CFEL SCIENCE

SEMINAR

14th January 2015 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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FEL-induced electron and atomic kinetics in solids

In this talk I will give an overview of our recent developments in theoretical treatment of transient nonequilibrium processes in solids after free-electron laser (FEL) irradiation. During FEL irradiation, photoabsorbtion excites electrons into high-energy states. Such highly energetic electrons produce electron cascades of impact ionizations and Auger-decay of core holes.

To study the electron kinetics in different materials, XCASCADE, a Monte Carlo model of X-ray-induced electron cascading, was recently developed. With this tool it was shown that the electron cascading duration is sensitive to material. A carefully selected target can significantly shorten the electron relaxation times. The obtained results suggested that with the choice of an appropriate material one could achieve monitoring of the pulse duration on a few-femtosecond time scale for photon energies up to 24 keV as will be produced by the European XFEL.

We also study atomic kinetics in silicon induced by an FEL pulse. Silicon under irradiation with intense femtosecond laser pulses can undergo a phase transition via two different channels: thermal (electron-phonon coupling) and nonthermal (change in the atomic potential). We developed a model to include both channels. Tight-binding molecular dynamics (TBMD) is used to model atomic dynamics with the potential energy surface dependent on the state of electronic system. Simultaneously, electronic state is traced with the Boltzmann equation for low-energy electrons, and with a Monte Carlo model for high-energy electrons. Our results show that electron-phonon coupling triggers phase transition into a low-density liquid phase for the deposited doses > 0.65 eV/atom. For deposited doses over 0.9 eV/atom, silicon undergoes a phase transition into high-density liquid phase triggered via interplay of thermal heating and the nonthermal change of the atomic potential. These thresholds are significantly lower than that obtained earlier within the Born-Oppenheimer approximation (2.1 eV/atom).

Host: Robin Santra – CFEL-DESY Theory Division