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Optical Properties of Indium Antimonide in the Region from 20 to 200 Microns

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The reflectivity and the transmission of InSb crystals (n-type) were measured between 20 and 200μ. The reflectivity curve has a sharp maximum at 54.6μ and the transmission curve shows a low transmission at the same wavelength due to lattice vibration of this crystal. The transmission curve shows a weak absorption at 28.3μ due to the overtone of that lattice vibration. The reflectivity curve shows another flat peak at longer wavelengths. The reflectivity minimum between these two peaks shifts from 160 to 72μ with increase of temperature from -35 to 130°C, and the maximum value of the flat peak increases with increase of temperature and is 80% at temperatures of 100°C or more.

The index of refraction n and the absorption constant K were calculated in the region in which both the reflectivity and the transmission were measured. Using the values of n and K thus obtained, the concentration of free electrons N and their mobility b were obtained, using the theory of free electrons. Then n, K, and the reflectivity, R, were calculated for the region in which the transmission could not be measured. The values of R thus obtained agree well with the observed values. This shows that the theory of free electrons holds in InSb except in the region in which the effects of lattice vibration in this crystal are dominant.

INTRODUCTION

INDIUM antimonide in its single-crystal form has many interesting properties, especially the unusually large mobility of free electrons. Many measurements of conductivity, Hall constant, and other electrical properties made on this material have been reported. A bibliography of these measurements is given by Madelung and Weiss.[1]

As to the optical properties, this crystal has one absorption in the region of a few microns which increases in intensity toward shorter wavelength and appears to be due to the transition of electrons to the conduction band. The wavelength of this absorption edge changes under different conditions from 2 to 7μ; several explanations to account for this have been proposed.[2–8]

Oswald and Schade[9] measured the index of refraction n and absorption constant K of this crystal for wavelengths as long as 16μ and made comparisons with the optical properties of AlSb, GaAs, GaSb, InP, InAs, and Ge.

In pure InSb crystals, the values of n and K are constant for wavelengths greater than 10μ, whereas in impure crystals the value of n is constant but K increases with increase of wavelength beyond 10μ. Recently Kaiser and Fan[10] measured the transmission of InSb crystals of n- and p-types between 3 and 35μ at different temperatures. They found that the absorption in the long-wavelength region could not be explained as the result of free carriers.

The InSb crystals used in the investigation reported here were made by T. C. Harman at the Battelle Memorial Institute. These are fairly large n-type single crystals. Using the far infrared grating spectrograph[11] in this laboratory, the reflectivity and transmission of these crystals in the region between 20 and 200μ were measured. The far infrared data show that this crystal has a sharp lattice vibration at 54μ, and make it clear that the absorption and transmission in this spectral region are not greatly affected by the presence of free electrons. The optical properties of this crystal in the longer-wavelength region are very sensitive to temperature changes, and the observed data are compared with calculated values.

EXPERIMENTAL RESULTS

The crystals used in the measurement of reflectivity were 2.5 by 1.8 cm in area and 3 mm thick. Two crystals used in the measurement of transmission had almost the same area and were 0.21 and 0.35 mm thick respectively. All crystals were sliced from one big InSb block, and their surfaces were ground and polished. Measurements made at the Battelle Memorial Institute show that these are all single (proved by the etching method) n-type crystals and have the values of resistivity ρ, mobility b of free electrons, and concentration N of free electrons shown in Table I.

TABLE I. Electrical properties of InSb sample.

Temperature	ρ (ohm-cm)	b^{a} (cm²/volt-sec)	N (cm^{-3})
83°K	6×10^{-3}		6×10^{15}
217°K	10×10^{-3}		6×10^{15}
300°K	4×10^{-3}	78 000	2×10^{16}
400°K		44 000	8×10^{16}
500°K		28 500	

[a] Effective mass of electron $=0.025\ m$.

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[1] O. Madelung and H. Weiss, Z. Naturforsch. **9a**, 527 (1954).

[2] H. Welker, Z. Naturforsch. **7a**, 744 (1952); **8a**, 248 (1953).

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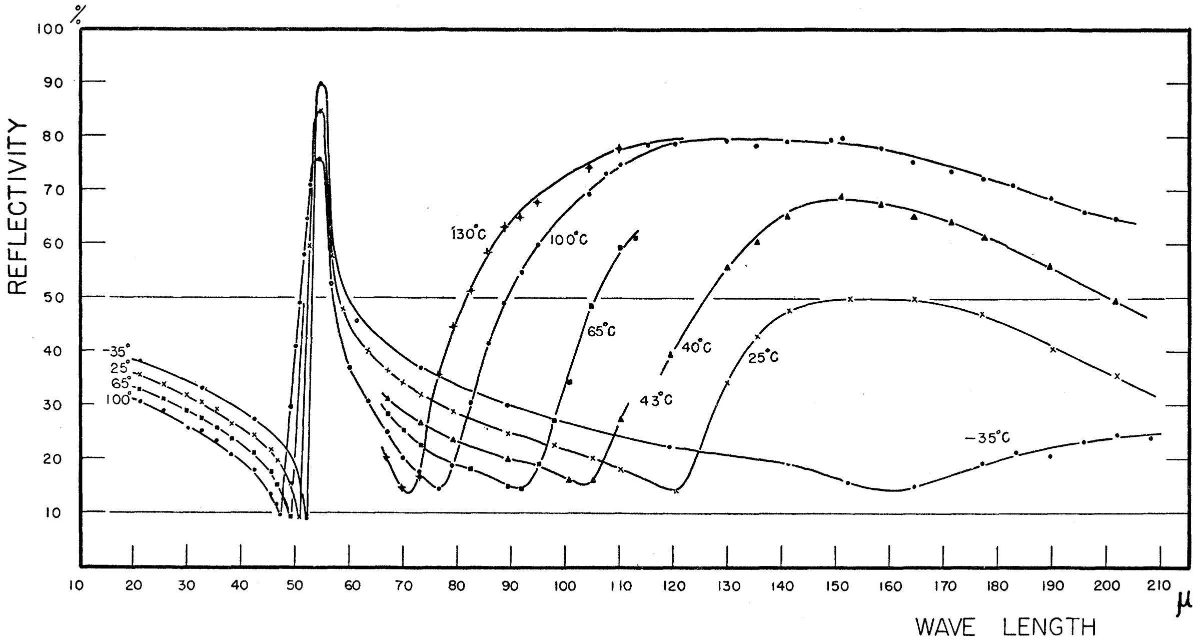

FIG. 1. Reflectivity of InSb crystal between 20 and 200μ at -35°C, 25°C, 43°C (part 40°C), 65°C, 100°C, and 130°C.

In the measurement of reflectivity, these crystals were put into the radiation beam between the chopper and the entrance slit of the spectrograph; this eliminated possibility of measurement of radiation emitted by these crystals. The incident angle was about 45°. The reflectivity of these crystals changes greatly with temperature. To vary their temperature, they were heated with an electric heater and cooled with dry ice. The temperature was measured using a thermocouple soldered to the crystals.

Figure 1 shows the reflectivity at -35°C, 25°C, 40° or 43°C, 65°C, 100°C, and 130°C. All curves have sharp peaks at 54.6μ of which the slope on the short-wavelength side is very steep. The wavelength of the maximum point of the peak does not change with temperature, but the intensity of the maximum increases with decrease of temperature and is 90% at -35°C. The minimum value of the reflectivity on the short-wavelength side of the peak is about 10% and is almost independent of temperature. The wavelength of minimum reflectivity varies from 51.2μ at -35°C to 46.7μ at 100°C. In the spectral region of wavelengths less than that of minimum reflectivity, the value of reflectivity decreases with increase of temperature.

In the region of wavelengths longer than that of the peak, the reflectivity curve shows another flat peak which is of interest, because this peak changes so greatly with temperature. The wavelength of the reflection minimum between these two peaks is 160μ at -35°C, 120μ at 25°C, 104μ at 43°C, 92μ at 65°C, 77μ at 100°C, and 72μ at 130°C. The intensity of the reflectivity maximum increases with increase of temperature and is 80% at temperatures of 100°C or more.

The transmission of the crystals of two different thicknesses was measured at -35°C, 25°C, 65°C, and 100°C. The results at -35°C, 25°C, and 100°C are shown in Fig. 2. These curves have the following characteristics. There is low transmissivity in the region corresponding to the sharp reflectivity maximum. A weak absorption is observed at 28.3μ; this wavelength is just half that of the strong absorption. Throughout the region in which measurements were made, the value of transmission decreases with increase of temperature. The absorption at 28.3μ becomes weak with increase of temperature. It was impossible to measure the transmission in the region of wavelengths greater than 120μ and at high temperatures, because the crystals available were too thick for this purpose.

In a recent note,[12] the authors reported far infrared reflectivity data for several materials. Comparison of the shape of the 54.6μ peak in InSb with a corresponding peak in ZnS at 25.6μ suggests that both are produced by lattice vibrations. The 28.3μ absorption in InSb is probably an overtone of the lattice vibration. On the other hand, PbS, PbSe, and TlCl crystals have the second peak. But the flat peak in InSb in the long-wavelength regions shows a different kind of temperature dependence and must have an origin different from that in the other crystals.

CALCULATION OF ABSORPTION COEFFICIENT AND INDEX OF REFRACTION

Because thick crystals were used in the measurement of reflectivity, the reflectivity R is given by

$$R = i_r / i_0, \qquad (1)$$

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[12] H. Yoshinaga, Phys. Rev. **100**, 753 (1955).

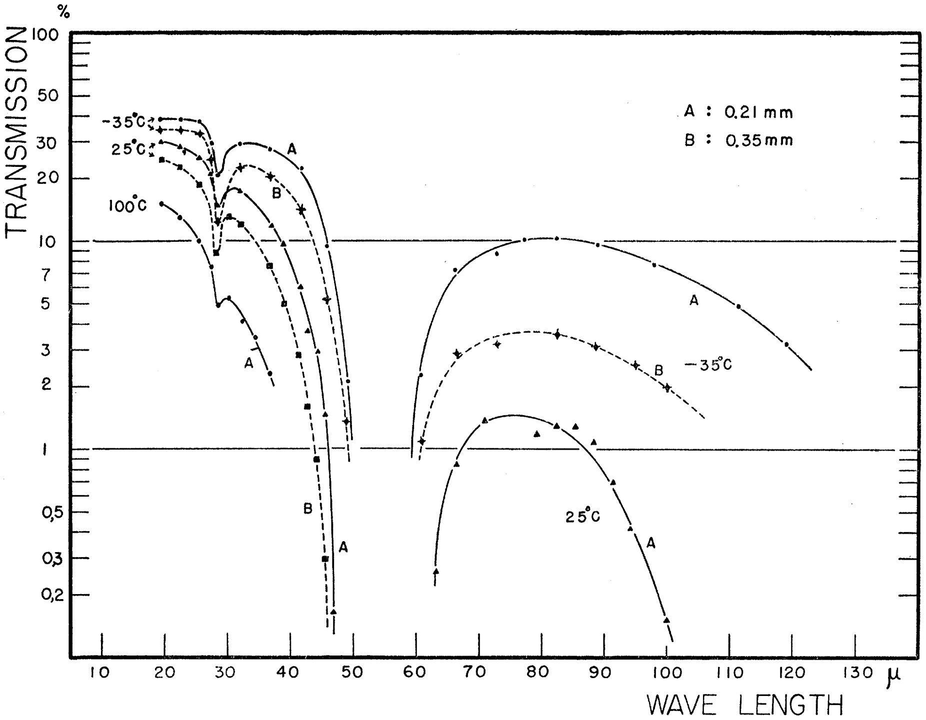

FIG. 2. Transmission of Insb crystals of 0.21- and 0.35-mm thickness at −35° C, 25°C, and 100°C.

where i_0 is the intensity of the incident radiation, and i_r is the intensity of the reflected radiation. The crystals used in the measurement of transmission were thin, so the transmission T is given by the following formula which takes into consideration the multiple reflections in the crystal

$$T=\frac{i_d}{i_0}=\frac{(1-R)^2e^{-Kd}}{1-R^2e^{-2Kd}}, \tag{2}$$

where i_d is the intensity of the transmitted radiation, K is the absorption constant, and d is the thickness of the crystal. From Eq. (2), one can calculate K and then the extinction coefficient κ:

$$\kappa=K\lambda/4\pi, \tag{3}$$

where λ is the wavelength.

In the region in which the transmission was measured, κ is small and the index of refraction n is about 3; therefore the difference in the intensities of radiation reflected when the incident angles are 0° and 45° respectively is negligible. The formula

$$R=[(n-1)^2+\kappa^2]/[(n+1)^2+\kappa^2], \tag{4}$$

which is strictly applicable in the case of normal incidence can be used to calculate n. The solid lines in Fig. 3 show the values of K and n obtained by using this method.

The values of K and n depend on the purity of InSb crystal. The values shown in Fig. 3 are quite reasonable compared to the values of Oswald and Schade[9] and Kaiser and Fan.[10] If the region of the absorption by the lattice vibrations is neglected, n decreases and K increases with increase of wavelength and temperature.

CALCULATION OF CONCENTRATION AND MOBILITY OF FREE ELECTRONS

Fan and Becker[13] calculated the reflectivity of Ge, using the following formulas proposed by Drude and Kronig:

$$n\kappa\nu=\frac{Neb}{1+(\nu/\gamma)^2}, \tag{5}$$

$$n^2-\kappa^2=\epsilon_0-\frac{Ne^2}{\pi m^*(\nu^2+\gamma^2)}, \tag{6}$$

where ν is the frequency, e is the charge on the electron, ϵ_0 is a constant, m^* is the effective mass of a free electron, N is the concentration of free electrons, b is the mobility of free electrons, and $\gamma=e/(2\pi m^*b)$. By the reverse process, we have calculated the values of N and b using the values of n and K shown in Fig. 3.

Table II shows the values of N and b for several wavelengths at −35°C and 25°C obtained using Eqs. (5) and (6). In these calculations, it was estimated that $m^*=0.03\ m$ (the value used in many other investigations), $\epsilon_0=15.5$ at −35°C and $\epsilon_0=17.0$ at +25°C. The values of N and b are fairly constant for wavelengths greater than 95μ at −35°C and greater than 90μ at 25°C. If different values of ϵ_0 are assumed, the con-

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[13] H. Y. Fan and M. Becker in *Semiconducting Materials* edited by H. K. Henisch (Academic Press, Inc., New York, 1951).

TABLE II. Concentration of free electrons and their mobility for each wavelength at different temperatures.

	−35°C		25°C	
λ (μ)	N (cm^{-3})	b (cm^2/volt-sec)	N (cm^{-3})	b (cm^2/volt-sec)
70			2.06×10^{16}	8 610
80	0.727×10^{16}	10 100	3.13×10^{16}	20 000
90	1.56×10^{16}	27 100	3.38×10^{16}	25 900
95	1.85×10^{16}	35 000	3.39×10^{16}	25 500
100	1.85×10^{16}	36 200	3.37×10^{16}	25 400
110	1.82×10^{16}	36 900		
120	1.81×10^{16}	36 900		

stancy of N and b decreases. Equations (5) and (6) do not hold for InSb crystal at 60 or 70μ owing to the lattice vibration, but they seem to hold very well in the long wave region where the effect of the lattice vibration is negligible. From the average values between 95 and 120μ for a temperature of −35°C and between 90 and 100μ for a temperature of 25°C, the results of this investigation give as best values for concentrations of free electrons and their mobilities the numbers presented in Table III.

COMPARISON BETWEEN CALCULATED VALUES AND OBSERVED VALUES

If values of N and b are known for a crystal, it is possible to calculate n and K in the wavelength region in which measurements of the transmission could not be made. The broken lines in Fig. 3 show the results of such calculation using the values of N and b given in Table III. The broken lines in the short-wavelength region also show the calculated values obtained using the same values of N and b. Calculated values of n agree well with the observed values, and calculated values of K differ from observed values by less than a factor of 2 except in the region in which the lattice vibration is effective.

Reflectivities in the region beyond 100μ (at 25°C) and 120μ (at −35°C) were calculated using the values of n and K shown in Fig. 3. In Fig. 4, the heavy parts of the solid curves show the observed data used in obtaining n and K, and thus N and b. These values of N and b were in turn used to calculate the reflectivities shown as the broken curves in Fig. 4. In this calculation, n is less than 3 and κ is not small, so that it is not proper to use the formula for normal incidence. Rather, the following formulas which hold at the incident angle of

TABLE III. Best values, as calculated from observed optical data.

Temperature	N (cm^{-3})	b (cm^2/volt-sec)	γ (sec^{-1})
−35°C	1.83×10^{16}	36 300	2.59×10^{11}
25°C	3.38×10^{16}	25 600	3.67×10^{11}

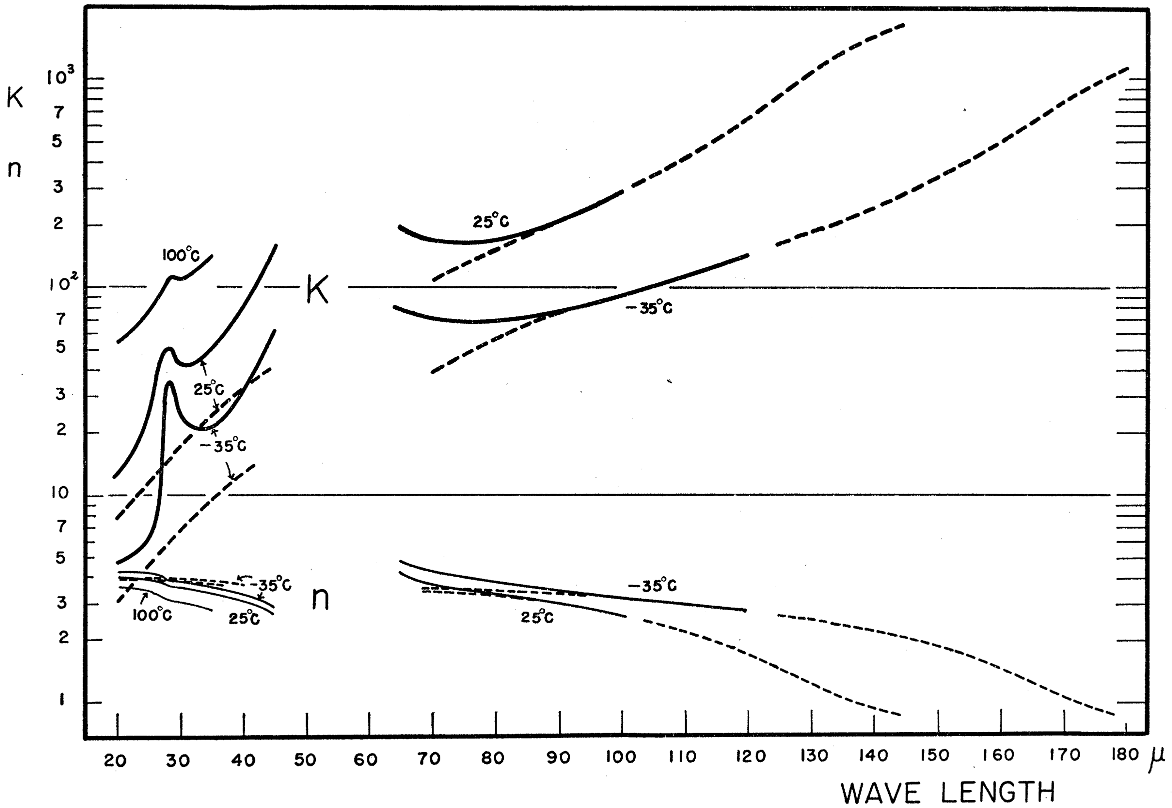

FIG. 3. Index of refraction and absorption constant of InSb crystal. Solid lines show observed data and broken lines show calculated values.

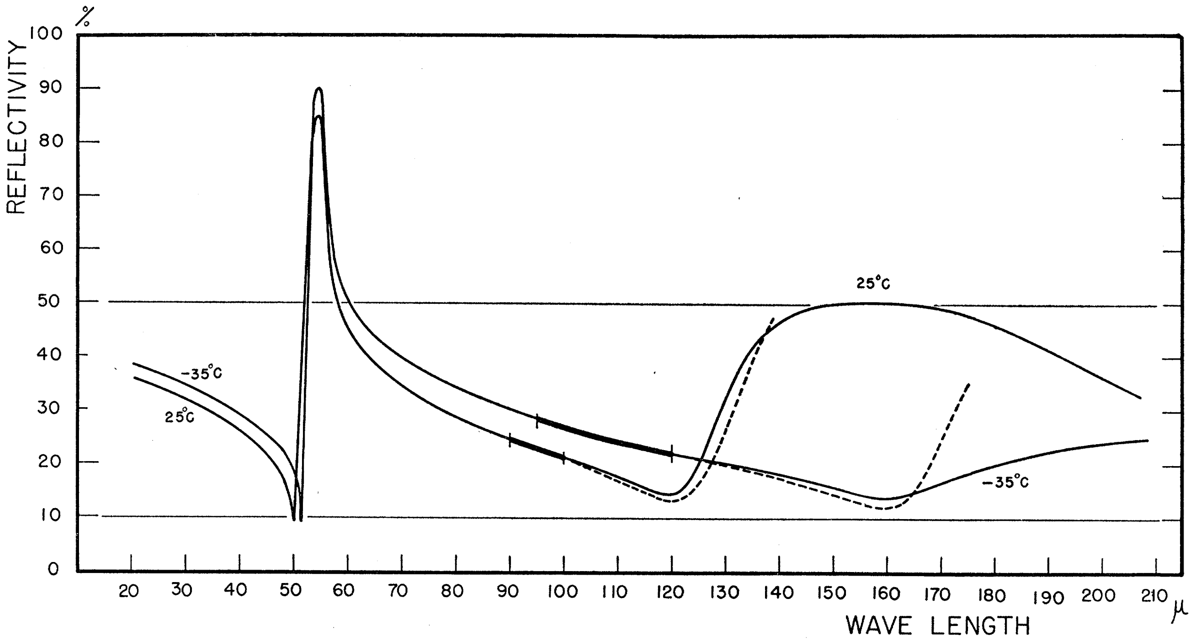

FIG. 4. Comparison of calculated reflectivity of InSb and observed data at −35°C and 25°C. Heavy parts of solid lines show the values used in that calculation, and broken lines show calculated reflectivities.

45° were used:

$$R_s = -E_s \frac{1-(2\epsilon'-1)^{\frac{1}{2}}}{1+(2\epsilon'-1)^{\frac{1}{2}}},$$
$$R_p = E_p \left[\frac{1-(2\epsilon'-1)^{\frac{1}{2}}}{1+(2\epsilon'-1)^{\frac{1}{2}}}\right]^2, \qquad (7)$$

where E is the amplitude of incident radiation, R is the amplitude of reflected radiation, and $\epsilon' = (n - i\kappa)^2$. At both 25°C and −35°C, the wavelengths of calculated minimum reflectivity coincide with observed values, and calculated reflectivities below this wavelength are close to the observed values. Beyond this wavelength, the calculated reflectivity increases faster than the observed reflectivity with increase of wavelength.

CONCLUSION

From the results shown above, it can be seen that the calculated reflectivities agree well with observed values, and the formulas (5) and (6) hold in the wavlength region where the effect of lattice vibrations is negligible. This is true even in the short-wavelength region where calculated and observed values have differed by more than a factor of 10^3 in the past.

The relation between the values of b at −35°C and 25°C gives

$$b \propto T^{-1.55}.$$

This relation is close to the well-known $b \propto T^{-\frac{3}{2}}$. Values of N and b obtained optically differ from values obtained using electrical properties by less than a factor of 3; these differences would be less if $m^* = 0.025\ m$ is used instead of $m^* = 0.03\ m$. Much consideration will be required in order to completely resolve these differences. These differences may be related to the fact that electrical data depend upon the characteristics of the whole volume of the crystals whereas optical data depend upon the characteristics of the thin surface-layer of crystals.

Equations (5) and (6) do not hold exactly at 90μ at −35°C, but hold very well at even this wavelength at 25°C due to the increase of the concentration of free electrons with increase of temperature. So those formulas may hold at wavelengths less than 90μ for temperatures of 65°C or 100°C. Calculation of b at these temperatures using the relation $b \propto T^{-1.55}$, assuming suitable values for N and ϵ_0, may yield values of reflectivity for these temperatures which are close to the observed data. We intend to develop techniques for making transmission measurements for thinner crystals and to compare data thus obtained with calculated values with the objective of resolving the differences between electrical data and optical data.

ACKNOWLEDGMENTS

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Deformation Potential Theory for *n*-Type Ge[†][*]

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The deformation potential theory has been re-examined for electrons in Ge to take into account the ellipsoidal nature of the energy surfaces, and the effect of shear wave scattering. The coupling between shears and the conduction band energy minima is calculated from Smith's piezoresistance data under the assumption that any changes in mobility due to strain may be neglected. The scattering by shears, which is the dominant mechanism, is strongly anisotropic and cannot be described by a simple relaxation time. We have shown that the distribution function for electrical conductivity has a tensor dependence on the orientation of the electric field. The mobility is calculated assuming several values of E_{1c}, the shift of the conduction band edge with dilation. The calculated values of the mobility are approximately $3\times10^{7}T^{-3/2}$ cm^2/v sec. Methods of accounting for discrepancies between the experimental and theoretical values of the mobility and its temperature dependence are discussed.

INTRODUCTION

THE lattice scattering mobility of carriers in nonpolar semiconductors was treated in the deformation potential theory of Bardeen and Shockley.[1] In this theory, scattering by long-wavelength acoustical modes is considered. The electron phonon coupling is the shift in the allowed energy bands due to the compressions and dilations produced by the longitudinal modes. The transverse modes cause no scattering since they produce no dilation.

It is now apparent, from the elastoresistance measurements of Smith,[2] that shifts in the conduction band minima or valleys in *n*-type Ge are caused by shears as well as by dilation. We should expect, therefore, that scattering of electrons will occur that is due to shears produced in the crystal by both longitudinal and transverse waves. In this paper, we wish to recalculate the mobility of electrons in Ge using the deformation potential theory and taking into account the effect of shear wave scattering.

It has been shown by Wannier,[3] and restated by Slater,[4] that in a periodic lattice, with a perturbing potential which varies slowly with position compared to the periodic potential, an electron may be treated essentially as a perturbed free particle with an appropriate effective mass. In the strained coordinate system of the crystal, the deformation potential due to long-wavelength acoustical modes is just such a slowly varying potential. We may therefore use the effective-mass theory to calculate the probability of transitions between momentum states. In such a treatment, any strain-induced changes in the effective mass will be of the order of the strain. Since the electrons are classically distributed, and are close to the conduction band bottom, changes in the effective mass may be ignored.

In principle, the deformation potential theory makes it possible to determine exactly the mobility of carriers in a semiconductor if one knows precisely how the edges of the allowed energy bands shift with strain. In reality, the shift with dilation of the individual band edges is not known; only the sum of shifts of the valence and conduction bands with dilatation has been determined. On the other hand, from the elastoresistance data on Ge, one can calculate uniquely[5] the shift with shear of the conduction band's energy minima. As we shall show, in *n*-type Ge the scattering due to shears is the dominant mechanism, so that one may calculate the mobility to within a small indeterminancy and compare it with the experimental values.

BAND STRUCTURE AND ELASTORESISTANCE IN *n*-TYPE Ge

Bardeen and Shockley assumed in their theory that the surfaces of constant energy in the Brillouin zone

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[1] J. Bardeen and W. Shockley, Phys. Rev. **80**, 72 (1950).

[2] C. Smith, Phys. Rev. **94**, 42 (1954).

[3] G. H. Wannier, Phys. Rev. **52**, 191 (1937).

[4] J. C. Slater, Phys. Rev. **76**, 1592 (1949).

[5] Actually there is a very weak dependence upon the dilation effect.