CHAPTER V

PRESSURE DERIVATIVES OF THE SECOND ORDER ELASTIC CONSTANTS OF HIGH TEMPERATURE SUPERCONDUCTOR $YBa_2Cu_3O_7$ AND $GdBa_2Cu_3O_7$.

5.1 INTRODUCTION

The experimental determination of the third-order elastic constants and the pressure derivatives of the effective second order elastic constants of solids have received considerable attention in the last four decades as these are a measure of the anharmonicity of a solid. However in the literature, we find that theoretical calculations or experimental measurements for the effective second order elastic constants of high Tc superconducting crystals are yet to come.

Rao and Menon [1,2,3,4,5,6,7] have obtained an expression for the effective second order elstic constants of tetragonal, trigonal, orthorhombic, monoclinic and triclinic systems based on the finite strain elasticity [8] theory in terms of the natural state second order elastic constants and third order elastic constants of the respective crystal systems. This method has been utilized to obtain the pressure derivatives of the effective second order elastic constants in this chapter. The basic importance of these expressions is that they enable one to fix up the first order anharmonic parameters in the potential energy expansion of a crystal.

5.2 PRESSURE DERIVATIVES OF THE SECOND ORDER ELASTIC CONSTANTS FROM THIRD ORDER ELASTIC CONSTANTS DATA

Let us consider an orthorhombic crystal subjected to a hydrostatic pressure p. Let a_i be the coordinates of a material point in the natural state and x_i the coordinates of the same material point after applying the pressure. The Jacobian

$J = | \partial x_i / \partial a_j |$ is given by

$$J = \begin{vmatrix} (1-\alpha_1) & 0 & 0 \\ 0 & (1-\alpha_2) & 0 \\ 0 & 0 & (1-\alpha_3) \end{vmatrix} \qquad 5.1$$

where every line element along a_i is reduced in length by a factor $(1-\alpha_i)$ in terms of the Lagrangian strain components η, ε, ζ.

$$(1 + \alpha_1)^2 = 1 + 2\eta$$

$$(1 + \alpha_2)^2 = 1 + 2\varepsilon$$

$$(1 + \alpha_3)^2 = 1 + 2\zeta \qquad 5.2$$

The density ρ_0 in the natural state changes to ρ in the deformed state as

$$\rho / \rho_0 = 1 / \det | J | \qquad 5.3$$

An infinitesimal stress is superimposed on this deformed state. The final coordinates of the material particle are given by

$$x_i' = x_i + \sum_j \beta_{ij} x_j \qquad 5.4$$

where β_{ij} are the infinitesimal strain parameters. The Lagrangian strain parameters η_{ij} in the final state are given by

$$\eta_{ij} = \frac{1}{2} \sum_{p=1}^{3} \left((\partial x_p' / \partial a_i) (\partial x_p' / \partial a_j) - \delta_{ij} \right) \qquad 5.5$$

and are obtained in terms of η, ε, ζ and β_{ij} . The strain energy density U can be written in power of η_{ij}

as

$$U = \frac{1}{2} \sum_{ijkl} c_{ijkl}\, \eta_{ij}\, \eta_{kl} + \frac{1}{6} \sum_{ijklmn} c_{ijklmn}\, \eta_{ij}\, \eta_{kl} \eta_{mn} \qquad 5.6$$

The stress tensor in the final state is given by Murnaghan as

$$\tau_{ij} = (\rho/\rho_o) \sum_{pq} (\partial x'_i / \partial a_p)\, (\partial U / \partial \eta_{pq})^* \, (\partial x'_j / \partial a_q) \qquad 5.7$$

The effective second order elastic constants $c'_{ij,pq}$ can be obtained to the first order in strain η, ε and ζ and by comparing with

$$\tau_{ij} = -p\, \delta_{ij} + \sum_{kl} c'_{ijkl}\, \beta_{kl} \qquad 5.8$$

where p denotes the pressure . Thus we find the expressions for the nine effective c'_{11}, c'_{12}, c'_{13}, c'_{22}, c'_{23}, c'_{33} , c'_{44} , c'_{55} and c'_{66} for orthorhombic crystal.

where

$$C'_{11} = C_{11} + \eta (5 C_{11} + C_{111}) + \varepsilon (-C_{11}$$

$$2 C_{12} + C_{112}) + \zeta (-C_{11} + 2 C_{13} + C_{113})$$

$$C'_{12} = C_{12} + \eta (C_{12} + C_{112}) +$$

$$\zeta (-C_{12} + C_{123}) + \varepsilon (C_{12} + C_{122})$$

$$C'_{13} = C_{13} + \eta (C_{13} + C_{113}) + \varepsilon (-C_{13}$$

$$+ C_{123}) + \zeta (C_{13} + C_{133})$$

$$C'_{22} = C_{22} + \eta (2 C_{12} - C_{22} + C_{122}) +$$

$$\varepsilon (5 C_{22} + C_{222}) + \zeta (2 C_{23} - C_{22} + C_{223})$$

$$C'_{23} = C_{23} + \eta (-C_{23} + C_{123}) +$$

$$\varepsilon (C_{23} + C_{223}) + \zeta (C_{23} + C_{233})$$

$$C'_{33} = C_{33} + \eta (2 C_{13} - C_{33} + C_{133}) +$$

$$\varepsilon (2 C_{23} - C_{33} + C_{233}) + \zeta (5 C_{33} + C_{333})$$

$$c'_{44} = c_{44} + \eta \left(\frac{1}{2} c_{12} + \frac{1}{2} c_{13} - c_{44} \right)$$

$$+ \varepsilon \left(\frac{1}{2} c_{22} + \frac{1}{2} c_{23} + c_{44} + c_{244} \right)$$

$$\zeta \left(\frac{1}{2} c_{23} + \frac{1}{2} c_{33} + c_{44} + c_{344} \right)$$

$$c'_{55} = c_{55} + \eta \left(\frac{1}{2} c_{11} + \frac{1}{2} c_{13} + c_{55} \right.$$

$$\left. c_{155} \right) + \varepsilon \left(\frac{1}{2} c_{12} + \frac{1}{2} c_{23} - c_{55} + c_{255} \right)$$

$$+ \zeta \left(\frac{1}{2} c_{13} + \frac{1}{2} c_{33} + c_{55} + c_{355} \right)$$

$$c'_{66} = c_{66} + \eta \left(\frac{1}{2} c_{11} + \frac{1}{2} c_{12} + \right.$$

$$\left. c_{66} + c_{166} \right) + \varepsilon \left(\frac{1}{2} c_{12} + \frac{1}{2} c_{22} + c_{66} \right.$$

$$\left. c_{266} \right) + \zeta \left(\frac{1}{2} c_{13} + \frac{1}{2} c_{23} - c_{66} \right) \qquad 5.9$$

where η ,ε, and ζ are given in terms of p and c_{ij} as

$$|a| = \begin{vmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{13} & C_{23} & C_{33} \end{vmatrix} \qquad \eta = -p \frac{\begin{vmatrix} 1 & C_{12} & C_{13} \\ 1 & C_{22} & C_{23} \\ 1 & C_{23} & C_{33} \end{vmatrix}}{|a|}$$

$$\varepsilon = -p \frac{\begin{vmatrix} C_{11} & 1 & C_{13} \\ C_{12} & 1 & C_{23} \\ C_{13} & 1 & C_{33} \end{vmatrix}}{|a|} \qquad \eta = -p \frac{\begin{vmatrix} C_{11} & C_{12} & 1 \\ C_{12} & C_{22} & 1 \\ C_{13} & C_{23} & 1 \end{vmatrix}}{|a|}$$

5.10

The pressure derivatives of the effective second order elastic constants of orthorhombic crystals have been calculated as

$$\partial(C'_{11})/\partial p, \quad \partial(C'_{12})/\partial p, \quad \partial(C'_{13})/\partial p$$

$$\partial(C'_{22})/\partial p, \quad \partial(C'_{23})/\partial p, \quad \partial(C'_{33})/\partial p$$

$$\partial(C'_{44})/\partial p, \quad \partial(C'_{55})/\partial p, \quad \partial(C'_{66})/\partial p$$

5.11

5.3 PRESSURE DERIVATIVES OF $YBa_2Cu_3O_7$ AND $GdBa_2Cu_3O_7$

Using the second and third order elastic constants of $YBa_2Cu_3O_7$ from the tables(3.1) of chapter III and (4.1) from chapter IV we hvae calculated the pressure derivatives of $YBa_2Cu_3O_7$, using (5.9) and are reported in table (5.1). Similarly using the second and third order elastic constants of $GdBa_2Cu_3O_7$ from tables (3.2) of chapter III and (4.2) of chapter IV we have calculated the pressure derivatives of $GdBa_2Cu_3O_7$.,using the expression (5.9) and are collected in table (5.2).

5.4 RESULTS AND DISCUSSIONS

From our calculated values, it is found that the pressure derivatives in the direction C_{55} , C_{11} and C_{22} are negative which means that these three elastic constants are decreasing with increasing pressure. But all other six pressure derivates are positive, which means that the other elastic constants are increasing with increasing pressure. However all nine pressure derivatives are small values which show that variation of elastic constants with pressue is small. Due to the non-availability of the large single crystals for the measurements of the elastic wave velocities under high pressure, complete experimental values of the elastic constants are not available in literature. However, such a measurement is highly anticipated.

Table(5.1)

Pressure derivatives of second order elastic constants of high temperature superconducting compound $YBa_2Cu_3O_7$.

Pressure derivatives of $YBa_2Cu_3O_7$ $\partial C'_{ij} / \partial p$	
$\partial C'_{55} / \partial p$	-0.1080
$\partial C'_{11} / \partial p$	-0.120
$\partial C'_{22} / \partial p$	-0.359
$\partial C'_{44} / \partial p$	-0.049
$\partial C'_{66} / \partial p$	-0.256
$\partial C'_{39} / \partial p$	-0.559
$\partial C'_{29} / \partial p$	-0.614
$\partial C'_{12} / \partial p$	-0.746
$\partial C'_{19} / \partial p$	1.053

Table(5.2)

Pressure derivatives of second order elastic constants of high temperature superconducting compound $GdBa_2Cu_3O_7$.

$\partial C'_{ij} / \partial p$	Pressure derivatives of $GdBa_2Cu_3O_7$
$\partial C'_{55} / \partial p$	-0.1178
$\partial C'_{11} / \partial p$	-0.8830
$\partial C'_{22} / \partial p$	-0.3649
$\partial C'_{44} / \partial p$	0.1221
$\partial C'_{66} / \partial p$	0.2515
$\partial C'_{33} / \partial p$	0.4500
$\partial C'_{23} / \partial p$	0.5865
$\partial C'_{12} / \partial p$	0.7419
$\partial C'_{13} / \partial p$	1.0347

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