COMPRESSIBILITY OF CARBON NANOTUBES FILLED WITH GASES AND FULLERENES

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Introduction

Several researchers have observed the intercalation of gases, metals and fullerenes into carbon nanotubes [1]. In this study we examine the compressibility of carbon nanotubes that have been filled with noble gases, methane and buckyballs and compare the values to the compressibility of empty nanotubes. The approach is classical molecular dynamics simulations.

Computational Details

The interatomic potential used in this study is the analytic reactive empirical bond-order potential of Abel-Tersoff that has been parameterized by Brenner (REBO), and coupled to a long range Lennard-Jones potential [2]. To treat intermolecular interactions with higher precision we also used adaptive intermolecular potential (AIREBO) [3]. In this study, (10,10) carbon nanotubes that are 100 Å and 200 Å long are filled with CH_4, Ne and C_{60}. Compression of the filled nanotube is performed by moving one end of the nanotube towards the other end with a constant velocity 41 m/s, while the other end is kept fixed. On every nanotube edge a layer that is several Å wide is subjected to Langevin frictional forces to maintain the nanotubes at a constant temperature and mimic the heat dissipation properties of a real nanotube bundle. No other constrains are applied to the system.

Results and Discussion

We have examined how the stiffness of the nanotubes during compression depends on different factors such as: the type of filling particles, the density of filling, the length of nanotube, and the temperature. Force plots for the compression of the nanotubes are shown in Figures 1,2 and 4. The simulations predict higher nanotube stiffness when the nanotube is filled with gases relative to the empty state. They also predict lower nanotube stiffness when the nanotube is filled with C_{60} relative to the empty state. Higher gas densities increase the buckling force of the nanotube (as shown in Fig.1) whereas a higher density of C_{60} decreases it (see Fig.2). One explanation for this prediction is that buckling requires a perturbation of some sort so that the nanotube knows in which direction to buckle and the presence of C_{60} which bounce off the inside walls increases the amount of perturbations in the direction transverse to the long axis (see Fig.3). We found that the longer nanotubes buckle at a lower compressive force than the shorter one nanotubes. Compression at higher temperature enables easier buckling (see Fig.4).

Conclusion

Compressibility of nanotubes filled with gases and fullerenes has been investigated. The simulations predict that the stiffness of the nanotubes changes with the temperature, type of filling particle, density of filling and the length of nanotube.

References

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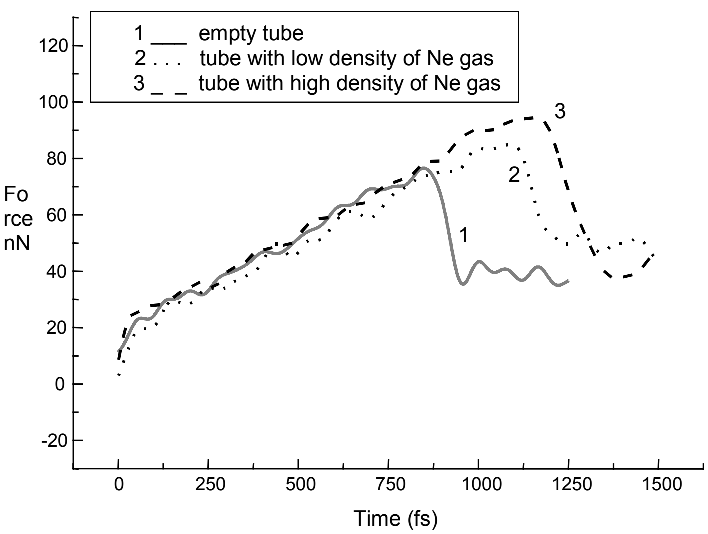

Fig.1 Force curves for the compression of a 100 Å long carbon nanotube filled with various densities of Ne.

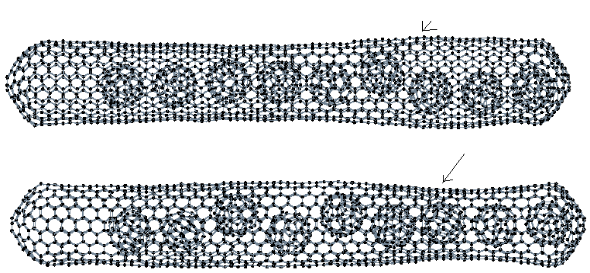

Fig.3 Side and top views of nanotube compression. The arrow indicates the moment before buckling.

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3. S.J. Stuart, A.B. Tutein, J.A. Harrisson, J. Chem. Phys. 2000; 112; 6472-6485.

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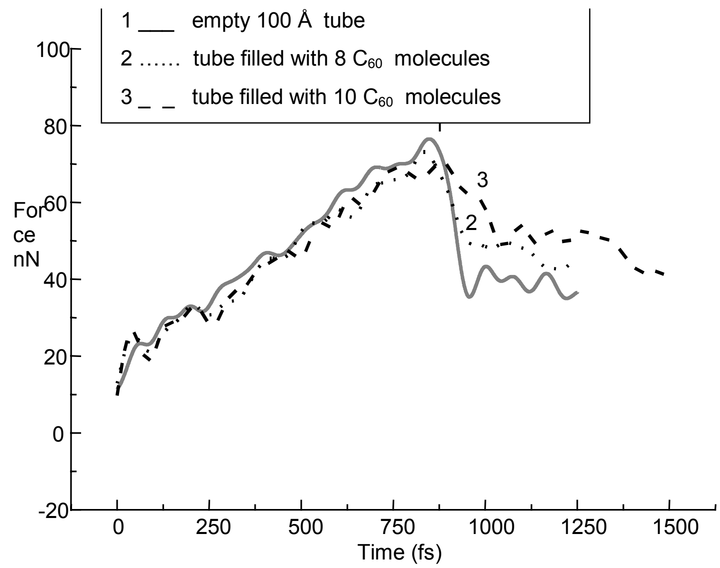

Fig.2 Force curves for the compression of a 100 Å long carbon nanotube filled with various densities of C_{60}.

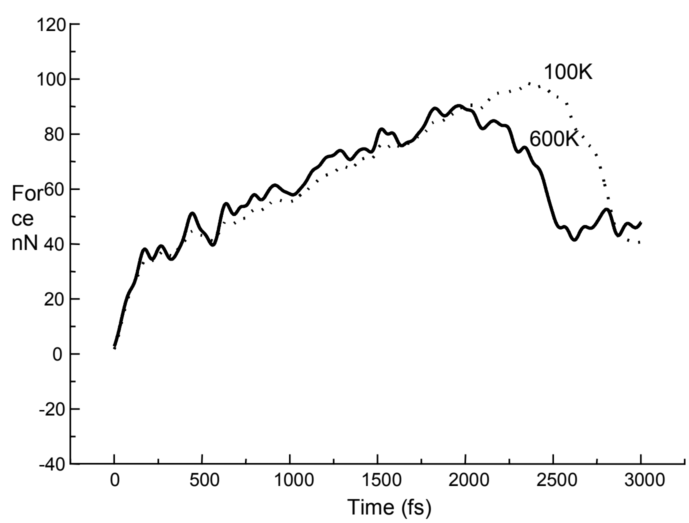

Fig.4 Force curves for the compression of a 200 Å long carbon nanotube filled with Ne at various temperatures