Ultrafast lasers, highly excited solids, and DFT-EAM-MD simulations

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Nowadays ultrafast infrared, optical and X-ray lasers have many applications from technology to medical treatments like cutting, drilling, micromachining of electronic devices, changes in colorizing and wettability due to appearance of nanoscale surface structures, keratotomy, LASIK, Epi-LASIK, CLEAR surgery and so on. Ultrafast means that duration of laser pulse τ_L is of the order of few picoseconds 10^{-12} s [ps] and less, down to few light oscillations. For infrared light with photon energy $h\nu = 1$ eV a period of oscillation is 0.7 fs; 1 fs = 10^{-15} s. In mentioned applications energies transferred to matter are in the range 0.1-1 eV/atom. A heated layer is extremely thin 10-100 nm, 30-300 interatomic spacings. Energy of pulse is absorbed by electron subsystem in intraband and/or interband transitions depending on electronic spectra of material and energy $h\nu$. Absorption strongly excite electrons, their temperatures T_e are 1-10 eV in our applications. Later electron-ion (e-i) relaxation, lasting few ps, equalizes electron and ion temperatures. To understand the processes, knowledge about equation of state (EOS), electron heat conduction coefficient κ, and e-i coupling parameter α, defining rate of e-i thermalization, is necessary for conditions of highly excited electron states of solids and liquids. EOS, κ, and α are applied to describe heating, melting, and motion of an irradiated target. We use DFT (Density Functional Theory) and kinetic equations to find energy, pressure (EOS), and kinetic characteristics (κ, α) of excited states. Those data are employed to run our hydrodynamic code. DFT is also used to find many-body interaction potential in frame of embedded atom model (EAM). Our EAM depicts all important parameters – bulk and shear modulus, vacancy formation energy, melting curve and so on. EAM potential is employed in large scale multi-processors molecular dynamics (MD) simulations. Combined hydrodynamic and MD codes describe full picture of many interlinked processes at different spatiotemporal scales from fs to ns. The processes are: absorption by electrons, conductive heating, e-i relaxation, hydromotion under action of electron and ion pressures, generation of superstrong elastic shocks (we have proved that ultrafast action keeps crystal in elastic uniaxially compressed state even near ultimate strength of solids), strong foaming of molten metals, and freezing of foam with creation of nanoscale structures containing ultrasmall bubbles frozen in solid matrix and frozen remnants of membranes of broken foam. The report gives a review of modern situation and is based on our recent papers:

[1] Agranat et al., Strength properties of an aluminum melt at extremely high tension rates under the action of femtosecond laser pulses, JETP Lett. 91, 471 (2010); [2] Zhakhovskii and Inogamov, Elastic-plastic phenomena in ultrashort shock waves, JETP Lett. 92, 521 (2010); [3] Demaske et al., Ablation and spallation of gold films irradiated by ultrashort laser pulses, Phys. Rev. B 82, 064113 (2010) [4] Ishino et al., Nanoscale surface modifications and formation of conical structures at aluminum surface induced by single shot exposure of soft x-ray laser pulse, J. Appl. Phys. 109, 013504 (2011); [5] Inogamov et al., Superelasticity and the Propagation of Shock Waves in Crystals, JETP Lett. 93, 226 (2011); [6] Zhakhovsky et al., Two-zone elastic-plastic single shock waves in solids, Phys. Rev. Lett. 107, 135502 (2011); [7] Ashitkov et al., Formation of Nanocavities in Surface Layer of Aluminum Target irradiated by Femtosecond Laser Pulse, JETP Lett. 95, 176 (2012); [8] Petrov et al., Thermal Conductivity and the Electron–Ion Heat Transfer Coefficient in Condensed Media with a Strongly Excited Electron Subsystem, JETP Lett. 97, 20 (2013); [9] Demaske et al., Ultrashort shock waves in nickel induced by femtosecond laser pulses, Phys. Rev. B 87, 054109 (2013).