THIRD ORDER ELASTIC CONSTANTS OF C_{60} IN Fcc PHASE

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ABSTRACT

We have applied an Extended Three Body Force Shell Model (ETSM) for the investigation of third order elastic constants of C_{60} in Fcc phase. The TOECs are responsible for finite elasticity, where the elastic stress is non-linear with elastic strain. The elastic shear behaviour is asymmetric with respect to shear displacements in certain crystallographic planes. The third order elastic constants pertain the knowledge about ion-core repulsive interactions, which varies with the interatomic separation. Here, we could compare our result with other available data for some properties only at room temperature.

I. INTRODUCTION

In the present decade, considerable interest has been taken in the investigation of anharmonic properties of materials of various kinds [1, 2]. Many workers have contributed in the field through their experimental and theoretical approach. Several efforts have been made in the study of physical and anharmonic properties of solids of different types [3-6]. Utilizing different physical conditions and using several techniques. Some interesting results have been presented by several investigators while studying the anharmonic properties of the substances possessing various crystal structures. Some have studied temperature variation of anharmonic properties of mixed alkali halides and cyanides of rare gas materials [9] of alkali halides [7, 8, 10] using ultrasonic [11, 12] and Brillouin scattering [13] methods.

The static and Dynamic structural properties of solid C_{60} are currently the subject of numerous investigations. At room temperature, the crystal has a face-centered cubic fcc structure, the fcc phase has the symmetry of the space group Fm3m with a lattice constant of $a_0=14.2$Å where the C_{60} molecules rotate freely. With decreasing temperature, the rotational degrees of freedom of the C_{60} molecules becomes more and more hindered and the solid C_{60} undergoes a first order structural phase transition from orientationally disordered fcc phase to an orientationally ordered simple cubic structures with four molecules per unit cell located on four different cubic sub lattices having different orientations[14].

Since the discovery of superconducting properties of C_{60} and the ability to prepare large quantities of this material [15, 16] an enormous amount of work has been carried out on it. Since Krastchmer *et al.* [14] produced macroscopic quantities of fullerene, knowledge of the molecular and solid state chemistry of C_{60} has had rapid growth. Solid C_{60} is a van der Waals bonded molecular crystal having a close packed face centered cubic structure at 300 K.

We have developed an Extended Three-Body Force Shell Model (ETSM), this model has successfully been applied to study the static, dynamic, dielectric, optical

and anharmonic properties of pure ionic crystals, cyanides and alkali halide- cyanide mixed crystals having NaCl structure, we have applied the ETSM to calculate the TOECs of C_{60}.

The essential formulation of the present model is given in the next section and the results obtained by us are presented and discussed in the subsequent section.

II. FORMULATION

The interaction potential used to derive the framework of the present ETSM can be expressed as [17, 18]

$$\phi = -\frac{e^2}{2}\sum_{kk'} Z_k\, Z_{k'} r_{kk'}^{-1}\left[1+\sum_{kk'} f_k(r_{kk'})\right]-\sum_{kk'} c_{kk'} r_{kk'}^{-6}$$

$$-\sum_{kk'} d_{kk'} r_{kk'}^{-8}-b\sum_{kk'}\beta_{kk'}\exp\left\{\frac{r_k+r_{k'}-r_{kk'}}{\rho}\right\} \qquad (1)$$

where the first two terms represent the long range Coloumb and Three Body Interaction [19]; the third and fourth terms are the van der Waals(vdW) interaction due to dipole-dipole(d-d) and dipole-quadrapole(d-q) attractions, the fifth term represents the Hafemeister Flygare [20] type short- range overlap repulsion extended up to second neighbour ions, $\beta_{kk'}$ are the Pauling coefficient [21,]; ρ and b are the range and hardness model parameters, respectively as defined earlier.

III. RESULTS & DISCUSSION

Using the input data given in Table 1 for fcc C_{60} [17, 18], we have calculated the model parameters listed in Table 2.

Table 1 Input data at 300K for C_{60}

S.No.	Properties	C_{60}
1	r (Å)	3.55 [a]
2	c_{11} (10^{11} dyn/cm^2)	2.64 [a]
3	c_{12} (10^{11} dyn/cm^2)	1.38 [a]
4	c_{44} (10^{11} dyn/cm^2)	1.17 [a]

a-[17]

Table 2 Model parameters at 300K for C_{60}

S.No.	Model Parameters	C_{60}
1	b (10^{12}erg)	4.164
2	ρ (Å)	0.2280
3	f (r)	-0.0041

Anharmonic elastic properties:

We have studied the anharmonic elastic properties by calculating Second Order Elastic Constants (SOECs), Third Order Elastic Constants (TOECs) as they provide physical insight into the nature of binding forces between the constituents of the crystal and are strongly related to other anharmonic properties, like thermal expansion, thermoelastic constants and thermal conductivity. The expression for these elastic constants and the pressure and temperature derivatives of SOECs are given by [22].

$$c_{11} = 32.237 Tb\beta_T + \frac{e^2}{4r_0^4}[-32.231B_1 - 34.48B_2 \\ + \frac{4C_1 - 12A_1 + C_2 - 3A_2}{4} + 13.4599B_1 \\ + 89.305r_0 f'(r_0)] \tag{2}$$

$$c_{112} = -4.15 Tb\beta_T + \frac{e^2}{4r_0^4}[4.151B_1 + 4.52B_2 \\ + \frac{C_2 - 3A_2}{8} + 4.6608r_0^2 f''(r_0) \\ - 18.640r_0 f'(r_0)] \tag{3}$$

$$c_{166} = -6.151 Tb\beta_T + \frac{e^2}{4r_0^4}[4.151B_1 + 4.52B_2 \\ + \frac{C_2 - 3A_2}{8} - 3.5377B_{21} - 5.56r_0 f'(r_0)] \tag{4}$$

$$c_{123} = 2.332 Tb\beta_T + \frac{e^2}{4r_0^4}[-2.332(B_1 + B_2) \\ + 16.692r_0 f'(r_0)] \tag{5}$$

$$c_{144} = 2.332 Tb\beta_T + \frac{e^2}{4r_0^4}[-2.332(B_1 + B_2) \\ + 5.564r_0 f'(r_0)] \tag{6}$$

$$c_{444} = 2.332 Tb\beta_T + \frac{e^2}{4r_0^4}[-2.332(B_1 + B_2)] \tag{7}$$

where $T\beta B_T = \frac{e^2}{4r^4}[1.165\varepsilon\{\varepsilon + 12f(r)\} + B_1 + B_2]$

and A_1, A_2, B_1, B_2 are the short range force parameters; $f(r)$ and $rf'(r)$ are the TBI parameters. The parameter $f(r)$ and its derivatives are calculated from the knowledge of elastic constants and the relation $f = f_0 \exp(-r/\rho)$. The values thus obtained are depicted in table 3. The present result on TOEC, on C_{60} are given in Table 3. These are the properties which are being reported by us, probably for the first time.

We have calculated the TOECs for C_{60} probably for the first time at 300K are listed in Table 3. It is found that at room temperature, the thermal effects are important and their contribution to SOECs and TOECs are significant [21].

Table 3 Values of pressure derivatives of SOECs and TOECs (10^{12} dyn/cm^2)of C$_{60}$ at 300K

Properties	Values
c_{111}	-7.997 **(6.240)**[a]
c_{112}	-3.830 **(-1.905)**[a]
c_{166}	-1.800 **(-1.605)**[a]
c_{123}	1.272 **(-1.80)**[a]
c_{166}	1.021
c_{456}	0.895

[a] –ref [22]

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