

Numerical Analysis of Producing SWNT from Graphite by Heating Processes

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There are several methods of producing carbon nanotubes. Mostly, it is produced with arc discharge method, besides relatively less used methods like laser ablation and chemical vapour deposition (CVD) [1]. Temperature takes very important part at each of these methods. Arc discharge and laser ablation methods have fewer structural defects than the other known methods, because of high-temperature processes. Although arc discharge and laser ablation methods both give less defects in SWNTs, arc discharge method is advantageous due to its cheapness. Hence, many theoretical and experimental works attempt to improve the SWNT yield [1] taking into account temperature effects [2].

In this work, formation of single wall nanotubes is investigated using molecular dynamics. Simulations include annealing and quenching processes of graphite consisting of 4 armchair edged graphene layers with 1920 atoms. Utilized MD simulation code uses modified form [3] of the Brenner potential [4]. Dependency of sp^2 and sp^3 bond formations are observed for annealing temperatures varying from 300 - 2400 K, and for quenching rates (Qr) between 0.05-0.2 K/fs ($1fs=10^{-15}s$).

One of the simulation results is shown in the Figure 1. The sample graphite at 600 K first annealed to 1600 K, and then quenched to 300 K with $Qr = 0.05$ K/fs, the formed structure is seen at the figure. The graphite was separated as layers at the very beginning of simulations. After the thermal processes explained above, atoms were bounded to form nanotubes, while few atoms make sp^3 bounds. Final form has not got a symmetric fullerene type. Instead, it resembles defected SWNTs which are bound to other SWNT on the defect side, which can be called as corridors.

Resulted slabs may be used as storage devices while the corridors being as flowing paths of possible filled material.

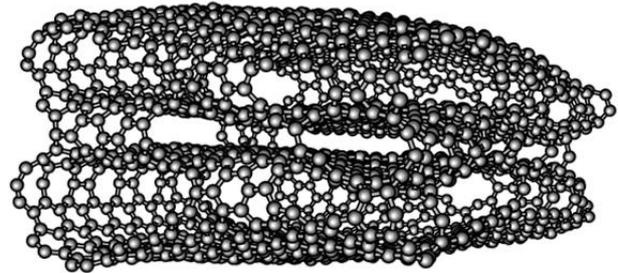


Fig. 1 Side view of the graphite C_{1920} . Resulted SWNT couple for the sample at 600 K was annealed to 1600 K thereafter quenched to 300 K.

References

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