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Opportunities for computational science in materials science

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Major computational challenges exist in the area of materials science. Examples include understanding processes far from equilibrium and the theory of nanostructured materials. The first topic includes the evolution of microstructure, fracture, friction and biological function. Being able to predict and control the microstructure developed during processing, for example, is critical to the determination of the properties of a system. This involves understanding the role of processing conditions in the nucleation and growth of the metastable phases involved in the microstructure selection. An understanding of this starting from an atomistic description poses a major challenge in computational science. One aspect of this involves determining the free energy landscape, including metastable and unstable states, for real systems

which are typically quite complex. Even “simple systems” such as those described by Lennard–Jones potential are not yet well understood.

The second topic involves understanding the formation of nanostructures in films, wires and dots. Such nanostructured materials typically are quenched in a metastable phase by the growth process. One can imagine forming an endless variety of such structures through different choices of materials and boundary conditions. The challenge here is to understand both the growth process as well as the relationship between the final structure and its material properties. Understanding these issues from a first principles atomistic description poses exciting opportunities to the computational science community.

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