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Atomistic studies of material dynamics: from petascale to exascale

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ABSTRACT

Computational materials science has provided great insight into the response of materials under extreme conditions that are difficult to probe experimentally. For example, shock-induced plasticity and phase transformation processes in single-crystal and nanocrystalline metals have been widely studied via large-scale molecular dynamics simulations, and many of these predictions are beginning to be tested at advanced fourth generation light sources such as Argonne's Advanced Photon Source and SLAC's Linac Coherent Light Source. I will give two examples from our work on the mechanical response of metals to shock loading: (i) copper and iron single crystals, probed via ultrafast in situ X-ray diffraction; and (ii) grain boundaries in copper, and deformation processes probed at an atomistic scale with post situ high-resolution TEM. I will then discuss outstanding challenges in modeling the response of materials to extreme mechanical and radiation environments, and our efforts to tackle these as part of the multiinstitutional, multidisciplinary Exascale Codesign Center for Materials in Extreme Environments (ExMatEx). As we look ahead from the current petascale (10–15 operations per second) era towards the exascale (10–18 operations per second) platforms expected to be deployed by the end of this decade, multiscale, or scale-bridging, techniques are particularly promising. ExMatEx is an effort to do this by initiating an early and extensive collaboration between computational materials scientists, computer scientists, and hardware manufacturers.