “Thermodynamics, the science of energy, is undoubtedly the most important branch of general science used in metallurgy,” and Robert DeHoff in 1993 [1993Deh] wrote “The practical everyday encounters with the question, ‘What determines how matter behaves?’ are best handled with phenomenological thermodynamics.” Clearly, a basic knowledge and understanding of thermodynamics and its application is an essential feature of a Materials Science education. However, it is also widely accepted that students find thermodynamics difficult to understand when first encountered—elegantly summarized by David Gaskell [1995Gas]: “Thermodynamics tends to be a confusing subject to the beginning student.” An obvious question to ask therefore is how and to what extent can recent developments in computational thermodynamics and access to powerful software and databases be used in teaching and in helping students understand this topic.

Traditional thermodynamics courses, now regarded as old-fashioned, consisted of statements of the laws of thermodynamics leading to the state functions, U , H , S , G , F plus derivation of equations and applications to practical problems. In many cases calculations were idealized/simplified due to their complexity. With this approach, many students become disillusioned due to the bewilderingly large number of equations and proofs involved. To overcome this, various types of diagrams were introduced for easier use and clarity—Ellingham Diagrams, Pourbaix Diagrams, Predominance Area Diagrams, Kellogg Diagrams, Schaeffler Diagrams, and so forth. Such diagrams enable conclusions based on thermodynamics to be made by inspection instead of by numerical calculation. With modern thermodynamics software, calculations on complex systems can be performed in an instant, provided the required Gibbs energy data are available.

The next question to ask is “at what stage should students be taught to use thermodynamics software?” There are many advantages in doing this at quite an early stage. For example, instant calculation and plotting of standard enthalpies, entropies, and Gibbs energies of reaction as a function of temperature focuses on the reaction itself. More time can then be spent on examining the conditions and feasibility of reaction, processing conditions, and so forth, rather than spending the time on lengthy numerical calculation. Using Gibbs energy minimization programs, one can immediately see which reaction is favored for a given set of conditions.

Gibbs energy software is particularly useful for teaching the thermodynamic basis of phase diagrams. With binary systems, molar Gibbs energy versus temperature versus composition diagrams for liquid and solid phases can be displayed, and their relation to the phase diagram, through the common tangent construction, can be seen by taking isothermal sections. This can be done for real systems selected to illustrate different types of behavior. The changes in shape of Gibbs energy surfaces with variation in interaction coefficients can be seen together with their effects on the phase diagram. The occurrence of miscibility gaps, eutectics, peritectics, and so forth, through interaction coefficients can be illustrated. Equilibrium and Scheil solidification, coring, and segregation effects can be demonstrated by calculation. Being able to select and display isothermal and isoplethal sections, liquidus projections, and phase fractions-temperature diagrams helps in the understanding of ternary phase diagrams. The latter illustrate microstructural development on equilibrium and non-equilibrium cooling of selected compositions from liquid phase. The different types of ternary phase reactions—eutectic, peritectic, and transition peritectics—can all be demonstrated.

Teaching material based on the above ideas will be available for use with the MTDATA thermodynamics software system produced by the National Physical Laboratory. It is envisaged that there will be three courses: Introductory Thermodynamics, Thermodynamics of Phase Equilibria, and Advanced Applications. Teaching material in the form of lecture notes and tutorial examples including a limited thermodynamics database will be available. Anyone wanting more information about this project or wishing to make suggestions concerning material to be included should contact Fred Hayes or John Gisby. Anyone wishing to contribute to this project is most welcome.

References

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