Elastic Constants of Indium Antimonide from 4.2°K to 300°K*

L. J. SLUTSKY† Department of Chemistry, University of Texas, Austin, Texas

AND

C. W. GARLAND, Department of Chemistry and Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts

(Received September 11, 1958)

The adiabatic elastic constants of a single crystal of indium antimonide have been measured by an ultrasonic pulse technique in which 10-Mc/sec acoustic waves were employed. The elastic constants extrapolated to 0°K are, in units of 10¹² dynes/cm², $c_{11}=0.6918$, $c_{12}=0.3788$, and $c_{44}=0.3132$. A Debye characteristic temperature, θ , of 205°±2°K at 0°K was calculated from these values of the elastic constants.

I. INTRODUCTION

THE ultrasonic pulse-echo technique provides a convenient method of measuring the elastic constants of a solid substance. In the case of a crystal with cubic symmetry, measurement of the velocities of longitudinal and transverse acoustic waves propagating in the [110] direction suffices to determine the three independent elastic constants c_{11} , c_{12} , and c_{44} ; the relations between the wave velocities (U) and the elastic constants being

$$\rho U_t^2 = \frac{1}{2} (c_{11} + c_{12} + 2c_{44}),$$

$$\rho U_t^2 = c_{44} \quad \text{(polarized parallel to [001])}, \qquad (1)$$

$$\rho U_t^2 = \frac{1}{2} (c_{11} - c_{12}) \quad \text{(polarized perpendicular to [001])},$$

where ρ is the density, and the subscripts *l* and *t* refer to the longitudinal or transverse character of the wave. In the [111] direction it is possible to propagate a longitudinal and a transverse wave with velocities given by

$$\rho U_t^2 = \frac{1}{3} (c_{11} + 2c_{12} + 4c_{44}),$$

$$\rho U_t^2 = \frac{1}{3} (c_{11} - c_{12} + c_{44}) \quad \text{(any polarization)}. \quad (2)$$

In this work the elastic constants of indium antimonide were determined over the temperature range 4.2°K to 300°K by fitting the measured velocities of longitudinal and transverse acoustic waves propagating in the [110] and [111] directions. The results obtained at room temperature are in good agreement with those of McSkimin, Bond, Pearson, and Hrostowski,¹ who used a phase-comparison technique employing ultrasonic waves of 50 Mc/sec. Our values of c_{11} and c_{12} are several percent higher, and our values of c_{44} somewhat lower, than those obtained by Potter,² who measured the elastic constants of indium antimonide from 77.6°K to 700°K, using the composite-oscillator technique with resonant frequencies of approximately 50 kc.

II. EXPERIMENTAL METHOD

The cryogenic technique used in this work has been described previously.⁸ In the ultrasonic pulse method,⁴ trigger pulses from a Du Mont 256-D oscilloscope are used to trigger an oscillator that applies a 10-Mc/sec pulse (approximately 2 μ sec in duration) to a quartz transducer cemented to the sample. The elastic wave so generated traverses the length of the sample, reflects off the far end, and on returning is partially reconverted into an electrical impulse by the quartz crystal. The interval between successive echo pulses gives the transit time of the pulse in the sample when a small correction is made for the delay of the pulse in the sample.

The sample was obtained in the form of a cylinder approximately 1 inch in diameter and 2 inches long, with the cylinder axis parallel to the [111] direction. Crystal orientation was determined in a back-reflection Laue apparatus, and pairs of (111) and (110) faces were ground off. At 300°K the distance between the (111) faces was 1.7879 inches, the distance between the (110) faces 0.8179 inch. Approximate values of the delay times associated with these path lengths are 23 μ sec for the longitudinal wave and 48 μ sec for the transverse wave in the [111] direction, 11 μ sec for the longitudinal wave and 18 and 25 μ sec for the two transverse waves in the [110] direction. The error in the orientation of the faces, and thus in the direction of propagation of ultrasonic waves, did not exceed 30'.

A Dow Corning 200 silicone fluid (viscosity 2.5×10^6 centistokes at 25°C) proved to be a satisfactory adhesive seal for work with longitudinal waves over the entire temperature range that was investigated. However, this material transmits transverse waves poorly above 215°K. Phenyl salicylate (Salol) gave good results in the temperature range 300°K to 230°K; below 230°K Fisher "NONAQ" stopcock grease was satisfactory for both longitudinal and transverse waves. Corrections of

^{*} This work was supported in part by the U. S. Army (Signal Corps), the U. S. Air Force (Office of Scientific Research, Air Research and Development Command), and the U. S. Navy (Office of Naval Research).

[†] Alfred P. Sloan Foundation Research Associate: Summer, 1958.

¹ McSkimin, Bond, Pearson, and Hrostowski, Bull. Am. Phys. Soc. Ser. II, 1, 111 (1956).

² R. F. Potter, Phys. Rev. 103, 47 (1956).

⁸ L. J. Slutsky and C. W. Garland, Phys. Rev. **107**, 972 (1957). ⁴ H. B. Huntington, Phys. Rev. **72**, 321 (1947).



FIG. 1. The values of ρU^2 for longitudinal waves in the [111] and [110] directions. The smooth curves are calculated from the elastic constants given in Table I.

0.03 μ sec for longitudinal and 0.04 μ sec for transverse waves³ were subtracted from the observed delay times to correct for the delay in the seal.

The density of InSb at 300°K was taken² to be 5.7751 g/cm³, and the density and path lengths were corrected for the effects of thermal expansion with the data of Hidnert and Kirby cited by Potter.² It was observed that below 100°K the attenuation increased considerably. Since it was desired to preserve this fairly large single crystal intact, it was not possible to reduce the path lengths in order to decide whether this increased attenuation was a characteristic of the sample or of the sealing compounds.

III. RESULTS

The independent elastic constants of indium antimonide are listed at 50°K intervals in Table I. The values of c_{44} were determined directly from a smooth curve through the experimental values of ρU^2 for the

TABLE I. The adiabatic elastic constants of indium antimonide. All entries are in units of 10^{12} dynes/cm².

$T(^{\circ}K)$	C11	C12	C44
0	0.6918	0.3788	0.3132
50	0.6899	0.3775	0.3123
77.6	0.6872	0.3753	0.3117
100	0.6847	0.3735	0.3111
150	0.6794	0.3698	0.3096
200	0.6744	0.3670	0.3076
250	0.6702	0.3652	0.3051
300	0.6669	0.3645	0.3020

[001] polarized transverse wave in the [110] direction. The values of c_{11} and c_{12} were obtained by a leastsquares fit to the measured values of $\frac{1}{2}(c_{11}+c_{12}+2c_{44})$, $\frac{1}{3}(c_{11}+2c_{12}+4c_{44})$, and $\frac{1}{2}(c_{11}-c_{12})$. Because of the small delay time and the consequently greater effect of the uncertainty in the seal correction, values of ρU_{l^2} in the [110] direction were given half weight in the leastsquares treatment. The experimental values of ρU^2 for longitudinal waves in the [111] and [110] directions are plotted in Fig. 1. Results for the two transverse waves in the $[1\overline{1}0]$ direction are given in Fig. 2. The smooth curves in these figures were obtained from the elastic constants in Table I by means of Eqs. (1) and (2). Measurement of the velocity of the transverse wave in the [111] direction at 300°K and 77.6°K provided an additional check on the internal consistency of the data. The experimental value of ρU^2 for this wave is, in units of 10^{12} dynes/cm², 0.2020 at 300°K and 0.2068 at 77.6°K, while the values calculated from the elastic constants given in Table I are 0.2015 and 0.2079, respectively. Values of c_{44} given by Potter² are plotted in Fig. 2. Our values of ρU^2 for the two longitudinal waves are consistently 3% higher and our values of $\frac{1}{2}(c_{11}-c_{12})$ are consistently 6.5% lower than those calculated from Potter's results.

The probable error in the measured values of ρU^2 as estimated from the average deviation among the time intervals between successive echo pulses and the uncertainty in the seal correction is $\pm 0.7\%$. In the measurement of $\frac{1}{2}(c_{11}-c_{12})$ below liquid nitrogen



FIG. 2. The values of ρU^2 for the two transverse waves in the $[1\overline{10}]$ direction. The smooth curves are calculated from the elastic constants given in Table I. Values of c_{44} given by Potter are shown as open circles.

TABLE II. The elastic constants of indium antimonide at room temperature obtained from the present measurements (SG) compared with values obtained by Potter^a (P) and McSkimin, Bond, Pearson, Hrostowski^b (M). Results are in units of 10¹² dynes/cm².

Obs.	Temp.	Freq.	C11	C12	C44
SG	300°K	10 Mc/sec	0.6669	0.3645	$\begin{array}{c} 0.3020 \\ 0.3018 \\ 0.3071 \end{array}$
M	298°K	50 Mc/sec	0.6717	0.3665	
P	300°K	50 kc/sec	0.6472	0.3265	

^a See reference 2. ^b See reference 1.

temperature the increased attenuation made the later echoes difficult to range. The uncertainty in ρU^2 for this wave below 77.6°K is estimated at $\pm 1.5\%$. The probable error in c_{11} and c_{12} is about $\pm 1\%$. The various checks on the internal consistency of the data are satisfied to within 0.5% over the entire temperature range.

The results of this work are compared with other determinations of the room temperature elastic constants of indium antimonide in Table II. A Debye characteristic temperature, θ , of $205^{\circ} \pm 2^{\circ}$ K was calculated from the 0°K values of the elastic constants with the aid of the tables given by de Launay.⁵ The calorimetric value is $200^{\circ} \pm 6^{\circ} K.^{2}$

ACKNOWLEDGMENTS

We wish to express our thanks to Dr. Edward P. Warekois and Mr. Paul Metzger of Lincoln Laboratory for the loan of a large single crystal of indium antimonide and for performing the x-ray orientation, and to Dr. Andrew C. Yang of Air Force Cambridge Research Center for advice and assistance in the preparation of the sample.

⁵ J. de Launay, J. Chem. Phys. 22, 1676 (1954).

PHYSICAL REVIEW

VOLUME 113, NUMBER 1

JANUARY 1, 1959

Compton Scattering of X-Rays from Nonspherical Charge Distributions

A. J. FREEMAN

Materials Research Laboratory, Ordnance Materials Research Office, Watertown, Massachusetts and Solid State and Molecular Theory Group, Massachusetts Institute of Technology, Cambridge, Massachusetts (Received July 8, 1958)

The Waller-Hartree theory for the incoherent Compton scattering of x-rays is extended to include the effects fo the inherent nonsphericity of atomic charge distributions. The dependence of the scattering on atomic orientation is treated by a general formalism which depends on the use of the matrix elements of a unitary representation of the group of three-dimensional rotations. Application is made to derive the oneelectron scattering matrix elements from atoms with s, p, and d electrons. It is shown that by a proper averaging over all orientations of the scattering vector, "mean" scattering formulas result which may be used directly for predicting the scattering from monatomic gases.

I. INTRODUCTION

QUANTUM-MECHANICAL theory of the scattering of radiation by a free atom has been given by several authors¹⁻⁴ to account for the observed coherent and incoherent parts of the scattered intensity. Since accurate crystal wave functions are not available, a valuable first approximation to the incoherent Compton scattering function for a crystal may be obtained by considering each atom in the crystal to behave independently of its neighbors, and hence the scattered intensity for the crystal will be given by that determined for the free atoms. This then gives added importance to the available formulas for the free-atom Compton scattering. Of these the one most frequently employed is the Compton-Raman-Wentzel1-3 equation for the intensity in electron units (e.u.):

$$I_{\text{e.u.}} = Z - \sum_{i=1}^{Z} |f_{ii}|^2, \qquad (1)$$

where Z is the number of electrons. To date the most accurate formula, which is based on a nonrelativistic wave equation and on a total atomic wave function expressed as a product of one-electron wave functions which specifically includes the effects of exchange, is that due to Waller and Hartree⁴:

$$I_{\text{e.u.}} = Z - \sum_{j=1}^{Z} |f_{jj}|^2 - \sum_{j} \sum_{k \neq j} |f_{jk}|^2, \qquad (2)$$

where

$$f_{jk} = \int \boldsymbol{\psi}_j^* \boldsymbol{\psi}_k \exp(i\kappa \mathbf{S} \cdot \mathbf{r}) dv, \qquad (3)$$

 $\kappa = 2\pi/\lambda$; λ is the wavelength of the incident radiation; $S = s - s_0$, where s, s_0 are unit vectors along the reflected and incident directions; and the ψ 's are appropriate

¹ A. H. Compton, Phys. Rev. **35**, 925 (1930). ² C. V. Raman, Indian J. Phys. **3**, 357 (1928). ³ G. Wentzel, Z. Physik **43**, 1 (1927).

⁴ I. Waller and D. R. Hartree, Proc. Roy. Soc. (London) A124, 119 (1929).