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Elastic wave surfaces for the (111) plane of cubic crystals

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Abstract. The nature of inverse velocity surfaces as well as energy surfaces for elastic wave propagation in the (111) plane have been studied for a number of cubic crystals. The sections of inverse velocity surfaces by the (111) plane exhibit six-fold symmetry in all cases. Cuspidal edges are exhibited with a six-fold symmetry by both the slow transverse and fast transverse shear modes in the (111) plane, unlike the case of the (100) and (110) planes for which only the slow transverse shear mode exhibits cuspidal edges. The slow transverse mode energy surface exhibits cuspidal edges along $(\bar{1}\bar{1}2)$ direction or an equivalent symmetry direction. The inverse velocity surfaces of the A-15 compounds exhibit unusually large inflexions for the slow transverse mode, whereas their energy surfaces have large cuspidal edges which intersect each other resulting in common regions of cusps.

Keywords. Inverse velocity surfaces; energy surfaces; A-15 compounds; cuspidal edges.

1. Introduction

The elastic wave surfaces of crystals have been attracting increasing attention in recent years. These investigations acquire a renewed importance in view of the vast research that is currently in progress in the fields of phonon focussing (Maris 1971; McCurdy 1974; Jacob Philip and Viswanathan 1977; Lax and Narayanamurti 1980) and the propagation of nonlinear pulses or solitons in solids (Toda 1967; Narayanamurti *et al* 1973; Bishop and Schneider 1978). Since elastic wave propagation is anisotropic in crystals, the energy surfaces exhibit cuspidal edges for a large number of crystals.

The elastic wave surfaces have been studied in the past by several workers (Miller and Musgrave 1956; Farnell 1961; Brugger 1965; Musgrave 1957) and an excellent introduction of the basic concepts can be obtained from the texts of Musgrave (1970) and Auld (1973). A very exhaustive study of the nature of the sections of the inverse velocity surfaces as well as energy surfaces by the (100) and (110) planes of over sixty five crystals has been made by Jacob Philip and Viswanathan (1977) and it has been found that a large number of cubic crystals exhibit cuspidal edges for the sections of energy surfaces along the (100), (110) and (111) directions. The most important symmetry planes for a cubic crystal are the (100), (110) and (111) crystallographic planes; but however, no work has so far been even attempted on the nature of the elastic wave surfaces by the (111) symmetry plane. A study of the sections of the inverse velocity surface as well as energy surface by this symmetry plane is necessary to complete our knowledge of the elastic wave surfaces of cubic crystals and it is for

this purpose that the present investigation has been undertaken. Unlike the case of the sections by the (100) and (110) planes which exhibit four-fold symmetry, the sections of the inverse velocity as well as energy surfaces by the (111) plane exhibit hexagonal symmetry and further both the quasi-shear modes exhibit cuspidal edges in this case. Some substances like V_3Si exhibit large cusps which are so large as to penetrate into each other resulting in common regions of cusps.

2. The dispersion equation in the (111) plane

Let($l\ m\ n$) denote the direction cosines of the wave vector of a wave propagating inside the crystal. Referred to the principal cubic axes of the crystal, the dispersion equation, determining the velocities of a wave propagating along ($l\ m\ n$) is then given by

$$\begin{vmatrix} (a_{11} - \rho v^2) & a_{12} & a_{13} \\ a_{12} & (a_{22} - \rho v^2) & a_{23} \\ a_{13} & a_{23} & (a_{33} - \rho v^2) \end{vmatrix} = 0, \qquad (1)$$

where $a_{11} = c_{11}l^2 + c_{44}(m^2 + n^2)$

$a_{22} = c_{11}m^2 + c_{44}(n^2 + l^2)$

$a_{33} = c_{11}n^2 + c_{44}(l^2 + m^2)$

$a_{12} = (c_{12} + c_{44})\, lm$

$a_{23} = (c_{12} + c_{44})\, mn$

and $a_{13} = (c_{12} + c_{44})\, ln$

In the above equation, ρ denotes the density of the material and v is the phase velocity of the acoustic wave.

In order to study the wave propagation in the (111) plane, it is convenient to transform to a new set of axes X', Y', Z' such that the X' axis coincides with the (111) direction of the cubic diagonal; then the $Y'Z'$ plane would represent the (111) symmetry plane. The OY' and OZ' axes refer respectively to the $(\bar{1}10)$ and $(\bar{1}\bar{1}2)$ directions of the crystal. If $(l'm'n')$ denote the direction cosines of the wave vector $\tilde{k}$ referred to $X'Y'Z'$ axes, we have

$$\begin{aligned} l' &= \frac{1}{\sqrt{3}}(l + m + n) \\ m' &= \frac{1}{\sqrt{2}}(-l + m) \\ n' &= \frac{1}{\sqrt{6}}(-l - m + 2n) \end{aligned} \qquad (2a)$$

and conversely $l = \frac{1}{\sqrt{6}}(\sqrt{2}l' - \sqrt{3}m' - n')$

$$m = \frac{1}{\sqrt{6}}(\sqrt{2}l' + \sqrt{3}m' - n') \tag{2b}$$

$$n = \frac{1}{\sqrt{6}}(\sqrt{2}l' + 2n')$$

For propagation in the (111) plane, we have $l' = 0$ and hence,

$$l = \frac{1}{\sqrt{6}}(-\sqrt{3}m' - n')$$

$$m = \frac{1}{\sqrt{6}}(\sqrt{3}m' - n') \tag{3}$$

$$n = \frac{2}{\sqrt{6}}n'$$

Substituting these in equation (1), we obtain the dispersion relation for the wave propagation in the (111) plane as $(\alpha - \rho v^2) = 0$ where the elements (α_{ij}) of the matrix are given by

$$\begin{bmatrix} \alpha_{11} \\ \alpha_{22} \\ \alpha_{33} \\ \alpha_{12} \\ \alpha_{13} \\ \alpha_{23} \end{bmatrix} = \begin{bmatrix} \frac{1}{2}(c_{11}+c_{44}) & \frac{1}{6}(c_{11}+5c_{44}) & (c_{11}-c_{44})/2(3)^{1/2} \\ \frac{1}{2}(c_{11}+c_{44}) & \frac{1}{6}(c_{11}+5c_{44}) & (c_{44}-c_{11})/2(3)^{1/2} \\ c_{44} & \frac{1}{3}(2c_{11}+c_{44}) & 0 \\ -\frac{1}{2}(c_{12}+c_{44}) & \frac{1}{6}(c_{12}+c_{44}) & 0 \\ 0 & -\frac{1}{3}(c_{12}+c_{44}) & -(c_{12}+c_{44})/2(3)^{1/2} \\ 0 & -\frac{1}{3}(c_{12}+c_{44}) & (c_{12}+c_{44})/2(3)^{1/2} \end{bmatrix} \begin{bmatrix} \\ (m')^2 \\ \\ (n')^2 \\ \\ 2m'n' \\ \end{bmatrix} \tag{4}$$

Writing $x = \rho v^2$, we find that the dispersion equation (1) reduces to the cubic equation

$$x^3 + a_2x^2 + a_1x + a_0 = 0. \tag{5}$$

The coefficients a_2, a_1 and a_0 are functions of the elastic constants and the direction cosines in the plane.

Considering the wave vector $\tilde{k}$ in the (111) plane, let θ denote the angle which the

vector $\tilde{k}$ make with the Z' axis so that $m' = \sin\theta$ and $n' = \cos\theta$. The components of the group velocity vector are given by Auld (1973).

$$\left.\begin{aligned} S_{x'} &= \partial\omega/\partial k_{x'} = \partial v/\partial l' = 0, \\ S_{y'} &= \partial\omega/\partial k_{y'} = \partial v/\partial m' \\ &= \frac{1}{2\rho v D}\left(x^2\frac{\partial a_2}{\partial m'} + x\frac{\partial a_1}{\partial m'} + \frac{\partial a_0}{\partial m'}\right) \\ S_{z'} &= \partial\omega/\partial k_{z'} = \partial v/\partial n' \\ &= \frac{1}{2\rho v D}\left(x^2\frac{\partial a_2}{\partial n'} + x\frac{\partial a_1}{\partial n'} + \frac{\partial a_0}{\partial n'}\right) \end{aligned}\right\} \quad (6)$$

where $D = (3x^2 + 2a_2x + a_1)$.

From the first of the equations (6), it follows that the energy flux vector lies in the $Y'Z'$ plane itself. The exact direction of the group velocity vector and the magnitude of the group velocity vector are given by

$$\left.\begin{aligned} \tan\theta_g &= (S_{y'}/S_{z'}) \\ S &= (S_{y'}^2 + S_{z'}^2)^{1/2} \end{aligned}\right\}. \quad (7)$$

Equations (5), (6) and (7) were solved using a TDC 316 computer for different values of θ from 0° to 180° in steps of 5° and sections of the inverse velocity as well as energy surfaces by the (111) planes of the following crystals were plotted: copper, gold, lithium, sodium, potassium, lead, molybdenum, tungsten, vanadium, niobium, PbS, V_3Si (transforming as well as nontransforming at 300°K and 4·2°K), NaCl, KI, RbF and some of the quantum crystals argon, krypton, xenon and neon.

3. Results and discussion

Figure 1 depicts a (111) section of the inverse velocity surface of potassium iodide. It is seen that the sections of inverse velocity surface of quasilongitudinal (L) and quasi-shear modes (T_1 and T_2) exhibit six-fold symmetry. The six-fold symmetry is exhibited sharply especially for the two shear modes. It can be noted that the position of a maximum inflexion for the slow transverse mode (T_1) corresponds to a minimum inflexion in the fast transverse mode (T_2) and vice versa. This is characteristic of the sections of the inverse surfaces of all the substances we have studied.

The criteria for the existence of inflexions and cusps for cubic and hexagonal crystal have been discussed in detail by Musgrave (1957, see also the footnote on page 903 of this paper). As pointed out by him, the inverse velocity surface is of degree six and it is not possible for a straight line to make more than six intersections with the inverse velocity surface. If the minimum occurred in the same direction,

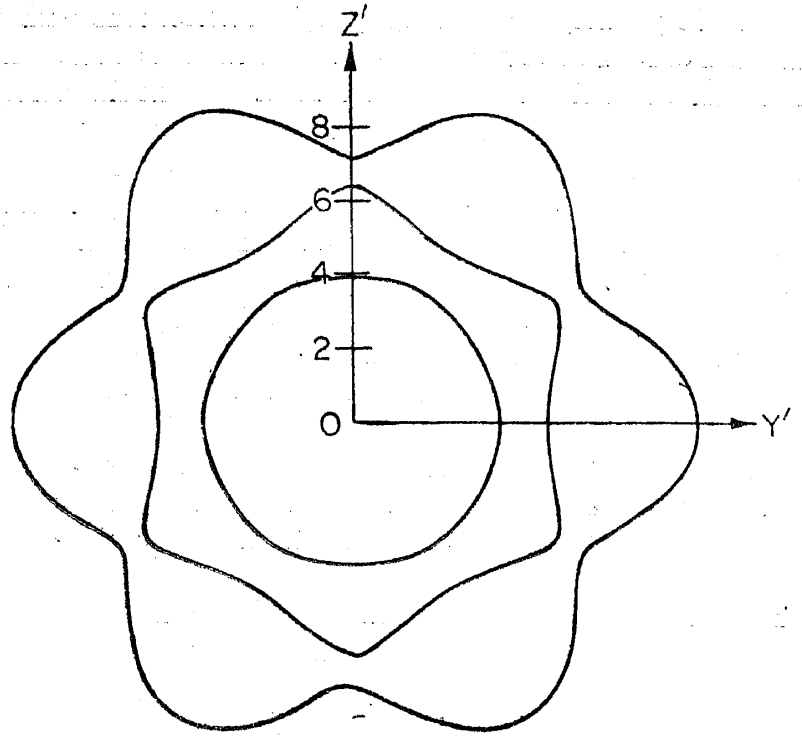

Figure 1. Section of the inverse velocity surface of the crystal potassium iodide in the (111) plane. Unit: 10^{-6} cm^{-1} sec. Y' and Z' refer to the $(\bar{1}10)$ and $(\bar{1}\bar{1}2)$ directions of the cubic crystal.

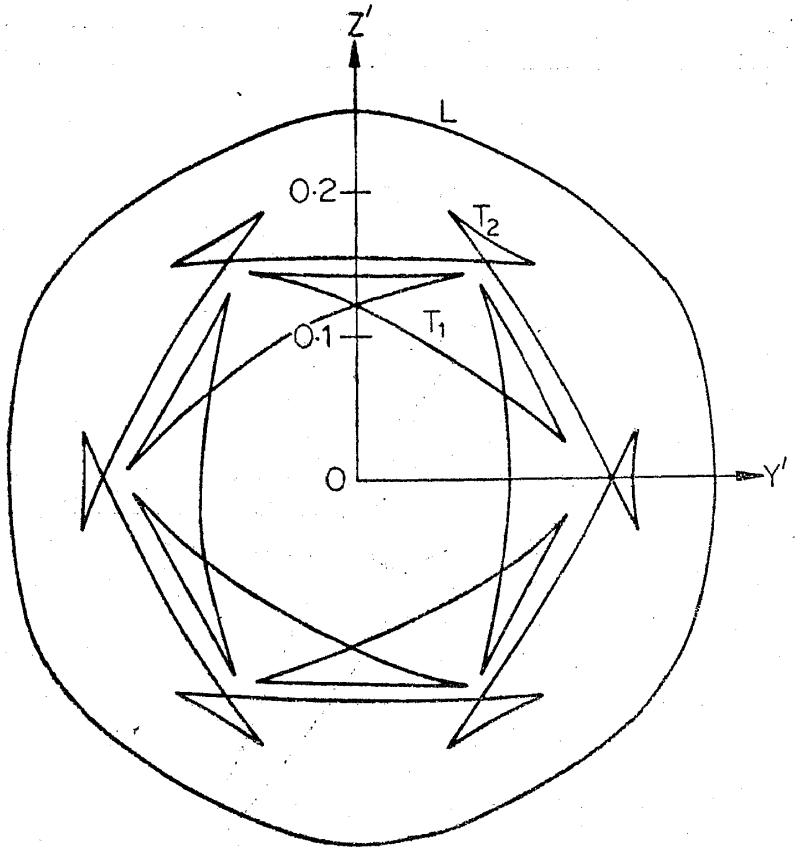

Figure 2. Section of the energy surface of potassium iodide in the (111) plane. Unit: 10 cms/sec. Y' and Z' refer to the $(\bar{1}10)$ and $(\bar{1}\bar{1}2)$ directions of the cubic crystal.

a straight line could possibly result making eight intersections with the surface. These mathematical conclusions are supported by our numerical computations which show that the minimum of the slow transverse mode (T_1) should correspond to the maximum of the fast transverse mode (T_2) or vice versa.

In figure 2, we reproduce the sections of the energy surfaces of KI. An interesting aspect of these figures is that cuspidal edges are exhibited by both the shear modes (fast transverse as well as slow transverse), unlike the case of the (100) and (110) planes for which only the slow transverse quasi shear mode exhibits cuspidal edges. The reason for this is that in the (111) plane both the transverse modes are quasi shear and not ' pure ' shear modes. For the case of (100) plane, both the inverse as well as the energy surfaces of the ' pure ' shear mode are circles, whereas they are ellipses for the (110) plane. For only the (111) plane do the section of the inverse velocity surfaces exhibit inflexions and hence the energy surface also exhibits cuspidal edges for both the quasi-shear modes. The cusps corresponding to the fast transverse mode are centred between the cusps for the slow transverse mode and vice versa.

Also, all the six inflexion maxima seen in figure 1 for the slow transverse mode correspond to the $(1\bar{1}0)$ or an equivalent symmetry direction as can be verified by substituting the corresponding direction in the transformation equation (3). The cusps for these slow transverse modes are centred along the direction $(\bar{1}\bar{1}2)$ or an equivalent symmetry direction. It is important to note that cusps could occur along directions like $(\bar{1}\bar{1}2)$ apart from the principal axes, face diagonals and cube diagonals. For fast transverse mode, the cusp occurs along the face diagonal.

As in the case of (100) plane, the inverse velocity surfaces of the A-15 compounds stand aloof distinctly and exhibit unusual characteristics at low temperatures. In

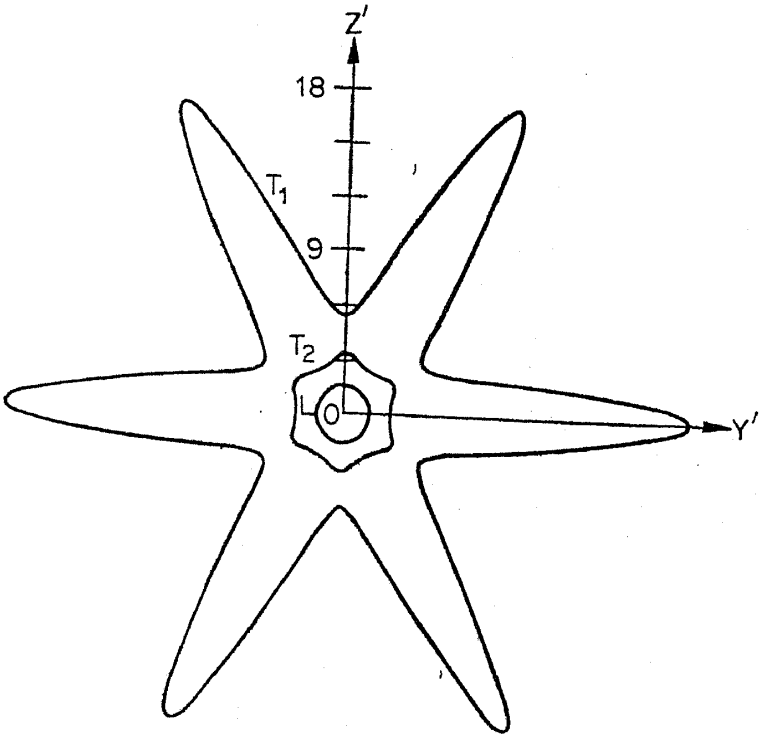

Figure 3. Section of the inverse velocity surface of V_3Si at 4·2°K. Unit: 10^{-6} cm^{-1} sec. Y' and Z' refer to the $(\bar{1}10)$ and $(\bar{1}\bar{1}2)$ dirctions of the cubic crystal.

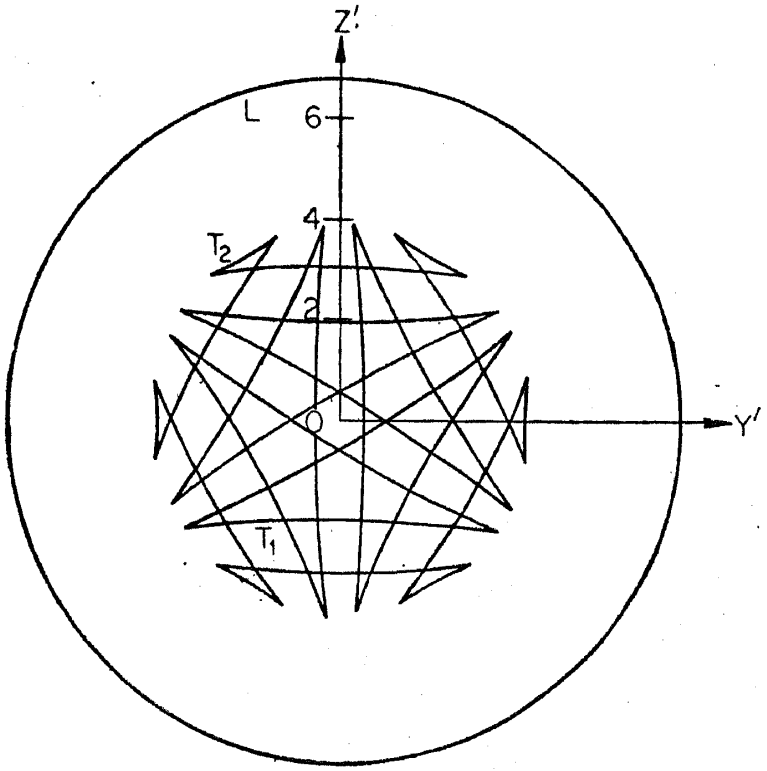

Figure 4. Section of the energy surface of V_3Si at 4·2°K. Unit: 10^6 cms/sec. Y' and Z' refer to the $(\bar{1}10)$ and $(\bar{1}\bar{1}2)$ directions of the cubic crystal.

Table 1. Elastic constant data

Substance	Elastic constants × 10^{12} dynes/cm²			Density g/cc
	C_{11}	C_{12}	C_{44}	
KI*	0·271	0·045	0·0364	3·13
V_3Si**	1·795	1·765	0·761	5·720

*Federov 1966
**Testardi *et al* 1965

figure 3 we reproduce sections of the inverse velocity surface of V_3Si (transforming) at 4·2°K. Since one of the quasi-shear modes propagating along the (110) direction with $(1\bar{1}0)$ polarization becomes soft for this material, the section of the inverse velocity surface for this mode exhibits very large inflexion. The other shear mode also has six-fold symmetry, but not pronounced peaks. Figure 4 gives the section of the energy surface of V_3Si (transforming) by the (111) plane. As stated before both the quasi-shear modes exhibit cuspidal edges and the cusps corresponding to the slow transverse mode (T_1) are very large, so large that the cuspidal edges cross each other resulting in common regions of the cusps.

In table 1, we have given the values of elastic constants and density used in our computations.

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