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Modeling, analysis and ultrafast imaging of lattice dynamics in core-shell bimetallic nanocrystals KIRAN SASIKUMAR, MATHEW CHERUKARA, Argonne Natl Lab, JESSE CLARK, None, THOMAS PETERKA, ROSS HARDER, SUBRAMANIAN SANKARANARAYANAN, Argonne Natl Lab — Energy transport via lattice vibrations play an important role in several applications such as heat dissipation in semiconductors, waste heat energy conversion via thermoelectric materials, and phase transitions in intensely heated nanofluids. Investigation of the temporal behavior of externally stimulated materials under severe thermal non-equilibrium conditions is, thus, crucial for energy research. Recently, advances have been made in experimental techniques to conduct time-dependent lattice dynamics measurements in nanomaterials. In particular, ultrafast laser pump and x-ray probe Bragg Coherent Diffraction Imaging (BCDI) has been used to directly image lattice distortions within nanocrystals. In particular, experiments on femtosecond laser heated bimetal (Au/Al) core-shell nanocrystals have revealed inhomogeneous effects in lattice breathing. Conventional theoretical models fail to explain the physics of the phenomena in such non-equilibrium environments, particularly in core-shell structures where interfacial effects can play an important role in phonon scattering. In this talk, we focus on multi-million-atom molecular dynamics (MD) simulations performed on core-shell bimetallic nanocrystals under the influence of extreme heat fluxes. We discuss how x-ray diffraction patterns are obtained from MD trajectories, which are directly compared with BCDI images to identify the origin of the inhomogeneous effects in lattice breathing.

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