

Public Abstract

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In this dissertation, the electron temperature dependent electron density of states, Fermi-Dirac distribution, and electron-phonon spectral function are computed as prerequisites before achieving the electron heat capacity, electron thermal conductivity and effective electron-phonon coupling factor. On the basis of ab initio quantum mechanics (QM) calculation, the obtained electron heat capacity, electron thermal conductivity and effective electron-phonon coupling factor, 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.

After successful construction of the QM-MD-TTM integrated framework, (1) this dissertation uses the QM-MD-TTM integrated simulation to investigate the difference of melting behaviors of picosecond laser irradiated copper film simulated by using ab initio calculated electron heat capacity and experimental electron heat capacity. The results show that even though significant difference of electron temperature response between the QM-MD-TTM simulation and conventional MD-TTM coupled simulation by substituting electron heat capacity from experimental result, there is slight difference between the final melting depths of the laser irradiated films. (2) By combining ab initio quantum mechanics (QM) calculation and Drude model, electron temperature and lattice temperature dependent electron thermal conductivity is calculated and implemented into the QM-MD-TTM multiscale model of laser material interaction. Comparisons of the simulations implementing the electron thermal conductivity determined in this letter and utilizing an empirically determined electron thermal conductivity are carried out. The results indicated that the electron thermal conductivity obtained from ab initio calculation leads to faster thermal diffusion than that using the electron thermal conductivity from empirical determination, which further induces deeper melting region, larger number of density waves travelling inside the copper film and more various speeds of atomic clusters ablated from the irradiated film surface. (3) A QM-MD-TTM integrated simulation probes the impacts of femtosecond laser heating by implementing the ab initio determined effective electron-phonon coupling factor and phenomenologically treated electron-phonon coupling factor. By monitoring temperature evolutions of electron and lattice subsystems, the result utilizing electron phonon coupling factor from ab initio calculation, shows a faster decrease of electron temperature and increase of lattice temperature than those using effective electron-phonon coupling factor from phenomenological treatment. (4) A finite-temperature density functional theory investigation of the ultrafast material response, induced by deposition of energy of femtosecond laser pulse in gold, is carried out. Obtained data demonstrate structural variations induced by large amounts of laser-energy deposition, bond hardening of laser-irradiated gold. (5) Laser heating with varying laser fluence is systematically studied to determine the thresholds of the observed melting, layer-ablation and vaporization, which provides a basis for interpreting the phase change process induced by laser heating, and facilitates the advancement of femtosecond laser pulse processing of material. (6) The effects of film thickness on femtosecond laser melting of silver film are studied, which show that when the film becomes thicker, the degree of heating becomes smaller, resulting in shallower the melting depth.

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.