The Role of Quantum Mechanics in “Virtual Aluminum Castings”

C. Wolverton
Ford Research Laboratories, Dearborn MI, USA
cwolvert@ford.com

Increasing demands to further reduce emissions and simultaneously improve fuel economy in automobiles has expanded the need for lightweight materials (such as Al, Mg, and their alloys). In order to optimize alloy design and processing conditions to quickly achieve Al-alloy castings with suitable mechanical properties, researchers at Ford Research Laboratory are developing the Virtual Aluminum Castings methodology: a suite of predictive computational tools that span length scales from atomistic to macroscopic to describe alloy microstructure, precipitation, solidification, and ultimately, mechanical properties. The role of first-principles atomistic computations in the Virtual Aluminum Castings methodology will be described. Because of their highly accurate and predictive nature, there is a growing desire to use these types of theoretical approaches to predict properties of new, experimentally unexplored, or difficult-to-synthesize solids. Application to problems of precipitation, thermal growth, and microstructure evolution during heat treatment has proved very fruitful. Combining these quantum-mechanical results with other modeling and experimental efforts, one can suggest heat treatments which optimize thermal stability and hardness of industrial alloys.