

# MULTISCALE MODELING AND SIMULATION OF LASER INTERACTION WITH METALS

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## ABSTRACT

The electron temperature dependent electron heat capacity, electron thermal conductivity and effective electron-phonon coupling factor are modeled and computed on the basis of ab initio quantum mechanics (QM) calculation. The obtained electron thermophysical parameters are implemented into energy equation of electron subsystem in two temperature model (TTM). Upon laser irradiation on metal, energy transfer from the electron subsystem to the lattice subsystem is modeled by including electron thermophysical parameters in molecular dynamics (MD) and TTM coupled simulation.

Phenomena, such as melting, layer-ablation, vaporization are found in the simulation results. In addition, bond hardening of femtosecond laser irradiated gold is observed. As the first work studying the laser interaction with metallic materials ranging from atomic scale to continuum scale, the successful construction of the QM-MD-TTM integrated simulation provides a general way that is accessible to other metals in laser heating. The simulation results highlight the promising application of the QM-MD-TTM integrated simulation. Obtained results from pure ab initio MD provide a better relation between microscopic processes and material response detected in experiments and serve for improved interpretation of experimental results on ultrafast laser-metal interactions. The results simulated and conclusion drawn will empower the multi-scale modeling of laser material interaction and be quite useful in helping to resolving the heat transfer and energy conversion problem during ultrashort laser processing of metals.