

CHAPTER III

SECOND ORDER ELASTIC CONSTANTS OF $\text{YBa}_2\text{Cu}_3\text{O}_7$ AND

$\text{GdBa}_2\text{Cu}_3\text{O}_7$



3.1 INTRODUCTION

Since the discovery of the new class of cuprate superconductors, it has been difficult to obtain a reliable information about the absolute values, the temperature dependence and anisotropy of the sound velocities. The experimental difficulties in measuring these parameters, for example, by means of ultrasound is mostly due to the small sample size of the available single crystals.

So far sound velocities of $\text{YBa}_2\text{Cu}_3\text{O}_7$ have been measured by means of ultrasonic techniques on polycrystalline materials[1-4] and in single crystals [5,6,7,16,17,18]. Elastic properties of these materials display unconventional behaviour [8-12]. Theoretical analysis of the elastic properties at the superconducting transition have been attempted by Mills and Alexandrov [13,14]. Here we derive the expressions for second order elastic constants. The calculated values of the elastic constants of $\text{YBa}_2\text{Cu}_3\text{O}_7$ is reported along with the available measured values for these compounds[15,16,17,18,7].



3.2 SECOND ORDER ELASTIC CONSTANTS

The finite deformation theory of Born and Huang [19] is made use of to determine the strain energy expression for the high temperature superconducting compounds and it is then compared with the strain energy expression from continuum theory to obtain expressions for the elastic constants. The potential energy per unit cell of a crystal can be written as

$$\phi = \frac{1}{2} \sum_{\substack{L L' \\ \nu \nu'}} \phi \left(\begin{matrix} L & L' \\ \nu & \nu' \end{matrix} \right) \quad 3.1$$

where ϕ is the potential energy. $\left(\begin{matrix} L \\ \nu \end{matrix} \right)$ represents the ν atom in the L^{th} cell and $\left(\begin{matrix} L' \\ \nu' \end{matrix} \right)$ represents the ν' atom in the L'^{th} cell. If we consider the central interaction under harmonic approximation, it can be then noted that $\phi \left(\begin{matrix} L & L' \\ \nu & \nu' \end{matrix} \right)$ depends only on the square of the vector distance

between the atoms $\left(\begin{matrix} L \\ \nu \end{matrix} \right)$ and $\left(\begin{matrix} L' \\ \nu' \end{matrix} \right)$.

Therefore we can write

$$\phi = \phi_0 + \phi_1 + \phi_2 \quad 3.2$$

where ϕ_0 is the static potential energy of the crystal and



$$\phi_1 = O' \phi \quad 3.3$$

$$\phi_2 = O'' \phi \quad 3.4$$

where $O' = (\partial/\partial r^2)$ and $O'' = (\partial/\partial r^2)^2$ are differential operators, r representing the interatomic distance. Under equilibrium conditions, ϕ_1 vanishes and the contribution to the change in the potential energy per unit cell is only from the ϕ_2 term which is the second order term.

When we consider only the nearest neighbour central interaction, the expression for the change in potential energy when the lattice is homogeneously deformed is given by

$$\Delta \phi = \frac{1}{2} \sum_{\substack{L L' \\ \nu \nu'}} O'' \phi \left(\begin{matrix} L & L' \\ \nu & \nu' \end{matrix} \right) \Delta R^2 \left(\begin{matrix} L & L' \\ \nu & \nu' \end{matrix} \right) \quad 3.5$$

where $\Delta R \left(\begin{matrix} L & L' \\ \nu & \nu' \end{matrix} \right)$ is the change in the interatomic vector distance between the atom $\left(\begin{matrix} L \\ \nu \end{matrix} \right)$ and $\left(\begin{matrix} L' \\ \nu' \end{matrix} \right)$.

Substituting for ΔR from equation (2.1) in equation (3.5)



and simplifying , we get

$$\Delta \phi = k_2 \sum \left[4 \sum_{ijkl} \eta_{ij} \eta_{kl} R_i R_j R_k R_l + \right. \\ \left. 4 \sum_{ij} \bar{W}_i \bar{W}_j R_i R_j + 8 \sum_{ijk} \eta_{ij} \bar{W}_k R_i R_j R_k + \right. \\ \left. 4 \sum_{ijk} \bar{W}_k^2 \eta_{ij} R_i R_j + 4 \sum_{ik} \bar{W}_i \bar{W}_k^2 R_i \right]$$

3.6

where $k_2 = O''\phi$ is the second order potential parameter. In the above expression

$$R_i = R_i \begin{pmatrix} L & L' \\ \nu & \nu' \end{pmatrix} \text{ etc. and } \bar{W}_i = \bar{W}_i (\nu, \nu') \text{ etc}$$

Carrying out the summations inside the square bracket of (3.6) we obtain the final expression for $\Delta\phi$ as

$$\Delta \phi = k_2 \sum_{\substack{L & L' \\ \nu & \nu'}} \left[4 \left[\eta_{xx}^2 R_x^4 + \eta_{yy}^2 R_y^4 + \right. \right. \\ \eta_{zz}^2 R_z^4 + 2 \eta_{xx} \eta_{yy} R_x^2 R_y^2 + 2 \eta_{xx} \eta_{zz} R_x^2 R_z^2 + \\ 2 \eta_{yy} \eta_{zz} R_y^2 R_z^2 + 4 \eta_{xy}^2 R_x^2 R_y^2 + 4 \eta_{xz}^2 R_x^2 R_z^2 + \\ \left. 4 \eta_{yz}^2 R_y^2 R_z^2 \right] + 4 \left[\bar{W}_x^{-2} R_x^2 + \bar{W}_y^{-2} R_y^2 + \bar{W}_z^{-2} R_z^2 + \right. \\ \left. 2 \bar{W}_x \bar{W}_y R_x R_y + 2 \bar{W}_x \bar{W}_z R_x R_z + 2 \bar{W}_y \bar{W}_z R_y R_z \right] +$$



$$\begin{aligned}
& \theta \left\{ \eta_{xx} \left[\bar{w}_x R_x^3 + \bar{w}_y R_x^2 R_y + \bar{w}_z R_x^2 R_z \right] + \right. \\
& \eta_{yy} \left[\bar{w}_x R_x R_y^2 + \bar{w}_y R_y^3 + \bar{w}_z R_y^2 R_z \right] + \eta_{zz} \left[\right. \\
& \left. \bar{w}_x R_x R_z^2 + \bar{w}_y R_y R_z^2 + \bar{w}_z R_z^3 \right] + 2 \eta_{xy} \left[\right. \\
& \left. \bar{w}_x R_x^2 R_y + \bar{w}_y R_x R_y^2 + \bar{w}_z R_x R_y R_z \right] + 2 \eta_{xz} \left[\right. \\
& \left. \bar{w}_x R_x^2 R_z + \bar{w}_y R_x R_y R_z + \bar{w}_z R_x R_z^2 \right] + 2 \eta_{yz} \left[\right. \\
& \left. \bar{w}_x R_x R_y R_z + \bar{w}_y R_y^2 R_z + \bar{w}_z R_y R_z^2 \right] \left. \right\} + 4 \left\{ \right. \\
& \left. \left\{ \bar{w}_x^{-2} + \bar{w}_y^{-2} + \bar{w}_z^{-2} \right\} \left\{ \eta_{xx} R_x^2 + \eta_{yy} R_y^2 + \eta_{zz} R_z^2 + \right. \right. \\
& \left. \left. 2 \eta_{xy} R_x R_y + 2 \eta_{xz} R_x R_z + 2 \eta_{yz} R_y R_z \right\} + 4 \left\{ \right. \right. \\
& \left. \left. \left\{ \bar{w}_x R_x + \bar{w}_y R_y + \bar{w}_z R_z \right\} \left\{ \bar{w}_x^{-2} + \bar{w}_y^{-2} + \bar{w}_z^{-2} \right\} \right\} \right\} .
\end{aligned}$$

where $R_i = R_i \begin{pmatrix} L & L \\ \nu & \nu' \end{pmatrix}$ and $\bar{w}_i = w_i (\nu \nu')$



This expression for $\Delta \phi$ for the superconducting compounds has been evaluated by making use of the position co-ordinates of the nearest neighbour atoms in the unit cell. The summations in eqn (3.7) are done for each atom separately taking into account of the nearest neighbour central interaction.

In the method of long waves or in the continuum model approximation, the relation between the elastic constants and the strain dependent lattice energy is written as

$$U = U_0 + \frac{1}{2} c_{ijkl} \eta_{ij} \eta_{kl} + \frac{1}{6} c_{ijklmn} \eta_{ij} \eta_{kl} \eta_{mn} \quad 3.8$$

Here the elastic constants of any order are defined as [20]

$$c_{ijklmn} = \left[\frac{\partial^2 U}{\partial \eta_{ij} \partial \eta_{kl} \partial \eta_{mn}} \right]_{\eta=0} \quad 3.9$$

Comparing equation (3.7) with equation (3.8) and on simplifying, we get the expressions for SOE constants.



3.3 SECOND ORDER ELASTIC CONSTANTS OF $\text{YBa}_2\text{Cu}_3\text{O}_7$

We make use of the deformation theory of Born and Huang to determine the strain energy for the high temperature superconducting compounds $\text{YBa}_2\text{Cu}_3\text{O}_7$ and it is then compared with the strain energy expressions for second order elastic constants.

Using the deformation theory the final expression for $\Delta\phi$ is given by

$$\begin{aligned} \nabla \phi = k_2 \left[& 8 a^4 \eta_{xx}^2 + 7 b^4 \eta_{yy}^2 + 10/2 (c/3)^4 \eta_{zz}^2 + \right. \\ & 4 a^2 b^2 \eta_{xx} \eta_{yy} + 2/3 a^2 c^2 \eta_{xx} \eta_{zz} + \\ & 2/3 b^2 c^2 \eta_{yy} \eta_{zz} + 8 a^2 b^2 \eta_{xy}^2 + 4/3 a^2 c^2 \eta_{xz}^2 + \\ & \left. 4/3 b^2 c^2 \eta_{yz}^2 \right] \end{aligned} \quad 3.10$$

In the continuum model approximation the second order term in the strain dependent lattice energy is written as

$$\phi = \frac{1}{2} c_{ijkl} \eta_{ij} \eta_{kl} \quad 3.11$$

Expression of (3.11) has been expanded and simplified for orthorhombic symmetry which reduces to



the following form

$$\begin{aligned}
 \nabla \phi = & \frac{1}{2} (c_{11} \eta_{xx}^2 + c_{22} \eta_{yy}^2 + c_{33} \eta_{zz}^2) + \\
 & 2 (c_{44} \eta_{yz}^2 + c_{55} \eta_{xz}^2 + c_{66} \eta_{xy}^2) + 4 (c_{46} \eta_{yz} \eta_{xy} \\
 & + c_{45} \eta_{yz} \eta_{xz} + c_{65} \eta_{xy} \eta_{xz}) + 2 (c_{14} \eta_{xx} \eta_{yz} \\
 & + c_{16} \eta_{xx} \eta_{xy} + c_{15} \eta_{xx} \eta_{xz} + c_{42} \eta_{yy} \eta_{yz} + \\
 & c_{43} \eta_{zz} \eta_{yz} + c_{62} \eta_{yy} \eta_{xy} + c_{63} \eta_{zz} \eta_{xy} + \\
 & c_{25} \eta_{yy} \eta_{xz} + c_{53} \eta_{zz} \eta_{xz}) + c_{12} \eta_{xx} \eta_{yy} + \\
 & c_{13} \eta_{xx} \eta_{zz} + c_{23} \eta_{yy} \eta_{zz}
 \end{aligned} \tag{3.12}$$

Comparing equation (3.10) and (3.12) we get the following expressions for the second order elastic constants of $\text{YBa}_2\text{Cu}_3\text{O}_7$ [21].



$$\begin{aligned}
C_{11} &= [16 a^4 / v_a] k_2 \\
C_{22} &= [16 b^4 / v_a] k_2 \\
C_{33} &= [16 (c/3)^4 / v_a] k_2 \\
C_{12} &= [4 (ab)^2 / v_a] k_2 \\
C_{13} &= [(2/9) (ac)^2 / v_a] k_2 \\
C_{23} &= [(2/9) (bc)^2 / v_a] k_2 \\
C_{66} &= [4 (ab)^2 / v_a] k_2 \\
C_{55} &= [(2/9) (ac)^2 / v_a] k_2 \\
C_{44} &= [(2/9) (bc)^2 / v_a] k_2
\end{aligned}$$

3.13

where v_a is the volume of the unit cell and a, b, c are the unit cell dimensions and

$$k_2 = \frac{1}{2} \left[\frac{\partial^2 \phi(r)}{\partial (r^2)^2} \right]_{\text{equilibrium}} \quad 3.14$$

Making use of the experimental values of C_{11} measured by Baumgart [7,16] we determine the interatomic potential parameters k_2 . This value of k_2 has been



used to evaluate the elastic constants of c_{11}, c_{22}, c_{33} , $c_{12}, c_{13}, c_{23}, c_{66}, c_{55}, c_{44}$, for $\text{YBa}_2\text{Cu}_3\text{O}_7$. Table (3.1) gives the calculated values of elastic constants of $\text{YBa}_2\text{Cu}_3\text{O}_7$ together with experimental values. The agreement between theoretical and experimental values is good.

3.4 SECOND ORDER ELASTIC CONSTANTS OF $\text{GdBa}_2\text{Cu}_3\text{O}_7$.

We have calculated the second order elastic constants of $\text{GdBa}_2\text{Cu}_3\text{O}_7$ by using the available sound velocity of the c_{44} mode of the single crystal [17] and density, $\rho = 6.942 \text{ gm/cm}^3$.

From the sound velocity of the c_{44} mode we have determined the interatomic potential parameters k_2 . This value of k_2 has been used to evaluate all the second order elastic constants of $\text{GdBa}_2\text{Cu}_3\text{O}_7$ and are reported in table (3.2). A comparison of these results with experimental values are not attempted as the same are not available.



3.5 RESULTS AND DISCUSSION.

The major objective of the work is to show how the deformation theory can be applied to the complicated structure like that of tripled ABO_3 perovskite compounds. In the determination of the elastic constants, we have considered only the central force interaction between nearest neighbours and hence neglected the electronic contribution. Even with these limitations we have got reasonably good results. In the next decade, the complete set of experimental measurements is hoped to come out for these crystals.



Table (3.1). Second order elastic constants of the high temperature superconducting compound $\text{YBa}_2\text{Cu}_3\text{O}_7$.

Elastic constants c_{ij}	Present work in $*10^{11}$ Pa	Baumgart in $*10^{11}$ Pa	Saint-paul in $*10^{11}$ Pa	Gavarri in $*10^{11}$ Pa
		(7,16)	(15,17)	(18)
c_{11}	2.11	2.11	2.3	--
c_{22}	1.95	--	--	--
c_{99}	2.71	1.59	1.6	2.87
c_{12}	0.54	--	0.82	--
c_{19}	0.82	--	--	1.23
c_{29}	0.84	--	--	--
c_{66}	0.54	--	0.66	--
c_{55}	0.82	--	--	--
c_{44}	0.84	0.3	0.25	--



Table(3.2). Second order elastic constants of $\text{GdBa}_2\text{Cu}_3\text{O}_7$

Elastic constants	Values in 10^{11} Pa
C_{ij}	
C_{11}	0.7085
C_{22}	0.6474
C_{33}	0.8825
C_{12}	0.1810
C_{13}	0.2721
C_{23}	0.2781
C_{66}	0.1810
C_{55}	0.2721
C_{44}	0.2781



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