Pressure Derivatives of Fullerene $C_{60}$

Vinu T P

Dept. of Physics, NSS Hindu College,
Changanacherry, Kerala, INDIA - 686 102

Abstract

The complete set of second - and third - order elastic constants of cubic fullerene $C_{60}$ is obtained using the finite strain elasticity theory by considering interactions up to three nearest neighbors of each molecule in the unit cell. The energy density is then compared with the strain dependent lattice energy density obtained from the continuum model approximation to obtain the expressions for the second-and third-order elastic constants of $C_{60}$. The second-order potential parameters are obtained from the measured second-order elastic constant of $C_{60}$ and the third order potential parameters are estimated from the Lennard-Jones type of inter atomic potential for $C_{60}$. We also determine the effect of pressure on the second-order elastic constants of $C_{60}$.

Key words- elastic constants, fullerene, potential parameters

I. INTRODUCTION

$C_{60}$ is the best-studied molecule of the newly discovered fullerene series. The $C_{60}$ molecule, which has icosahedral symmetry, are bound together by weak Van der Waal’s interactions and form a close-packed array of a face-centered-cubic (fcc) lattice\(^1\)\(^-\)\(^3\), with a lattice constant of 14.2 Å\(^0\).\(^4\)\(^-\)\(^7\)

Higher order elastic constants and their pressure derivatives provide insight in to the nature of binding forces between molecules since they are represented by the
derivative of the internal energy of the crystal\textsuperscript{8}. The response of a material to an applied stress is determined by the elastic constants and their pressure derivatives.

II. THEORY

A. Procedure to obtain elastic constants

The method of homogenous deformation\textsuperscript{9} is used for the determination of the strain energy density of $C_{60}$. The elastic properties are expressed by means of the derivatives of $\phi$ with respect to atomic displacements when the lattice is deformed. Expressions for the elastic constants are obtained in terms of parameters of the generalized theory\textsuperscript{10}. The potential $\phi$ of the lattice can be expanded in Taylor series as

$$\phi = \phi_0 + O\phi \left[ \sum_l \Delta R^2(l) \right] + \frac{1}{2} O\phi \left[ \sum_l [\Delta R^2(l)]^2 \right] + \frac{1}{6} O\phi \left[ \sum_l [\Delta R^2(l)]^3 \right] + \cdots \quad (1)$$

where $l$ refers to the nearest neighbors. $O\phi, O^2\phi, O^3\phi$ are the first, second and third-order coordinate derivatives of the potential function $\phi$.

If the atoms suffer displacement because of the deformation of the lattice, the potential due to two-body interactions arising from three nearest neighbors can be written as

$$\phi' = \phi + \frac{1}{2} \sum_{N=1}^{3} \sum_{\mu=1}^{4} \left\{ \frac{1}{2} k_2 \left[ R \left( \frac{L}{\mu} \frac{L+N}{\mu'} \right) - R \left( \frac{L}{\mu} \frac{L}{\mu'} \right) \cdot R \left( \frac{L}{\mu} \frac{L+N}{\mu'} \right) \right]^2 + \right\}$$

$$\frac{1}{6} k_3 \left[ R \left( \frac{L}{\mu} \frac{L+N}{\mu'} \right) - R \left( \frac{L}{\mu} \frac{L}{\mu'} \right) \cdot R \left( \frac{L}{\mu} \frac{L+N}{\mu'} \right) \right]^3 \right\}$$

where $k_2$ and $k_3$ are second- and third-order potential parameters respectively.

On comparing with the strain dependant lattice energy density expression from the continuum model approximation\textsuperscript{10},

$$U = \frac{1}{2} \sum_{ijkl} C_{ijkl} \eta_{ij} \eta_{kl} + \frac{1}{6} \sum_{ijklmn} C_{ijklmn} \eta_{ij} \eta_{kl} \eta_{mn} + \cdots \quad (3)$$
Equating coefficients of similar terms in $\eta_2^2 \eta_{kl}$, we get the expression for the second order elastic constants as

$$
\begin{align*}
C_{11} &= 276k_2' \\
C_{12} &= 114k_2' \\
C_{44} &= 114k_2'
\end{align*}
$$

(4)

where $k_2' = \frac{k_2 a^4}{V_z}$ and $V_z$ is the volume of unit cell of $C_{60}$.

The potential parameter $k_2$ has been obtained by substituting the value of $C_{11}$ in equation (4). The values of second order elastic constants for $C_{60}$ are obtained from equation (4) and are given in table [I] along with reported values. Here we have chosen $C_{11}$ calculated by R.V Gopala Rao to determine the potential parameter $k_2$.

The expressions for the third order elastic constants are also obtained by equating the coefficients of $\eta_2^2 \eta_{kmn}$ as

$$
\begin{align*}
C_{111} &= 1494k_3' \\
C_{112} &= 387k_3' \\
C_{123} &= 252k_3' \\
C_{144} &= 252k_3' \\
C_{155} &= 252k_3' \\
C_{456} &= 387k_3'
\end{align*}
$$

(5)

where $k_3' = \frac{-k_3 a^6}{V_z}$, $k_3$, the third order potential parameter and is evaluated by assuming a Lennard-Jones type of inter atomic potential.

$$
\phi(r) = 4\epsilon \left[ \left( \frac{\sigma}{R} \right)^{12} - \left( \frac{\sigma}{R} \right)^{6} \right]
$$

(6)

where $4\epsilon \sigma^6 \equiv A$ and

$$
\phi(r) = \frac{B}{R^{12}} - \frac{A}{R^6}
$$

We obtain, $k_3 = \left[ \frac{1}{6} \left( \frac{d^2 \phi}{dx^2} \right) \right]_{r=a} = -\frac{4k_2}{a^2}$

Using the values of $k_2$ and $k_3$ all the six third order elastic constants of $C_{60}$ are obtained and are given in Table [II].
B. Procedure to obtain the pressure derivative of the elastic constants.

Consider a cubic lattice subjected to a hydrostatic pressure $P$. An infinitesimal stress is superimposed on this deformed state. The expressions for the pressure derivatives of the second-order elastic constants are given in Equation (7).

$$\frac{dC_{11}}{dP} = \frac{-1}{C_{11} + 2C_{12}} [C_{111} + 2C_{112} + 3C_{11} + 4C_{12}]$$

$$\frac{dC_{12}}{dP} = \frac{-1}{C_{11} + 2C_{12}} [2C_{112} + C_{123} + C_{12}]$$

$$\frac{dC_{44}}{dP} = \frac{-1}{C_{11} + 2C_{12}} [C_{144} + 2C_{155} + C_{44} + C_{11} + 2C_{12}]$$

(7)

Substituting the values of second-and third-order elastic constants of $C_{60}$ in equation (7) we get the pressure derivatives of the second-order elastic constants of $C_{60}$.

III. RESULTS AND DISCUSSIONS

The results of the second order elastic constants as obtained from this theory are in good agreement with the results obtained by R.V Gopala Rao$^{12}$ and other theoretical results$^{13-15}$. The value of the second-order elastic constant $C_{11}$, obtained in the present work is in good agreement with corresponding value obtained by J.P Lu$^{20}$ and E. Burgos$^{11}$. We apply Martin’s$^{21}$ criteria for testing the numerical validity of SOEC’s. According to Martin the following equation should be satisfied by the elastic constants. The equation is

$$(7/6) \frac{2}{C_{44}} \left( C_{11} + \frac{2}{7} C_{12} \right) / \left( (C_{11} + 2C_{12})(C_{11} - C_{12}) \right) = 1.$$ 

Putting the present calculated values we get the left side as equal to 0.98.

The calculated values of the third order elastic constants of $C_{60}$ are given in Table [II]. All the results are negative and are in agreement with the values obtained by Vekatesh$^{14}$. The constant $C_{111}$ is the largest as in the case of diamond which shows anisotropy$^{18}$ of $C_{60}$.

Table [III] gives the calculated values of the pressure derivatives of the second-order elastic constants of $C_{60}$. It is found that the pressure derivatives of the elastic constants in the directions $C_{11}$, $C_{12}$ and $C_{44}$ are positive in the present work, which means that these three elastic constants are increasing with increasing pressure. The results obtained are in good agreement with the experimental values as reported by Duclos$^{16}$. 
**Pressure Derivatives of Fullerene \( C_{60} \)**

### Table [I]. Second order elastic constants of \( C_{60} \) in units of \( 10^{12} \text{ dyn/cm}^2 \)

<table>
<thead>
<tr>
<th></th>
<th>( C_{11} )</th>
<th>( C_{12} )</th>
<th>( C_{44} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Present work</td>
<td>0.37</td>
<td>0.15</td>
<td>0.15</td>
</tr>
<tr>
<td>R.V Gopala Rao(^{12})</td>
<td>0.37</td>
<td>0.15</td>
<td>0.17</td>
</tr>
<tr>
<td>E.Burgos(^{11})</td>
<td>0.14</td>
<td>0.07</td>
<td>0.07</td>
</tr>
<tr>
<td>X. Li(^{13})</td>
<td>0.30</td>
<td>0.14</td>
<td>0.16</td>
</tr>
<tr>
<td>R.Venkatesh(^{14})</td>
<td>0.22</td>
<td>0.11</td>
<td>0.11</td>
</tr>
<tr>
<td>Jin Yu(^{15})</td>
<td>0.26</td>
<td>0.14</td>
<td>0.12</td>
</tr>
</tbody>
</table>

### Table [II]. Third order elastic constants of \( C_{60} \) in units of \( 10^{12} \text{ dyn/cm}^2 \)

<table>
<thead>
<tr>
<th></th>
<th>( C_{111} )</th>
<th>( C_{112} )</th>
<th>( C_{144} )</th>
<th>( C_{155} )</th>
<th>( C_{123} )</th>
<th>( C_{456} )</th>
</tr>
</thead>
<tbody>
<tr>
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<td>-800</td>
<td>-210</td>
<td>-210</td>
<td>-210</td>
<td>-140</td>
<td>-140</td>
</tr>
<tr>
<td>R.Venkatesh(^{14})</td>
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<td>-190.5</td>
<td>-161.4</td>
<td>-160.5</td>
<td>-180</td>
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### Table [III]. The pressure derivative of the second-order elastic constants of \( C_{60} \)

<table>
<thead>
<tr>
<th></th>
<th>( \frac{dC_{11}}{dP} )</th>
<th>( \frac{dC_{12}}{dP} )</th>
<th>( \frac{dC_{44}}{dP} )</th>
</tr>
</thead>
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<td>8.1</td>
<td>7.1</td>
</tr>
<tr>
<td>R.Venkatesh(^{14})</td>
<td>25</td>
<td>14</td>
<td>12</td>
</tr>
<tr>
<td>R.V GopalaRao(^{12})</td>
<td>6.7</td>
<td>3.3</td>
<td>3.1</td>
</tr>
</tbody>
</table>

**REFERENCE**
