parameters the better the "goodness" of the fit should be.

From this model the agreement between theory and experiment for beryllium exhibits the greatest disparity. Schmunk[2] has compared his data to the theoretical calculations of Gupta and Dayal,[17] Iyengar *et al.*,[6] and DeWames *et al.*[19] concluding that the last model gives the best agreement with the data but that further improvements are desired. This best agreement when compared to the results of this model, on the same scale, is only slightly better but utilizes thirteen adjustable parameters compared to only five in this model.

For magnesium and zinc the goodness of fit between theory and experiment is just as good if not better for this model when compared to the models of Iyengar *et al.*,[6] DeWames *et al.*,[19] Collins,[3] Squires,[8] and Borgonovi *et al.*[10] All of the other models utilize many more atomic force constants than the five used with this model.

A modification of the elastic constants by a consideration of the contribution of the electron gas on them could lead to dispersion relations, where the atomic force constants have been evaluated by these new elastic constants, that correlate well to experimental observations. One such modification, proposed by Gupta and Dayal,[17] has been criticized[2,22,23] because of its assumption that the electron gas term is shear free, a position which is untenable for the hcp divalent metals. The modification has also been criticized because it violates symmetry requirements.[24] A slight innovation of this model making it compatible to the hcp metals might lead to new elastic constants that imply theoretical dispersion relations in good agreement with experimental dispersion relations.

The questions of the number of neighbors needed to truly represent the lattice and of the types of interactions between atoms is not fully resolved although the results of this investigation indicate that it is better at the outset to include angular forces in the model of the hcp crystal lattice rather than simply extending the sphere of interaction to include more and more neighbors.

ACKNOWLEDGMENT

The author is grateful to Professor Edwin R. Fitzgerald who suggested the problem and who aided the author by discussions and critiques.

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PHYSICAL REVIEW VOLUME 177, NUMBER 3 15 JANUARY 1969

Optical Properties of Tellurium in the Fundamental Absorption Region*

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(Received 12 August 1968)

An analysis has been made of the optical absorption edge and reflectivity spectrum of single-crystal tellurium. Transmission measurements, using polarized light, were made between 10 and 300°K covering a range of absorption coefficient from 0.4 cm^{-1} to 5×10^3 cm^{-1}. Below 100°K a sign reversal of the temperature coefficient of the absorption edge was observed for both directions of polarization. The low-absorption region for $\mathbf{E}\parallel c$ showed behavior indicative of indirect transitions, while the absorption edge for $\mathbf{E}\perp c$ varied exponentially with photon energy for over two decades. These features, together with the observation of an exciton at 0.336 eV for $\mathbf{E}\perp c$, are similar in nature to those previously reported for trigonal selenium. Optical constants, such as the real and imaginary parts of the dielectric constant, have been calculated over a wide range of wavelengths at 10°K, as well as at 300°K, by applying the Kramers-Kronig relation to the reflectivity spectrum.

I. INTRODUCTION

The present paper is concerned with the experimental investigation of the optical properties of Te single crystals in the fundamental absorption region. Optical constants such as the real and imaginary parts of the dielectric constant have been calculated over a wide range of wavelengths, at 10°K as well as at 300°K, by applying the Kramers-Kronig relation to the reflectivity spectrum. The temperature and polarization dependences of the absorption edge have been studied between 300 and 10°K in order to elucidate the nature of the transitions involved at the band edge. In extending previous optical data on Te, which facilitate comparison with theoretical attempts to determine its precise energy band configuration, our investigations have shown several interesting features. These include

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* Preliminary results were presented at the Washington, D.C., April, 1968, A.P.S. Meeting.
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the observation of a sign reversal of the temperature coefficient of the absorption edge for both directions of polarization and behavior indicative of indirect transitions for **E**$\|c$.

Extensive literature exists concerning the optical properties of Te. In the highly absorbing region, several workers[1–3] have measured the reflectivity at room temperature while the temperature dependence of the absorption edge has been studied at room and liquid-nitrogen temperatures using transmission techniques.[4,5] Exciton peaks have been observed at 10°K for both directions of polarization.[6–8] These authors made oscillatory magnetoabsorption experiments on Te which yielded a band-gap energy, 0.335 eV, for this crystal. Two other features of the experimental studies relating to the electronic structure are the occurrence of a strong absorption peak at 0.1 eV,[9–11] due to intravalence-band transitions for light polarized with E parallel to the c axis, and a recombination radiation polarized perpendicular to the c axis which has been observed at low temperatures at the band edge.[12] The earlier semiempirical attempts to evaluate the band structure have been supplemented in recent years by more sophisticated numerical calculations.[13–19] Most of these band theories agree as to the general band structure and the location of the band extrema in k space.[16,17,19] They are also able to account for some of the characteristic properties revealed by experimental work.

II. EXPERIMENTAL

Te is an elemental semiconductor which has D_3 point group symmetry and is optically uniaxial.[20] Therefore, its optical properties depend on the plane of polarization of the light with respect to the optical axis (the c axis). Accordingly, all measurements were made using light polarized perpendicular (**E**$\perp c$) and parallel (**E**$\|c$) to the c axis. The experiments were carried out in two parts; the absorption measurements at the band edge (0.3–0.5 eV), and the reflectivity measurements over a wider spectral range in the fundamental absorption region.

The single crystals used in our experiment were grown by the Czochralski process in a hydrogen atmosphere. Spectral analysis indicated a total impurity content less than 6ppm. The hole concentration measured at 77°K was 8×10^{13} cm^{-3}, a value typical of the Te crystals used by other workers.[21]

The absorption measurements were made on 19 different samples covering a range of thickness 6μ–7.3 mm. The samples were prepared by cleaving the crystal along two parallel $(10\bar{1}0)$ planes. Only those crystals with mirrorlike cleavage surfaces were investigated. Thin samples were prepared from cleaved crystals by chemical polishing with a methanol solution of bromine. Lapping and optical polishing were avoided because of their undesirable effects.[5] The reflectivity measurements were made on cleaved $(10\bar{1}0)$ surfaces. Those which were etched chemically after cleaving yielded results that, within experimental error, were identical to those obtained on cleaved smooth surfaces.

The experimental techniques employed were similar to those described elsewhere.[22,23] For the infrared range between 0.25 and 1 eV, a double-plate transmission polarizer was constructed with two optically polished silicon plates, $1\times20\times50$ mm. Owing to the uniform transmission and high refractive index[24] in this region, silicon plates proved to be an excellent material for the polarizer, producing a degree of polarization better than 97%. Similar polarizers using germanium plates have been reported previously.[25] A Leiss single monochromator with a LiF prism was used in conjunction with a glow-bar light source, an indium antimonide detector and a phase-sensitive amplifier. For the spectral range between 5.5 and 12 eV, a biotite plate[26] was used as a Brewster angle reflector polarizer; this provided a degree of polarization of better than 95% when combined with the partly polarized output of the vacuum uv monochromator (McPherson 0.5-m monochromator with a 600-line/mm grating blazed at 1500 Å). Because of gas-condensation problem on the sample crystal at low temperatures, measurements in the vacuum uv range were only possible at room temperature.

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III. RESULTS AND DISCUSSION

A. Absorption Edge

The dichroism of the optical absorption edge of Te is apparent from Fig. 1, which illustrates the variation of absorption coefficient with photon energy at 300 and 196°K for both directions of polarization. The temperature dependence of the edge for individual polarizations is displayed in Fig. 2 ($\mathbf{E}\perp c$) and in Fig. 3 ($\mathbf{E}\parallel c$). Our results are in general agreement with the less extensive data compiled by previous authors.[5] However, an apparent difference in the low-absorption region may be explained. In our measurements the residual absorption at low energy (0.3 eV), which may be due to impurities and structural defects, remains constant with temperature. In Blakemore and Nomura's[5] analysis, the apparent residual absorption varied by more than an order of magnitude between 300 and 100°K. The variance stems from the fact that they applied the room-temperature reflectivity, which was obtained from the room-temperature refractive index, to calculate the absorption coefficient at lower temperatures for each polarization. This is inadmissible, however, for, as shown in Table I, the reflectivity is a function of temperature. The values given in Table I were measured at 0.3 eV and used in our analysis to compute the absorption coefficient α, which is expressed by the relationship

$$\frac{I}{I_0}=\frac{(1-R)^2\exp(-\alpha d)}{1-R^2\exp(-2\alpha d)}, \tag{1}$$

where I/I_0 is the ratio of transmitted to incident intensity, R is the reflectivity, and d is the specimen thickness.

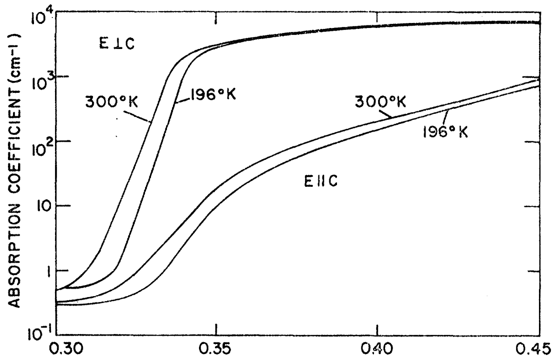


FIG. 1. Edge absorption spectra for Te at 196 and 300°K for light polarized $\mathbf{E}\perp c$ and $\mathbf{E}\parallel c$.

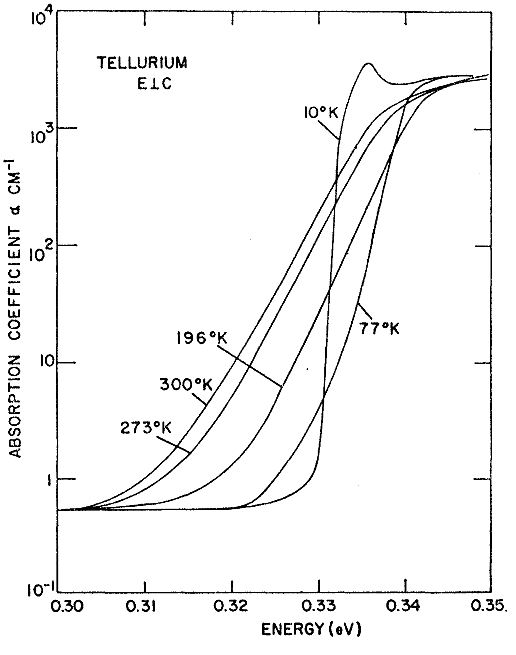


FIG. 2. Absorption coefficient for Te as a function of photon energy for light polarized $\mathbf{E}\perp c$.

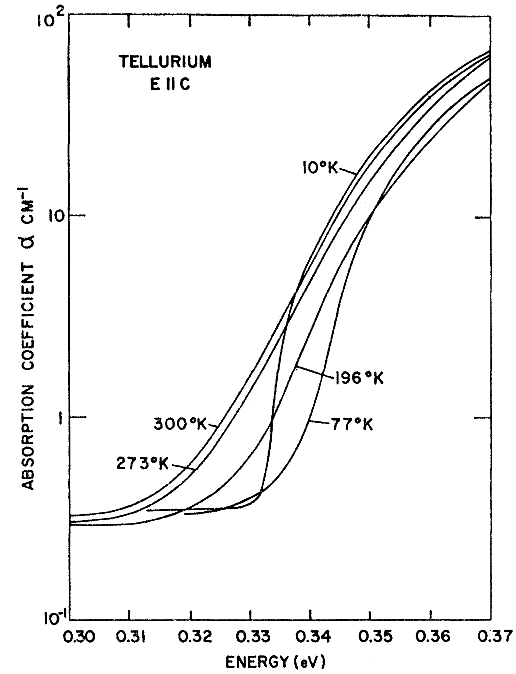
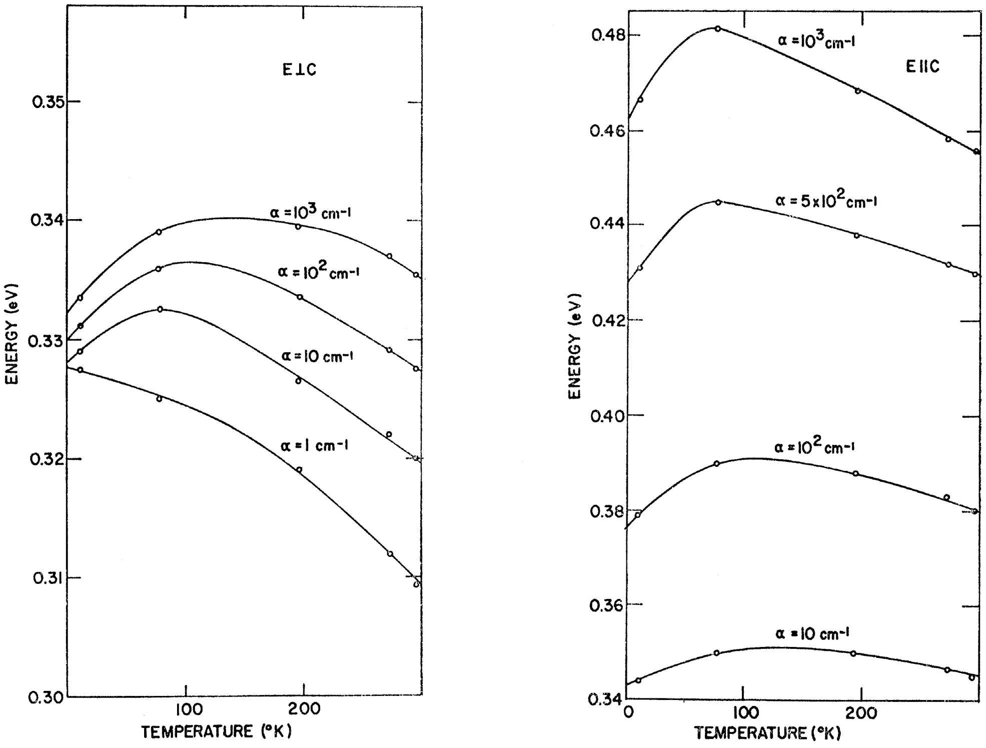


FIG. 3. Absorption coefficient for Te as a function of photon energy for light polarized $\mathbf{E}\parallel c$.

It may be seen from Table I that the reflectivity at the absorption edge experiences a minimum between 300 and 10°K. The reflectivity is related to the refractive index n and to the extinction coefficient k by the

TABLE I. Reflectivity of tellurium at 0.3 eV.

Temp. (°K)	$R_{\mathbf{E}\perp c}$	$R_{\mathbf{E}\parallel c}$
300	0.43	0.53
273	0.40	0.49
196	0.39	0.49
77	0.37	0.51
10	0.41	0.52



(a) (b)

FIG. 4(a). Isoabsorption curves for several values of absorption coefficient; $\mathbf{E}\perp c$. (b) Isoabsorption curves for several values of absorption coefficient; $\mathbf{E}\|c$.

expression

$$R=(n-ik-1)^2/(n-ik+1)^2. \tag{2}$$

Therefore, the minimum reflects the fact that, when the crystal temperature is lowered from room temperature, the absorption edge at first shifts toward higher energies (blue shift) with diminishing temperature, but as the temperature is lowered further, it reverses itself and shifts towards lower energies (red shift). This anomalous variation is seen clearly in Figs. 2 and 3 and is also evident in the complementary isoabsorption curves for $\mathbf{E}\perp c$ and $\mathbf{E}\|c$ shown in Figs. 4(a) and 4(b), respectively.[27] At 300°K for $\alpha=10^2$ cm^{-1}, where these curves may be approximated to a straight line, one obtains

$$(\partial E/\partial T)_\perp=6.3\times10^{-5}\text{ eV/°K}$$

and

$$(\partial E/\partial T)_\|=6.7\times10^{-5}\text{ eV/°K},$$

in good agreement with the values reported by Blakemore and Nomura.[5] In both cases the apparent edge shows a blue shift with decreasing temperature above 100°K and a red shift below 100°K for values of α above unity. Similar behavior which was observed several years ago in TlCl remains unexplained.[28,29]

The temperature dependence of the band-gap energy E_g is given by the relationship

$$\frac{dE_g}{dT}=\left(\frac{\partial E_g}{\partial T}\right)_V-\frac{a}{b}\left(\frac{\partial E_g}{\partial P}\right)_T, \tag{3}$$

where a and b are the volume thermal-expansion coefficient and compressibility, respectively, P is the pressure, and T is the absolute temperature. At higher temperatures, the first term on the right-hand side of Eq. (3), which represents the thermal broadening of the edge due to electron-lattice interactions, generally dominates the absorption edge. This term is for most crystals negative, and this accounts for the blue shift of the absorption edge upon cooling near room temperature. However, as the crystal cools, the thermal-broadening term diminishes in magnitude and eventually the second term begins to dictate the position of the edge. The pressure coefficient of the band gap, $(\partial E_g/\partial P)_T$, has been reported to be negative at room temperature in Te,[30–32] which could account for the reversal of the edge shift at low temperatures in this material. An alternative mechanism for the anomalous behavior in Te is that two different processes are superimposed at the

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[27] This effect has been noted by H. W. Buhren and K. Winzer of the University of Cologne (unpublished); see Ref. 10.

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band edge, each dominating the absorption process in separate temperature regions.

An exciton peak was observed for $\mathbf{E}\perp c$ at 0.336 eV at 10°K (Fig. 2) which is in agreement with the data reported by Alpert and Rigaux[7] and by Grosse and Winzer[8]; this confirms their interpretation that the transitions for $\mathbf{E}\perp c$ at the band gap are allowed and direct. However, in contrast to our results for the $\mathbf{E}\perp c$ polarization, no exciton peak was observed for $\mathbf{E}\parallel c$ (Fig. 3). This observation is in disparity with previous work.[6,8] It is not possible to account for the absence of an exciton for this direction of polarization by speculating that our crystals were strained. This is because direct comparison with Grosse and Winzer's[8] curve for $\mathbf{E}\parallel c$ at 10°K shows that although the shapes of the two curves are in general agreement for $E > 0.34$ eV, the values of α in our experiment were always lower than those reported by these authors. Direct comparison with the data reported by Rigaux and Drilhon[6] is not possible because they discussed their results in terms of arbitrary units. Furthermore, these authors were able to fit their results to Elliott's[33] theoretical expression for direct forbidden transitions. Between 0.335 and 0.45 eV our data for $\mathbf{E}\parallel c$ do *not* fit Elliott's theory for the direct-forbidden case but rather fit the expression for nondirect transition processes.[34] It should also be mentioned that Grosse's data for $\mathbf{E}\parallel c$ could not be explained simply in terms of forbidden direct transitions.

If the transition involved is forbidden and direct, then the absence of an exciton for $\mathbf{E}\parallel c$ may easily be understood. It has been shown[33,35] that the oscillator strength of excitons due to forbidden transitions is weaker than that of allowed transitions by at least a factor of $(a_0/a_B)^2$, where a_0 is one-half of the nearest-neighbor distance and a_B is the exciton Bohr radius. In Te, $a_0 \approx 2$ Å and $a_B \approx 410$ Å,[8] and, therefore, one would expect the ratio of the absorption coefficient of excitons for $\mathbf{E}\parallel c$ to that for $\mathbf{E}\perp c$ to be approximately 2×10^{-5}. Since the observed absorption peak height of allowed excitons ($\mathbf{E}\perp c$) is only in the vicinity of 5×10^3 cm^{-1}, it is reasonable that we do not find an exciton peak associated with a direct, forbidden transition at the absorption edge for $\mathbf{E}\parallel c$ polarization.

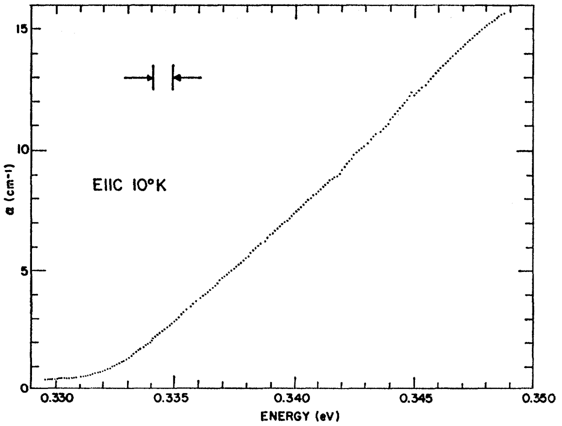

FIG. 5. Absorption curve for Te with $\mathbf{E}\parallel c$ at 10°K showing lack of fine structure in the energy range 0.33–0.35 eV.

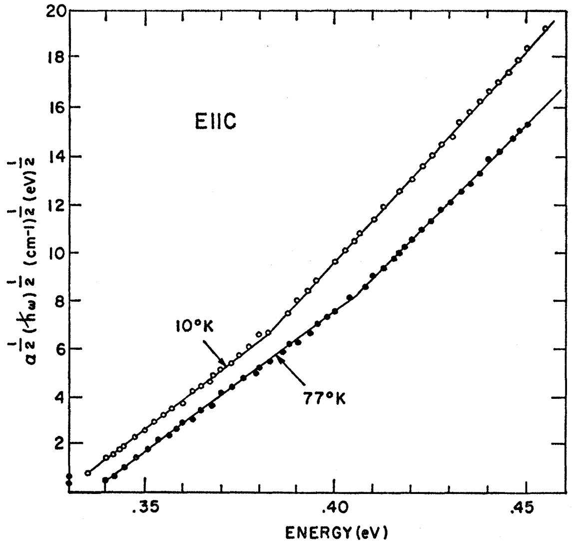

FIG. 6. Absorption plot, representative of allowed indirect transitions, for Te with $\mathbf{E}\parallel c$ at 77 and 10°K.

Figure 5 shows in some detail the absorption edge of one of our samples (2.2-mm thick) between 0.33 and 0.35 eV for $\mathbf{E}\parallel c$ at 10°K. The curve itself is noticeable for its lack of fine structure, even in the range $\alpha \approx 0.4$. No steps are observed in the absorption curve which would indicate the start of various processes involving phonons. For a more extended energy range, however, some structure is observed in a plot of $(\alpha\hbar\omega)^{1/2}$ versus energy which is indicative of phonon-assisted allowed transitions within the forbidden gap. This is shown in Fig. 6, from which we estimate the energy gap for the indirect transitions to be 0.337 eV at 10°K.

The differences between our results and those obtained by Rigaux and Drilhon[6] and by Grosse and Winzer[8] is nonetheless perplexing. However, the structure we observed for this direction of polarization coupled with the implications of recent band-structure calculations[17,36] on Te that indirect transitions can exist at the band edge, compel us to favor the interpretation presented in this section.

In a previously published paper[23] we analyzed the absorption tail of trigonal Se in terms of Urbach's rule. A study of the temperature dependence yielded a phonon energy in agreement with that obtained from

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infrared reflectivity.[37] It may be seen from Fig. 2 that the absorption edge of Te for $\mathbf{E}\perp c$ for over two decades is essentially exponential.

Urbach's empirical relationship has been generalized to the form[38]

$$\alpha=\alpha_0(T)\exp[\sigma_0(E-E_0(T)/kT^*]. \qquad (4)$$

The value of σ_0 is indicative of the steepness of the absorption curves, while its reciprocal may be taken as a reflection of the strength of the exciton-lattice interaction.[39] T^* is an effective temperature, which is related to the absolute temperature by the equation

$$T^*=\hbar\omega'/2k\coth(\hbar\omega'/2kT). \qquad (5)$$

The energy $E'=\hbar\omega'$ may be interpreted as the energy associated with an appropriate average of the zero-point vibration frequencies of the thermal vibrations responsible for the absorption tail. $E_0(T)$ and $\alpha_0(T)$ are temperature-dependent parameters characteristic of the crystal and are related, respectively, to the energy gap and the matrix element for optical absorption.

For Te, the anomalous temperature dependence of the edge discussed earlier in this section complicates the Urbach-rule behavior and prevents estimation of the zero-point energy E' of the crystal and thus an accurate determination of σ_0. The value of the latter parameter may, however, be estimated by taking $T=T^*$ at 300°K. In comparison to the value $\sigma_0=0.64$ for trigonal Se,[23] we calculate σ_0 for Te at 300°K to be approximately 7.8. In a recent publication, Hopfield[40] stressed the importance of establishing whether or not materials existed with exponential tails giving values of σ_0 *not* close to unity. The limited range of α which shows an exponential dependence with photon energy that is covered by our transmission measurements is restricted at one end by the exciton peak ($\alpha\approx5\times10^3$ cm^{-1}) and at the lower end by residual absorption and possibly indirect transitions. This is unfortunate because it precludes our stating with any certainty that Te ($\sigma_0=7.8$) is one such material.

B. Optical Constants in Fundamental Absorption Region

Reflectivity measurements were made at approximately 5° angle of incidence in the spectral range 0.35–5.5 eV and at 20° angle of incidence above 5.5 eV. Between 0.35 and 5.5 eV, the data we show represent the average values obtained from the four most flawless specimens. The uncertainty in the value of the reflectance data in this range is estimated to be within ±5%. In the energy range above 5.5 eV, three samples were studied, the accuracy being within ±10%.

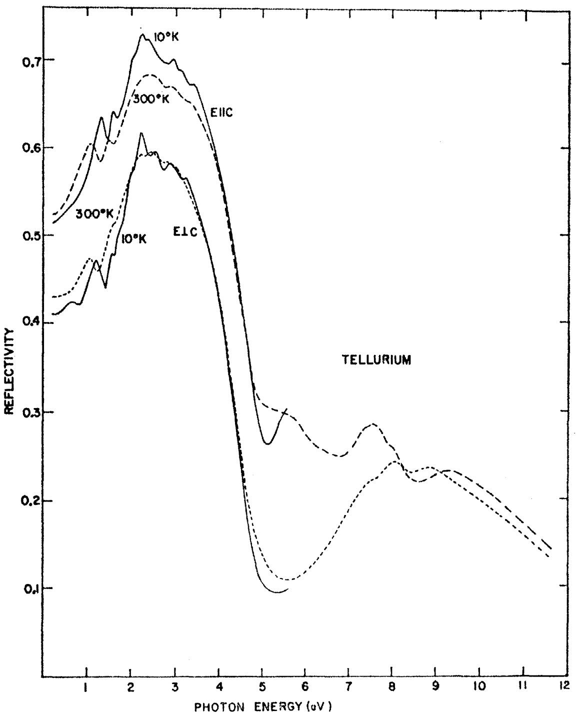

FIG. 7. Reflectivity spectra of Te for the two main polarizations at 300 and 10°K.

The reflectivity spectra of Te are displayed in Fig. 7, where the data for 10°K are shown as solid lines and those for 300°K as broken lines. The curves at 300°K agree well with previously published work.[2,3] The solid curves together with all subsequent curves at 10°K represent the first extended reflectivity data on Te at this temperature. The derivation of other useful optical parameters has been accomplished by applying the Kramers-Kronig analysis to the reflectivity data. Since no reflectivity data were available above 5.5 eV at

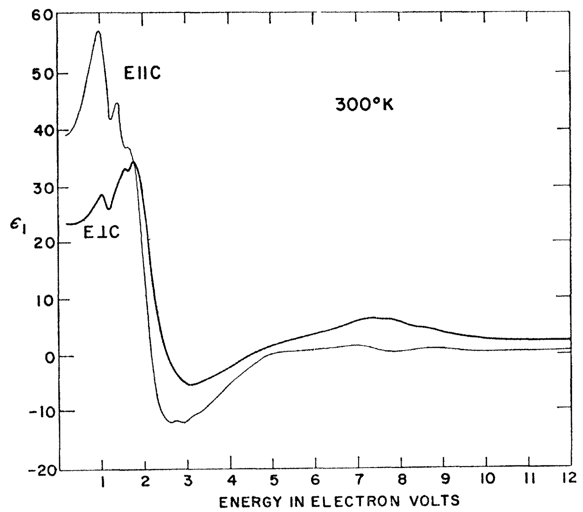

FIG. 8. Real part of the dielectric constant ϵ_1 of Te at 300°K for both directions of polarization.

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10°K, the room-temperature data in this range were substituted as a best approximation for the 10°K analysis. Approximately 210 points were used to compute the phase shift θ for each mode of polarization at each temperature. The real and imaginary parts of the dielectric constant, ϵ_1 and ϵ_2, respectively, thus calculated are displayed in Figs. 8–11 for 300 and 10°K.

The majority of the recent band calculations[16,17,19] for Te agree that the direct band gap is located at the corner of the Brillouin zone edge, $H(k=\pi/c)$. We have seen, however, that the absorption coefficient at H is too small ($\sim 10^3$, Fig. 1) to create any structure in the reflectivity spectrum (Fig. 7). Thus, in Figs. 9 and 11, the first significant structure that appears at 10°K is a rather broad but low bump at 0.7 eV for $\mathbf{E}\perp c$. The proximity of this value to the gap energy and also the fact that it appears more prominently for $\mathbf{E}\perp c$ suggests that transitions in the vicinity of H are probably responsible for this structure. The two peaks in the $\mathbf{E}\|c$ spectrum between 1.0 and 1.5 eV and the peak at 1.27 eV in the $\mathbf{E}\perp c$ spectrum (Fig. 11) show a blue shift with decreasing temperature. In view of the fact that the band-gap transitions show a red shift, these three distinct peaks probably originate from transitions remote from H. On the whole the Te spectra, e.g., Fig. 11, show far less structure than those of Se.[22] Another difference is the relatively high value of ϵ_2 for Te. In recent publications, Picard and Hulin[17] and Sandrock and Treusch[16] have shown that the upper valence-band triplet levels and the lower conduction-band triplet levels of Te are rather flat and parallel to each other along the Δ and S axes (Sandrock's notation).[16] Thus the oscillator strengths integrated over wide k space can account for the rather high peak values of ϵ_2 shown in Figs. 10 and 11.

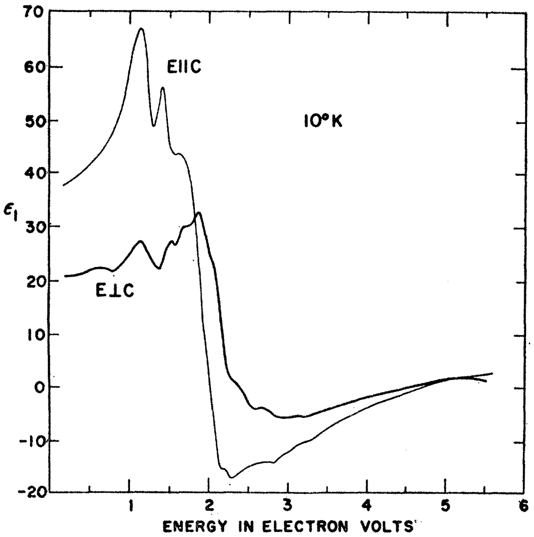

FIG. 9. Real part of the dielectric constant ϵ_1 of Te at 10°K for both directions of polarization.

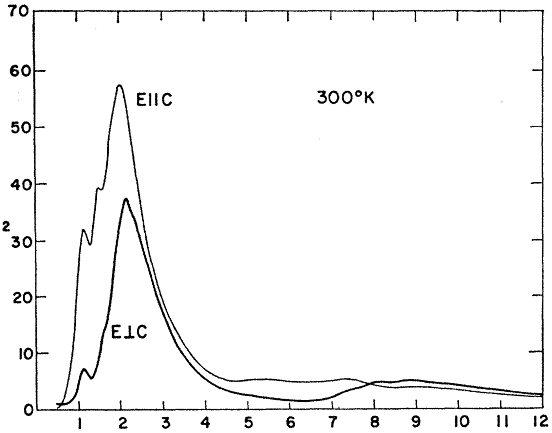

FIG. 10. Imaginary part of the dielectric constant ϵ_2 of Te at 300°K for both directions of polarization.

Sandrock[36] has recently published a band calculation on trigonal Se in which he demonstrated that the spectrum of Se is determined not only by the joint density of states but also strongly by the variation of the oscillator strength in k space. Accordingly, it is not possible to classify the various peaks in the optical spectrum of trigonal Se in terms of direct interband transitions localized at specific points in k space. Since Te is isomorphic to trigonal Se in its crystal structure and their electronic configurations are similar, one would expect an analogous situation to exist for Te. For this reason we have not attempted to carry out a group-theoretical study of the electronic energy levels of Te along the lines followed for trigonal Se.[22] Knowledge of a complementary band calculation that used approximate wave functions is necessary for any further interpretation of the spectra shown in Figs. 8–11.

The absorption coefficient for Te was also calculated from the reflectivity data and is shown in Fig. 12 for 300°K. The minimum in the neighborhood of 6.0 eV is similar to that observed[41] in trigonal Se, and may be a

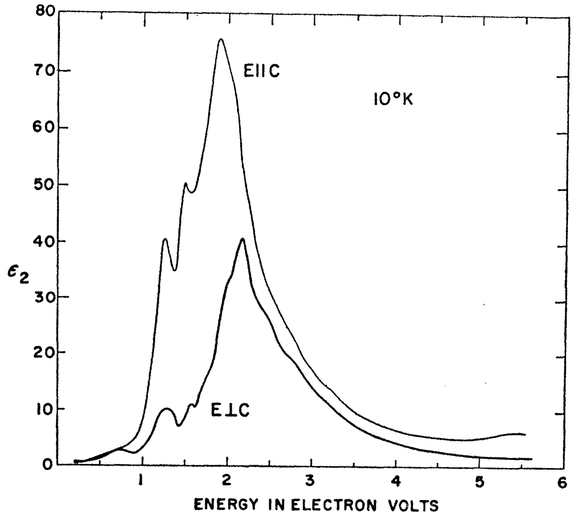

FIG. 11. Imaginary part of the dielectric constant ϵ_2 of Te at 10°K for both directions of polarization.

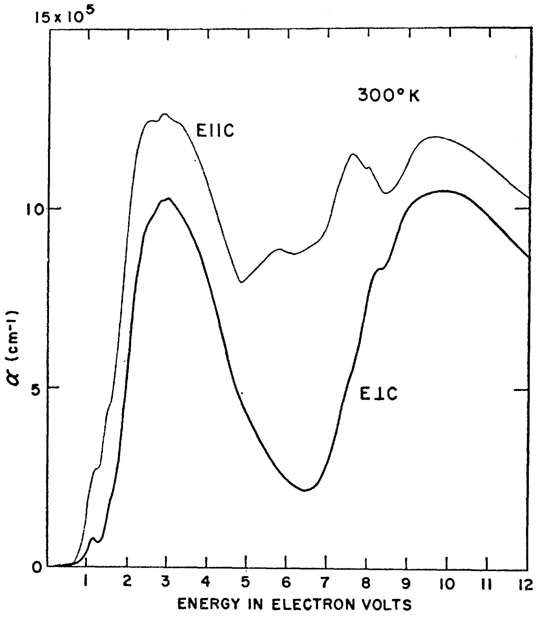

FIG. 12. Absorption coefficient of Te at 300°K for both directions of polarization.

consequence of the gap between the two groups of valence triplets.[36,41] The spectrum above 6.0 eV resembles that[41] of Se in the same energy range and is presumably due to transitions from the lower valence triplets to the lower conduction-band triplets.

Figure 13 exhibits the energy-loss function as a function of photon energy. From fast-electron-scattering experiments at room temperature on thin samples of Te, Leder[42] reported a major peak at 17.9 eV and a minor peak at 5.6 eV. The peak we observe at approximately 4.8 eV for both directions of polarization, which is clearly the subsidiary peak, is in surprisingly good agreement with the value 5.6 eV obtained using fast-electron techniques. Following the method of Ehrenreich,[43] we interpret this peak as being due to plasma oscillations modified by the existence of certain levels above 6.0 eV.

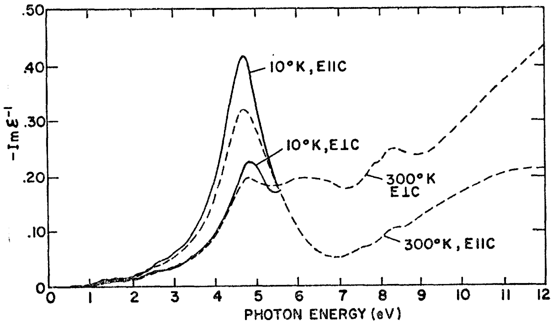

FIG. 13. Energy-loss function $-\mathrm{Im}\,\epsilon^{-1}$ for Te at 300 and 10°K for both directions of polarization.

IV. SUMMARY

Figure 14 displays the absorption spectrum of single-crystal Te at 10°K; this is a composite curve obtained from the combined results of our absorption and reflectivity study. The pronounced dichroism of the band edge, including the existence of an exciton peak for **E**⊥*c*, parallels closely the behavior previously reported for Se.[22,23] The anomalous temperature dependence of the absorption edge below 100°K for both directions of polarization is interesting but, unfortunately, is also responsible for obscuring the absorption processes in this region. For example, it would be desirable to make a detailed study of the exponential edge for **E**⊥*c* along the lines adopted for trigonal Se.[23] In the low-absorption region, our results suggest the presence of an indirect edge; this must be established by further measurements on thick samples of Te which exhibit a lesser amount of residual absorption than the ones used in our investigation. Also, in order to establish definite relationships between characteristic features of the optical spectra and the main predictions of band-structure calculations, it is imperative that theoretical curves for the dielectric functions, etc., be calculated for Te.

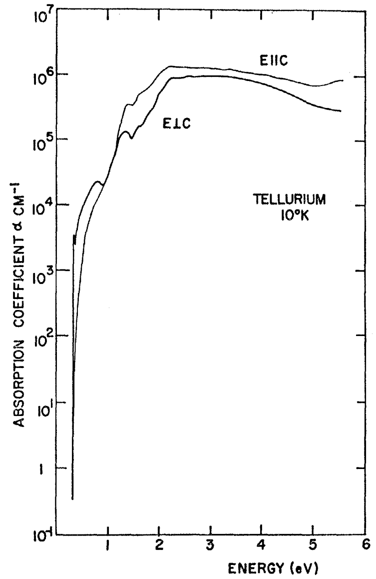

FIG. 14. Composite curve of absorption coefficient versus photon energy obtained from transmission and reflectivity data for Te at 10°K for **E**⊥*c* and **E**∥*c*.

ACKNOWLEDGMENTS

We wish to thank G. Charnitski for his able assistance with the experimental work and Miss B. Van Yserloo for her assistance with the computer programming.

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