European XFEL Theory Seminar

Thursday 20th February 2020, 16:00

Campus Schenefeld, main building (XHQ) room E1.172

Vladimir Lipp

Center for Free-Electron Laser Science CFEL, DESY, Hamburg, Germany

Modelling the evolution of X-ray-irradiated materials on femtosecond to nanosecond timescales

Modern X-ray free-electron lasers (XFELs) produce intense femtosecond X-ray pulses able to modify material properties. Energetic photoelectrons created upon the X-ray absorption and Auger electrons emitted after relaxation of core-hole states trigger secondary electron cascades, which contribute to the increasing transient free electron density. Further evolution may involve energy/particle diffusion, creation of point defects, and lattice heating. In this talk, we discuss the effect of X-ray irradiation in LiF and silicon, both materials highly relevant for the XFEL beam diagnostics. We show predictions obtained with classical Monte Carlo simulations and long-timescale continuum approach. The electron cascades developing on femtosecond timescales are simulated with our in-house Monte Carlo code XCascade3D [1]. It provides temporal and spatial characteristics of the excited electrons and holes. Within the underlying atomistic approximation any material can be efficiently treated. The predicted spatial distribution of the valence holes in LiF shows a reasonable agreement with the measured positions of long-living defects called color centers. It was suggested that the latter reflect the lateral shape of the X-ray beam and, therefore, may serve as an efficient and precise diagnostic tool to estimate spatial pulse profile [2]. The long-timescale (nanosecond) X-ray-induced dynamics is simulated on the example of silicon in two-dimensional (e.g. cylindrical) geometry. The XCascade3D code provides initial conditions on the energy deposition in Si by an X-ray beam on femtosecond timescales, while extended Two-Temperature model with electron density dynamics, nTTM [3], describes further relaxation of the sample on nanosecond timescales. It takes into account ambipolar carrier diffusion, electronic and atomic heat conduction, as well as the electron-phonon coupling. To solve the nTTM system of equations in two dimensions, we developed a dedicated finite-difference integration algorithm based on Alternating Direction Implicit method with an additional predictor-corrector scheme. We show first results obtained with the model and discuss its possible applications. In particular, the model can estimate the timescale of material excitation relevant for beam diagnostic applications during high repetition-rate operation of XFELs.

[1] V. Lipp, N. Medvedev, B. Ziaja, Proc. SPIE 10236, 102360H (2017). [2] T. Pikuz, A. Faenov, Takeshi Matsuoka, et al., Scientific Reports 5, 17713 (2015). [3] H. van Driel, Phys. Rev. B 35, 8166 (1987).

Host: Ruslan Kurta