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**Understanding the Evolution of Microstructure: What is the Role of Molecular Dynamics?<sup>1</sup>**

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The microstructure of a material, as characterized for example by grain size, determines a wide range of materials properties such as strength, toughness, and corrosion resistance. Understanding how the microstructure influences properties and how to obtain a desired microstructure are some of the enduring central problems of materials science. This challenge is inherently multi-scale since the fundamental mechanisms by which microstructures change occur at the atomic scale while the network of interfaces is on a scale of microns and up. In this talk, the role of molecular dynamics (MD) simulations in understanding the evolution of microstructure will be examined. The successes and outstanding challenges of using MD simulations to determine the properties of grain boundaries, in particular free energy and mobility, will be described. Further, microstructures with nanoscale grains evolve in times accessible to MD simulation. The insights into grain growth and deformation that can be obtained from such simulations will be described.

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