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First Principles Simulation of the Dynamics of Warm Dense Matter during Femtosecond Laser Damage using a Particle-in-Cell Method with Pair-Potential Interactions and Direct Comparison to Experiment

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Understanding of the warm dense matter (WDM) state is of fundamental importance in the modeling of femtosecond laser damage because laser electron coupling and subsequent electron lattice coupling can rapidly increase the material temperature at the laser focal region to on the order of an eV, producing WDM not well described by standard liquid and solid equations of state. By modifying the particle-in-cell formalism designed for plasmas to include a pair-potential interaction model, we have created the first fundamental simulation method for modelling ultrashort pulse laser damage that can treat large scale (micron sized) damage morphology and resolves dynamics spanning over six orders of magnitude in time from the femtosecond to the nanosecond scale. We confirm the accuracy of our algorithm by comparing simulated crater profiles on copper against those produced from precision experiment and then show the dynamics of transient warm dense matter formation in aluminum. This material is based upon work supported by the Air Force Office of Scientific Research under award number FA9550-16-1-0069 and computing time from the Ohio Supercomputer Center.

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