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Simulating Picosecond X-ray Diffraction from Shocked Crystals using FFT Methods on MD Output GILES KIMMINAU, ANDREW HIGGINBOTHAM, WILLIAM MURPHY, JUSTIN WARK, University of Oxford, UK, JAMES HAWRELIAK, DAN KALANTAR, HECTOR LORENZANA, BRUCE REMINGTON, LLNL, NIGEL PARK, AWE, Aldermaston, UK — Multi-million atom non-equilibrium molecular dynamics (MD) simulations give significant insight into the transient processes that occur under shock compression. Pico-second X-ray diffraction enables the probing of materials on a timescale fast enough to test such effects. In order to simulate diffraction patterns, Fourier methods are required to gain a picture of reciprocal lattice space. We present here results of fast Fourier transforms of atomic coordinates of shocked crystals simulated by MD, and comment on the computing power required as a function of problem size. The relationship between reciprocal space and particular experimental geometries is discussed.

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