This is an example of modeling irradiation of solid diamond with a soft X-ray (or XUV) pulse of 92 eV photon energy, 10 fs FWHM duration, absorbed dose of 1 eV/atom, with XTANT-3 code[[1]](#footnote-1).

1. The files INPUT.txt and dt\_grid.txt must be placed inside of the directory INPUT\_DATA [read the manual !XTANT\_3\_manual.docx or !XTANT\_3\_manual.pdf for more details on the input files]. This example input-file described the irradiation with a single pulse of a gaussian temporal shape with 10 fs FWHM, 92 eV photon energy, and 1 eV/atom of the absorbed dose. The number of atomic in the simulation box with periodic boundary conditions (NVE ensemble) is 216 (defined by 3x3x3 orthogonal unit cells, each containing 8 atoms). The time-step is defined in the file dt\_grid.txt (starting with 1 fs, and changing to 0.1 fs before the beginning of irradiation).
2. The files C\_C\_TB\_Hamiltonian\_parameters.txt, C\_C\_TB\_Repulsive\_parameters.txt, Diamond.cdf, Unit\_cell\_atom\_relative\_coordinates.txt and Unit\_cell\_equilibrium.txt must be placed in the directory Diamond (the name given in the first line in INPUT.txt) inside the directory INPUT\_DATA (by default, these files are already present in this directory as distributed together with the XTANT-3 code). They contain the description of the elementary unit cell, the parameters of the TB Hamiltonian (from [1]), and the parameters of the electron scattering cross section in the CDF formalism (see [2]).
3. Compile the code by calling Make.exe (under Windows) or make (under Unix) [read the manual !XTANT\_3\_manual.docx or !XTANT\_3\_manual.pdf for more details on how to compile the code, which compilers are needed; the compilation file assumes that all the path to compilers are set in your system].
4. Run the compiled code XTANT.exe or XTANT.x. It will create output directory with all the output files and plots created with gnuplot (if it is installed in your computer and the paths to it are set in the system).

[1] C.H. Xu, C.Z. Wang, C.T. Chan, K.M. Ho, A transferable tight-binding potential for carbon, J. Phys. Condens. Matter. 4 (1992) 6047–6054. https://doi.org/10.1088/0953-8984/4/28/006.

[2] N.A. Medvedev, R.A. Rymzhanov, A.E. Volkov, Time-resolved electron kinetics in swift heavy ion irradiated solids, J. Phys. D. Appl. Phys. 48 (2015) 355303. https://doi.org/10.1088/0022-3727/48/35/355303.

1. <https://github.com/N-Medvedev/XTANT-3> [↑](#footnote-ref-1)