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Slowness surfaces, ray velocity surfaces and phonon focussing in high T_c superconductor crystals

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Abstract. This paper reports the results of the study of anisotropy in elastic wave propagation in single crystal superconducting BSCCO. The inverse and group velocities of elastic waves propagating in different directions have been computed and the corresponding slowness and ray velocity surfaces plotted, taking elastic constant data from literature. In addition, the phenomenon of phonon focussing has been investigated in this material by computing the phonon enhancement factor along different directions in spherical polar coordinates. The abnormally high values in phonon enhancement factor exhibited in certain directions for the phonon modes are interpreted as due to caustics occurring in the geometrical acoustics approximation adopted in the computational analysis. The results in LSCO and YBCO are found to be similar to those in BSCCO.

Keywords. High T_c superconductors; slowness surfaces; ray velocity surfaces; phonon focussing catastrophes.

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1. Introduction

It is well known that a detailed description of the nature of elastic wave propagation in anisotropic solids can be done by plotting the phase velocity, slowness and ray velocity surfaces [1]. Of these, the ray surface is physically the most meaningful one because it represents the wave front of equal phase for an oscillatory disturbance a unit time interval after it has been created at the origin. Several papers and books have appeared in literature depicting the features of these surfaces in different crystal systems and it is found that several crystals exhibit cuspidal edges in ray velocity surfaces along specific directions for selected modes [1–3]. The slowness surface, which is the polar reciprocal of the ray surface, plays an important role in the discussions that follow since one can trace all the important features of ray surfaces from the corresponding slowness surfaces. The analytical techniques for generating slowness and ray surfaces are well established and the conditions for the existence of cuspidal edges in ray surfaces have been worked out for different crystal classes.

Another important feature of elastic anisotropy is 'phonon focussing', which arises due to the non-collinearity of the ray and phase velocities. Whenever the slowness surface is nonspherical in shape in any direction, more than one wave vector may correspond to a single ray velocity vector and the corresponding ray surface will contain folds or cuspidal edges in that direction. Consequently, energy flow in that direction is enhanced compared to other directions. This effect, known as phonon focussing, is now well understood and has been a subject of intense research for the past two decades or so both theoretically and experimentally [4–7].

Several workers have carried out heat pulse experiments in ultrapure single crystals of Ge, GaAs, Si etc. and have demonstrated phonon focussing effects along selected directions for transverse acoustic modes. Most of these experiments exploit temporal analysis of the heat pulse intensity. Results of ballistic phonon imaging experiments carried out on Ge [7], GaAs [8] and KDP [9] show striking differences in the intensity of phonons propagating along different directions which have correspondence with phonon enhancement calculations in these crystals. Ballistic phonon imaging offers a geometric visualization of anisotropic phonon propagation in crystals.

The mechanism of superconductivity and the role played by phonons in superconducting transition in high T_c superconductors remain unclear even today. Of late, with the success in growing single crystals of many of the high T_c superconductors, it has become possible to get a better insight into these materials with the aid of fine experiments. The resonant ultrasound technique has been used to isolate the independent elastic constants of many of these materials [10–12]. However, all the independent elastic constants are available only for a few high T_c superconductor crystals, that too only at room temperature. The only material for which all the elastic constants above and below T_c have been reported is a textured BSCCO (2212) crystal with cylindrical symmetry about the c-axis [13]. Assumption of cylindrical symmetry merges some of the elastic constants resulting in only five independent ones.

In this paper, we trace the slowness and ray surfaces of single crystal BSCCO, taking elastic constant data from literature [13]. Phonon enhancement factors have been evaluated in spherical polar coordinates and plotted. An outline of the computational procedure, results obtained and a discussion of the results are given in the following sections. Even though results have been obtained on YBCO and LSCO, they are not reported here as these are similar to those of BSCCO.

2. Slowness and ray surfaces for BSCCO above and below T_c

The Christoffel equation for the propagation of elastic waves through a crystal is of the form [1]

$$\Omega(\omega, k_x, k_y, k_z) = 0. \tag{1}$$

A vector $\mathbf{m}$, with $\mathbf{m} = \mathbf{n}/v$, having the direction of the wave normal and magnitude equal to the reciprocal of the phase velocity v, is known as the reciprocal velocity vector or slowness vector.

The ray velocity or the velocity with which energy is transported is given by [1]

$$\mathbf{S} = -\frac{\nabla_{\mathbf{k}}\Omega}{(\partial\Omega/\partial\omega)}. \tag{2}$$

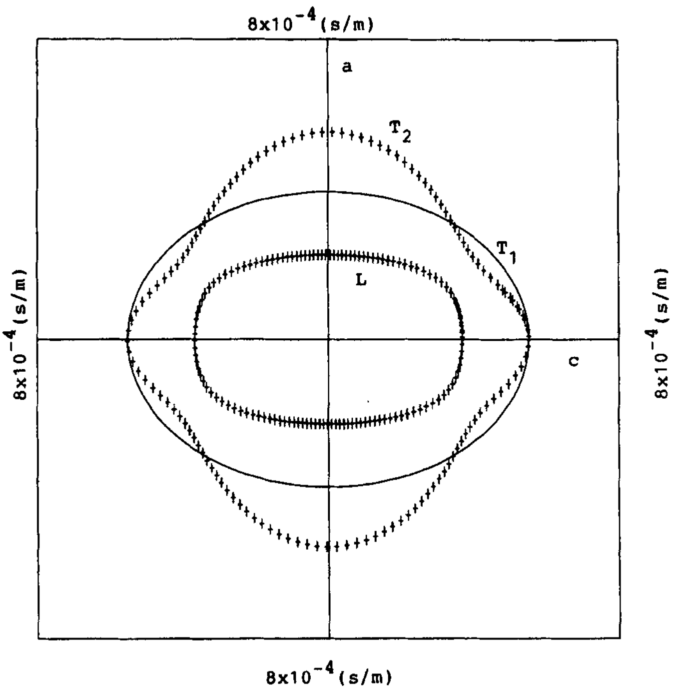

Figure 1. Sections of the slowness surfaces for BSCCO in the $a-c$ plane at 20 K. L, T_1 and T_2 denote the quasilongitudinal, pure shear and quasishear modes respectively. Because of transverse isotropy assumed, the surfaces are concentric circles in the $a-b$ plane. Surfaces for $a-c$ and $b-c$ planes are identical.

Expressions for the components of the slowness and ray velocities for wave propagation in different planes for orthorhombic symmetry have been used to plot the corresponding surfaces for high T_c superconductor crystals. Corresponding to the three solutions of equations (1) and (3), three modes of elastic waves propagate in any direction, which correspond to quasilongitudinal, pure shear and quasishear modes. The slowness and ray velocity surfaces have been plotted for the high T_c superconductor BSCCO in different symmetry planes at two temperatures, one above and the other below T_c, taking elastic constant data from literature [13].

As is expected for an orthorhombic crystal with cylindrical symmetry, wave propagation in the $a-b$ plane is isotropic and the corresponding slowness and ray surfaces are simply concentric circles. The surfaces have been plotted for the $a-c$ plane at 290 and 20 K and those at 20 K are shown in figures 1 and 2. It may be noted that the slowness surface for the quasishear mode deviates from circular shape and contains regions of positive and negative curvatures which give rise to cuspidal edges or folds in the ray surface.

3. Computation of phonon enhancement factor for BSCCO

The direction of energy flux (θ_s, ϕ_s) is obtained from the ray velocity components which in turn depend on the corresponding directions of the phase velocity (θ_k, ϕ_k). This **k** space

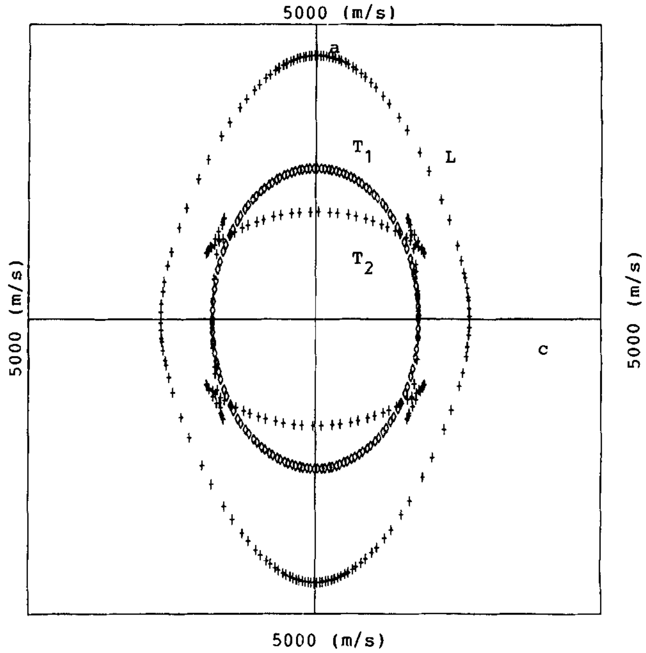

Figure 2. Sections of the ray velocity surfaces for BSCCO at 20 K in the a–c plane. L, T_1 and T_2 have the same meaning as in figure 1.

to s space transformation may be expressed as

$$\cos\theta_s = f(\cos\theta_k, \phi_k),$$
$$\phi_s = g(\cos\theta_k, \phi_k), \tag{3}$$

where the functions f and g are determined from the components of s. Equations (3) are basically a mapping of one two-dimensional space (θ_k, ϕ_k) into another two-dimensional space (θ_s, ϕ_s). The ratio of the product of the differentials in these two spaces is the Jacobian of the functions f and g. This can be written as

$$\mathrm{d}\Omega_s = \mathrm{d}(\cos\theta_s)\mathrm{d}\phi_s = J\mathrm{d}(\cos\theta_k)\mathrm{d}\phi_k = J\mathrm{d}\Omega_k, \tag{4}$$

where the Jacobian is given by

$$J = \begin{vmatrix} \partial f/\partial\cos\theta_k & \partial f/\partial\phi_k \\ \partial_g/\partial\cos\theta_k & \partial_g/\partial\phi_k \end{vmatrix}. \tag{5}$$

This equation provides the desired link between the mathematical formalism and the phonon intensities. The phonon enhancement factor A, defined as the ratio of the solid angle in the phase velocity space to the corresponding solid angle in the ray velocity space, is now related to the Jacobian by the relation [2]

$$A = \left|\frac{\Delta\Omega_k}{\Delta\Omega_s}\right| = \frac{1}{|J|}. \tag{6}$$

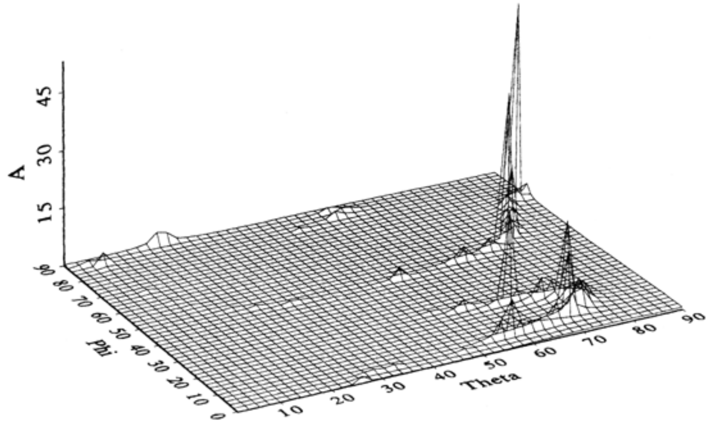

Figure 3. Pseudo-3D representation of the distribution of phonon intensities for the quasishear mode of BSCCO at 20 K. A is the phonon enhancement factor, with θ (theta) and ϕ (phi) designating the polar and azimuthal angles in spherical polar coordinates.

The geometrical interpretation of the Jacobian J is that $J = K|k^2|\cos\zeta$, where K is the Gaussian curvature of the slowness surface and ζ is the angle between the phase velocity vector and ray velocity vector. The Gaussian curvature is the product of the two extremal curvatures (inverse radii) of an elemental surface. If either or both of the extremal curvatures vanish, J and K will vanish. The Jacobian is dimensionless and is directly related to the phonon enhancement factor A by (6).

We have computed the phonon enhancement factors for single crystal BSCCO at 290 and 20 K following the method outlined above. Computations have been performed varying θ_k and ϕ_k from 0 to $\pi/2$, each in steps of 2° resulting in performing the computation at 2025 points in the wave vector space. Figure 3 gives a pseudo-3D view of the phonon intensities distributed in the first quadrant of the wave vector space for the quasishear mode in BSCCO at 20 K. Even though we have done the computation for the pure shear and quasilongitudinal modes as well, these are not reproduced here as no anomalous features are expected to be exhibited by these modes in phonon intensity distribution. However, similar to the peaks observed in the quasishear mode, very sharp peaks are seen in the enhancement factors for the pure shear and quasilongitudinal modes as well, but in other directions. Mirror reflections of this figure give a complete pseudo-3D representation of the phonon intensities distributed in the wave vector space for quasishear mode.

Phonon enhancement factor is found to take physically unrealistic values for all the modes of wave propagation in certain directions. In certain cases the values run into several thousands, particularly for the pure shear mode. This can be attributed only to singularities occurring in the phonon enhancement factor. As has been described by several workers before [14, 15], these singularities are a consequence of the geometrical acoustics approximation used in the definition and evaluation of phonon enhancement factor. Note that the ray surfaces for the pure shear mode do not contain folds or cusps and so one cannot expect any anomalous values for the phonon enhancement factor for

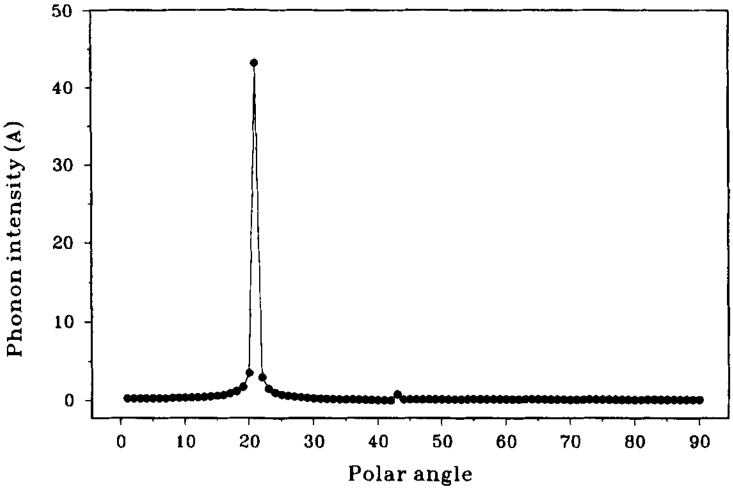

Figure 4. Variation of phonon intensity with the polar angle θ for the propagation of quasishear mode in the a–c plane of BSCCO at 20 K. The peak in the figure corresponds to the point at which caustics intersect the a–c plane.

this mode. This is true for the quasilongitudinal mode as well. The only mode for which we can expect to see interesting features in phonon enhancement is the quasishear mode.

We have computed the phonon enhancement factors along the cusp directions for the quasishear mode. The general program developed to compute phonon enhancement factors along general directions has been modified to compute phonon enhancement factors along the directions in which cusps occur in the ray velocity surface. The computation have been performed on BSCCO and the 20 K result is shown in figure 4. The directions in which peaks in phonon intensities occur in this figure correspond to the points at which the caustics intersect the (101) plane in this crystal. A qualitative analysis of the positions of these peaks in comparison with the directions in which cusps occur indicate that these are the directions along which the phonon intensity is getting amplified. The values of phonon enhancement factors are not abnormally high, and these are the directions in which one should look for phonon focussing effects in an experiment. Since the results in YBCO and LSCO are similar to these, they are not reproduced here.

4. Conclusions

We have computed and plotted the slowness surfaces, ray surfaces and phonon enhancement factors in single crystals of the high T_c superconductors BSCCO, YBCO and LSCO. The results bring out the changes that the slowness and ray surfaces undergo when the material undergoes superconducting transition. The results indicate that there are no significant changes in these surfaces due to superconducting transition or superconducting transition does not significantly affect the elastic anisotropy of these materials.

It is known that phonon focussing does not have any direct bearing on superconducting transition. All we see is a change in the magnitude of the phonon enhancement factor at temperatures above and below T_c. This change merely reflects the changes that the elastic constants undergo over this temperature range. We have identified the directions in which folds occur in the ray velocity surfaces and verified that phonon intensity for the quasishear mode gets enhanced in these directions. The phonon mean free path near T_c is very small in these materials and one cannot expect to see phonon focussing effects at such elevated temperatures. One must look for these effects in ultrapure single crystals at ultralow temperatures, or under the boundary scattering regime.

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