

## P R E F A C E

This thesis presents an attempt to calculate the interlattice displacements, second order elastic constants, third order elastic constants, first order pressure derivatives of second order elastic constants and the anisotropic thermal expansion of high temperature superconducting compounds  $\text{YBa}_2\text{Cu}_3\text{O}_7$  and  $\text{GdBa}_2\text{Cu}_3\text{O}_7$ .

The thesis is divided into six chapters. Chapter I contains, the theory of elasticity, experimental set-up used in studying elastic properties of crystals, the theory of thermal expansion in the quasiharmonic approximation of the orthorhombic crystals and a review about the basic structure, phase transformation and the rare earth substitution of 123 compounds.

In chapter II, we have determined the general expressions for interlattice displacements of  $(\text{R})\text{Ba}_2\text{Cu}_3\text{O}_7$  ( where  $\text{R} = \text{Sm}, \text{Eu}, \text{Gd}, \text{Dy}, \text{Y}, \text{Ho}, \text{Er}, \text{Tm}$  )



in terms of the strain components, making use of the deformation theory. The nature of the interlattice displacements of all 13 atoms in the unit cell is discussed. It is found that the interlattice displacements occur in such a way that pair of atoms along any linear chain move in opposite direction with equal magnitude.

In chapter III we have derived an expression for the strain energy of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  and  $\text{GdBa}_2\text{Cu}_3\text{O}_7$  using the deformation theory and this is compared with the strain energy expression from continuum theory to obtain the values of the second order elastic constants. Theoretical values of the second order elastic constants of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  is compared with experimental values and are found to agree satisfactorily.

In Chapter IV, we have determined the third order elastic constants of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  and  $\text{GdBa}_2\text{Cu}_3\text{O}_7$  on the basis of the deformation theory. General expressions have been derived for the third order elastic constants of these compounds taking into account the nearest



neighbour central interaction. The individual room temperature third order elastic constants of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  and  $\text{GdBa}_2\text{Cu}_3\text{O}_7$  have been calculated and reported for the first time. We have shown how the deformation method could be applied to determine the higher order elastic constants of complicated perovskite structure.

From the strain elasticity theory, expressions for the effective second order elastic constants in terms of the second and third order elastic constants of the respective crystals in their natural state have been derived. These expressions have been used to evaluate the pressure derivatives of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  and  $\text{GdBa}_2\text{Cu}_3\text{O}_7$  and are given in chapter V.

Chapter VI deals with the finite elasticity theory for the calculation of the generalized Grunesien parameters for the acoustic waves in orthorhombic crystals of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  and  $\text{GdBa}_2\text{Cu}_3\text{O}_7$  from its third order elastic constants. From the acoustic modes the low temperature limits  $\bar{\gamma}_{\perp}^{(-3)}$  and  $\bar{\gamma}_{\parallel}^{(-3)}$  of the Grunesien gammas have been obtained parallel and



perpendicular to the  $c$ -axis of the crystal. Also the variation of  $\gamma'$  and  $\gamma''$  for the three acoustic branches are presented. The anisotropy in the different directions are discussed.



Most of the work reported in this thesis are either published, presented in conferences or in the process of publication.

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2. "Pressure derivatives of the elastic constants of high temperature superconductor  $\text{YBa}_2\text{Cu}_3\text{O}_7$ ." Proceedings of the Fourth Kerala Science Congress, N.V. Eldhose and C.S. Menon, 1992, P.217.

3. "Pressure derivatives of the elastic constants of high temperature superconductor  $\text{GdBa}_2\text{Cu}_3\text{O}_7$ ". Proceedings of the Fifth Kerala Science Congress, N.V. Eldhose and C.S. Menon, 1993, P. 360.

4. "Higher order elastic constants of high temperature superconductor  $\text{GdBa}_2\text{Cu}_3\text{O}_7$ ". Solid State Communications, N.V. Eldhose and C.S. Menon, (Communicated).

5. "Pressure derivatives of elastic coefficients of



$\text{YBa}_2\text{Cu}_3\text{O}_7$  and  $\text{GdBa}_2\text{Cu}_3\text{O}_7$ ". Journal of Physics C (U.K),  
C.S. Menon and N.V. Eldhose, (Communicated).

6. "Low temperature thermal expansion of  $\text{YBa}_2\text{Cu}_3\text{O}_7$   
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7. "Low temperature thermal expansion of  
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