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Atomistic Computational Model of Ultrafast Response of Complex Systems in Intense X-rays[1] PHAY HO, WEI JIANG, LINDA YOUNG, Argonne National Laboratory — We present a combined Monte-Carlo/Molecular-dynamics (MC/MD) computational model for treating ultrafast electronic damage processes and the subsequent structural distortion on complex systems exposed to femtosecond, high-intensity x-ray free-electrons laser pulses. Our first target systems are nickel nanoparticles since the range for self-seeded LCLS operation (7.1-9.5 keV) spans the nickel K-edge (8333 keV). Our MC/MD method includes the contribution of photoelectrons, Auger electrons, fluorescence photons and secondary electrons. It goes beyond the earlier particle approaches by tracking the electronic configuration of each charged particle throughout the x-ray pulse. With this new capability, we present the impact of both transient core-hole states and delocalized electrons, which may exist within, or within the proximity, of the nanoparticle, on the measured coherent x-ray diffraction pattern.

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