Computational Materials Science – Applications at a National Laboratory

The development of computational models for the simulation and prediction of the structure, properties and behavior of heterogeneous materials is advancing our understanding of materials science and engineering at an increasing rate. In most cases, it requires the use of a variety of computational methods that span from an atomistic description of interactions to a continuum numerical modeling that include: first principles calculations, structural relaxations, lattice and molecular dynamics, and kinetic Monte Carlo, among others. This is particularly true at a National Laboratory, where research has applications in future energy production, engineering innovations, materials strength, and national security.

In this presentation I will show a set of examples of my research at LLNL that combine both, theoretical and computational modeling techniques including: a mesoscale particle-based model of colloidal suspensions that undergo electrophoretic motion, atomistic simulations of nucleation and growth of Cu from the melt, and phase transformation of Ti under extreme conditions where the structural transition from the hcp phase into the omega phase, a martensitic transformation, is investigated as a function of increasing shock strength.

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