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

Modern X-ray free-electron lasers (XFELs) produce femtosecond X-ray pulses sufficiently intense to modify material properties or damage the target. On the femtosecond timescales, 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. We simulate these cascades using an in-house classical Monte Carlo code XCascade3D [1], which can provide temporal and spatial characteristics of the excited electrons, including their energy distribution. The latter can serve as initial conditions for further simulation on longer timescales.

On the nanosecond timescales, the target evolution may involve energy/particle diffusion and lattice heating. We simulate it on the example of silicon using an extended Two-Temperature Model with electron density dynamics, nTTM [2]. It takes into account electron-hole 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.

In this work, the student should help us connect the two above computer programs by generating the output files from the XCascade3D and reading them in nTTM, thus making it possible to provide a more consistent simulation results, which would be compared with the experiments. Programming skills in Fortran 90 would be very helpful.

The full combined model would then be able to reliably evaluate timescales of material excitation during high-repetition-rate operation of XFELs, which is relevant for beam diagnostic applications.

[1] Lipp, Milov, Medvedev, J. Synchrotron Rad. 29, 323 (2022).
[2] Lipp, Rethfeld, Garcia, Ivanov, Appl. Sci. 10, 1853 (2020).

Field

A6: Theory and computing

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Special Qualifications:

Programming skills in Fortran would be very helpful.

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