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Atomistic Computational Model of Radiation Damage of Nano-sized Systems in Intense X-ray Pulses[1] PHAY HO, WEI JIANG, KAR CHUN LAU, LINDA YOUNG, Argonne National Laboratory — We present a combined Monte-Carlo/molecular- dynamics (MC/MD) computational model that is suitable for monitoring the physics of intense, femtosecond XFEL pulses interacting with complex systems of various sizes, from nanometers to micrometers, and matters of various compositions. In this model, the occurrences of x-ray absorption, ionization, relaxation and electron-impact processes are treated by a MC method, and the subsequent dynamics of the all the electrons, ions and atoms are tracked using an MD method. Our model extends the previous MC/MD model [1] and provides new capabilities to probe the impacts of transient states on radiation damage dynamics. Recently, we have added LAMMPS as the driver of MD dynamics. This is a critical addition as now our code can run on Mira, a new petascale supercomputer with 786K core processors at the Argonne Leadership Computing Facility. Also, it can treat micron-sized systems with trillions of particles and both homogeneous and heterogeneous composition. Using our model, we examine the ionization dynamics of Argon clusters in an XFEL pulse as a function of particle sizes and pulse parameters, and we compare our results with the experimental data [2].

[1] Z. Jurek *et al.*, Eur. Phys. J. D **29**, 217 (2004).
[2] S. Schorb *et al.* PRL **108**, 233401 (2012).

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