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Consequences of Anisotropic Sound Velocities in hcp Solid He^4 †

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The elastic constants for hcp solid He^4 recently published by Crepeau, Heybey, Lee, and Strauss are used for calculating the wave surfaces associated with elastic waves, according to the recent method of Wanner. The deviation of the energy path or ray from the wave normal is calculated and is correlated with experimental sound-velocity data previously obtained by the authors.

Wanner[1] has recently analyzed some of the early sound-velocity data on bcc solid He^3 and He^4 in which the crystal orientation was unknown and has shown that the observations can be used to estimate the elastic constants for these solids. Part of his arguments were based on the fact that the observed sound velocities in some of the earlier data were restricted to a few rather widely separated values, rather than a smoothly varying continuum. This behavior was shown to result from the nature of sound propagation in highly anisotropic media rather than from preferred crystal orientation as supposed by some of the earlier investigators.[2] Using an analysis similar to that used by Wanner,[1] we consider the recent sound-velocity results obtained for hcp solid He^4 in oriented crystals by Crepeau *et al.*[3] It is shown that the data are entirely consistent with this type of analysis.

When discussing sound velocities in anisotropic solids, the three surfaces generally referred to are the velocity, inverse, and wave surfaces.[4,5] From the point of view of an experimentalist measuring sound velocities in a crystal, the velocity surface is the one most directly useful.

Figure 1 shows a typical experimental setup for measuring sound velocities. Sound transducers are affixed to either side of the experimental crystal, and with one transducer as a source of sound waves in the crystal and the other as a receiver, the time for a sound pulse to traverse the crys-

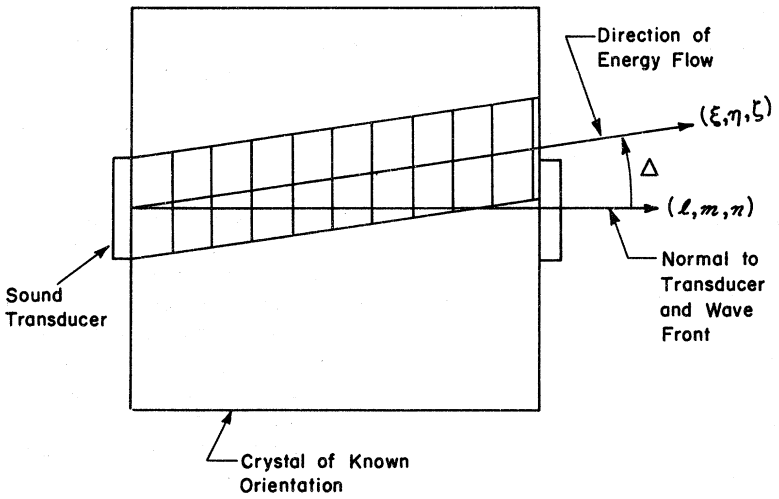

FIG. 1. General experimental design for measuring sound velocities.

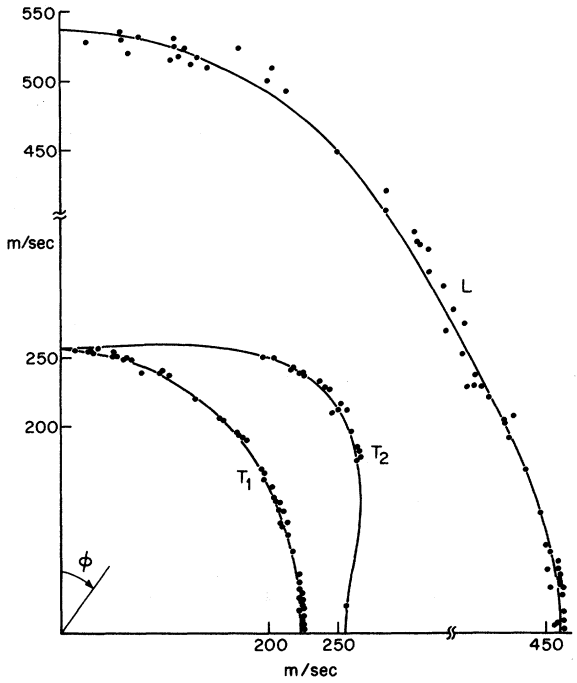

FIG. 2. Polar plot of the various sound velocities as a function of angle ϕ, the angle between the sound propagation direction and the c axis of the helium crystal. T_1 corresponds to a pure transverse mode whereas T_2 and L are quasitransverse and quasilongitudinal modes, respectively.

tal is measured.

Knowing the separation of the sending and receiving transducers thus allows calculation of the velocity of propagation perpendicular to the transducers. As seen in Fig. 1 this measured velocity corresponds to the phase velocity or the component of the velocity with which the wave front traverses the crystal in the direction (l, m, n) normal to the wave front or transducer. In an isotropic substance, this velocity would also be the group velocity and would be found to be independent of the sample orientation. In general, for an anisotropic medium the path of the sound ray does not coincide with the normal to the wave front. A knowledge of the orientation of the crystal with respect to the transducers for hcp crystals then allows a plot of the phase velocity as a function of ϕ, the angle between the c axis and the wave normal, to be made. Figure 2 is a polar plot of this velocity in a plane containing the c axis for solid He^4 showing the published experimental points. This plot is a cross section of the velocity surface with $l = 0$ and the c axis of the crystal along the vertical axis.

While the velocity surface is easily measured, the wave surface has the clearest physical meaning. This is the surface which represents the expanding wave front of a point disturbance occurring at the origin, one unit of time after that disturbance has taken place. Another way to say this is that the wave surface is the locus at time $t = 1$ of all possible plane waves which passed through the origin at time $t = 0$. Since the wave surface describes what is actually happening in a crystal, and the velocity surface describes what is measured in an experiment, both of these surfaces are necessary for a full understanding of sound propagation in an anisotropic crystal. Because in an anisotropic medium the path of the sound ray does not coincide with the normal to a wave front, the velocity surface does not in general coincide with the wave surface, in such a medium. The inverse or slowness surface is also important for some considerations, [6] but we shall not make use of it here.

For greater intuitive grasp of the relation between the velocity surface and the wave surface, we shall here describe a graphical construction that will enable the wave surface to be constructed from the velocity surface or vice versa. We use the notation (l, m, n) and (ξ, η, ζ) to represent the coordinates of a point on the velocity surface and wave surface, respectively; or, if the quantities are normalized, to represent the direction cosines of those points. If the wave surface and the velocity surface are drawn to the same scale in polar coordinates on one sheet of paper, then any tangent to the wave surface at a point (ξ, η, ζ) will intersect the velocity surface at the corresponding point (l, m, n) such that the line from the origin to the point $(l, m, n,)$ on the velocity surface is perpendicular to the tangent line. To apply this idea to find the velocity surface from the given wave surface, simply draw a tangent line to some point on the wave surface. The normal to this tangent line (the wave front) from the origin intersects the tangent at a corresponding point on the velocity surface. Starting with a velocity surface, the method is a little more difficult but follows from the above idea. At any point on the velocity surface, construct a line perpendicular to the radius vector. This line will form a tangent to the required wave surface. It may be necessary to draw many of these tangent lines from neighboring points on the velocity surface to map the wave surface.

The above description is given only as an aid to seeing the relation between the two surfaces, and for any serious consideration it is necessary to give the equations of the two surfaces. The following equations have come from Musgrave's comprehensive work on the propagation of elastic waves. [4,5] Starting with the five reduced elastic constants (elastic constants divided by the density) needed to describe a medium of hexagonal symmetry, c_{11}, c_{12}, c_{13}, c_{33}, and c_{44}, we define a, c, d, h, and H as follows in order to simplify the necessary

equations:

$$a = c_{11} - c_{44}, \quad c = c_{11} - c_{12} - c_{44}, \quad d = c_{13} + c_{44},$$

$$h = c_{33} - c_{44}, \quad H = v^2 - c_{44}.$$

Here v is the phase velocity with direction cosines (l, m, n). Because of the symmetry of the hcp crystal structure, we limit the discussion to the plane containing the c axis for which $l = 0$. By rotation of this plane about the c axis the total surfaces may be reconstructed.

In this plane the equations for plane-wave solutions to the stress-strain Hooke's law equations are

$$(m^2c/2 - H)A_x = 0,$$

$$(m^2a - H)A_y + dmnA_z = 0,$$

$$dmnA_y + (n^2h - H)A_z = 0.$$

In these equations A_x, A_y, A_z are the x, y, and z components, respectively, of the displacement vector for elastic-wave propagation. By setting the determinant of the coefficients in the above set of equations equal to zero, we obtain a cubic equation for H (and thus for v^2) whose three solutions correspond to one longitudinal and two transverse wave solutions. The three solutions H_L, H_{T_1}, and H_{T_2} are

$$H_{L,T_2} = \tfrac{1}{2}\{m^2a + n^2h \pm [(m^2a + n^2h)^2 - 4m^2n^2(ah - d^2)]^{1/2}\}$$

and

$$H_{T_1} = \tfrac{1}{2}m^2c \ .$$

Solving for the displacements A_x, A_y, and A_z, we find for L, the longitudinal mode,

$$A_x = 0, \quad p_L = 0, \quad \frac{A_y}{A_z} = \frac{H_L - n^2h}{mnd} = \frac{q_L}{r_L} \ ,$$

for T_2,

$$A_x = 0, \quad p_{T_2} = 0, \quad \frac{A_y}{A_z} = \frac{H_{T_2} - n^2h}{nmd} = \frac{q_{T_2}}{r_{T_2}} \ ,$$

and lastly for T_1,

$$A_x \neq 0, \quad A_y = A_z = 0$$

or

$$p_{T_1} = 1, \quad q_{T_1} = r_{T_1} = 0.$$

In the above equations p, q, and r are the direction cosines for displacement vector A. Using the above three solutions for H_{L_1}, H_{T_1}, and H_{T_2} and the published elastic constants,[3] the solid lines of Fig. 2 were calculated.

The coordinates of any point on the wave surface of wave normal $(0, m, n)$ are[7]

$$\xi = 0,$$

$$\eta = m\left(v - \frac{H}{v}\right) + \frac{p^2mc + (2q^2H/m)}{2v} \ ,$$

$$\zeta = n\left(v - \frac{H}{v}\right) + \frac{r^2H}{nv} \ .$$

Two additional parameters of interest are δ_L, the angle between A_L and (l, m, n) and Δ_{L,T_1}, T_2, the deviation of the energy path from (l, m, n). In an hcp crystal it can be shown[4] that A_{T_1}, A_{T_2}, and A_L are mutually perpendicular and that A_{T_1} is perpendicular to (l, m, n). In other words, T_1 is a pure transverse mode and $\delta_L = \delta_{T_2}$, where δ_{T_2} is the angle between A_{T_2} and the plane perpendicular to (l, m, n). The fact that δ_L and δ_{T_2} are nonzero is an indication that the L and T_2 modes are *not* pure longitudinal and pure transverse, respectively. The equation for δ_L is

$$\cos\delta_L = lp_L + mq_L + nr_L \ .$$

Since Δ_{L,T_2,T_1} is the angle between the radius vector to a point on the wave surface and the radius vector to a point on the velocity surface, it is given by

$$\Delta_i = \arccos(l\xi_i + m\eta_i + n\zeta_i).$$

Using the above equations, the given elastic constants for hcp solid helium, and a desk computer, (ξ, η, ζ), δ_L, and Δ_i were calculated. The section of the wave surfaces in the plane $(0, m, n)$ is shown in Fig. 3. Figure 4 is a plot of Δ_L, Δ_{T_1}, and Δ_{T_2} as a function of ϕ measured from the c

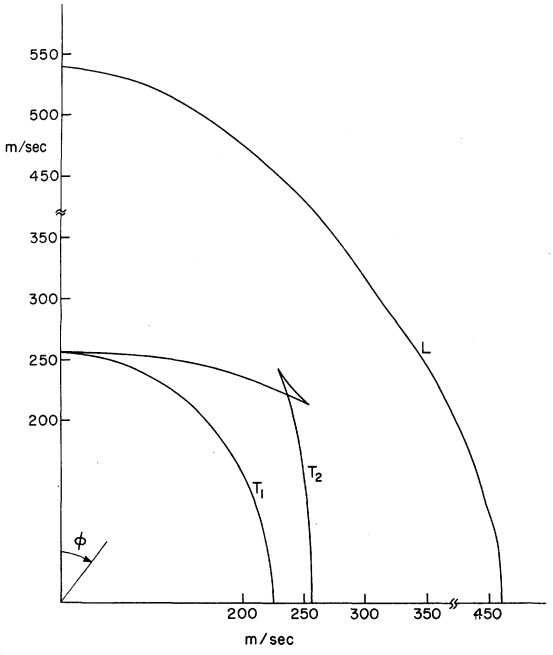

FIG. 3. Cross section of the wave surfaces of hcp solid He^4.

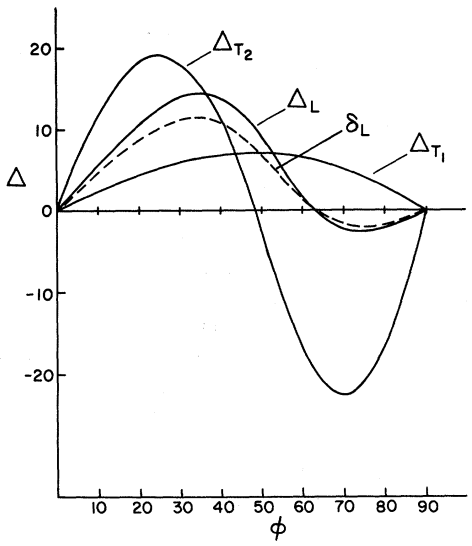

FIG. 4. Plot of the deviations Δ_L, Δ_{T_1}, Δ_{T_2}, and δ_L as a function of ϕ, the angle between the wave normal and the c axis.

axis. The quantity δ_L is also shown in Fig. 4 as the dashed line.

Using the method of analysis of Wanner,[1] we can explain the regions of missing data along the T_2 curve of Fig. 2. A consideration of Fig. 1 leads to the conclusion that if the angle Δ between the wave normal and the direction of propagation (ray) is too large, then the sound beam emitted by the transmitting quartz crystal will not be intercepted by the receiving transducer. For the apparatus of Crepeau *et al.*,[3] where the diameter of the transducers is 0.310 in., if the angle Δ the sound ray makes with the wave normal is greater than 17 deg, the direct sound signal will not reach the receiving transducer and hence a sound velocity will not be recorded. It can be seen from the graph of Fig. 4 that this occurs between values of $\phi = 17$ and 32 deg and again between $\phi = 60$ and 80 deg for the curve Δ_{T_2}. A quick glance at Fig. 2 shows that these are approximately the regions on the T_2 curve where no data have been recorded. For all values of ϕ for the T_1 and L curves it is to be expected that data will be measured because Δ is less than 17 deg.

We have examined the propagation of sound in solid helium crystals using the published data and elastic constants. The wave surfaces and values of the deviation of the sound ray from the wave normal have been calculated and used to explain the regions of missing data in the results of Crepeau *et al.*[3]

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Realistic Single-Function Potential Model for the Noble Gas Hydride Ions†

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Only for HeH^+ of the noble-gas hydride ions have accurate Born-Oppenheimer energies been found,[1] and these over a small range (1.1–1.8 bohr) near the equilibrium separation $r_m = 1.462$ bohr. Michels[2] has delineated the shape of the curve over the larger range 0.1–6 bohr, albeit with less accurate absolute values. Peyerimhoff[3] has made approximate calculations for NeH^+ extending from 1.35–4.5 bohr. For the heavier systems, only crude approximations for the quantities r_m, D_e (the potential-well depth), and k (the force constant) exist. In view of this sparsity of information and the current interest[4,5] in these systems, it would seem useful to have mathematical models for their inter-