From Microstructures to Predict Properties of Materials KE-GANG WANG, Florida Institute of Technology — Understanding the precise and fundamental manner in which materials structures (nanostructures or microstructures) and their evolution influences properties and service lifetimes of advanced materials profoundly impacts material design and today materials design plays an increasingly important rôle in many engineering applications. Linking structures to properties and predicting properties of materials is fundamental step for materials design. First, a framework of applications of multiscale modeling to property prediction of advanced materials will be briefly presented. As an example, a methodology will be shown to link micro-scale to the continuum scale, integrating microstructure modeling with the large Thermo-Calc$^{\circledR}$ database. This paradigm was successfully applied to the case of Fe-12Ni-6Mn maraging steel. Next, methodology for integrating first-principle calculation into simulations of microstructure evolution will be reviewed. Our methods are sufficiently reliable to permit control and fabrication of quantum-dots structures, nanocrystals, and particle-reinforced nanocomposites, as well as assist in the predictive behavior of macro-scale colloids, aerosols, and other soft matter systems.

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