From solids to warm dense matter: various processes at play

This talk will review the results of our theoretical research on damage mechanisms in materials irradiated with femtosecond free-electron-laser pulses at fluences ranging from mild excitation of the target to warm dense matter formation. Various damage mechanisms are discussed on examples of diamond, amorphous carbon, C60 crystal, graphene sheets, silicon, and gold targets. They are studied with a developed hybrid approach, XTANT (X-ray-induced Thermal And Nonthermal Transitions [1]), which includes nonequilibrium kinetics, nonthermal effects, and nonadiabatic dynamics.

We analyze the effects of thermal melting of targets as a result of electron-ion energy exchange; nonthermal phase transitions due to modification of the interatomic potential; Coulomb explosion due to accumulated net charge in finite-size systems; spallation or ablation at higher fluences due to detachment of sample fragments; and a complex kinetics of warm dense matter formation. We calculate transient optical coefficients to be compared with experimental data whenever available, which provide interesting insights into evolution of the target properties. In particular, we demonstrate that the electron-ion (electron-phonon) coupling parameter can be accessed in highly-excited samples via time-resolved measurements of optical properties.