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Sub-Picosecond Dynamics of Displacement Cascades[1]

BENNETT LARSON, JON TISCHLER, ROGER STOLLER, YURI OSETSKIY, Oak Ridge National Laboratory, CHRISTIAN DAVID, Paul Scherrer Institute — Sub-picosecond x-ray pulses produced by the Linac Coherent Light Source (LCLS) now enable real time experimental measurements of atomic displacement cascade structure and dynamics on sub-picosecond time scales. Such measurements will make possible the first direct experimental test of molecular dynamics (MD) displacement cascade simulations. Here we will discuss the potential to use single, seeded, 100-fs LCLS hard x-ray pulses focused to ∼100 nm diameter by diamond-based Fresnel zone plate optics to make real-time diffuse scattering measurements on 50 keV Ar-ion-induced cascades in thin single-crystal samples. We will present x-ray Bragg diffuse scattering calculations based on ∼ 4M atom, 25 keV primary knock-on energy MD cascade simulations demonstrating that temporally-random, 100 fs LCLS x-ray pulse measurements of diffuse scattering near low index Bragg reflections can be time-ordered from sub-picoseconds to a few picoseconds. Time ordering is made possible in this regime by the distinct nature of diffuse scattering profiles as a function of time that are produced by shock-induced pressure waves according to MD cascade simulations in Fe. The expected results and the experimental challenges anticipated to perform such measurements will be discussed.

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