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Energetics of carbon nanotubes

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Abstract. We have investigated the energetics of carbon nanotubes. Calculations have been performed by using the empirical many-body potential energy function developed by Tersoff for carbon.

PACS. 61.48.+c Fullerenes and fullerene-related materials – 61.46.+w Clusters, nanoparticles, and nanocrystalline materials – 31.15.Ct Semi-empirical and empiricalculations (differential overlap, Hückel, PPP methods, etc.)

The carbon tubule research was greatly stimulated by the initial report of the existence of carbon nanotubes [1], and the subsequent report of conditions for the synthesis of large quantities of nanotubes [2]. Various experiments carried out thus far are consistent with identifying the carbon nanotubes with cylindrical graphene sheets of carbon atoms [3].

Formally, from the theoretical point of view, carbon nanotubes are modeled as single-wall tubules, cylindrical in shape, namely a single graphene sheet rolled to form the cylinder. The various types of cylindrical shells are possible [4]; armchair tubule, zigzag tubule, and chiral tubule. If a C_{60} molecule is bisected normal to a fivefold axis, the armchair tubule is formed, and if the C_{60} molecule is bisected normal to a threefold axis, the zigzag tubule is formed. Chiral carbon nanotubes can be formed with a screw axis along the axis of the tubule and with a variety of hemispherical-like caps. The carbon nanotubes could be either open ended or with caps at each ends, such that the two caps can be joined to form a fullerene. A detailed information about the various properties of carbon tubules can be found in [5].

In this paper we have investigated the energetics of carbon nanotubes in zigzag model with open ended forms. Although it is possible, in principle, to calculate quantum mechanically the interaction energy of a nanotube, it requires a large computational effort and it is limited to small systems. On the other hand, empirical many-body potential energy functions can be applied to larger systems.

In the present calculation we have used the Tersoff empirical many-body potential energy function (PEF) [6], which was developed for covalent systems, and parameterized for carbon.

The carbon nanotube considered in this work is represented by two parameters. L represents the number of hexagons along the length, and W represents the number of hexagons around the circumference of the nanotube. A model nanotube with $L = 5$ and $W = 7$ is shown in Figure 1. Total number of hexagons, H, forming the nanotube is equal to the product of L and W, namely $H = LW$. In this work the carbon-carbon distance, or the side of each hexagon has been taken as the nearest-neighbour distance of carbon atoms in graphite with $d_{nn} = 2.456$ Å. All nanotubes generated for the present calculations are assumed to be ideal, and not relaxed. The results of the calculations correspond to the unrelaxed carbon nanotubes. We believe that the choose of the ideal model will not change the trends seen in the calculations.

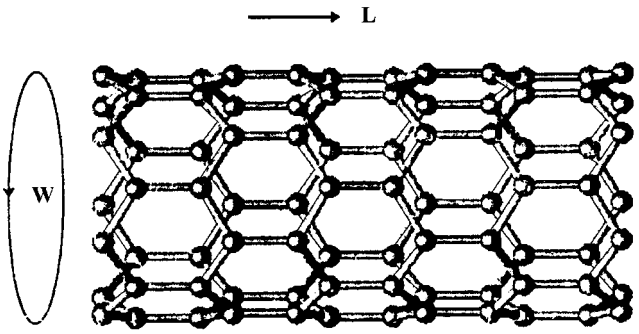

Fig. 1. Geometry of the nanotube in zigzag model with open ended. L represents the number of hexagons along the length of the nanotube, and W represents the number of hexagons around the circumference of the nanotube. In this model $L = 5$, and $W = 7$.

We have calculated the total interaction energy of a given nanotube using the Tersoff PEF. The variation of binding energy, E_b (average interaction energy per atom), with respect to L, the number of hexagons along the length of the nanotube is shown in Figure 2. The variation of E_b with respect to W, the number of hexagons around the circumference of the nanotube is shown in Figure 3.

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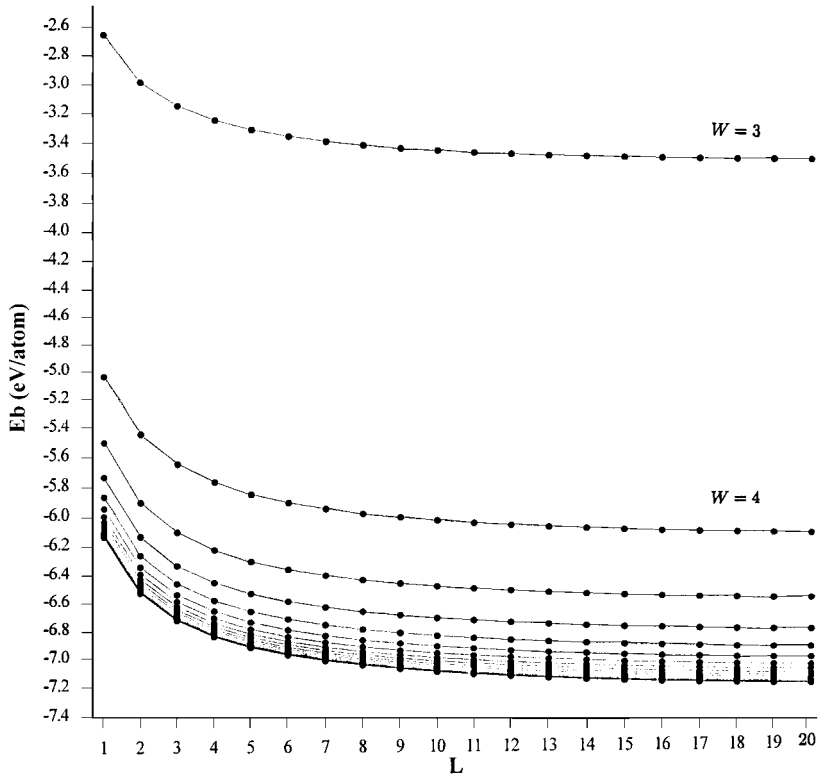

Fig. 2. Variation of binding energy, E_b (average interaction energy per atom) with respect to L. Each curve corresponds to different W.

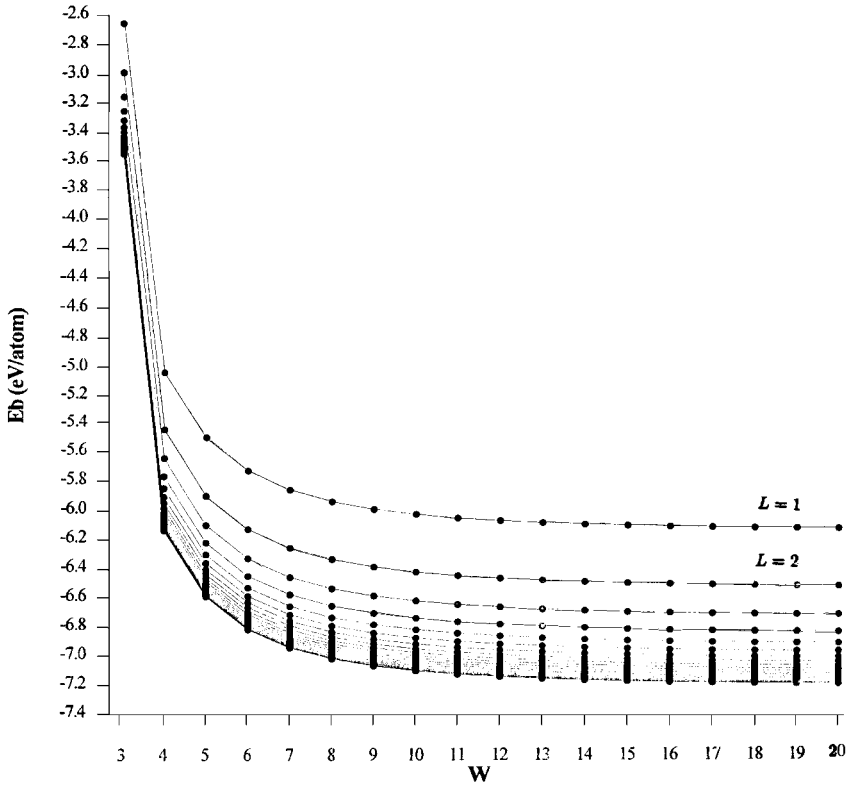

Fig. 3. Variation of binding energy, E_b (average interaction energy per atom) with respect to W. Each curve corresponds to different L.

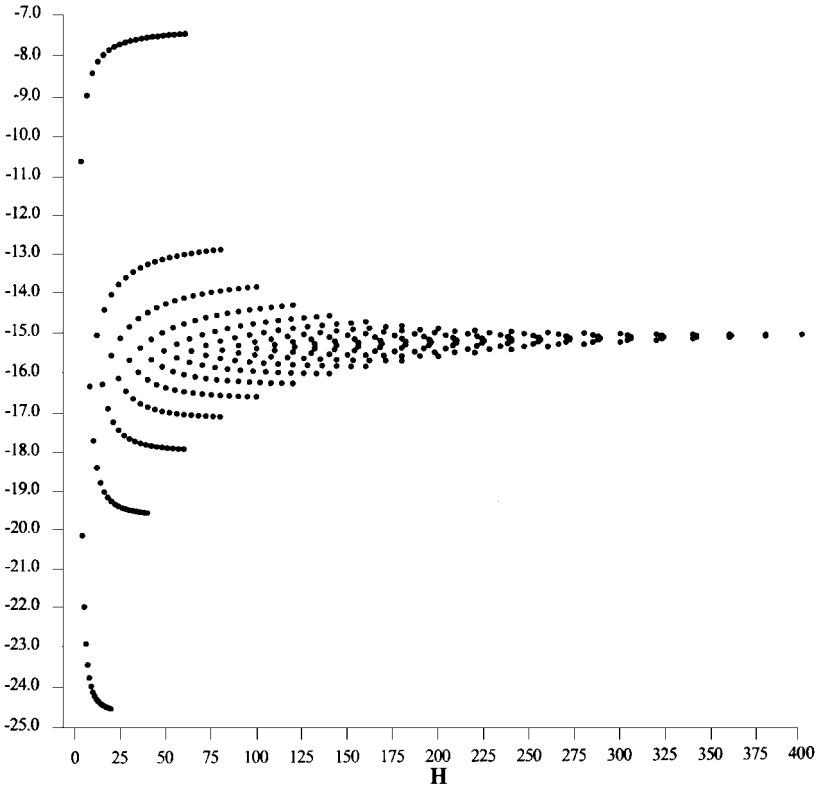

Fig. 4. Variation of hexagon energy, E_h (average interaction energy per hexagon) with respect to H, number of hexagons in the nanotube, $H = LW$.

On the other hand, we also plotted the variation of hexagon energy, E_h (average interaction energy per hexagon) with respect to H, the number of hexagons in the nanotube, in Figure 4.

As seen from Figure 2, E_b *versus* L varies smootly and binding energy degreases very slowly as L increases. Each curve in Figure 2 corresponds to a different W value starting from $W = 3$ up to $W = 20$. On the other hand, the curves for separate W are almost parallel to each other. Separation between successive curves degreases and converges smoothly. The relative separation between the curves is largest between $W = 3$ and 4. This means that the nanotube with $W = 3$ might be very difficult practically to produce.

The variation of E_b *versus* W, in Figure 3, shows a similar trend as seen in E_b *versus* L in Figure 2. In Figure 3 each curve corresponds to a different L value, starting from $L = 1$ upto $L = 20$. The energy positions for $W = 3$ are separated from the rest of them; here again one can see that the nanotube with $W = 3$, whether L is small or large, seems to be very difficult to produce experimently. In both cases, Figures 2 and 3, average binding energy per atom converges to the value of -7.20 eV/atom for the largest size considered in this work ($L = 20$, $W = 20$).

Variation of average interaction energy per hexagon, E_h, with respect to the number of hexagons, H, in carbon nanotubes shows an interesting feature, which is shown in Figure 4. Distribution of average hexagon energies shows three different patterns. For the number of hexagons less than 75 ($H < 75$), E_h varies in the range -25 and -7 eV per hexagon ($-25 < E_h < -7$). On the other hand for the nanotubes with the number of hexagons larger than 100 ($H > 100$), the range of E_h becomes narrower, and reaches a single value of -15.12 eV/hexagon.

In an infinitly large graphene plane or tube, the average interaction energy per hexagon (E_h) should be equal to the twice of the average interaction energy per atom (E_b). Each atom has three bonds in the tube or in the graphene plane, energy per bond is $E_{bond} = E_b/3$. On the other hand, each hexagon has six bonds, energy per bond in this case is $E_{bond} = E_h/6$. From these results one can write that $E_h = 2E_b$. Using this relation one can predict the average binding energy per atom in large tubes as $E_b = E_h/2 = -7.56$ eV/atom. This value should correspond to the asymptotic values of Figures 2 and 3, which represent the infinitely large tube.

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