This is an example of creation of a relaxed crystalline polyethylene structure using XTANT-3 code[[1]](#footnote-1). This should be done in two steps [1]:

1. Quenching MD (analogous to zero-temperature MD, or steepest descent)
2. Relaxation to the room temperature.

It can be done with the following steps:

Steps from the point I:

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 polyethylene in ideal structure, but unrelaxed absolute positions of atoms. The number of atoms in the simulation box with periodic boundary conditions (NPH ensemble) is 288 (defined by 4x3x2 orthogonal unit cells, each containing 12 atoms). The time-step is defined in the file dt\_grid.txt (starting with 1 fs, and changing to 0.1 fs). Note that in this case, it can be changed to just 1 fs as a constant value in line 24 in INPUT.txt.
2. The files TB\_Hamiltonian\_parameters.txt, TB\_Repulsive\_parameters.txt, Unit\_cell\_atom\_relative\_coordinates.txt and Unit\_cell\_equilibrium.txt must be placed in the directory C2H4n (the name given in the first line in INPUT.txt – may be renamed, but the directory name must coincide with the name given in this line) 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 (in the DFTB form in matsci-0-3 parameterization [2]). Note that the directory DFTB with the subdirectory matsci-0-3 must exist inside the directory INPUT\_DATA, containing the Slater-Koster .skf files (provided together with XTANT-3, or may be downloaded from DFTB.org).
3. Compile the code by calling Make.exe (under Windows) or make (under Unix); it also compiles the post-processing subroutines in the directory !XTANT\_ANALYSIS\_SUBROUTINES [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).

Steps from the point II:

1. Once you have the results stored in directory starting with OUTPUT\_C2H4n\_..., copy the files SAVE\_atoms.txt and SAVE\_supercell.dat from this results-folder to the directory C2H4n inside of INPUT\_DATA. These SAVE-files contain the final positions of atoms and the vectors of the supercell from the quenching-MD simulation, to be used as initial conditions for the Step II simulation run, relaxing them to the room temperature in NVE ensemble.
2. Rename the file INPUT\_Step\_II.txt into INPUT.txt, and replace with it the one in the directory INPUT\_DATA.
3. Run XTANT-3 again with these new simulation parameters and new atomic coordinates. The results will be the relaxed supercell of polyethylene, relaxed at the room temperature (273 K).

Note that if the system is not fully relaxed, or a simulation had a random fluctuation changing the properties to some undesired state, you may rerun the same simulations but for longer time (increase it in the line 6 in INPUT.txt), in either or in both steps, I or/and II.

[1] N. Medvedev, I. Milov, Electron-Phonon Coupling and Nonthermal Effects in Gold Nano-Objects at High Electronic Temperatures, Materials (Basel). 15 (2022) 4883. https://doi.org/10.3390/MA15144883.

[2] J. Frenzel, A.F. Oliveira, N. Jardillier, T. Heine, G. Seifert, Semi-relativistic, self-consistent charge Slater-Koster tables for density-functional based tight-binding (DFTB) for materials science simulations., Dresden, 2009. http://www.dftb.org/parameters/download/matsci/matsci-0-3-cc/.

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