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Simulation of Forward and Inverse X-ray Scattering From Shocked Materials JOHN BARBER, QUINN MARKSTEINER, CRIS BARNES, Los Alamos National Laboratory — The next generation of high-intensity, coherent light sources should generate sufficient brilliance to perform in-situ coherent x-ray diffraction imaging (CXDI) of shocked materials. In this work, we present beginning-to-end simulations of this process. This includes the calculation of the partially-coherent intensity profiles of self-amplified stimulated emission (SASE) xray free electron lasers (XFELs), as well as the use of simulated, shocked moleculardynamics-based samples to predict the evolution of the resulting diffraction patterns. In addition, we will explore the corresponding inverse problem by performing iterative phase retrieval to generate reconstructed images of the simulated sample. The development of these methods in the context of materials under extreme conditions should provide crucial insights into the design and capabilities of shocked in-situ imaging experiments.

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