



ICAMS special lecture

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CALPHAD databases for commercial alloys and applications

The Calphad method has been identified in a recent report by the US National Academies as one of the cornerstones of Integrated Computational Materials Engineering (ICME). The strengths of the Calphad method are that it allows obtaining information on phase equilibria, thermochemical and other properties of multicomponent materials and can be coupled with other computational methods for the simulation of materials processes.

Core of the Calphad method are thermodynamic databases. In these databases the Gibbs energy of each phase is described as function of concentration, temperature and, if needed, pressure. Thermodynamic databases have been constructed at the Metallurgy Division of NIST for the calculation of superalloys, solder alloys, light weight hydrogen storage materials and the construction of databases for several other materials is in progress. In addition to the thermodynamic databases the Calphad method has been applied to the construction of diffusion mobility databases for the simulation of diffusion processes.

In this presentation the strategy for the construction of Calphad databases will be briefly illustrated and examples from the application for a variety of commercial materials will be presented.