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Atomistic Simulations of High-intensity XFEL Pulses on Diffractive Imaging of Nano-sized Systems[1] PHAY HO, CHRISTOPHER KNIGHT, LINDA YOUNG, Argonne National Laboratory, MIKLOS TEGZE, GYULA FAIGEL, Institute for Solid State Physics and Optics of the Wigner Research Centre for Physics — We have developed a large-scale atomistic computational method based on a combined Monte Carlo and Molecular Dynamics (MC/MD) method to simulate XFEL-induced radiation damage dynamics of complex materials. The MD algorithm is used to propagate the trajectories of electrons, ions and atoms forward in time and the quantum nature of interactions with an XFEL pulse is accounted for by a MC method to calculate probabilities of electronic transitions. Our code has good scalability with MPI/OpenMP parallelization, and it has been run on Mira, a petascale system at the Argonne Leardership Computing Facility, with particle number >50 million. Using this code, we have examined the impact of high-intensity 8-keV XFEL pulses on the x-ray diffraction patterns of argon clusters. The obtained patterns show strong pulse parameter dependence, providing evidence of significant lattice rearrangement and diffuse scattering. Real-space electronic reconstruction was performed using phase retrieval methods. We found that the structure of the argon cluster can be recovered with atomic resolution even in the presence of considerable radiation damage.

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