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Editorial

With this issue, the name of this Journal becomes *Journal of Phase Equilibria and Diffusion.* This name change was made to keep abreast of the changes that are occurring in our area of interest. In the calculation of phase equilibria, there has been a remarkable growth and development of programs and databases since the publication of Larry Kaufman's book with Nessor, *Calculation of Phase Diagrams*, in 1970. One might categorize present-day programs as second-generation programs, and they are in the early stages of incorporating both kinetic data through utilization of diffusion data and estimation of physical properties of the phases of a selected phase diagram. The emphasis on calculations in these statements is not meant to denigrate experiment nor theory, and the Journal will continue to publish articles in those areas with full recognition that calculated results mirror the quality of the input data. Certainly experimental data tempered by theory provides that input. This tempering can be seen by an analogy with crystal structure determination. In determining positional parameters for the crystal loci of the atoms in a structure, the crystallographer prefers data for 10 or more diffraction intensities per adjustable parameter because of the limited precision of intensity measurements. In assessing phase equilibria by the Calphad method, the assessor considers all available experimental data concerning the thermodynamics and phase equilibria for the system of interest. The assessor then fuses all data to find a mathematical "best fit" for describing the phase equilibria of the system. Today the field has progressed to a stage in which a large fraction of the economically important binary systems have been assessed and progress is being made on ternary and higher order systems. The goal is to maintain consistency among the assessments so that simpler systems can be combined for the prediction of more complicated systems.

The majority of present day Calphad-type calculations are assessments of equilibrium diagrams, and, though such calculations are a necessary first step, a fact of life is that a very large fraction of the materials of commerce and industry are used in non-equilibrium states. Thus, the next step in the calculating procedure is to incorporate the kinetic factors that control the distribution of the phases that should be present after a given set of processing steps. Rather obviously, diffusion is the major rate limiting factor in most solids, so the incorporation of diffusion data into the calculating process should be very useful in predicting ways of achieving desirable non-equilibrium states. Ideally, if an exact thermodynamic description of a system were available, one could predict the paths by which phase distributions would develop by maximizing the time rate of entropy production. In essence, just as a ball will roll in the direction of the steepest elevation gradient, phases will develop along the steepest enthalpy gradient. Unfortunately, Utopia is a dream and thermodynamic descriptions of such precision are not currently available. Progress will be made in incremental steps toward the ideal. It is encouraging that the early steps toward incorporating diffusion data into calculations are being taken with programs such as that now being developed by Sundman and coworkers in Sweden. This Journal plans to encourage the incorporation of kinetic factors for predicting phase distributions by publishing pertinent diffusion articles, compilations, etc. Certainly the original scope statement describing the goals of the Journal included a statement that articles related to "facilitating the achievement of or mitigating against the achievement of phase equilibrium" would be considered acceptable, but a negligible number of such articles were submitted. Hopefully, the addition of "Diffusion" to the Journal's title will emphasize the interest in this area.

Finally, it is generally recognized that the ultimate goal of the materials specialist is the *a priori* design of materials for specific applications. For this, it will be necessary to add to a description of the phase distribution an estimate of the properties of a material. Again, work aimed in that direction is developing, e.g., the work of Miodownik and Saunders in Britain. Therefore, articles on materials properties as related to phase compositon and distribution are certainly of interest and their submission is encouraged.

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Editor
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