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Toroidal forms of graphitic carbon. II. Elongated tori

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An elongated toroidal cage form of graphitic carbon C_{240} that has an elliptical cross section is proposed. The elongated toroidal form consists of pairs of pentagons and heptagons among the hexagons of carbon atoms. The rotational symmetry, the cohesive energies, and thermal stabilities of the elongated toroidal forms derived from C_{240}, as well as other various toroidal forms are studied by molecular dynamics. It is found that the sevenfold rotational symmetry is the most stable for the elongated toroidal forms derived from C_{240}, although both fivefold and sixfold rotational symmetries are the most stable for the toroidal forms derived from the tori C_{360} previously proposed by us and from C_{540} proposed by Dunlap. This indicates that five and seven pentagon (on the outer rim) -heptagon (on the inner rim) pairs might also appear in the turnover edge of carbon nanometer-sized tubes, even though only hexagonal pairs are experimentally observed by transmission electron microscopy. The distortion energies of the elongated tori are estimated from the cohesive energies of the series of the tori C_n, where n ranges from 80 to 1680. The proposed structures are found to be thermodynamically stable by the finite-temperature simulations.

I. INTRODUCTION

Various forms of carbon have recently been discovered by experiments: fullerene C_{60},[1] fullerenes of higher order C_{70}, C_{78}, C_{82}, C_{84}, C_{94}, and C_{96},[2] multilayered fullerenes,[3] and carbon nanometer-sized tubes.[4] There are many proposals for other new structures of graphitic carbon: spherical fullerenes of much higher order,[5] such as C_{1500}, nanometer-sized capsules,[6] periodic minimal surfaces (schwarzite) having negative curvature,[7] and toroidal forms[8,10] and helically coiled forms,[11] both of which have the positively curved surface of fullerenes and the negatively curved surfaces of minimal surfaces. Since the cohesive energies of those proposed structures are lower than that of fullerene C_{60}, these structures are expected to exist. Among these, toroidal forms, which have the positively and the negatively curved surfaces, have interesting characters, since they can be expected to have intermediate characters between the isolated fullerene molecule and the extended structures of nanometer-sized tubes or the helically coiled forms.

Topologically, toroidal forms can be constructed from the tubes in the following ways: (1) connecting small sliced parts of the tubes, (2) bending a tube section around and connecting its ends together, and (3) connecting two sections of identical turnover bilayer tube ends at the equator of the resulting torus. By connecting the sliced parts of tubes, Dunlap proposed toroidal structures C_{540} and C_{576},[8] both of which have sixfold rotational symmetry. By using the fivefold rotational symmetric surface of C_{60}, we proposed a fivefold symmetric toroidal form of C_{360} (Ref. 9) (and a series derived from it),[10] as the form connecting a single-layered tube at one edge. The tori proposed by Dunlap contain twelve pairs of pentagons and heptagons in their equators, but our structures consist of ten pairs of pentagons and heptagons, none of which lie on the equator.

Transmission electron microscopy (TEM) images taken by Iijima, Ajayan, and Ichihashi[12] recently provided experimental evidence of the existence of the pairs of pentagons (outer rim) and heptagons (inner rim) in the turnover edge (or turn around edge[12]) of carbon nanotubes. They suggested that the pairs of pentagons and heptagons, appearing in the turnover edge of carbon nanotubes, have sixfold symmetry along the tube axis (thus the number of pairs of pentagons and heptagons is six). These pairs are the essential ones in forming the theoretically proposed toroidal structure. However, parallel fringes appearing in the turnover edge of carbon nanotubes have a separation of 0.34 nm,[12] which is small compared to the distance between outer and inner surface of the previously proposed toroidal structure.[7-9] Thus, in this paper we propose an elongated toroidal structure which has a small separation between parallel fringes. The elongated toroidal structures C_{240} proposed here can be considered as a greatly shortened (0.88-nm length) tube consisting of double layers with two turnover edges as observed by TEM. Hereafter, we use the elongated torus as the torus which has an elliptic cross section whose longer axis is parallel to the rotational axis of the torus. The various symmetric elongated toroidal structures derived from C_{240} and tori derived from Dunlap's torus C_{540} were generated by a similar method to that used to create various toroidal forms from torus C_{360}.[13] The symmetry dependencies of the various tori generated from tori C_{240}, C_{360}, and C_{540} are studied. With the use of the Goldberg algorithm,[14,15] the distortion energies of the series of fivefold symmetric tori generated from torus C_{240} and torus C_{360}, as well as the spherical series created from the spherical fullerene C_{60},[16] are also studied.

II. CONSTRUCTION OF ELONGATED TORI

We provide a method of construction of the elongated toroidal forms of graphitic carbon whose cross section is elliptical. The forms of the proposed elongated tori are different from those of the previous ones, though these structures have a local topology similar to those of other fullerene structures. The outermost and innermost circles in the elongated tori consist of positive and negative curvatures, respectively. The outermost circle contains pentagons and the innermost heptagons. The positively curved surface with fivefold rotational symmetry obtained from the equator (here, the pole is in the center of the pentagon) of spherical C_{240} was used for the outer surface, while for the negative inner surface, the surface of the spherical fullerene C_{60} with the pentagons replaced by heptagons, was used. Thus, the elongated toroidal form of C_{240} is created. In the torus C_{240}, the number of the heptagons is ten, which is equal to that of pentagons to eliminate the excess dangling bonds on the surface. The distortion that is introduced by forming the torus is topologically relaxed by the inclusion of both pentagons and heptagons. This makes it possible to retain a bond distance almost equal to that of the fullerenes.

The elongated torus form has 240 carbon atoms, and it belongs to the point group D_{5d}, since fivefold symmetric surfaces of spherical fullerenes C_{60} and C_{240} were used. The coordinates for the 24 inequivalent sites in the torus are given in Table I. The remaining coordinates of 96 (120 minus 24) atoms on the upper half of the torus are generated by applying four operations of rotating $2\pi/5$ around the center of the torus (or the fivefold rotational axis). The other remaining coordinates of 120 atoms on the lower half of the torus are generated by inverting the upper half of the torus, and rotating by $2\pi/10$ around the center of the torus. As mentioned before, torus C_{240} is constructed from the spherical fullerenes C_{60} and C_{240}. On the other hand, the outer surface of torus C_{360} is obtained from the cluster C_{360}, which is derived from the spherical cluster form C_{540} by removing the parts on either side of its equator,[17] while for the inner surface, the surface of spherical fullerene C_{60} with pentagon-heptagon replacement is used.

TABLE I. Relaxed positions of inequivalent atoms in the C_{240} toroidal structure, given in units of Å. Here, the origin is the center of the torus.

No.	x	y	z
1	7.614	0.805	0.028
2	3.118	6.993	0.028
3	3.549	1.590	0.689
4	2.609	2.884	0.689
5	5.251	5.831	1.331
6	7.168	3.193	1.331
7	3.903	6.726	1.385
8	7.603	1.633	1.385
9	1.891	3.268	2.070
10	3.692	0.789	2.070
11	5.981	5.355	2.665
12	6.942	4.034	2.665
13	3.129	6.978	2.764
14	7.604	0.820	2.764
15	4.211	1.405	3.455
16	2.637	3.571	3.455
17	3.935	2.859	3.922
18	3.568	5.969	3.928
19	6.779	1.549	3.928
20	5.031	5.279	3.950
21	6.576	3.154	3.950
22	2.422	4.927	4.216
23	5.434	0.781	4.216
24	5.152	3.743	4.436

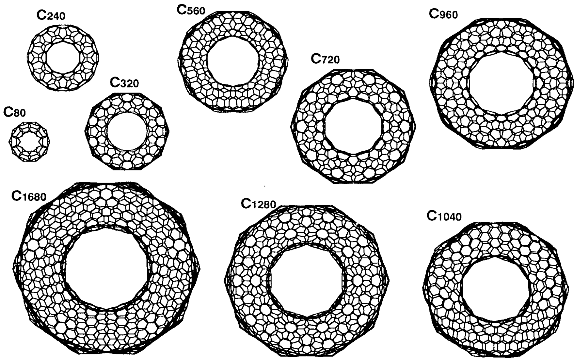

FIG. 1. Top views of the elongated toroidal cage forms of carbon. The subscript of C represents the number of atoms in the toroidal structure. The depicted net represents the nearest-neighbor bonding between the carbon atoms.

The k-rotational symmetric structures were prepared by cutting the k_0-symmetric torus along the radius of curvature into k_0 equal pieces, and by continuously combining the k pieces. Since torus C_{240} has fivefold symmetry ($k_0=5$), each piece contains 48 atoms. Thus, we generated C_{192}, C_{288}, C_{336}, and C_{384} for $k=4$, 6, 7, and 8. For other toroidal forms, such as Dunlap's torus C_{540} which has sixfold symmetry ($k_0=6$), a similar procedure was used to generate various rotational symmetric forms.

Using the prescription of Goldberg, which was also used in deriving the large-scale fullerenes[16] and tori,[10] we can automatically generate large toroidal forms. In the Goldberg transformations,[15] hexagons are inserted into (or removed from) the original C_{240} toroidal structure, and the directions of the pentagons and heptagons are turned appropriately as the toroidal cage changes in size. Each structure thus obtained from torus C_{240} has N carbon atoms, where $N=Nb\,(n^2+nm+m^2)$ ($Nb=80$, n and m are non-negative integers). The elongated toroidal forms containing N atoms obtained from torus C_{240}, where $N=80$, 240, 320, 560, 720, 960, 1040, 1280, and 1680 (see Fig. 1), are thus generated. It is highly likely that the structures will be stable, as in other experimentally discovered carbon forms.

III. METHOD OF CALCULATION

Molecular dynamics is a powerful method for studying both structural and dynamical properties without requiring precise initial geometrical information. Thus, molecular-dynamics methods were used to confirm the stability of the toroidal structures proposed here. The empirical interatomic potential of the carbon atoms was as follows: Stillinger-Weber–type three-body potentials[18] were used to take account of the covalently bonded characters between carbon atoms.[19] Parameters used in these forms were taken from those for graphite proposed by Abraham and Batra:[20] $A=5.373\,2037$, $B=0.508\,245\,71$, $a=1.894\,3619$, $\lambda=18.707\,929$, and $\gamma=1.2$. Here, the constant in the three-body term of one-third is replaced by one-half to represent a graphite sheet (the two-dimensional honeycomb structure). The efficiency of the potential used in the simulations was checked and its validity was confirmed by evaluating the stability and the cohesive energy in the spherical fullerenes as well as in a graphite sheet, as discussed in a previous paper.[9]

The simulation procedures were the same as in previous papers.[10,11] Thus, we briefly comment: The integration of equations of motion for atomic coordinates was performed by the leapfrog algorithm with a time step of 0.36 fs. For the calculation of the ground state of the cohesive energy, the system was eventually cooled down to 0 K by using the first-order equations of motion (dynamical steepest descent method). Less than 10^{-12} J/m of force acting on an atom was used as the convergence criterion. When usual second-order equations of motion were employed for the finite-temperature simulations having more than 20 000 steps, the temperature was gradually raised up to 2000 K using 15 000 steps with the total energy being conserved after 16 000 steps.

IV. RESULTS AND DISCUSSION

A. Symmetry

For the relaxed structure of torus C_{240}, the parallel fringes which correspond to the distance between the outer and inner surface of the torus have a separation of 0.37 nm, which is close to the observed value of the separation (0.34 nm) of those appearing in the turnover edge of carbon nanotube.[12] (The distance between the outer and inner surface of the relaxed structure of tori C_{360} and C_{540} is 0.74 and 0.58 nm, respectively.)

We will discuss the relationship between the rotational symmetry of the pentagon and heptagon pairs and the thermodynamical stability of the toroidal structures. Figure 2 shows the top and side views of the relaxed structures of the various (rotational) symmetric toroidal forms, obtained by steepest decent molecular-dynamics simulations. It can be seen from Fig. 2 that the top surface becomes convex in torus C_{240}, in contrast to the torus C_{360} where the top surface becomes planar as discussed fully later.

For the elongated tori C_{192}, C_{240}, C_{288}, C_{336}, and C_{384} derived from torus C_{240}, the values of the cohesive energies per atom are -7.25, -7.33, -7.37, -7.38, and -7.37 eV (for $k=4$, 5, 6, 7, and 8), respectively. For the potential used here, the sevenfold rotational symmetry is found to be the most stable for these elongated toroidal forms, whereas either fivefold or sixfold rotational symmetry is the most stable for the toroidal forms derived from tori C_{360} and C_{540}. This difference may arise from the fact that the elongated toroidal forms derived from torus C_{240} come closer and closer to the ideal toroidal forms as the rotational symmetrical parameter k approaches 7 (this value of 7 causes the top surface to become wavy). On the other hand, values of k smaller or larger than 6 increase the stress on the surface for tori C_{360} and C_{540}.

In the forms derived from Dunlap's sixfold symmetric torus, C_{540},[8] which contain twelve pairs of pentagons and heptagons in their equators, the fivefold and sixfold symmetric forms are the most stable. For the tori C_{360}, C_{450}, C_{540}, C_{630}, and C_{720} derived from torus C_{540}, the values of lowest cohesive energies per atom are -7.38, -7.40, -7.40, -7.38, and -7.35 eV (for $k=4$, 5, 6, 7, and 8), respectively. (Note that the value for the other sixfold symmetric torus C_{576} of Dunlap is -7.39 eV/atom according to our calculations. In addition, it should be noted that in this work C_{576} is found to be less stable than C_{540}.) There seem to be no substantial changes in the shape of the torus form for tori derived from torus C_{540}. Fivefold and sixfold symmetric toroidal structures C_{450} and C_{540} are the most stable among them, although these are derived from the sixfold symmetric torus C_{540}.

Fivefold and sixfold symmetric toroidal structures C_{432} and C_{360} are the most stable in tori derived from the torus C_{360} (Ref. 9) which, in a sense, consists of two $\pi/5$ rotated turnover edges of tubes, giving 12 and 10 pairs of pentagons and heptagons, respectively. The values of energies per atom of tori derived from torus C_{360}—C_{288}, C_{360}, C_{432}, C_{504}, and C_{576}—are -7.37, -7.41, -7.41, -7.37, and -7.33 eV (for $k=4$, 5, 6, 7, and 8), respectively. For the tori derived from torus C_{360}, although the energies of other symmetric structures are similar, the top surface becomes planar in the sixfold symmetric torus C_{432}, convex in the fivefold symmetric torus C_{360}, and wavy in the sevenfold and eightfold symmetric torus C_{504} and C_{576}.

Since the cohesive energy of the fullerene C_{60} is -7.29 eV/atom and that of the graphite sheet is -7.44 eV/atom, the toroidal forms proposed here (except torus C_{192}) are more energetically stable than C_{60}. Finite-temperature molecular-dynamics simulations also show that all the toroidal structures proposed here (except torus C_{192}) are thermodynamically stable.

From the stress consideration, the ordered pairs of pentagons and heptagons are essential in forming toroidal structures. By TEM experiments, the sixfold rotational symmetric appearance of ordered pairs of pentagons and heptagons is observed in the turnover edges of nanotubes.[12] On the other hand, we showed that the fivefold, sixfold, and sevenfold symmetric pairs of pentagons and heptagons is likely to appear in a toroidal form, from the symmetrical consideration of the tori proposed here. Thus, it is likely that fivefold, sixfold, and sevenfold pairs of pentagons (outer rim) and heptagons (inner rim) may also appear in the turnover edge of carbon nanotubes although only sixfold symmetric pairs have been observed by TEM experiments.[12]

B. Distortion energies of series of tori

In order to compare the series of toroidal forms derived from torus C_{360}, we calculated the cohesive energies of the series of tori derived from fivefold symmetric torus

C_{240} by applying the Goldberg algorithm. We also found that the generator of the series of tori derived from torus C_{240} is torus C_{80} (though it turns out to be unstable as discussed later). Since in our series of toroidal structures the numbers of pentagons and heptagons are kept constant, the local curvatures near the pentagons and heptagons deviate further and further from the global ideal curvature of the torus, with increasing number of carbon atoms N.

The edges of the toroidal structures derived from torus C_{240} (or C_{80}) become wavy with increasing N, as one can see from Fig. 1. The various radii (see the inset of Fig. 3) versus N are given in Fig. 3. As expected from the topological considerations, the radii of the tori increase with $\sqrt{N}$, which is consistent with the series of tori of C_{360} whose generator is the torus C_{120}.

The N dependencies of the cohesive energy of the various toroidal carbon forms are given in Fig. 4. The cohesive energies per atom of tori, as well as spheres, decrease with increasing N. Here, N for the tori derived from C_{240} varies as $N=80$, 240, 320, 560, 720, 960, 1040, 1280, and 1680. For the tori derived from C_{360}, $N=120$, 360, 480, 840, 1080, 1440, 1560, and 1920. For spherical fullerenes, $N=60$, 80, 180, 240, 320, 540, 720, 960, and 1280.

Figure 4 shows the cohesive energy dependence on N for (spherical) fullerenes derived from C_{60} (whose generator is an icosahedron C_{20}) and tori derived from tori C_{240} and C_{360}. (Similar N dependence has been studied using semiempirical electronic potentials.[5] However, it is difficult to discuss the stability of the tori by comparing these results, since the accuracy of the potential leads to different values of the cohesive energies.) Although the elongated tori derived from torus C_{240} are much higher in

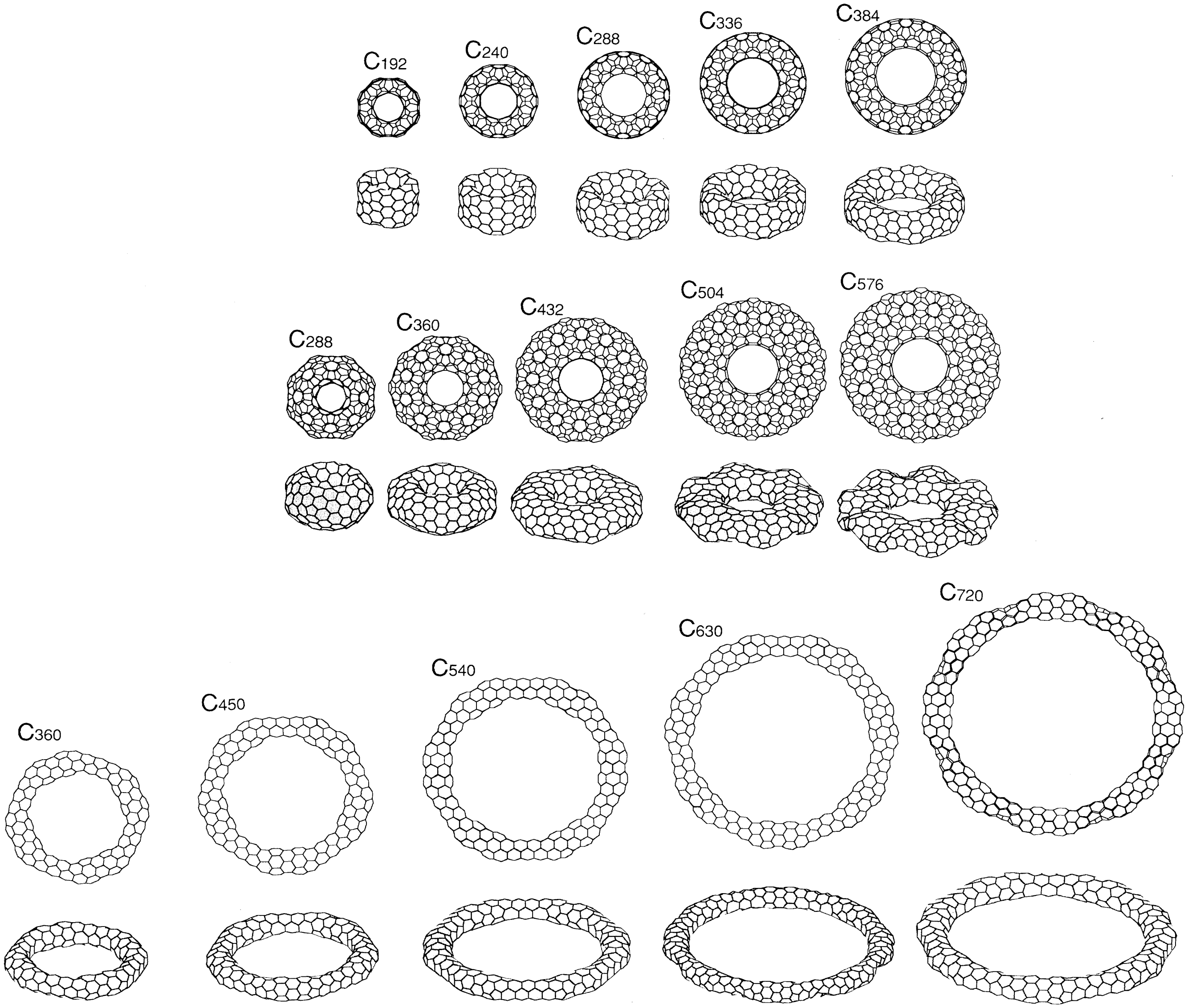

FIG. 2. The symmetric dependencies of the top and side views of the various toroidal structures. From left to right, rotational symmetric parameter k varies from 4 to 8.

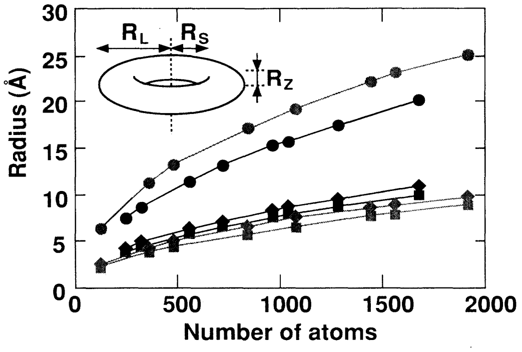

FIG. 3. The radii of the elongated toroidal structures vs the number of atoms in the toroidal structures derived from torus C_{240}. R_L (●), R_S (■), and R_Z (◆) are the lengths of the radii shown in the inset. Those for the toroidal structures derived from torus C_{360} are also shown by gray symbols.

energy than spherical fullerenes or the tori derived from torus C_{360} for given number of N, these elongated tori may exist. This is because the values of the cohesive energies per carbon atom of these toroidal forms are lower than that of the stable fullerene C_{60}, whose cohesive energy is -7.29 eV/atom. (Note that the cohesive energy of the graphite sheet is 7.44 eV/atom.) Thus, the elongated tori are predicted to be energetically stable. The increase in N, which means an increase in the number of hexagons, leads to cohesive energies of the elongated toroidal forms much closer to that of graphite. It should be noted that the cohesive energy per atom E becomes linear in $1/N$ for large N.

The distortion energy of a given structure δE is determined as the energy difference of the energy of a structure per atom E from that of a graphite sheet E_0,

$$\delta E = N(E - E_0) ,$$

where N is the number of carbon atoms in a structure. Here, $E_0 = -7.44$ eV. For large N, the E values for these structures become similar to each other. This indicates that the pentagons and heptagons among the hexagons become independent with increasing N, though they interact with each other when N is small. This is reasonable from the rules of the Goldberg transformation, where only hexagons between the pentagons and heptagons are introduced. The difference in the shape of the tori derived from torus C_{240} and torus C_{360} arises from the difference in the outer surface of these tori as shown in the cross-sectional view of the tori (see Fig. 5). Since the inner surfaces of both tori C_{240} and C_{360} are derived from the surface of the spherical fullerene C_{60} with the same pentagon-to-heptagon replacement, the difference between tori C_{240} and C_{360} arises from the difference in the outer surfaces: Pentagons are located closer to the great circle (or equator) in torus C_{360}, while they are located in the circle of the higher meridian in torus C_{240}. Thus, the shape of the cross section of torus C_{360} is closer to a circle, but that of torus C_{240} is closer to an ellipse. This geometrical difference leads also to the difference in the distortion energies: the distortion energies for C_{60}, C_{240}, and C_{360}, are 9.0, 19.5, and 13.0 eV, respectively. Of these, torus C_{240} has the highest distortion energy. This can also be seen from the angle between pentagons and hexagons. These values are 142.6°, 98°, and 129° for C_{60} and the most bent part of C_{240} and C_{360}, respectively. The largest deviations of the angle for C_{240} and C_{360} from that for C_{60} are 45° and 14°, respectively.

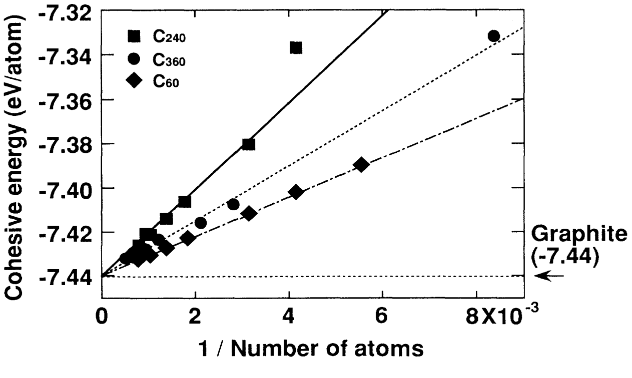

FIG. 4. The cohesive energy per atom of the toroidal structures and fullerenes vs the number of atoms in the torus. The distortion energy of a torus δE is determined as the energy difference of the energy of a torus per atom E from that of a graphite sheet E_0, $\delta E = N(E - E_0)$, where N is the number of carbon atoms in the torus. Here the energies for smaller structures are not plotted.

To confirm the thermodynamical stability, simulations at higher temperatures were also performed. As we heated them up to 2000 K, the geometrical structures retained their stability, though their vibrational amplitude increased with increasing temperature. Thus, we can conclude that elongated toroidal forms of carbon proposed here, except for C_{80} and C_{192}, are thermodynamically stable. Thus, the elongated torus C_{240} and its derivatives will be viable once they are created. The synthesis of the elongated torus C_{240} can be expected in the near future, since the essential parts of the structures have already been observed by TEM experiments in the turnover edges in the nanotubes.[12]

Because we used an empirical interatomic potential for the carbon atoms, the electronic, optical, and chemical properties of toroidal carbon forms remain unexplored. However, as far as thermodynamics are concerned here, the essential part of our study obtained by the Stillinger-Weber potential should not change if more elegant quantum-mechanical calculations or more complicated

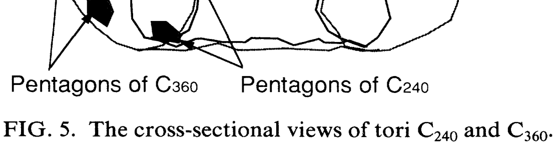

FIG. 5. The cross-sectional views of tori C_{240} and C_{360}.

empirical potential calculations are performed. It is quite interesting to study the properties of the combined forms of the toroidal structures: one-, two-, and three-dimensional crystals, molecules, the extended structures (such as helically coiled forms), and also the nesting form of the tori. We suggest that the structures proposed here are candidates for further theoretical investigations and attempts at synthesis. We think that these structures will become promising for building parts, such as gears and bearings, in nanotechnology.[21]

V. SUMMARY

We have proposed an elongated toroidal form of the carbon structure C_{240} whose parallel fringes have a separation of 0.37 nm which is in good agreement with the value of that of turnover edge in nanotubes observed by TEM. The tori derived from the torus C_{240} have similar geometrical characteristics to the toroidal fullerenes C_{360} and C_{540}, where pentagons and heptagons are introduced into the hexagons. The sevenfold rotational symmetry is the most stable for the elongated toroidal form C_{240}, although both fivefold and sixfold rotational symmetry is the most stable for the toroidal forms derived from tori C_{360} and C_{540}. Thus, it is likely that fivefold, sixfold, and sevenfold pairs of pentagons (outer rim) and heptagons (inner rim) may also appear in the turnover edge of carbon nanotubes although only hexagonal pairs have been observed by TEM experiments.[12] Those elongated toroidal forms proposed here are predicted to be energetically and thermodynamically stable.

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