

Abstract Submitted  
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**Combined Hydrodynamic and Diffraction Simulations of Femtosecond X-Ray Scattering from Laser-Shocked Crystals** JUSTIN WARK, ANDREW HIGGINBOTHAM, University of Oxford, DESPINA MILATHIANAKI, LCLS, SLAC, ARIANNA GLEASON, Stanford University — We describe a simple hydrocode based on a two-step integration scheme that models the evolution of elastic and plastic strains in crystals subject to rapid laser-shock loading. By monitoring the elastic strains during plastic flow we track the rotation and spacing of lattice planes within the polycrystalline sample, and can thus predict the signal that would be produced by X-ray diffraction in a variety of experimental geometries. By employing a simple Taylor-Orowan dislocation model we simulate diffraction patterns from in a Debye-Scherrer geometry to track the orthogonal strain states within a laser-shocked sample. The yielding rate is approximately matched to those observed in multi-million atom MD simulations, allowing movies to be made of the diffraction images that would be seen in a real experimental geometry, and illustrating the pertinent experimental requirements, including target texture. Judicious choice of geometry allows clear demarcation of the initial elastic response of the target to be made from the subsequent plastic relaxation. We discuss the simulations in the context of the novel experimental capabilities that have recently become available with the advent of 4th generation light sources, which allow single-shot diffraction with sub-100-fs resolution.

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