

## Some Optical Properties of Cadmium Telluride

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(Received December 28, 1959)

Some optical properties of CdTe samples having a carrier concentration of the order of  $10^{15} \text{ cm}^{-3}$  were measured. The index of refraction in the infrared was determined to be 2.61. Values of the absorption coefficient  $\alpha$  as a function of frequency were obtained at various temperatures. By plotting  $\alpha^1$  and  $\alpha^2$  against frequency, it was found that at room temperature the minimum energy for direct transitions is 1.50 eV; that for indirect transitions is 1.44 eV. The temperature dependencies between 77°K and 373°K are given by  $(1.66 - 5.6 \times 10^{-4}T)$  eV for direct transitions and  $(1.56 - 4.1 \times 10^{-4}T)$  eV for indirect transitions.

### INTRODUCTION

ALTHOUGH considerable electrical work has been done on CdTe<sup>1,2</sup> and the absorption edge has been measured at room temperature<sup>3</sup> and over a range of temperatures<sup>4</sup> there has not, to the authors' knowledge, been a careful study of the absorption edge at reasonably high resolutions. Such a study has been carried out in this laboratory.

The CdTe used was prepared by direct fusion of the elements in an evacuated quartz tube, followed by zone melting for purification. Samples from the resulting ingot were annealed for 48 hours at 900°C in a cadmium atmosphere of 0.8 atm pressure. This had been found previously to raise the transmission considerably at longer wavelengths (2–15 microns). The samples selected for measurement were all *n* type with carrier concentrations of the order of  $10^{15} \text{ cm}^{-3}$ . They gave quite flat transmission of about 70% from near the absorption edge out to 15 microns and beyond. The lattice constant of CdTe was found to be  $6.4815 \pm 0.0005 \text{ \AA}$ .

### EXPERIMENTAL DETAILS

Samples were prepared for optical measurements by standard techniques. Final surface polish was achieved with 0.1-micron alumina. For the very thinnest samples, the CdTe was polished on one face and then mounted on a glass microscope slide, ground to about 0.001-inch thickness on a grinder, and then lapped to the required thickness with 1-micron alumina polish. The mounting substance was crystal cement, which was found to have no absorption at wavelengths in the region of the absorption edge of CdTe.

Transmission measurements were made using a Model 83 Perkin-Elmer monochromator fitted with an NaCl prism. This instrument was modified by the addition of a focusing mirror after the exit slit, so that the exit slit could be imaged several inches behind the monochromator. An evacuable low-temperature cell with rock salt windows was placed here. The cadmium telluride sam-

ples were mounted in the Dewar flask on a slotted copper block with ordinary rubber cement. This method was found to be satisfactory over the range of temperature considered.

When the thicker samples were used, a thermocouple was inserted in a small hole drilled into the slotted copper block. Because of the intimate contact between the sample and the copper block, the thermocouple gave the sample temperature quite accurately. The thin samples were mounted on glass slips which were attached to the copper block. In this case, the thermocouple was indium-soldered to the glass surface just adjacent to the sample. Approximately 20 minutes were allowed to assure that the front surface of the glass (and also, presumably, the sample) had come to equilibrium. These temperatures, although stable, were considerably above the coolant temperatures in the Dewar.

### RESULTS

The transmissions of the samples were measured point by point as a function of wavelength. No provision existed with the apparatus for the measurement of reflections, and so the method adopted was to determine the index of refraction from the measurement of interference fringes at about 10 microns wavelength in a sample of known thickness. A value of 2.61 was thus found for the high-frequency index of refraction. The relationship between reflectivity,  $R$ , and refractive index,  $n$ , is given by

$$R = [(n-1)^2 + \kappa^2] / [(n+1)^2 + \kappa^2]. \quad (1)$$

Very low absorption coefficients in the 2 to 15 micron region make the extinction coefficient,  $\kappa$ , negligible. Equation (1), therefore, yields a value of 0.20 for the reflectivity. This was used in calculations of absorption coefficients.

In order to confirm these results, the approximate reflectivity was measured between 2 and 13 microns on a Perkin-Elmer 21-B spectrometer. It was found that the reflectivity agreed approximately with the above value and was essentially constant throughout the wavelength range. A further check was made using absorption coefficients at 1.18 microns calculated on the basis of the above reflectivity for various thicknesses of sample.

<sup>1</sup> F. A. Kröger and D. de Nobel, *J. Electronics* **1**, 190 (1955).

<sup>2</sup> J. L. Stull, thesis, State University of New York College of Ceramics, Alfred, New York, July, 1958 (unpublished).

<sup>3</sup> D. A. Jenny and R. H. Bube, *Phys. Rev.* **96**, 1190 (1954).

<sup>4</sup> C. Z. van Doorn and D. de Nobel, *Physica* **22**, 338 (1956).

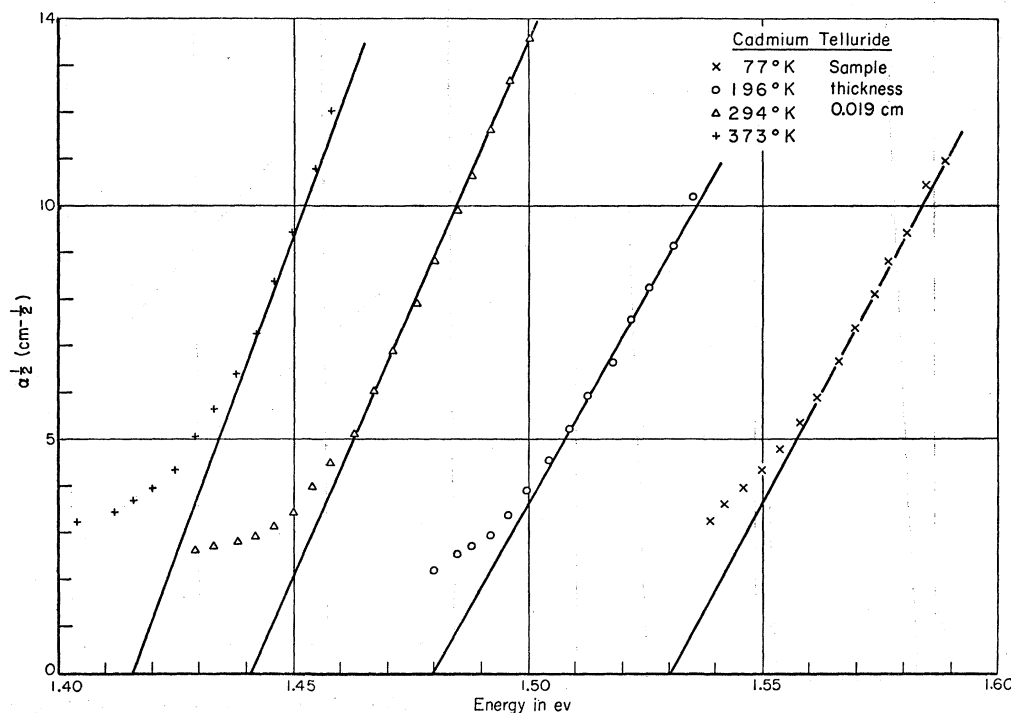


FIG. 1. Temperature dependence of indirect transitions in *n* type cadmium telluride.

Here, again, the agreement was excellent, and so the conclusion that the reflectivity remains unchanged, in the samples used, from the absorption edge to 15 microns seems warranted.

It was assumed that values of absorption coefficient less than a few hundred  $\text{cm}^{-1}$  represented indirect interband transitions and that these transitions vary in probability approximately as  $(h\nu - E_G)^2$ , where  $E_G$  is the minimum energy separating the two bands.<sup>5</sup> Accordingly, for the smaller values of absorption coefficient,  $\alpha^{1/2}$  is plotted against the photon energy in Fig. 1 for various temperatures. The straight-line portions are extrapolated to zero and the values obtained are taken as the absorption edge for indirect transitions at the temperature given.

It was assumed that the probability of indirect transitions occurring continues to follow a law  $(h\nu - E_G)^2$  for a considerable distance into the higher frequency range. Thus, the "indirect absorption coefficient",  $\alpha_i$ , was calculated in the region of large absorption coefficients, the  $\alpha_i$  being then subtracted from the measured  $\alpha$ . In Fig. 2 the values of  $(\alpha - \alpha_i)^{1/2}$  for various temperatures are plotted against photon energy. In this region we assume that we are entering the region of direct transitions whose probability follows  $(h\nu - E_G)^{1/2}$  approximately.<sup>5</sup> Again, the extrapolated straight-line intercepts are as-

sumed as the energies for direct transitions at the temperatures given.<sup>6</sup>

These transition energies are found to vary linearly with temperature in the range 77–373°K and give the following values for the absorption edges as a function of the absolute temperature,  $T$ , as shown in Fig. 3.

$$\text{Direct transitions } E_D = 1.66 - 5.6 \times 10^{-4} T \text{ ev.}$$

$$\text{Indirect transitions } E_G = 1.56 - 4.1 \times 10^{-4} T \text{ ev.}$$

## DISCUSSION

de Nobel and Hofman report a low-frequency dielectric constant of  $11.0 \pm 0.3$  from electrical measurements on CdTe<sup>7</sup> which corresponds to a refractive index of about 3.32. A comparison of this value with the optical refractive index (2.61) determined in the present work suggests that bonding in CdTe is somewhat ionic. This conclusion, as well as the value of the optical refractive index, is at variance with the observations of Garlick et al.<sup>8</sup> but is supported by earlier estimates of de Nobel<sup>9</sup> and by recent detailed measurements of Fisher and Fan.<sup>10</sup>

<sup>6</sup> The spectral slit width of the instrument was about  $1.7 \times 10^{-3}$  ev for all of the measurements of the absorption edges given here.

<sup>7</sup> D. de Nobel and D. Hofman, *Physica* **22**, 252 (1956).

<sup>8</sup> G. F. J. Garlick, J. M. Hough, and R. A. Fatchally, *Proc. Phys. Soc. (London)* **72**, 925 (1958).

<sup>9</sup> D. de Nobel, *Philips Research Repts.* **14**, 361 (1959); **14**, 320 (1959).

<sup>10</sup> P. Fisher and H. Y. Fan, *Bull. Am. Phys. Soc.* **4**, 409 (1959).

<sup>5</sup> H. Y. Fan, *Reports on Progress in Physics* (The Physical Society, London, 1956), Vol. 19, p. 107.

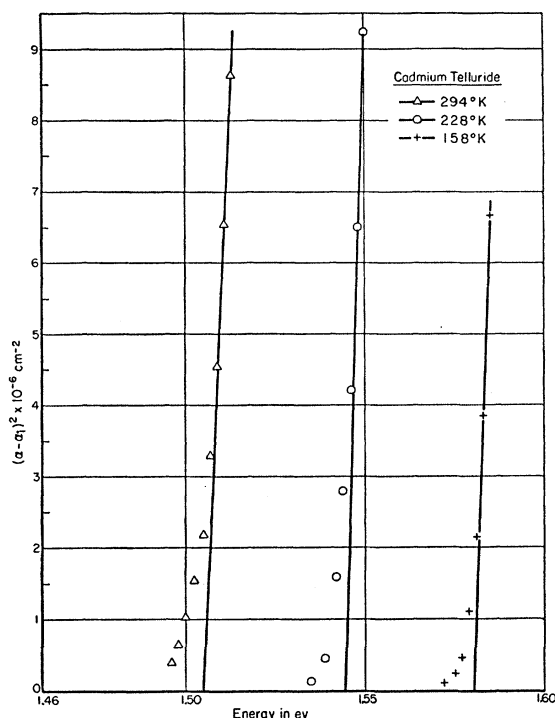


FIG. 2. Temperature dependence of direct transitions in *n* type cadmium telluride.

With regard to the temperature dependence of the absorption edge, the results of Bube, taken from photoconductivity maxima, give  $1.52 - 3.6 \times 10^{-4}T$  eV for temperatures from 77°K to 330°K.<sup>11</sup> Van Doorn and de Nobel,<sup>4</sup> using infrared transmission measurements, obtain slightly different results for a similar range of temperatures.

Bube's value presumably represents indirect transitions, and our constant for the temperature variation is slightly different from his. It is to be noted that the temperature variation for the direct transition edge is substantially different from the indirect.

A calculation was made to fit the thermal shift of the absorption edge to some of the known constants of the crystal. In view of the above discussion, it was assumed that the crystal bonding was predominantly ionic and that, consequently, the shift could be calculated from<sup>12</sup>

$$E_G = -\frac{\pi(ee^*)^2 \hbar^{\frac{1}{2}}}{a^3 M \omega_l^{\frac{1}{2}}} \left[ \left( \frac{2m_e^*}{\hbar^2} \right)^{\frac{1}{2}} + \left( \frac{2m_v^*}{\hbar^2} \right)^{\frac{1}{2}} \right] (n+1), \quad (2)$$

where  $e^*$  is the effective charge of the ion,  $\omega_l$  is the frequency of the longitudinal optical mode of the crystal,  $a$  is the interionic distance,  $M$  is the reduced

<sup>11</sup> R. H. Bube, Phys. Rev. **98**, 431 (1955).

<sup>12</sup> H. Y. Fan, Phys. Rev. **82**, 900 (1951).

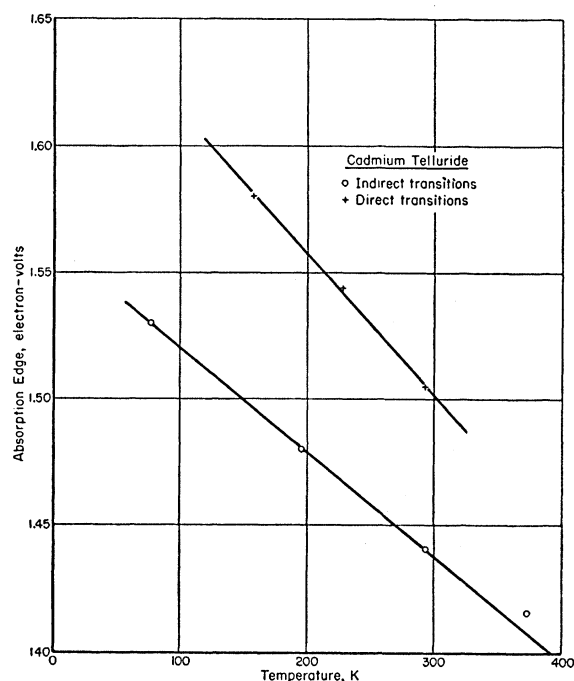


FIG. 3. Variation of absorption edges with temperature in *n* type cadmium telluride.

mass of a cadmium-tellurium pair,  $m_e^*$  and  $m_v^*$  are electron and hole effective masses, respectively, and  $n = [\exp(\hbar\omega_l/kT) - 1]^{-1}$ .

To assure a self-consistent set of optical parameters for the calculation, values cited in reference 9 were used. Effective masses were those reported in reference 1. The frequency of the longitudinal optical mode was calculated from the relation<sup>13</sup>  $\omega_l^2 = \omega_0^2 \epsilon_0 / \epsilon_\infty$ , where  $\omega_0$  is the frequency of the fundamental optical mode and  $\epsilon_0$  and  $\epsilon_\infty$  are respectively the low and high-frequency dielectric constants. For the shift at room temperature, the calculation yields

$$\partial E_G / \partial T = -7.5 \times 10^{-4} \text{ eV}/^\circ\text{C},$$

which compares favorably with our experimental value of  $-4.1 \times 10^{-4} \text{ eV}/^\circ\text{C}$ .

#### ACKNOWLEDGMENTS

The authors are indebted to Professor H. Y. Fan for valuable consultation and criticism of this work, C. S. Peet and A. C. Beer for encouragement, support, and discussion during its undertaking, and H. L. Goering and his staff for making the CdTe available. We are indebted to Battelle Memorial Institute for the fundamental research grant which supported this work.

<sup>13</sup> R. H. Lyddane, R. G. Sachs, and E. Teller, Phys. Rev. **59**, 673 (1941).