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Precipitation modeling of multi-component commercial alloys

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ABSTRACT

In this presentation, we propose a practical and scientifically sound modeling approach for precipitation simulation of multi-component alloys under the framework of the Integrated Computational Materials Engineering (ICME). In this approach, the Calphad method is adopted to provide the necessary mobility data and thermodynamic properties. The modeling of microstructural evolution is based on the KWN approach, which considers the concurrent nucleation, growth, and coarsening of multi-phase and multi-component alloys. Consequently, the mechanical properties, such as yield strength and hardness, are estimated from the simulated microstructure. The present study shows the promise of using an integrated modeling framework to comprehend the relationship between the chemistry/processing – structure – properties. This will be demonstrated by the simulation of precipitation hardening behavior of a number of multi-component Ni-based superalloys as well as a series of Al alloys.

KEYWORDS: precipitation modeling, KWN, multi-component alloys, ICME, calphad, yield strength