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Simulation of X-ray Diffraction Patterns from Arbitrary Targets
JOHN BARBER, Los Alamos National Laboratory — I describe recent advances in simulation methods for the generation of X-ray diffraction patterns from an arbitrary sample. The sample consists of a set of N atomic positions, which in practice is most often generated via molecular dynamics simulation. Unlike some commercially-available diffraction software, the sample need not be crystalline: Any set of atomic coordinates may be considered. The methods used include fast Fourier transform techniques which yield $\mathrm{O}\left(\mathrm{N}\log\mathrm{N}\right)$ scaling, as opposed to the $\mathrm{O}\left(\mathrm{N}^2\right)$ scaling of a brute-force approach. This allows, for example, the simulation of in-situ experiments on the dynamically-changing diffraction pattern due to a shock front passing through a crystal, along with the attendant phase transitions. I will discuss several mathematical solutions and outstanding challenges to the problem of fast generation of such patterns from very large atomic coordinate data sets, and I will present various results in the form of diffraction patterns from some moderately-sized and large systems.

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