



# Temperature-dependent thermal expansion of graphene

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## HIGHLIGHTS

- The CTE of Graphene is calculated by an exact method.
- The Brenner many-body potential and harmonic oscillator model are employed.
- CTE of graphene is negative and tends toward zero by increasing the temperature.
- The model can be used to predict theoretically the CTE of other carbon structures.

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## ABSTRACT

In this paper the coefficient of thermal expansion of graphene is calculated by a new method based on the thermodynamics parameters. First, the graphene is investigated at zero temperature and then the changes made by temperature are studied. The Brenner many-body potential and harmonic oscillator model are employed to describe the interactions between carbon atoms in the graphene. The results show that the coefficient of thermal expansion of graphene is negative and tends toward zero by increasing the temperature which is in good agreement with reported experimental results. The approach presented in this paper can be used to predict theoretically the CTE of other structures of carbon such as nanotubes and composites.

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## 1. Introduction

Graphene was discovered in 2004 [1] and due to its unique thermal, electrical and mechanical properties [2–9] including high intrinsic mobility and thermal conductivity and good electrical conductivity, has attracted a lot of attention in recent years [10–13]. Two of the most important issues in design, manufacturing and usage of graphene-based nano devices are recognizing and controlling the temperature-dependent properties of graphene. One of the mentioned properties is thermal expansion of the graphene. There are different methods for investigation of coefficient of thermal expansion (CTE) of graphene. Mounet and Marzari used the density functional perturbation theory to investigate CTE of graphene [14]. Their study's results showed a distinctive in-plane negative CTE for graphene. Nonequilibrium Green's function approach is employed by Jiang et al. which shows a negative CTE for graphene in absence of interaction between graphene and its substrate [15]. The negative CTE of graphene is experimentally estimated by using temperature-dependent Raman spectroscopy in the temperature range between 200 and 400 K [16]. The results of molecular dynamics simulations carried out by Zahabul Islam et al. [17] show that the CTE of graphene is negative over a temperature range of 0–500 K. Silva

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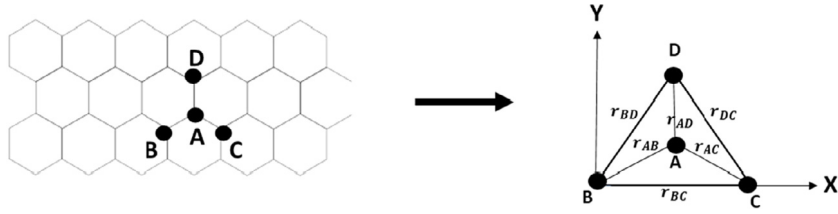


Fig. 1. (Left) a carbon atom in the graphene and its nearest neighbors and (Right) the geometry parameters of the problem.

et al. obtained a negative value for the CTE of graphene at room temperature by extension of the unsymmetrized self-consistent field method [18]. Also the negative CTE of graphene is obtained by the equation of state based on thermodynamic variables [19].

However there is not an exact physics-based theoretical model to describe and calculate the CTE of graphene. In this paper, a theoretical approach based on Brenner many body potential [20] and harmonic oscillator model [21] is presented to calculate the temperature-dependent CTE of graphene. According to the results obtained in next sections, the CTE of graphene is negative in a wide range of temperature and tends toward zero by increasing the temperature which is in agreement with experimental reports.

## 2. Theoretical calculations

### 2.1. Geometry of problem

Graphene is a two dimensional sheet of carbon atoms which are arranged in a honeycomb lattice due to their  $sp^2$  hybridization and each of atoms is connected to three other atoms by covalent bonds. Fig. 1 shows the atom A with its three nearest neighbor atoms.

Due to the periodic properties of atoms in the graphene, the position of all atoms can be achieved by the translation of these four atoms. The bond length between any two atoms,  $r$ , e.g. W and Z with coordinates  $(x_w, y_w)$  and  $(x_z, y_z)$  is given by

$$r_{wz} = \sqrt{(x_w - x_z)^2 + (y_w - y_z)^2} \quad (1)$$

The angles between atoms are expressed by

$$\cos(\angle BAD) = \frac{r_{DA}^2 + r_{AB}^2 - r_{BD}^2}{2 r_{DA} r_{AB}} \quad (2)$$

$$\cos(\angle BAC) = \frac{r_{AB}^2 + r_{AC}^2 - r_{BC}^2}{2 r_{AB} r_{AC}} \quad (3)$$

$$\cos(\angle CAD) = \frac{r_{DA}^2 + r_{AC}^2 - r_{DC}^2}{2 r_{DA} r_{AC}} \quad (4)$$

### 2.2. Brenner many-body potential

In this section, the Brenner potential is introduced and rewritten for graphene. According to the Brenner potential, the energy saved in a carbon bond,  $V$ , depends on the bond length and the angles between bonds, means that [20]

$$V(r_{ij}, \theta_{ijk}) = V_R(r_{ij}) - \bar{B}_{ij} V_A(r_{ij}) \quad (5)$$

where  $V_R$ ,  $V_A$  and  $\theta_{ijk}$  are repulsive pair term of the potential, attractive pair term of the potential and the angle between the bond  $i-j$  and bond  $i-k$ , respectively. The repulsive and attractive pair terms are given by

$$V_R(r) = \frac{D^{(e)}}{s-1} e^{-\sqrt{2s}\beta(r-R^{(e)})} f_c(r) \quad (6)$$

$$V_A(r) = \frac{D^{(e)}s}{s-1} e^{-\sqrt{\frac{2}{s}}\beta(r-R^{(e)})} f_c(r) \quad (7)$$

$D^{(e)}$ ,  $R^{(e)}$ ,  $\beta$  and  $s$  depend on the physical properties of various type of carbon atoms and their values are given in Table 1. The cut-off function,  $f_{ij}(r)$ , which restricts the pair potential to nearest neighbors, is given by

$$f_c(r) = \begin{cases} 1 & r < R^{(1)} \\ \frac{1}{2} \left( 1 + \cos \left( \frac{\pi(r-R^{(1)})}{(R^{(2)}-R^{(1)})} \right) \right) & R^{(1)} < r < R^{(2)} \\ 0 & r > R^{(2)} \end{cases} \quad (8)$$

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