Simulations of short pulse laser-matter interaction

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Laser-matter interaction and its branch connected with the ultrafast lasers are now areas of scientific researches and important technological applications. They cover cutting, drilling, molding in a motor industry, aircraft- and shipbuildings, together with applications in metaoptics, nanoplasmonics, nanoparticles production, biomedicine (e.g., delicate laser transfer of living tissues) and others. New devices are created combining a femtosecond (fs) laser and an electron microscope in one chamber (TriBeam Tomography). Processes in condensed matter triggered by fs action are fast. The only way to follow them in the course of their existence is the pump-probe experimental technique. It supplies us with information about evolution of the optical properties of an irradiated target caused by the fs action, see [1]. But this information is indirect. Physical models unified with the computer simulation based approaches are necessary to transit from the measured data about the current variation of intensity and phase of the reflected probe light wave to the data concerning the current internal state of matter in a target.

The second large source of data is the post-mortem analysis of the irradiated substance. Here a large variety of different techniques of the microscopic studies is available. They include a scanning electron microscope (SEM); a focused ion beam (FIB) used for preparation of a lamella and subsequent analysis of the lamella by a transition electron microscopy (FIB/SEM cross-sectioning); an atomic force microscope; an energy dispersive x-ray spectroscopy; electron backscatter diffraction and others. Using of these techniques allows studying strong modification of matter after the fs action. The dislocation non-homogeneous concentration, formation of a subsurface porous layer [2] and surface nanostructures [2,3] were observed thanks to those studies. But all these observations of the final complicated states say nothing about the way and hierarchy of processes which finalize in these states. Again physical models and computer sciences are needed for understanding and description.

In the report the approach with a chain of models and computer programs is presented. They accompany the chain of the physical processes caused by the fs laser action. The dream to create the computer program for one pass-through from the beginning-to-end description of results of the fs action is unachievable for today. We have to present (i) the two-temperature (2T) state (when electrons in metal are much hotter than ionic subsystem) with heat flux propagation through electron subsystem and transfer of energy from electrons to ions; (ii) melting at the 2T state and with high overheating above melting temperature $T_m(p)$; (iii) formation of shocks [1] due to compression and nucleation of voids as result of stretching; (iv) diffusion limited crystallization of the non-equilibrium strongly overcooled (hundreds K below T_m) liquid; (v) dynamics of the (partially crystallized and partially disrupted) foam where capillarity interplays with elastic reaction of the solidified parts. To present the (i-v) phenomena we use (I) the ab-initio quantum simulations [4] to describe electron and phonon spectra, interatomic potentials, equation of thermodynamic state, transport coefficients, and electron-ion coupling [4]; (II) molecular dynamics including heat conduction through the Monte-Carlo block [2,3]; (III) 2T hydrodynamics including light absorption, heat conduction, electron-ion coupling with phase transitions. Work is supported by RBRF 16-02-00864.

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