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Simulations of transient electronic and atomic kinetics: energy dissipation in highly excited dielectrics

Tuesday, 19 May 2015 08:30 (30 minutes)

In this talk I will give an overview of the transient nonequilibrium electron and atomic kinetics after high-energy deposition in dielectric. An ultrafast energy deposition can be made my means of x-ray free-electron laser (FEL) irradiation or swift-heavy ion (SHI) beams. The differences between the two methods will be discussed. In both cases, first, the electron subsystem of a dielectric is excited. Electrons are provided with energy up to a few tens of keV, which initiates nonequilibrium electron kinetics. High-energy electrons then perform secondary cascading and exchange energy with the lattice. The different channels of scattering and their simulation challenges will be addressed.

Dielectrics and semiconductors under irradiation with intense femtosecond laser pulses can undergo a phase transition via two different channels: thermal and nonthermal. Their difference will be discussed in detail. The first one occurs if the lattice is heated strongly enough by electron-ion (electron-phonon) coupling. The second one results from the modification of the atomic potential energy surface by excitation of electrons from the valence to the conduction band. I will present our developed approach to include both channels within a consistent framework.

The developed hybrid model consists of tight-binding molecular dynamics (TBMD) for modeling atomic system with the potential energy surface dependent on the state of electronic system [1]. Simultaneously, electronic state is traced with the Boltzmann equation for low-energy electrons, and with a Monte Carlo model for high-energy electrons. With this model it is possible to study different channels of energy dissipation in dielectrics. Examples of thermal and nonthermal melting and their interplay will be presented for silicon and diamond.

[1] N. Medvedev, H.O. Jeschke, B. Ziaja, New Journal of Physics 15, 015016 (2013)

Primary author: Dr MEDVEDEV, Nikita (Center for Free Electron Laser Science, DESY)

Presenter: Dr MEDVEDEV, Nikita (Center for Free Electron Laser Science, DESY)

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