

Editorial



The coupling of thermodynamics and phase equilibria is now a successfully established method, and credit has to be given to Larry Kaufman, who first focused these activities in the CALPHAD circle in the mid-1970s. Sophisticated models for complex solution phases and carefully tested software for the calculation of multicomponent phase equilibria have been developed since then.

Today the next level of applying the thermodynamics of alloys is under way in process development and reactor modeling. The key advantage of this approach is that it minimizes the number of process model parameters by exploiting the knowledge of the thermodynamics of the materials.

Applications at such a high level or generally in multicomponent systems must be based on the strong foundation of a standardized thermodynamic database. A substantial effort has to be devoted to the generation of these data by assessment of individual binary or higher order systems. It is of utmost importance to prepare these data in a compatible manner in order to make them useful for multicomponent applications. The recent progress on this route has been clearly pointed out by Ansara in the February 1994 issue on this page.

The extension of the growing databases (steels, light metals, superalloys, semiconductors) and the expansion to new areas (ceramics, ceramic-metal interactions) requires a coordinated effort and a cooperation between many research groups. How should this cooperation be organized, beyond joint research projects among individual groups?

Let me envision an *International Center for Thermodynamic Data of Alloys (ICTDA)*. The two main objectives of an ICTDA could be 1) the coordination of research input, and 2) the interface to potential applicants of the data.

The coordination of research input for assessment could initially comprise information on compatible models and lower-order data and eventually the management of data transfer for assessments (interface to assessors). The interface to the "user" world may work in public relations and in seminars on user applications, and eventually a coordinated marketing of the databases may be found useful.

Such an ICTDA could be organized as an open cooperative of interested research groups, including at least all of the major groups active in the field.

We cannot and should not simply copy the structure of mature organizations like the *International Center for Diffraction Data*: however, this example could give a reasonable inspiration for a future development. The specific features of our field, the thermodynamics and phase equilibria of alloys, have to be accounted for in our case.

This sketch of some of my personal ideas and views on this topic may stimulate a discussion and I would appreciate receiving comments or other views. I am convinced that we have to be concerned about the link between high quality scientific results and their application and usefulness for a greater scientific and engineering community.

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