

# Coupled MD/NEGF simulation of transport properties under straining of a graphene bridge

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## Abstract

Recent years have seen a rapid progress in the application of graphene in flexible displays, which are supposed to be able to be subjected to a large mechanical deformation without affecting the fundamental operation of the device. The challenge is, however, that the active components – the transistors or light-emitting diodes – are an integrated part of the flexible substrate itself. It is therefore crucial to understand how these electronic components behave under non-ideal conditions, such as strain, temperature, or other external influence.

In this work we have performed a molecular dynamics (MD) simulation of how the electronic transport properties of a graphene-like bridge between two capped carbon nanotubes (Fig. 1) change as the system is adiabatically stretched in the transport direction.

The nanotubes are pulled apart slowly enough (0.1 Å/ps) that the structure has time to equilibrate adiabatically in the MD routine, which uses a Verlet integration with time step 1 fs, initialized with a room-temperature Maxwell–Boltzmann distribution of the ion velocities. The entire simulation is run for 40 ps, at which point the graphene bridge begins to break away from the nanotubes.

The calculation is made possible by integrating two separate codes – and also two separate computational approaches – into a single simulation framework. The MD part is performed using a classical Tersoff potential [1] as implemented in Tremolo-X [2], whereas the electronic transport properties are evaluated using a non-equilibrium Green's function (NEGF) approach [3], in which the electronic structure part is computed with a semi-empirical Slater–Koster method [4], as implemented in our software package Atomistix ToolKit (ATK) [5]. The entire computation is driven by a single Python script, where the NEGF calculation is inserted as a “hook” into the MD simulation that is called after a specified number of MD steps.

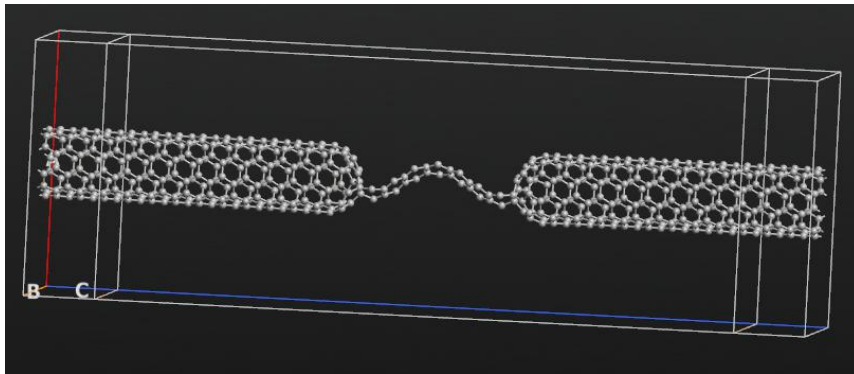
The results show that the electronic properties are remarkably stable when the system is strained, up until the point where the graphene bridge begins to tear apart from the nanotubes. The change in the linear response current at 0.5 V bias, as the strain increases, is comparable to the variations caused by pure temperature fluctuations (without any strain applied). At the same time, those variations in the current are almost 10% (standard deviation), at an average current of 3.7  $\mu$ A.

The presented methodology is generic and can easily be applied to any type of device structure, based on graphene or other materials, and it is possible to freely mix and match the methods used for the force evaluation in the MD part and the electronic structure calculation for the NEGF, choosing between DFT, extended Hückel, Slater-Koster tight binding as desired.

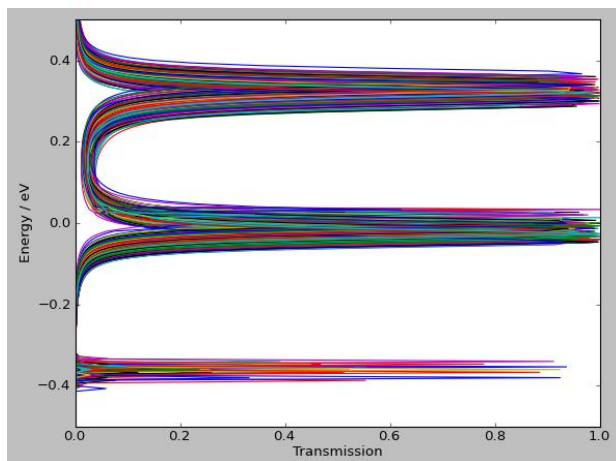
## References

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- [5] Atomistix ToolKit, QuantumWise A/S ([www.quantumwise.com](http://www.quantumwise.com)).

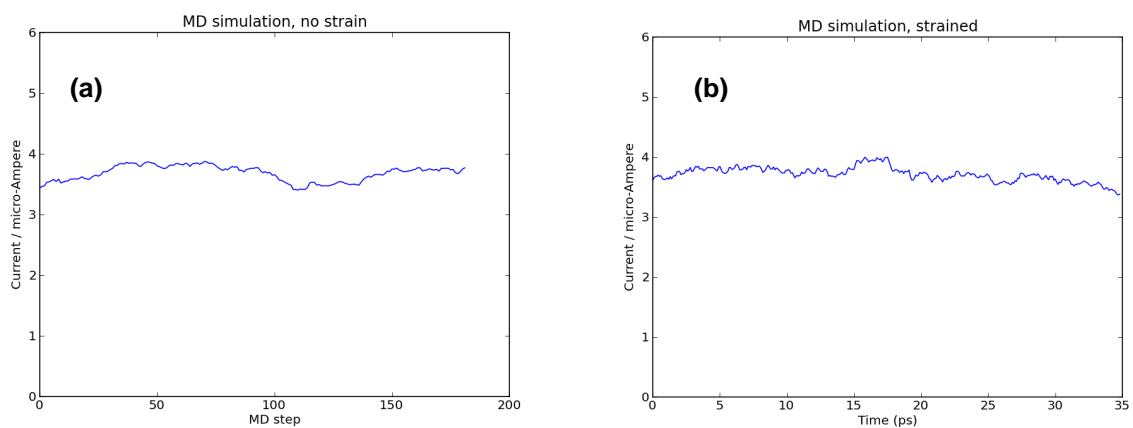
## Figures



**Figure 1:** The initial ( $t=0$  sec) device structure used for the coupled MD/NEGF simulation, consisting of two capped (5,5) carbon nanotubes joined by a 2 atom wide zigzag graphene nanoribbon. The structure shown in the figure is the result of a combined force/stress optimization which minimized the forces to  $0.05 \text{ eV/\AA}$  and the stress to  $0.0005 \text{ eV/\AA}^3$ , starting with the graphene bridge being flat.



**Figure 2:** Transmission spectrum, in units of the quantum conductance, evaluated at 0.1 ps interval during the MD run. Essentially all transmission spectra are identical, except for the precise position of the Fermi level (dotted). This causes a large (and growing with time) fluctuation in the *conductance* (the transmission at the Fermi level), but when the spectrum is integrated to obtain the linear response current, the variation more or less disappears (Fig. 3).



**Figure 3:** Running average (window=20 samples) of the linear response current at 0.5 V source-drain bias as a function of the simulation time for **(a)** a pure MD simulation without straining the sample (time step 1 fs), and **(b)** the case where strain is adiabatically applied.