MM 32 Invited Talk Chen (SYMM)

Time: Thursday 14:00–14:30 Room: IFW A

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From First-Principles Calculations to Precipitate Microstructure Evolution in Alloys — •Long-Qing Chen — Department of Materials Science and Engineering, Penn State University, University Park, PA 16802, USA

Precipitation reaction is one of the most important processes utilized to strengthen various engineering alloys, and the control of precipitate microstructures is the key to achieve desired mechanical properties. Various computational models have been applied to studying the thermodynamics and kinetics of precipitation reactions at different length and time scales. Examples include first-principles calculations of structural and thermodynamic properties of precipitate phases, phenomenological modeling of thermodynamics and phase equilibria in alloys with precipitates, and mesoscale models for predicting precipitate microstructure evolution. This presentation will discuss a number of approaches of integrating these different models through information passing at different scales with the objective to understand the relationships among the chemistry, microstructure and properties of materials. Examples of predicting the precipitate microstructure evolution in Al- and Ni-alloys will be presented.