Calphad-based Computational Precipitation Kinetics

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Precipitate microstructure is probably the most important and most studied materials microstructure. Precipitation hardening has been employed for more than one century to improve the strength and toughness of various high performance alloys. With the advance of computational thermodynamics, computer simulation of precipitation kinetics in industry relevant alloys is now possible on the basis of Langer-Schwartz theory and Kampmann-Wagner numerical (KWN) method. This approach provides materials scientists and engineers an efficient and cost-effective way to tailor precipitate microstructures for maximizing the strengthening effect via the optimization of alloy composition and heat treatment schedule.

Computational tools, such as Thermo-Calc and Dictra, have developed for several decades and are now routinely utilized in materials research in both academia and industry. Their success relies on their capability to provide fundamental phase equilibrium and phase transformation information in multicomponent materials, which is possible due to the adopted CALPHAD methodology where free 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.

In this presentation, we introduce TC-PRISMA, a recently developed software package that extends the Thermo-Calc and Dictra approach with additional interface 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 presented. Application examples will be demonstrated with focus on simulating precipitate microstructure evolution in Nickel-base superalloys under arbitrary heat treatment conditions. In particular, the effects of alloy chemistry and cooling rates on the formation of multimodal microstructures are closely examined in order to understand the underlying thermodynamics and kinetics. Practical issues that are critical to the accuracy and applicability of the current simulation technique will also be discussed.