Bridging the timescale gap between simulations and experiments using Accelerated Molecular Dynamics

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One of the major difficulty in using fully dynamical atomistic simulations like Molecular Dynamics to assist in the interpretation of time-resolved experiments is the very small range of timescales that are typically accessible (μs or less). This often limits direct comparison to extreme conditions of strain rates, temperatures, deposition rates, irradiation doses, etc. Over the last decade, Accelerated Molecular Dynamics methods that aim at bridging that gap were developed at LANL by Arthur Voter and collaborators. I will briefly review the basics of these methods and demonstrate their usefulness to investigate the kinetics of material's evolution. Drawing from our own research, I will discuss specific examples where the convergence of high-resolution time-resolved x-ray measurement and of modern simulations techniques would provide a unique opportunity to further the understanding of the dynamical behavior of materials out of equilibrium. Specifically, I will address the failure of materials under stress, both in slowly strained nanostructured systems, where current experiments cannot spatio-temporally resolve the processes leading to failure, and in shocked bulk materials, where the initial stages of nucleation and growth of defects is largely unknown, as well as the evolution of damage in irradiated materials, where the atomistic characteristics conferring radiation tolerance remain elusive.