The modelling of phase diagrams and thermodynamic properties in multicomponent systems – crucial tool for the development of new materials

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Abstract:

The knowledge of the alloy thermodynamics and phase equilibria involved in the multicomponent alloy system is crucial in the design of new advanced materials. Traditional methods of experimentation for the choice of appropriate compositions are both costly in terms of time and money and are clearly no longer applicable owing to the increasing complexity of materials involved.

A semi-empirical approach, referred to as the CALPHAD method is widely used for the modelling of thermodynamic properties and for the calculation of phase diagrams in such systems both by scientists and in engineering practice. Its main feature is the combination of experimental observation and theoretical modelling and it can significantly decrease the amount of necessary experimental work.

Over the past 30 years, the construction of thermodynamic databases for the calculation of complex phase equilibria by the CALPHAD method has become more important. Along with appropriate software, it is possible to predict the stable phase equilibria in multicomponent alloy systems as a function of temperature, pressure and composition. This has obvious implications not only by full understanding of the underlying chemistry of an alloy system, but also by being able to predict likely scenarios whilst kinetic constraints may mask the true nature of the equilibrium. The basic principles of database development will be described in the lecture, particular attention will be given to the creation of proper thermodynamic assessments of simpler systems and their exploitation for the creation of consistent thermodynamic database with some practical examples about ternary Al-Si-V system.