# Atomistic and Heat Dissipation Modelling of Carbon Nanostructures

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## I. Potential of Mean Force Calculations

- Classical molecular dynamic (MD) simulations (LAMMPS code [1]) have been employed to study dimer interaction in carbon fullerenes.
- Forces between particles are obtained with interatomic potentials: Adaptive Intermolecular Reactive Empirical Bond Order potential with nondivergent Morse potential (AIREBO/M) [2].
- The Langevin thermostat [3] was considered to sample equilibrium configurations at a given temperature.
- The Potential of Mean Force (PMF(**r**)) between the two centres of mass (CoM), was obtained by employing the Weighted Histogram Analysis Method (WHAM) [4].

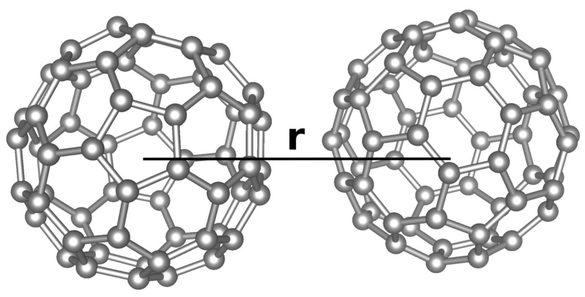


**Fig. 1:** Two $C_{60}$ molecules with the CoM at a distance **r**.

Our interest is mainly focused on the behaviour of PMF(**r**) as a function of distance, its dependence with temperature and the formation of dimers by covalent bonding. The interaction of rotational and vibrational degrees of freedom with the CoM distance may lead to a temperature dependence of PMF(**r**).

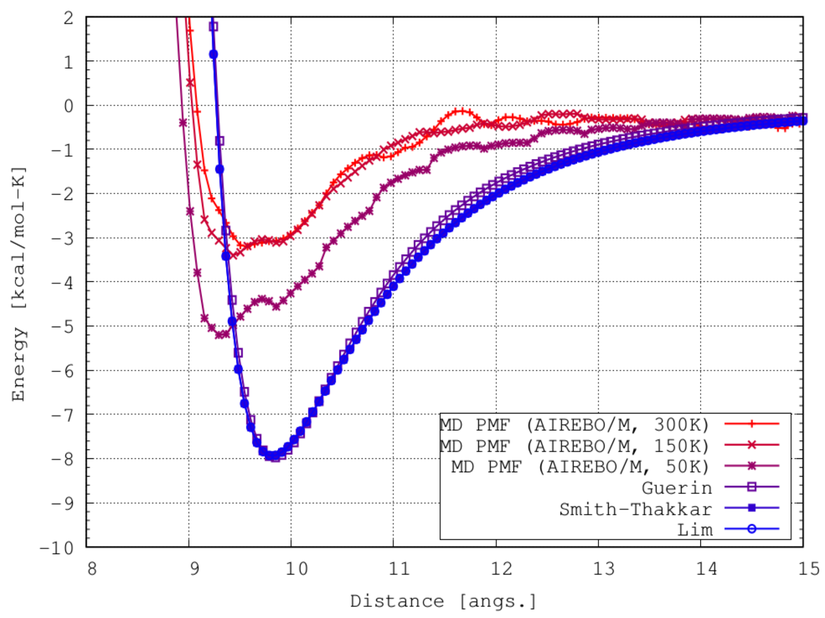


**Fig. 2:** PMF(**r**) obtained from molecular dynamics simulations, for three different temperatures, namely 300K, 150K and 50K. Comparison is made between effective potentials of Guerin, Smith-Thakkar and Lim, which were fitted to data points calculated by DFT-based symmetry-adapted perturbation theory (SAPT) (obtained from Ref [5]).

Preliminary MD temperature-dependent calculations (Fig. [2]) shows the PMF(**r**) with shallow potential depths (PD), which deepen when the temperature decreases:

- 300 K: **r**=9.58 Å; PD=-3.2 kcal mol$^{-1}$
- 150 K: **r**=9.44 Å; PD=-3.4 kcal mol$^{-1}$
- 50 K: **r**=9.30 Å; PD=-5.2 kcal mol$^{-1}$

By comparing to the effective potentials fitted to DFT-SAPT (Ref. [5]), the potential energy minimum is at longer distances of **r**=9.85 Å, and deeper potential depth with -8.0 kcal mol$^{-1}$.

## II. Heat Dissipation Modelling

The purpose of this study is to model the heat dissipation properties of nanostructured carbon materials with high surface area to volume ratio. The vertically aligned hybrid material comprising diamond thin platelets (DP) covered by a crystalline graphite layer was produced in a single run by tuning the CVD synthesis conditions [6]. The finite element method was used to study the heat dissipation, by air convection, of a simplified model placed over a heat source.

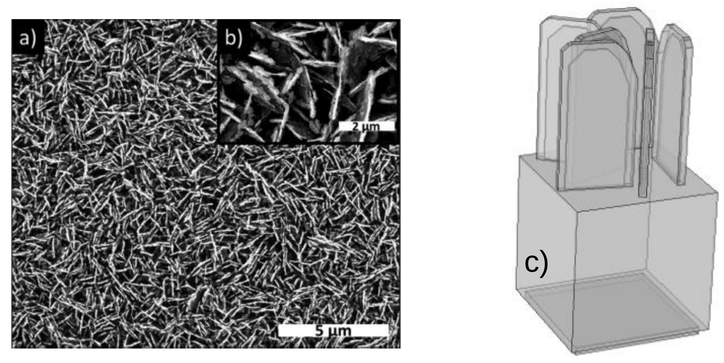


**Fig. 3:** a) Low magnification SEM image of the sample; b) High magnification SEM image of the sample; c) Geometry used in finite element simulations.

The initial approach was to use a system with just a few platelets with homogenous diamond composition. Different box sizes and convection conditions, both natural and forced, were considered. The effect of the value of the heating power was also analysed. Subsequently, systems with a larger number of DPs, and, as a consequence, of larger horizontal dimensions, were studied. It was found that presence of the nanoplatelets increases the coefficient of heat transfer from 25% to 40% compared with the uncovered diamond base. A larger density of DPs over the diamond surface, has also positive effects on the heat dissipation performance.

A more realistic composition of the system, taking into account the crystalline graphite layer is being modelled.

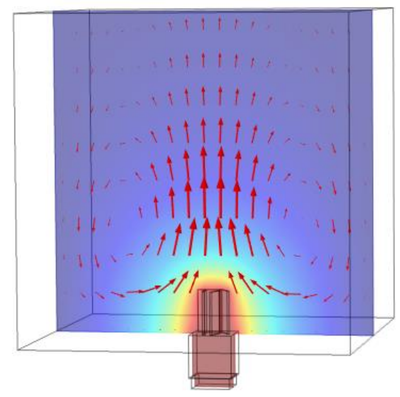

**Fig. 4:** Heat dissipation by natural convection. The system is in a stationary state.

The microscale transmission of heat is expressed by the Fourier's law and the Newton's law of cooling. Due to the systems dimensions these laws can become invalid. Further studies will have to take this into account.

Focussing in the fluids behaviour one way of deciding the analytical approach is using the Knudsen number [7].

- ($0.001 < K_n < 0.1$) is considered slip flow. In this case, a continuum modelling approach is used. However, adjustments are made in the boundary conditions.
- ($0.1 < K_n < 10$) is considered transition flow, and the Lattice Boltzmann method can be used.
- ($K_n > 10$) is considered free molecular flow, and the angular coefficient method can be used.

[1] S. Plimpton, J. Comp. Phys. 117, 1 (1995); http://lammps.sandia.gov.
[2] T. C. O'Connor, J. Andzelm and M. O. Robbins, J. Chem. Phys. 142, 024903 (2015).
[3] Schneider and Stoll, Phys. Rev. B 17, 1302 (1978).
[4] Grossfield, A, http://membrane.urmc.rochester.edu/content/wham/, Version 2.0.9., and references therein.
[5] D. I. Sharapa, J. T. Margraf, A. Hesselmann and T. Clark, J. Chem. Theory Comput. 13, 274 (2017).
[6] N. F. Santos, T. Holz, T. Santos, A. J. S. Fernandes, T. L. Vasconcelos, C. P. Gouvea, B. S. Archanjo, C. A. Achete, R. F. Silva, and F. M. Costa, ACS Appl. Mater. Interfaces 7, 24772 (2015).
[7] C. B. Sobha and G.P. Peterson, Microscale and Nanoscale Heat Transfer, CRC Press, 2008.

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