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Molecular dynamics study of the C_{60} molecule

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Abstract

Tight-binding molecular dynamics calculations were performed for 60 carbon atoms. Under helium atmosphere, cage like structures were obtained independent of the initial arrangement of the carbon atoms, but in the case of bulk simulation the final structure was determined by the density of the carbon atoms. After a simulation time of 30.8 ps in helium atmosphere of temperature 4000 K, a C_{60} cage structure of 11 pentagons, 19 hexagons, one tetragon and one heptagon was obtained.

Keywords: C_{60}; Carbon structure; Molecular dynamics

1. Introduction

Since the discovery of the buckminsterfullerene [1] one of the interesting problems of fullerene research is the explanation of the formation of this remarkable molecule. From the molecular dynamics calculations [2] we mention here the papers of Ballone and Milani [3], Chelikowsky [4] and Wang et al. [5]. In all of these simulations of C_{60} formations, however, there were applied some artificial conditions in order to obtain the closed cage like structures. Ballone and Milani kept the carbon atoms on the surface of a sphere for $T > 4000$ K, Chelikowsky removed and replaced randomly the energetically unfavorable atoms and Wang et al. Confined them into a sphere and obtained closed cage only for $R = 3.832$ Å. In the present work we used a more natural boundary condition. In the first part of our work we put namely the 60 carbon atoms into helium atmosphere and the temperature of the helium gas was controlled with Nosé–Hoover thermostat [6,7]. In the second part of our calculation we studied the formation of amorphous graphite and diamond structures.

2. Results and discussions

The carbon–carbon interaction was calculated from the tight binding Hamiltonian of Xu et al. [8] and the carbon–helium and helium–helium interactions were described through Lennard–Jones two-body potentials [2]. Our unit cell of side 25.0 Å contained 60 carbon atoms and randomly distributed 1372 helium atoms. We prepared four initial arrangements for the carbon atoms. The first one was Kroto's four-deck model 6:24:24:6 [9] and for the others we put 60 carbon atoms randomly in cubes of sides 8.424, 8.00 and 6.4 Å. In this way we obtained the macroscopic densities of $\rho = 2.03$, 2.335, and 4.56 g/cm^3 according to the amorphous, graphite and diamond structures. In each molecular dynamics run one of these structures was evaporated by giving an initial kinetic energy of 13000 K to the carbon atoms. At the same time the Nosé–Hoover temperature of the helium atoms was the constant $T = 4000$ K. For the unit cell of side 25.0 Å periodic boundary condition was applied. In the case of the bulk simulations the same amorphous, graphite and diamond initial structures were used, but

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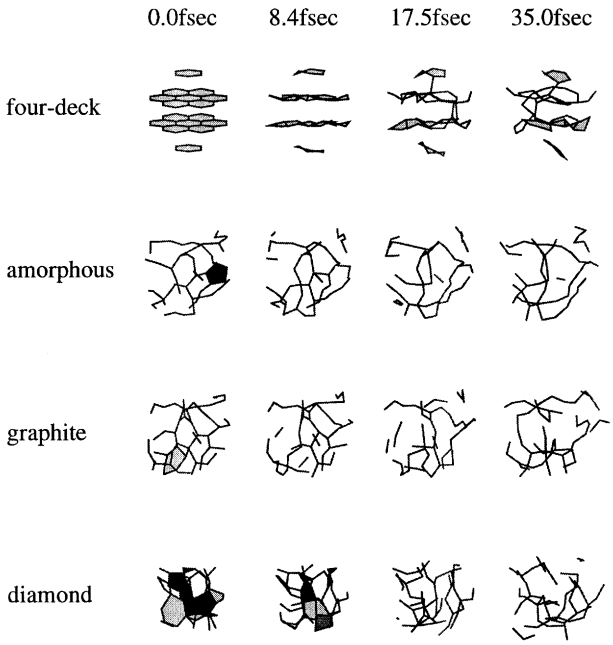

Fig. 1. Snapshots at 0.0, 8.4, 17.5 and 35.0 fs of the 6:24:24:6 four-deck amorphous, graphite and diamond structures. The carbon atoms are connected by straight lines when the interatomic distances are less than 1.8 Å. The helium gas temperature is $T = 4000$ K.

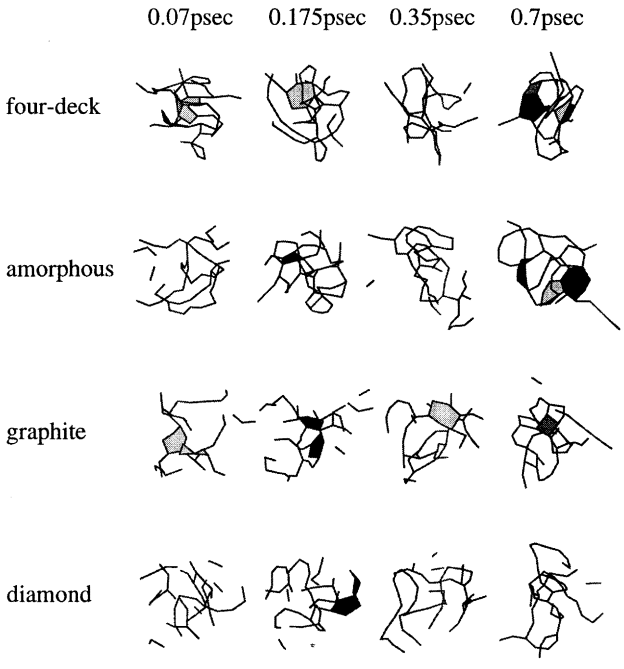

Fig. 2. Snapshots at 0.07, 0.175, 0.35 and 0.7 ps of the 6:24:24:6 four-deck, amorphous, graphite and diamond structures. The carbon atoms are connected by straight lines when the interatomic distances are less than 1.8 Å. The helium gas temperature is $T = 4000$ K.

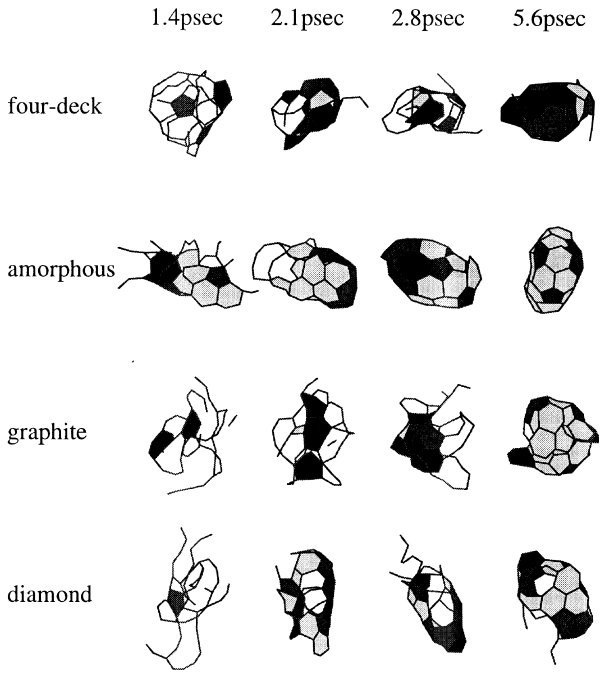

Fig. 3. Snapshots at 1.4, 2.1, 2.8 and 5.6 ps of the 6:24:24:6 four-deck, amorphous, grahite and diamond structures. The carbon atoms are connected by straight lines when the interatomic distances are less than 1.8 Å. The helium gas temperature is $T = 4000$ K.

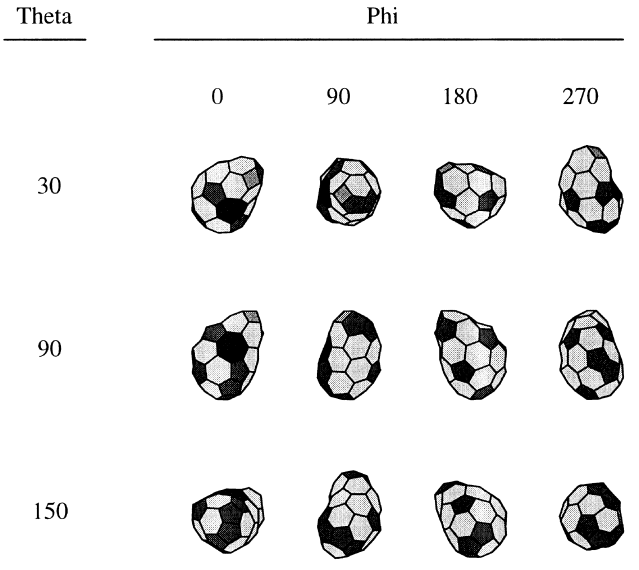

Fig. 4. Different views of the C_{60} cage structure obtained from the 6:24:24:6 four-deck arrangement after the simulation time of 30.8 ps. Theta and Phi describe the directions of the views in polar co-ordinates.

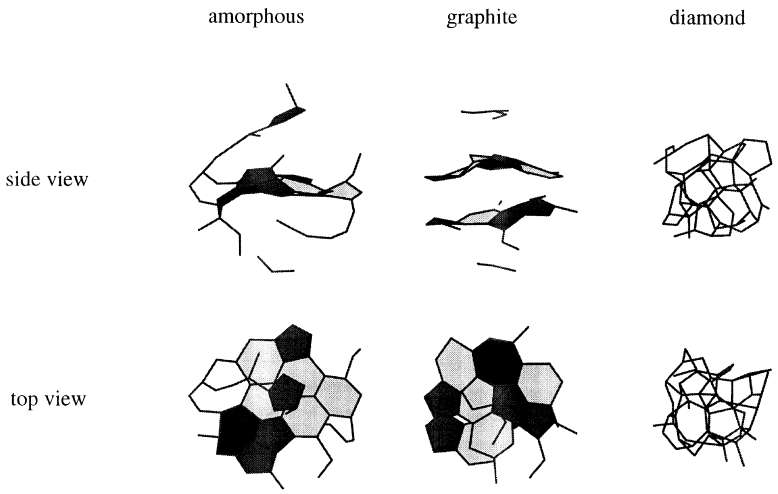

Fig. 5. Amorphous graphite and diamond structures after a simulation time of 5.6 ps under the carbon densities of amorphous, graphite and diamond structures.

without the helium atmosphere, as periodic boundary condition was taken into account for the carbon unit cells.

Figs. 1–3 show the evolutions of the carbon structures. In the first 0.35 ps we obtained the disintegration of the various initial arrangements (1). In the range of 0.7–1.4 ps new poligons were created (2), and for 5.6 ps cage like structures were developed in initial states (3). We continued the simulation for the four-deck model until 30.8 ps and Fig. 4. Depicts the final cage structure of C_{60}. It contains 11 pentagons, 19 hexagons, 1 tetragon and 1 heptagon.

In the second part of our calculation we studied the bulk formation of amorphous, graphite and diamond structures by applying periodic boundary conditions with unit cells of sides 8.424, 8.00 and 6.4 Å for the carbon atoms. The final structures of amorphous graphite and diamond densities are in Fig. 5. In the case of amorphous and graphite densities we can see the plane structures of sp^2 atoms in initial state, and at diamond densities mostly sp^3 atoms were obtained. The number of onefold, twofold, threefold and fourfold co-ordinated sites are in order 0.0%, 10.0%, 86.7% and 3.3% for the amorphous; 3.3%, 10.0%, 86.7% and 0.0%. For the graphite; and 0.0%, 0.0%, 10.0% and 90.0% for the diamond density. In these simulations the temperature of the Nosé–Hoover thermostat was $T = 3500$ K.

In conclusion we can say that under helium atmosphere we obtained cage like structures independent of the initial arrangement of the carbon atoms, but in the case of bulk simulation the final structure depends on the density of the carbon atoms.

Acknowledgements

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