FUNDAMENTAL OPTICAL ABSORPTION IN β-SILVER TELLURIDE*

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There has been considerable interest lately in the electrical properties[1] of β-Ag_2Te, the monoclinic polymorph of silver telluride stable below 133°C. A recent value[2] of the thermal energy gap E_0^t at 0°K, obtained from an analysis of Hall-coefficient data, is 0.064 eV. However, the only reported[3] study of the optical absorption proposed a value of the energy gap of 0.67 eV at room temperature. These results were obtained on evaporated films. In view of the discrepancy between the optical and thermal energy-gap values, we have investigated the optical absorption of β-Ag_2Te at room temperature.

The samples used were thin layers prepared by evaporation of β-Ag_2Te in vacuum. Alkali halide (KBr and CsI) substrates were used and the thicknesses were calculated by weighing the samples, measuring their areas, and assuming bulk density. X-ray powder-pattern analysis of the specimens showed both to be β-Ag_2Te; however, one contained a few percent of the hexagonal "empressite" modification of silver telluride. Transmission spectra of each sample were taken using the conventional "sample-in, sample-out" method. The spectrometer used was a single-beam recording instrument whose dispersing element was a Leiss double-prism monochromator; conventional amplification and phase-sensitive detection were employed. Using the relation $T = F(R) \times \exp(-\alpha t)$ [where T is the transmissivity, $F(R)$ is a function of the reflectivity R, t is the sample thickness, and α is the absorption coefficient], the transmission spectra of the two samples of different thicknesses allowed calculation of absorption coefficients. In this way, the absorption spectrum was calculated and is shown in Fig.1 from 0.08 to 0.15 eV. We note that the shape is characteristic of the absorption of a semiconductor in the region of the fundamental absorption edge. The sharp increase in α with increasing photon energy beginning at about 0.1 eV is believed to be due to band-to-band transitions across the energy gap. The increasing absorption at photon energies below 0.1 eV is due to absorption by free carriers; a plot of absorption coefficient

α vs λ^2, where λ is the wavelength, was linear. This is shown in Fig. 2. In order to obtain a value of the 300°K optical energy gap E_{300}^0 from the data, it is necessary to extrapolate the absorption curve to $\alpha = 0$. While the absorption edge in Fig. 1 is sharp, a more reliable method of extrapolation is desirable. It has been shown[4] that the functional dependence of the absorption coefficient on photon energy will vary with the type of transition being observed. In general, for a parabolic band model, $\alpha^n = A(h\nu - E_g)$, where $n = 2$ or $\frac{2}{3}$ for direct transitions and $n = \frac{1}{2}$ or $\frac{1}{3}$ for indirect transitions. While the shapes of these curves would be modified by the effect of thermal broadening of the distribution of final states,[5] we have plotted these powers of α vs $h\nu$ and find that a plot of α^2 vs $h\nu$ gave the best straight line. This plot is shown in Fig. 3, as is the extrapolation to $\alpha = 0$. In addition to supporting the belief that
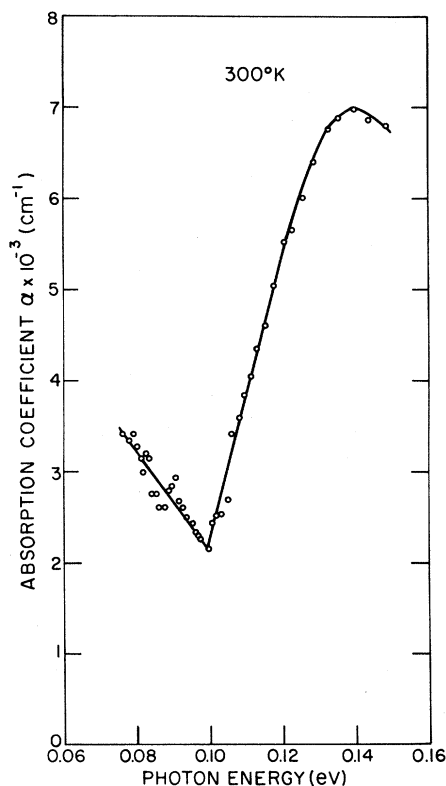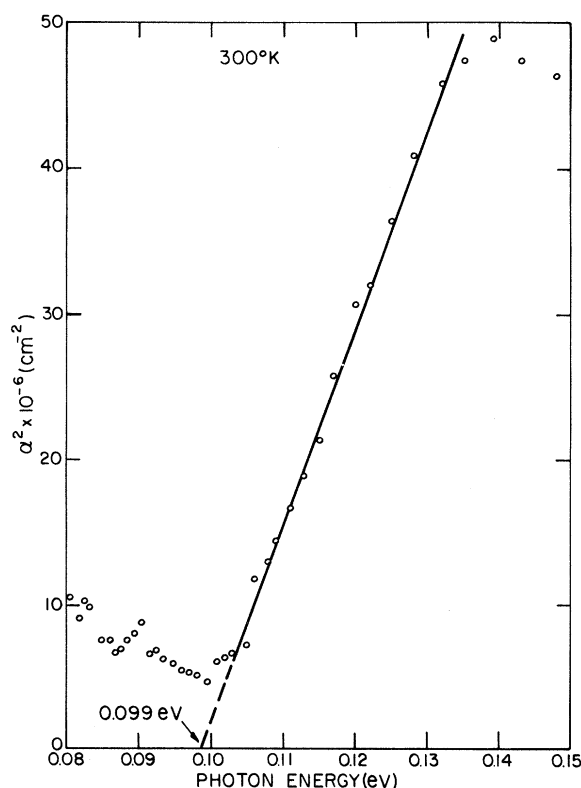

FIG. 1. Optical absorption in β-Ag_2Te.
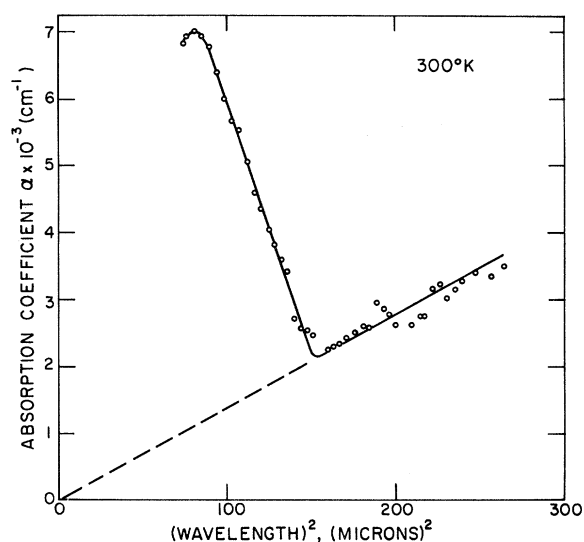
FIG. 2. Free-carrier absorption in β-Ag$_2$Te.

FIG. 3. α^2 vs $h\nu$ for β-Ag$_2$Te.

these data show the fundamental absorption edge, the linearity of this plot offers a method of extrapolation giving the most reliable value of the intercept I on the $h\nu$ axis. We find $I = 0.099$ eV.

In order to relate this value of I to $E_{300}{}^0$, we note that the linearity of the α^2-vs-$h\nu$ plot suggests that the optical transitions being observed are direct ($\Delta \vec{k} = 0$). If this is indeed the case, the thermal and optical energy gaps will be the same at a given temperature. Hence, the 300°K thermal gap is $E_{300}{}^t = E_{300}{}^0$ and, assuming $E_0{}^t > E_{300}{}^t$, as is the case for most semiconductors, we have $E_{300}{}^0 < E_0{}^t$ and hence $E_{300}{}^0 < 0.064$ eV. In addition, $E_0{}^0 = E_0{}^t$ and thus $E_0{}^0 = 0.064$ eV. Since the transitions are direct, the intercept I cannot contain a phonon-energy term, and we ascribe the difference $(I - E_{300}{}^0)$ to a Burstein shift E_B of the absorption edge. Hence, $E_B = (I - E_{300}{}^0)$ and thus $E_B > 0.035$ eV. From electrical measurements, it is known that the β-Ag$_2$Te from which the samples were prepared was n type with a 300°K electron concentration of about 10^{18} cm^{-3}. Hence, expecting a small density of conduction band states, this value of E_B is reasonable and may be compared with a value[6] of E_B of about 0.10 eV for InSb at ~10°K containing about 5×10^{17} electrons cm^{-3}.

In summary, we believe our results agree with the picture of β-Ag$_2$Te as a conventional semiconductor and provide the first optical evidence supporting the values reported for the thermal energy gap. The optical-absorption data have been interpreted in terms of a 300°K optical energy gap of less than 0.064 eV and a Burstein-effect shift of more than 0.035 eV.

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[3]J. Appel, Z. Naturforsch. 10a, 530 (1955).

[4]See, for example, R. A. Smith, Wave Mechanics of Crystalline Solids, (John Wiley & Sons, Inc., New York, 1961), Chap. 13.

[5]See Ref. 4, pp. 412-413. The author would like to thank Dr. R. E. Simon for pointing out this possibility.

[6]J. O. Pehek and H. Levinstein, Phys. Rev. 140, A576 (1965).