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Abstract

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Nested boron nitride and carbon-boron nitride nanocones

D. Baowan and J.M. Hill

Abstract: In this letter we extend previously established results for nested carbon nanocones to both nested boron nitride and carbon-boron nitride nanocones. Based purely on mechanical principles and classical mathematical modelling techniques, we determine the energetically favourable structures for nested boron nitride and carbon-boron nitride nanocones. While only three apex angles for boron nitride tend to occur, we also consider the other two angles corresponding to the equivalent carbon nanocones. Two nanocones are assumed to be located co-axially in a vacuum environment. The Lennard-Jones parameters for boron nitride and carbon-boron nitride systems are calculated using the standard mixing rule. For the boron nitride cones, numerical results indicate that the interspacing between two cones is approximately 3.4 Å which is comparable with the experimental results. For the hybrid carbon-boron nitride cones, the numerical results essentially depend on the outer cone angle, and the interspacing distance is also obtained to be approximately 3.4 Å. Moreover, the equilibrium position is such that one cone is always inside the other, and therefore nested double-cones are possible in practice.

1 Introduction

Carbon nanostructures have been widely studied because they are believed to be unique materials which may be used as components to create many future nanodevices. Because of their unique mechanical and physical properties, as well as their simple structures, comprising of pentagonal and hexagonal lattices, carbon nanostructures have stimulated considerable interest because of their capacity to form many novel structures such as carbon nanotori [1] and carbon nanocones [2]. Nanocones may be viewed as an intermediate structure between a graphene sheet and a nanotube [3]. Interatomic potentials such as the Lennard-Jones potential and the Tersoff-Brenner potential have been successfully utilised to investigate ideal arrangements, defects and dynamical properties for such structures [4–10]. In this paper we extend the results of [11] to boron nitride and carbon-boron nitride for nested conical structures formed from nanocones.

The aim of this paper is to utilise the Lennard-Jones potential function and the continuum approximation to determine equilibrium locations for nested boron nitride cones and carbon-boron nitride cones. Boron nitride is a good semiconducting compound which is second only to diamond in hardness. Furthermore, the large band gaps in this material may produce better electronic properties than those of carbon structures [12]. There are two crystal structures for boron nitride which are the cubic and the hexagonal structures, but here we only consider the hexagonal boron nitride which is comparable with a carbon graphene sheet [13].

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For carbon nanocones, there are five possible structures depending on the number of pentagons which are needed to close the vertex [2]. The five cone angles α can be obtained from $\sin(\alpha/2) = 1 - N_p/6$ where N_p is the number of pentagons. Most research deals with the electronic structure of carbon nanocones [14, 15] since they might be regarded as ideal candidates for nanoprobes in scanning tunnelling microscopy [14]. For boron nitride cones, Bourgeois *et al.* [16] investigate the conical structure of boron nitride using transmission electron microscopy and they measure their angles using an electron diffraction technique. From an analysis of the diffraction patterns, they observe a layer of nanocones and two possible models are proposed, which are the monolayer boron nitride cones one inside the other and cones formed from helical overlapping sheets. Moreover, they find that generally apex angles of 84° occur because of a stable square ring at the vertex. Bourgeois *et al.* [17] also observe two other conical structures which have apex angles of 19.2° and 38.9° arising from 300° and 240° disclinations, respectively. They suggest that these two configurations arise because of the different stiffness of the chemical bonds in boron nitride compounds, and square rings which are the favoured ring defects in boron nitride. Furthermore, Han *et al.* [18] study conical nanotubes using highresolution transmission electron microscopy and electron energy loss spectroscopy, and suggest that nested cones occur with the same apex angle as for boron nitride. Xu *et al.* [19] successfully synthesise conical helices of graphitic boron nitride and they theoretically examine their elastic properties. These helices hold considerable promise for potential applications in new-generation high-performance composite materials.

The Lennard-Jones potential function is utilised by Lee [20] who determines gigahertz frequencies for boron nitride oscillators and finds that the frequencies generated by the boron nitride nanotubes are higher than those generated by the corresponding carbon nanotubes. Lee [20] also examines hybrid carbon-boron nitride nanotube oscillators by applying a well known mixing rule for the Lennard-Jones

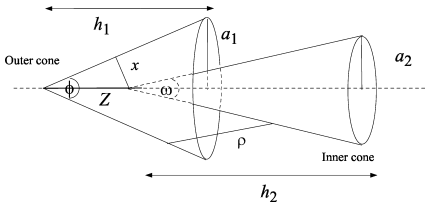

Fig. 1 *Two nested nanocones*

parameters. Baowan and Hill [11] undertake the continuum approximation and the Lennard-Jones potential function to investigate the energetically most favourable structures for any two carbon nanocones. They find that the equilibrium location occurs such that one cone is always inside the other so that nested double-cone configurations are likely to occur in practice.

In this paper, we further examine equilibrium structures for two nested nanocones comprising either boron nitride or carbon-boron nitride, again using the well known Lennard-Jones potential function and the continuum approximation. We exploit analytical expressions obtained previously in [11] and numerical results are determined for the equilibrium distance Z between two vertices and the perpendicular distance x between the inner cone vertex and the surface of the outer cone as shown in Fig. 1. For the hybrid carbon-boron nitride nanocones, the same numerical results are obtained irrespective of which cone is inside the other.

2 Model formation

In [11] for carbon nanocones, the well known Lennard-Jones potential function and the continuum approximation are utilised to determine the energetically most favourable structures for nested cones. Here, we extend those results to both boron nitride and carbon-boron nitride cones. Using the continuum approximation which assumes that the discrete atoms may be replaced by a uniform surface density of atoms over the surface, the total potential energy of the system is obtained by performing double-cone surface integrals. Two Lennard-Jones parameters, the well depth $\varepsilon = A^2/(4B)$ and the van der Waals diameter $\sigma = (B/A)^{1/6}$, for carbon, boron and nitrogen atoms are taken from Lee [20] and shown in Table 1 where A is the attractive constant and B the repulsive constant. Noting that the constants for boron nitride and carbon-boron nitride systems are obtained from the mixing rules which are given by $\varepsilon_{12} = \sqrt{(\varepsilon_1\varepsilon_2)}$ and $\sigma_{12} = (\sigma_1 + \sigma_2)/2$ [21].

We consider two cones not necessarily with the same vertex angle which are located co-axially. The distance between their vertices is denoted by Z and the perpendicular distance from the vertex of the inner cone to the surface of the outer cone at the equilibrium location is denoted by x, as illustrated in Fig. 1. The outer cone has the vertex angle ϕ with base radius a_1 and height h_1, and $r_1 = \beta z_1$ where $\beta = \tan(\phi/2)$. The inner cone has the vertex angle ω with base radius a_2 and height h_2, and $r_2 = \gamma z_2$ where $\gamma = \tan(\omega/2)$. With reference to a rectangular Cartesian coordinate system (x_1, y_1, z_1) with origin located at the vertex of the outer cone, a typical point on the outer cone surface has coordinates $(r_1 \cos\theta_1,\ r_1 \sin\theta_1,\ z_1)$. Similarly, with reference to the same rectangular Cartesian coordinate system $(x_2,\ y_2,\ z_2)$, a typical point on the inner cone surface has coordinates $(r_2 \cos\theta_2,\ r_2 \sin\theta_2,\ Z + z_2)$. The distance between two typical points on the outer and the inner cones is then given by $\rho^2 = (\beta^2+1)z_1^2 + (\gamma^2+1)z_2^2 - 2z_1z_2(\beta\gamma+1) - 2Z\ (z_1 - z_2) + Z^2 + 4\beta\gamma z_1 z_2 \sin^2[(\theta_1 - \theta_2)/2]$, and the total Lennard-Jones potential energy can be written as

$$E = \eta_1\eta_2\left(\frac{a_1a_2\sqrt{(a_1^2+h_1^2)(a_1^2+h_1^2)}}{h_1^2h_2^2}\right) \times \int_0^{h_2}\int_0^{h_1}\int_0^{2\pi}\int_0^{2\pi} z_1z_2\left(-\frac{A}{\rho^6}+\frac{B}{\rho^{12}}\right) \times \mathrm{d}\theta_1\,\mathrm{d}\theta_2\,\mathrm{d}z_1\,\mathrm{d}z_1$$

where η_1 and η_2 denote mean atomic surface densities of the outer and the inner cones, respectively. Analytical expressions for the θ_1 and θ_2 integrals can be evaluated either in terms of hypergeometric functions or Legendre functions and we refer the reader to Baowan and Hill [11] for the details of these calculations. Integrations with respect to z_1 and z_2 need to be performed numerically using the algebraic package MAPLE.

3 Numerical results

Following the work of Bourgeois *et al.* [16, 17], the apex angles α assumed for the three different boron nitride cones which tend to occur in practice are 19.2°, 38.9° and 83.6°. The height h is assumed to be 50 Å which corresponds to base radii of 8.338, 16.649 and 33.327 Å, respectively, which are determined from $a = h\tan(\alpha/2)$. Numerical values for the equilibrium distance Z between the two vertices and the perpendicular distance x at the equilibrium location between the vertex of the inner cone and the surface of the outer cone for any two of the above three boron nitride cones are presented in Table 2. Moreover, the other two vertex angles for boron nitride cones corresponding to the equivalent carbon nanocones are also considered and shown in Table 2. Corresponding values for any of the five possible carbon-boron nitride cones are shown in Table 3. For the carbon-boron nitride cones, the numerical results essentially depend on the outer cone angle and they indicate that the same results are obtained irrespective of which cone is inside the other.

For two identical cones, we observe that the equilibrium distance Z decreases for increasing cone angle, which is due

Table 1: Lennard-Jones constants

	C	B	N	BN	C-BN
ε(eV)	0.002635	0.004116	0.006281	0.005085	0.003660
σ (Å)	3.369	3.453	3.365	3.410	3.390
A (Å^{-6})	15.412	27.907	36.475	32.005	22.220
B (Å^{-12})	22 534.750	47 303.611	52 955.321	50 364.986	33 723.874

Table 2: Equilibrium distance Z (Å) between two vertices and the perpendicular distance x (Å) for boron nitride cones

Outer angels / Inner angels		19.2°	38.9°	60.0°	83.6°	112.9°
19.2°	*Z*	20.317	8.324	5.901	4.746	4.143
	x	3.388	2.772	2.951	3.163	3.453
38.9°	*Z*	34.378	10.708	5.823	4.718	4.097
	x	5.733	3.566	2.912	3.145	3.414
60.0°	*Z*	39.926	23.363	7.586	4.646	4.051
	x	6.658	7.780	3.793	3.097	3.376
83.6°	*Z*	42.800	30.344	17.873	6.146	3.995
	x	7.138	10.104	8.937	4.097	3.329
112.9°	*Z*	44.603	34.625	24.619	14.672	5.320
	x	7.438	11.530	12.310	9.779	4.434

Table 3: Equilibrium distance Z (Å) between two vertices and the perpendicular distance x (Å) for carbon-boron nitride cones

Outer angels / Inner angels		19.2°	38.9°	60.0°	83.6°	112.9°
19.2°	*Z*	20.188	8.278	5.863	4.732	4.101
	x	3.367	2.756	2.936	3.154	3.418
38.9°	*Z*	34.321	10.667	5.754	4.685	4.070
	x	5.724	3.552	2.877	3.123	3.392
60.0°	*Z*	39.873	23.316	7.554	4.630	4.025
	x	6.650	7.764	3.777	3.086	3.354
83.6°	*Z*	42.772	30.316	17.835	6.099	3.962
	x	7.133	10.095	8.918	4.065	3.302
112.9°	*Z*	44.560	34.598	24.592	14.642	5.282
	x	7.431	11.521	12.296	9.759	4.402

to the repulsive force arising from the vertices. The inter-spacing distance x is found to be approximately 3.4 Å which is in excellent agreement with Bourgeois *et al.* [17] for nested cones. Furthermore, the equilibrium distance Z decreases for the case when the inner cone angle is smaller than that of the outer cone. This is because the inner cone can move closer to the outer vertex for the distance x to attain the value 3.4 Å. In this case, the perpendicular distance x which is illustrated in Fig. 1 is the shortest distance between the inner vertex and the outer wall. Consequently, the equilibrium distance Z is increased when the inner cone angle is larger than that of the outer cone, and the distance x between the inner vertex and the outer wall is actually the greatest distance between the two surfaces.

The relation between the cone angles and the distance Z for boron nitride nanocones is shown in Figs. 2–4. For two identical boron nitride cones, we observe that at the equilibrium location the system is more stable for the larger apex angle as shown in Fig. 2. This is because the large apex angle reduces the repulsive force arising from the vertex. In the case when the outer cone has a larger apex angle than that of the inner cone, the stability of the system also increases for increasing inner cone angle as shown in Fig. 3. On the other hand, the system is less

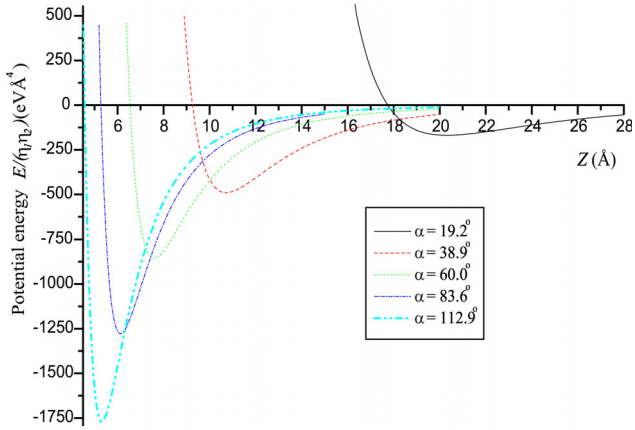

Fig. 2 *Potential energy against the distance Z between two vertices for five identical possible boron nitride nanocones*

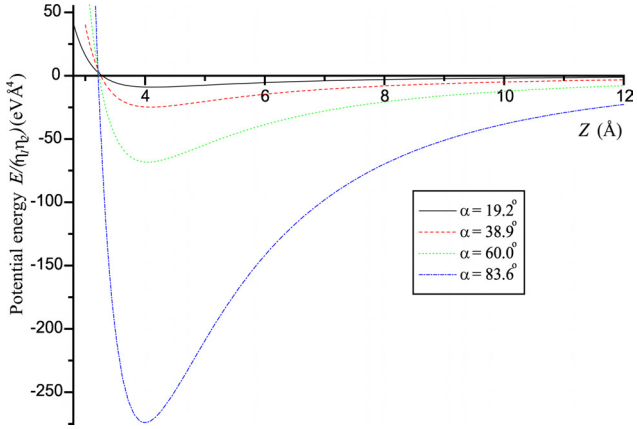

Fig. 3 *Potential energy against the distance Z between two vertices for boron nitride cones when the outer cone angle α = 112.9° and the inner cone angles α = 19.2°, 38.9°, 60.0° and 83.6°*

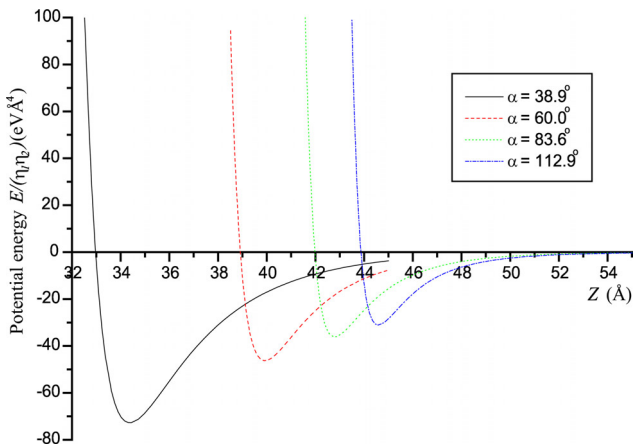

Fig. 4 *Potential energy against the distance Z between two vertices for boron nitride cones when the outer cone angle α = 19.2° and the inner cone angles α = 38.9°, 60.0°, 83.6° and 112.9°*

stable at the equilibrium location if the outer cone angle is smaller than that of the inner cone as illustrated in Fig. 4. This indicates that the nested cones are less likely to occur when the vertex angle of the outer cone is smaller than that of the inner cone. We note that the energy profiles for the carbon-boron nitride nanocones are similar to those for boron nitride nanocones and we do not repeat them here.

4 Summary

The major contribution of this letter is to extend the results of [11] derived for carbon nanocones to both boron nitride and carbon-boron nitride nanocones. The energetically favourable structures for nested boron nitride and carbon-boron nitride cones in a vacuum environment are investigated by employing the Lennard-Jones potential function and the continuum approximation. The Lennard-Jones parameters for boron nitride and carbon-boron nitride systems are obtained using a standard mixing rule to determine the Lennard-Jones constants, A and B. For both boron nitride and carbon-boron nitride nanocones, we examine all five possible vertex angles which occur for carbon nanocones. The interspacing between two monolayer cones is obtained to be approximately 3.4 Å for both systems, and this result is in excellent agreement with the finding of Bourgeois *et al.* [17]. Furthermore, the equilibrium location always occurs with one cone inside the other, so that nested double-cones might be expected to form in practice.

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