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ELASTIC CONSTANTS OF α-ZnS*

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Abstract—The elastic constants of hexagonal zinc sulfide were measured at room temperature. Velocity measurements used for computing the elastic constants were made at 10 mc/sec using a coherent pulse/cw technique. The derived values of the elastic constants, in units of 10^{12} dyn/cm^2 are: $c_{11} = 1{\cdot}312$, $c_{12} = 0{\cdot}663$, $c_{13} = 0{\cdot}509$, $c_{33} = 1{\cdot}408$ and $c_{44} = 0{\cdot}286$. Curves of intersection of the velocity surfaces with the XZ plane are given and compared with similar curves for hexagonal cadmium sulfide.

1. INTRODUCTION

THE WORK reported here was undertaken primarily to measure the velocities of propagation of pure compressional and pure shear elastic waves along the c axis of zinc sulfide, required for determining the thickness of half-wavelength vapor deposited ZnS piezoelectric transducers.(1) As the ZnS sample obtained was large enough to propagate elastic waves along three suitable separate crystallographic directions, all five independent elastic constant (c_{11}, c_{12}, c_{13}, c_{33} and c_{44}) were determined from the eight independent velocity measurements made. In addition, three internal checks on the accuracy of the results were obtained. The velocities were measured by a coherent pulse/cw technique(2) which permitted a simultaneous comparison with the conventional pulse/echo technique.

2. RELATIONS BETWEEN ACOUSTIC VELOCITIES AND ELASTIC CONSTANTS

For propagation of plane elastic waves in hexagonal crystals, MUSGRAVE(3) has derived the following wave equation

$$\begin{vmatrix} l^2a+m^2(c/2)-H, & lm(a-(c/2)), & n\,l\,d \\ lm(a-(c/2)), & l^2(c/2)+m^2a-H, & m\,n\,d \\ n\,l\,d & m\,n\,d, & n^2h-H \end{vmatrix} = 0 \tag{1}$$

where l, m, n are the direction cosines of the wave normal, c_{ij} are elastic constants, v is acoustic velocity, ρ is density and

$$a = c_{11}-c_{44} \tag{2}$$

$$c = c_{11}-c_{12}-2c_{44} \tag{3}$$

$$d = c_{13}+c_{44} \tag{4}$$

$$h = c_{33}-c_{44} \tag{5}$$

$$H = \rho v^2-c_{44} \tag{6}$$

It can be shown from equation (1) that circular symmetry about the X_3 or Z axis exists for both the velocity and wave surfaces. Thus the circles of intersection of the free velocity surfaces with the basal plane are the roots of the equation

$$H^3-(a+\tfrac{1}{2}c)H^2+\tfrac{1}{2}acH = 0 \tag{7}$$

which is obtained from equation (1) by allowing n to become zero.

The elastic constants c_{11}, c_{12}, c_{44} can be obtained by measuring the velocities of propagation of the three acoustic modes in the basal plane. The appropriate equations are

$$\rho v_L{}^2 = c_{11} \tag{8}$$

$$\rho v_{T_1}{}^2 = \tfrac{1}{2}(c_{11}-c_{12}) \tag{9}$$

$$\rho v_{T_2}{}^2 = c_{44} \tag{10}$$

In these equations L refers to the compressional mode, T_1 to the shear mode with displacement

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vector parallel to the basal plane and T_2 to the shear mode with displacement vector normal to the basal plane as shown in Fig. 1. Propagation along the hexad axis yields c_{33} and an internal check on c_{44} as shown in the following equations

$$\rho v_L^2 = c_{33} \tag{11}$$

and

$$\rho v_T^2 = c_{44} \tag{12}$$

The last of the five independent elastic constants c_{13} can only be derived from the equations for propagation at some angle between the hexad axis and the basal plane. For propagation at 45° to the hexad axis one obtains for the T_1 mode

$$\rho(v_{T_1})^2 = \tfrac{1}{4}(c_{11}-c_{12}+2c_{44}) \tag{13}$$

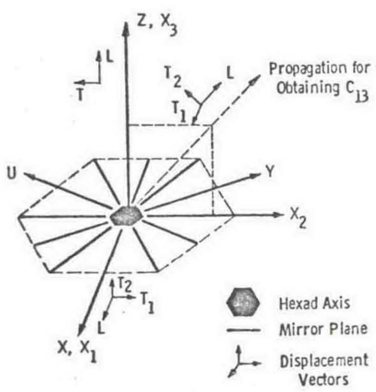


FIG. 1. Hexagonal ZnS symmetry element.

and for the L and T_2 modes

$$\rho v^2 = \tfrac{1}{4}(c_{11}+c_{33}+2c_{44}) \pm \tfrac{1}{4} \times \{(c_{11}-c_{33})^2+4(c_{13}+c_{44})^2\}^{1/2} \tag{14}$$

In this equation the positive second term applies to the L mode and the negative to the T_2 mode.

The equations for the curves of intersection of the velocity surfaces of the three acoustic modes with any plane containing the hexad axis can be obtained from equation (1) into which the computed values of the c_{ij} have been substituted. The appropriate equation is

$$[H-\tfrac{1}{2}c(1-n^2)] \times [H^2-\{n^2h+(1-n^2)a\}H+n^2(1-n^2) \times (ah-d^2)] = 0 \tag{15}$$

where n is allowed to assume all values between $+1$ and -1.

3. VELOCITY MEASUREMENTS

A single crystal of hexagonal ZnS, grown in these Laboratories, was cut and polished to have pairs of parallel faces normal to the X_1 and X_3 axes and to a direction in the X_2X_3 plane at 45° to either of these axes as shown in Fig. 1. The directions of the displacement vectors are shown in this diagram for each propagation direction used in these measurements. The transducers used were 10 mc/sec x- or y-cut quartz plates obtained from Valpey Crystal Corp. The pulse/cw technique used has been described elsewhere.(2) Table 1

Table 1. Velocity measurements

Mode	Propagation direction (along axis)*	Displacement direction (along axis)*	Velocity $\times 10^5$ cm sec^{-1}
L	X_3	X_3	5·868
T†	X_3	X_1	2·645
L	X_1	X_1	5·667
T_1	X_1	X_2	2·815
T_2	X_1	X_3	2·644
L	45° to X_3	43° to X_3	5·469
T_1	45° to X_3	X_2	2·717
T_2	45° to X_3	−47° to X_3	3·224

* See Fig. 1.
† Shear modes degenerate.

lists the eight independent velocity measurements used for calculating the elastic constants given in Table 2 and the curves of intersection of the velocity surfaces with any plane containing the Z or X_3 axis shown in Fig. 2.

Table 2. Elastic constants in units of 10^{12} dyn cm^{-2}

c_{11}	c_{12}	c_{44}	c_{33}	c_{13}
1·312	0·663	0·286	1·408	0·509

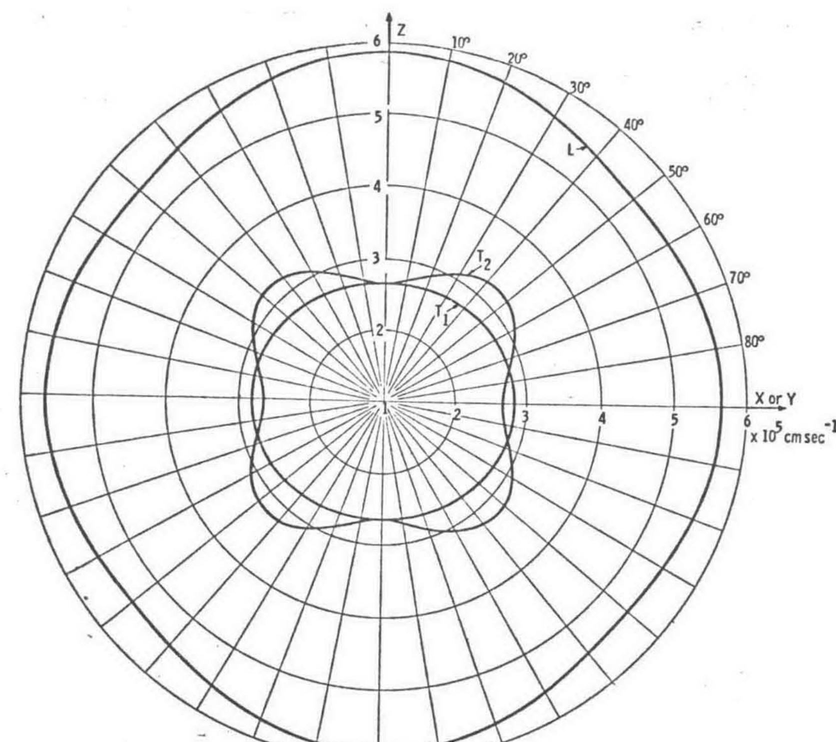


FIG. 2. Curves of intersection of velocity surfaces with any plane containing the Z axis.

4. WAVE SURFACES

The curves of intersection of the wave surfaces(3) with any plane containing the Z axis are loci of points R such that

$$R_i^2 = \frac{(v_i-A_i')^2}{(\cos\epsilon_i)^2}+2A_i'v_i-A_i'^2$$

or

$$R_i^2 = \left(\frac{H_i}{(\rho v_i\cos\epsilon_i)}\right)^2+2A_i'v_i-A_i'^2 \tag{16}$$

where

$$i = L,\quad T_1,\quad T_2$$

$$\cos\epsilon_i = \left\{\frac{m^2n^4d^4}{[(H_i-m^2a)^2+m^2n^2d^2]^2}+\frac{(H_i-m^2a)^4}{n^2[m^2n^2d^2+(H_i-m^2a)^2]^2}\right\}^{-1/2} \tag{17}$$

and

$$A_i' = \frac{c_{44}}{\rho v_i} \tag{18}$$

and H_i is as defined in equation (6). The parameters R_i, ϵ_i, A_i' and v_i are as defined in Fig. 3. The angle Δ between the wave normal and the direction of energy flow is defined by

$$\tan\Delta_i = \left(\frac{v_i-A_i'}{v_i}\right)\tan\epsilon_i \tag{19}$$

Figure 4 shows how the ray direction, or energy flow, deviates from the wave normal for each of the modes L, T_1 and T_2 as a function of θ, which is the angle between the Z axis and the wave normal, in any plane containing the Z axis. Figure 5 shows a plot of $(\Delta+\theta)$ as a function of θ for all three modes. The section of the T_2 mode curve for $20° < \theta < 70°$ corresponds to the cusp between 40° and 50° in Fig. 6, in which are shown the curves of intersection of the wave surfaces with any plane containing the Z axis. As indicated earlier, this is a plot of R_i as a function of $(\Delta+\theta)$.

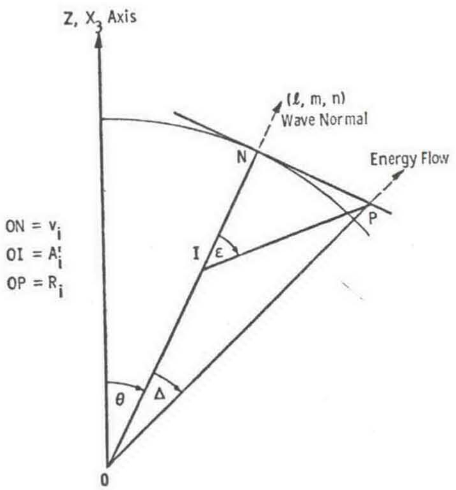


FIG. 3. Relation between wave normal and energy flow direction.

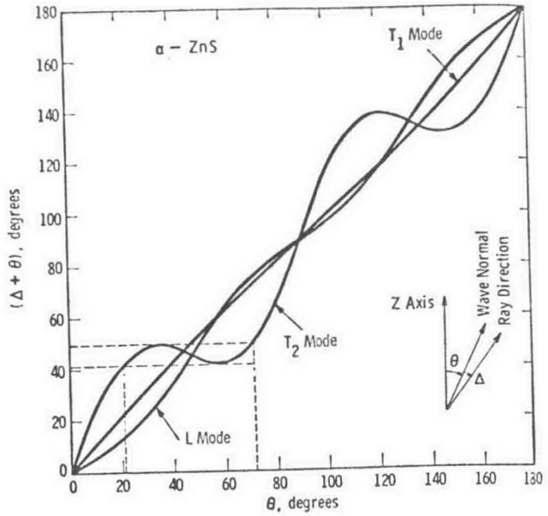


FIG. 5. $(\Delta+\theta)$ plotted as a function of θ for modes L, T_1 and T_2.

The T_1 mode is always a pure mode and hence the associated displacement vector is always parallel to the basal plane. The L and T_2 modes are

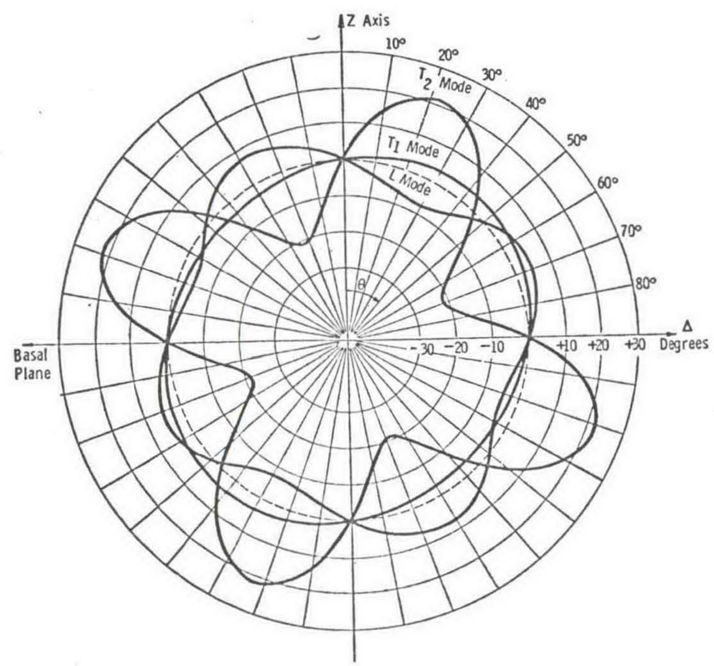


FIG. 4. Deviation of ray from wave normal in ZnS for L, T_1 and T_2 modes in any plane containing Z axis.

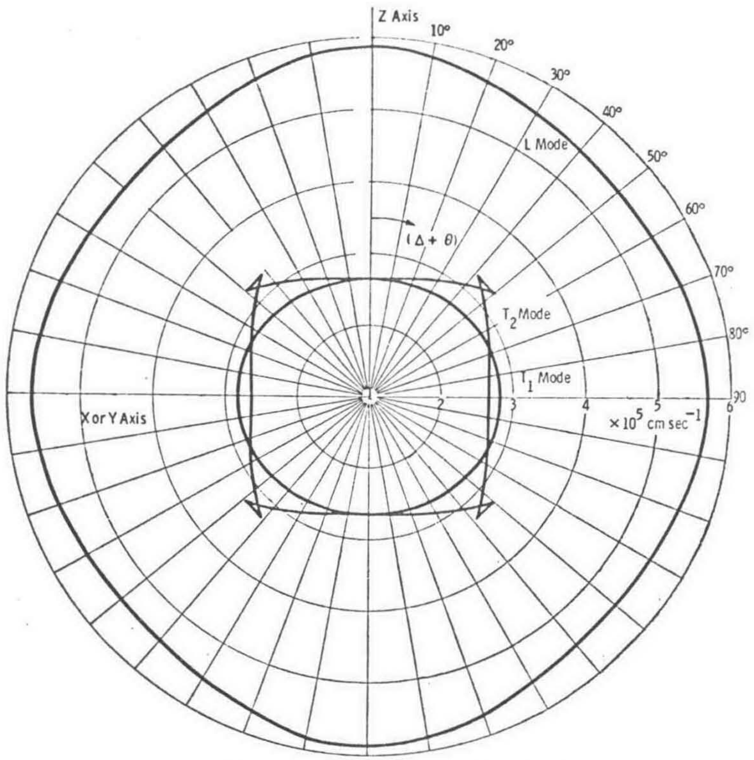


FIG. 6. Curves of intersection of wave surfaces for ZnS with any plane containing the Z axis.

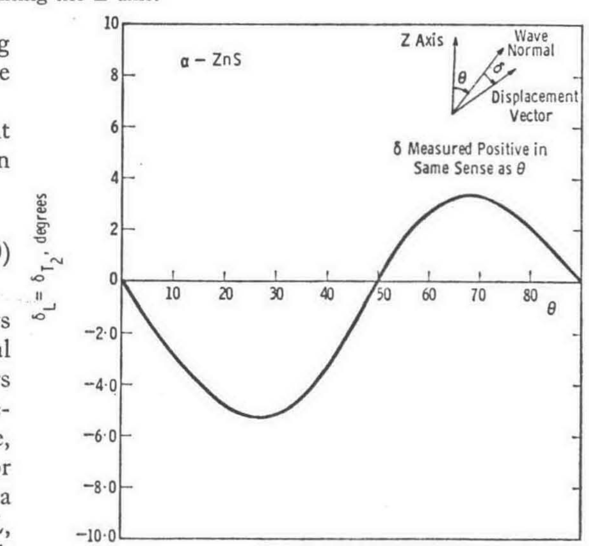
not pure modes except in the basal plane, along the Z axis, and along the cone mentioned in the next paragraph.

The deviation, δ, of the L mode displacement vector from the wave normal for propagation in any plane containing the Z axis is given by[(3)]

$$\cos\delta_L = \frac{m^2nd+n(H_L-m^2a)}{[(H_L-m^2a)^2+m^2n^2d^2]^{1/2}}. \quad (20)$$

The L and T_2 mode displacement vectors always remain in the plane containing the wave normal and the Z axis. As the three displacement vectors are mutually orthogonal and the T_1 mode displacement vector is always parallel to the basal plane, equation (20) will also give the deviation, δ_{T_2}, for the T_2 mode. Figure 7 indicates how δ varies as a function of θ. This figure indicates that other L, T_1, T_2 pure mode directions will form a cone, with axis along the hexad axis, and the semi-angle of 50°.

As a comparison with CdS, Fig. 8 shows the curves of intersection of the velocity surfaces with



Deviation of displacement vector of quasi-longitudinal wave (L mode) from wave normal

FIG. 7. Deviation of displacement vector of quasi-longitudinal wave (L mode) from the wave normal.

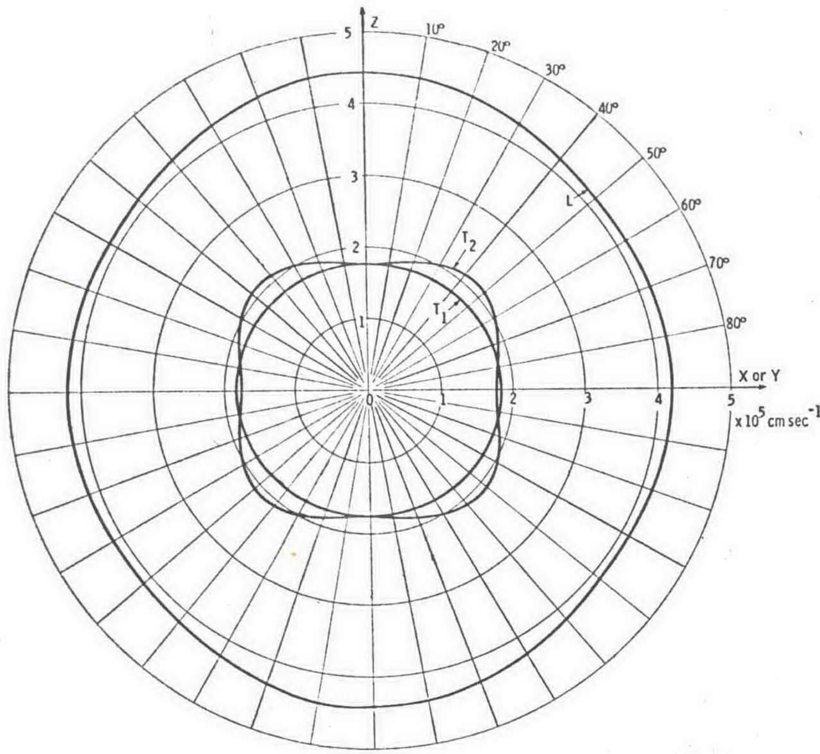


FIG. 8. Curves of intersection of velocity surfaces for CdS in any plane containing the Z axis.

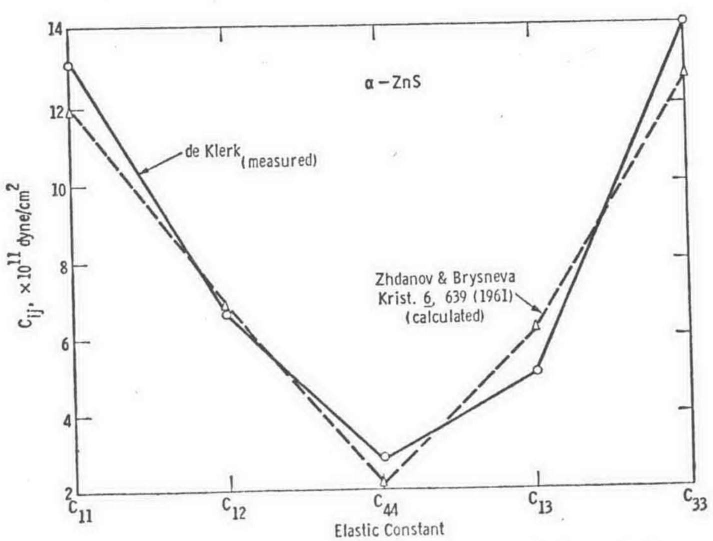


FIG. 9. Comparison of experimental and theoretical values of c_{ij}.

any plane containing the Z axis. Data used for this curve were obtained from measurements made by BOLEF, MELAMED and MENES.[5] The anisotropy is slightly greater in ZnS than in CdS. Figure 9 compares the measured values of c_{ij} with theoretical values calculated by ZHDANOV and BRYSNEVA[6] from measurements on cubic ZnS made by BHAGAVANTAM and SURYANARAYANA.[7]

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