Abstract Submitted
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Atomistic simulation of the ultrafast melting of gold: Benchmarking to experiments[1] JACOB MOLINA, THOMAS WHITE, University of Nevada, Reno — With the advent of ultrafast MeV electron diffraction, experiments are now able to probe the structure of matter on a nanometer scale. Such techniques have recently been used to observe the transition from heterogeneous to homogeneous melting in gold irradiation with an ultrafast optical laser pulse. On a picosecond timescale these systems form a complex non-equilibrium state of matter that cannot be fitted with a simple linear equilibration model. Due to the commensurate spatial and temporal scales between these experiments and classical molecular dynamics, such simulations provide an ideal test-bed where additional non-linear effects can be included. However, current simulations fail to match the experimental results due to over the simplification of the general properties and behavior of the electronic and atomic subsystems. We perform new simulations that improve on those in the literature by introducing a variable electron specific heat capacity, a more physically accurate potential, and the correct thin-film geometry. As a result of these improvements, our simulations better match experimental results and more accurately predict the transition between homogeneous and heterogeneous melting.

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