PRECIPITATION SIMULATION ENABLED BY THERMODYNAMIC AND KINETIC DATABASES

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Computational tools, such as Thermo-Calc and Dictra, have been developed for several decades and are now routinely utilized in materials research in both academia and industry. Their success is rooted in their capability to provide indispensable phase equilibrium and phase transformation information for simulating microstructural evolution in commercial multicomponent alloys, which was made possible by the adoption of the CALPHAD methodology where the Gibbs energy or atomic mobility of each phase can be modelled hierarchically from low-order systems to high-order ones, and model parameters can be evaluated by considering both ab-initio and various experimental data. A collection of sets of optimal thermodynamic or atomic mobility model parameters for all phases in binary and ternary systems forms a CALPHAD thermodynamic or kinetic database. Over the years, databases containing up to 35 elements for various alloys, such as steels, light metal alloys, Ni-based superalloys, etc., have been developed. By using Thermo-Calc and Dictra together with such databases, phase equilibria, driving forces, and diffusivities necessary for simulating diffusion-controlled phase transformation in multicomponent systems can be calculated without resorting to ad hoc approaches that require fitting parameters varying from one alloy to another, and therefore diffusion-controlled microstructural evolution in multicomponent systems can be predicted.

Precipitation gives many alloys their desired strength and toughness. A precipitate microstructure consists of dispersed second phase particles embedded in a solution phase matrix and is a product of diffusion-controlled solid state phase transformation fully governed by system (bulk and interface) thermodynamics and kinetics. With the advance of CALPHAD and widely available databases, computer simulation of the precipitate microstructure in multicomponent alloys is readily feasible on the basis of Langer-Schwartz theory and Kampmann-Wagner numerical (KWN) method. In this talk, we present TC-PRISMA, now fully integrated into Thermo-Calc as the Precipitation Simulation module, that extends the Thermo-Calc and Dictra approach with additional thermophysical property data to simulate the concurrent nucleation, growth, and coarsening of second phase particles. Nucleation and growth rate models implemented in the software will be elaborated. Engineering applications of precipitation modelling and challenges will also be shown and discussed as well.