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Dynamic materials response at multiscales: Experiments and simulations[1]

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One of the grand challenges in materials physics is dynamic responses to impulsive loading, including shock waves, radiation, and pulsed fields, due to their highly transient nature and extremely complex microstructure effects. Dynamic responses, such as plasticity, damage, cavitation, phase changes, and chemical reactions, are inherently multiscale and heavily dependent on microstructure. One has to resort to a suite of tools, including experiments, modeling and simulations, and theory. However, the gaps in spatial or temporal scales between experiments and simulations are still wide, while cross-scale theories are still in early development. To this end, we exploit large-scale molecular dynamics simulations, electron microscopy, and ultrafast synchrotron X-ray imaging and scattering, to probe materials response at length scales ranging from lattice to micron, and time scales, from picosecond to second. For examples, simultaneous, high-speed, X-ray imaging (mesoscale strain-field mapping) and diffraction measurements along with macroscopic measurements have been achieved. Based on classical nucleation theory and large-scale molecular dynamics simulations, we demonstrate the equivalence between length and time scales for nucleation events, which provides a framework to bridge different scales. Certainly, advancing multiscale science requires sustained, concerted, experimental, modeling and theoretical efforts.

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