INTRODUCTION

Graphene is a two dimensional crystalline material and discovered in 2004. It has exceptional mechanical properties investigated by the different researchers during recent past years. It has been found that electronic structure of graphene depends on the strain produced at different temperatures in it. Graphene band structure can be changed by applying strains larger than 15% \(^7\). In addition to that it is noted that a compressed monolayer of graphene with size 30×100 µm\(^2\) is fastened with 0.7% strain approximately. There are two widely used theoretical approaches available to study the various mechanical properties. These theories are based on elastic continuum and the interatomic potentials (EP)\(^4, 9, 10\) such as the Brenner potential (REBO)\(^11, 12\) and the LCBOPII potential\(^13\).

Due to instability coupled with stretching modes, the graphene is expected to be strongly anharmonic. This coupling plays an important role to prevent the cracking in crystal and stabilize the flat phase as confirmed by atomistic simulations for graphene at room temperature. This is well established that anharmonicity is of general importance in condensed matter in relation to structural phase transitions, soft modes in ferroelectrics, melting, and other related phenomena. Since the anharmonicity in crystals is very weak, it can be explained within the framework of quantum theory of perturbation\(^16, 20\).
However, this is not true for graphene which is a strongly anharmonic crystal. Therefore, the atomistic simulations offer the possibility to study anharmonic effects for a specific material without the need of perturbation theory. A very accurate description of thermodynamic properties of different allotropes of carbon including graphene is provided by the empirical bond order potential LCBOPII.

Many interatomic potentials have been used to calculate the thermal and bending modulus properties of graphene at zero temperature. In the present study we have applied for the first time, the potential free model to analyze the thermal expansion behavior of graphene with varying temperature from room temperature to higher temperature range. The mathematical formulation is described in section 2 and the results are discussed in section 3.

Mathematical formulation

Considering the product of thermal expansion coefficient \( \alpha = \frac{1}{V} \left( \frac{dV}{dT} \right)_p \) and bulk modulus \( K_T \) remains constant under the effect of temperature i.e.,

\[
\alpha K_T = \text{Constant} \quad \ldots (1)
\]

On the basis of equation (1) Singh and Gupta [29] derived the equation of state to determine the values of \( \alpha_T \) and \( V/V_0 \). These expressions are given below:

\[
\alpha_T = \alpha_0 \left[ \frac{\delta_T^0 \alpha_0}{T_0^k} \right]^{1/2} \left[ T_0^{k-1} - T_T^{k-1} \right]^{-1} \quad \ldots (2)
\]

and

\[
\frac{V}{V_0} = \exp \left[ \int_{T_0}^{T} \frac{\alpha_0}{1 - \alpha_0 \delta_T^0 \left( T_0^{k-1} - T_T^{k-1} \right)} \right] dT \quad \ldots (3)
\]

Or

\[
\frac{V}{V_0} = \exp \left[ \int_{T_0}^{T} \frac{\alpha_0}{1 - A \left( T_0^{k-1} - T_T^{k-1} \right)} \right] dT \quad \ldots (4)
\]

Table 1: Input data used in present work for Graphene at room temperature

<table>
<thead>
<tr>
<th>( \alpha_0 (\text{Å}) )</th>
<th>( \alpha_4 \left( 10^4 \text{K}^{-1} \right) )</th>
<th>( K_0 \left( \text{eV Å}^{-2} \right) )</th>
<th>( \alpha_T )</th>
</tr>
</thead>
</table>

Table 2: Calculated values of thermal expansion coefficient \( (\alpha_T) \), volume thermal expansion \( (V/V_0) \) and bulk modulus \( (K_T) \) with varying temperature

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>( \alpha_T (10^4 \text{K}^{-1}) )</th>
<th>( V/V_0 )</th>
<th>( K_0 \left( \text{eV Å}^{-2} \right) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>-4.8</td>
<td>0.9975</td>
<td>0.9969</td>
</tr>
<tr>
<td>400</td>
<td>-4.46</td>
<td>0.9969</td>
<td>0.9962</td>
</tr>
<tr>
<td>500</td>
<td>-3.36</td>
<td>0.9963</td>
<td>0.9957</td>
</tr>
<tr>
<td>600</td>
<td>-3.21</td>
<td>0.9954</td>
<td>0.9951</td>
</tr>
<tr>
<td>700</td>
<td>-2.85</td>
<td>0.9947</td>
<td>0.9945</td>
</tr>
<tr>
<td>800</td>
<td>-2.5</td>
<td>0.9941</td>
<td>0.9938</td>
</tr>
<tr>
<td>900</td>
<td>-2.35</td>
<td>0.9936</td>
<td>0.9935</td>
</tr>
<tr>
<td>1000</td>
<td>-2.20</td>
<td>0.9938</td>
<td>0.9935</td>
</tr>
</tbody>
</table>
conformed with the temperature dependent Raman spectroscopy and in good agreement with those values obtained from QHA-GGA ab-initio study. This confirms the validity of the equation of state used in the present investigation to analyze the thermal expansion behavior of graphene at high temperature.

On the basis of overall descriptions it is emphasized that a simple and straightforward method used in the present study is capable of explaining the temperature dependent properties of graphene successfully. The methodology adopted in the present work may be of current interest to those researchers engaged in the study of mechanical properties of nanomaterials and alike materials.

REFERENCES

18. Souvatzi, P.; Erixsson, O.; Katsnelon, M.I.;


