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Fundamental Absorption and Franz-Keldysh Effect in Silicon Telluride

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The optical constants of crystalline Si-Te compounds have been investigated by several authors (1 to 5), the interpretations of the results, however, appear to be controversal. No optical determination of effective masses has been published up to now. In this paper we report on reflectivity and transmission of Si_2Te_3 single crystals. From the experimental data the temperature dependence of the absorption coefficient could be calculated. We also present the first Franz-Keldysh results obtained for this material.

The single crystals used for our measurements were grown from the vapor phase as described by Bailey (6). To avoid decomposition of the surface the samples were handled with great care in a glove box which was filled with dry argon. Before each measurement the surface of the samples was cleaned by the annealing procedure which was used by Ziegler and Birkholz (7). The absorption coefficient K as a function of energy for different temperatures is shown in Fig. 1. Two regions can be distinguished: At high energies the absorption coefficient exhibits an exponential increase with energy (Urbach's rule). In the low energy region the curve flattens. This is more pronounced at low temperatures. There is a strong variation of the absorption edge with temperature. From the energy shift of the absorption curves at $K = 5x10^2\ cm^{-1}$ we obtain a temper-

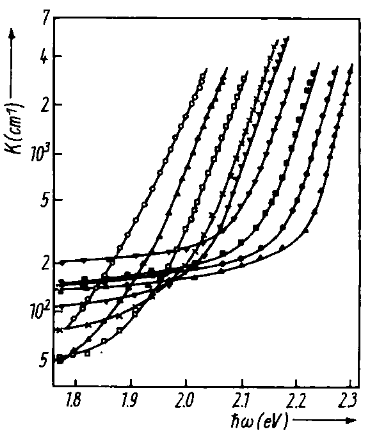

Fig. 1. Absorption coefficient as a function of photon energy for different temperatures; o 476 K, △ 426 K, □ 373 K, × 323 K, ▽ 298 K, ▼ 250 K, ■ 200 K, ● 150 K, ▲ 104 K

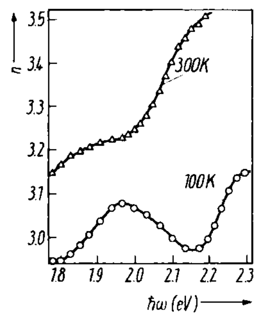

Fig. 2. Refractive index as a function of photon energy

ature coefficient of the band gap $dE_g/dT = -0.93\times10^{-3}$ eV/K. The refractive index for 100 and 300 K is shown in Fig. 2. In the low temperature curve, a maximum is observed near 2 eV.

According to Lucovsky (8) the behavior of the absorption coefficient at low energies can be interpreted as impurity center absorption; the temperature variation being due to the temperature dependent occupancy of the traps and recombination centers. The high energy results can be explained by Dow and Redfield's theory for optical absorption in the presence of an electric field (9). This model assumes a broadening of an exciton line under the influence of an internal electric field. The origin of the field may be related to the defect structure of Si_2Te_3.

For the investigation of the transmission under the influence of an external electric field (Franz-Keldysh effect) we applied semitransparent gold electrodes to the samples. With a sample thickness of 20 to 30 μm it was possible to use periodic electric fields up to 170 kV/cm at a frequency of 220 Hz. The signal was detected by a lock-in amplifier. The observed red shift of the absorption edge as a function of the field obeys a square law (Fig. 3). The reduced effective mass μ of electrons and holes can therefore be calculated by Franz' formula (10):

$$\mu = 6.4\times10^{-17} \frac{(\mathrm{eV})^3}{(\mathrm{V/cm})^2} \frac{S^2F^2}{\Delta E} m_o$$

($S = d\ln K/dE$, F electric field, ΔE red shift, m_o free electron mass).

We find for Si_2Te_3 parallel to the c-axis $\mu = 2.7\ m_o$. If the effective masses of electrons and holes are assumed to be equal, it follows $m_{e,h} = 5.4\ m_o$ corresponding to an effective

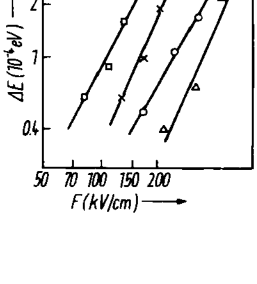

Fig. 3. Field-broadening of the absorption edge for different energies (log log plot); □ E = 2.084 eV, slope 2.0; × E = 2.108 eV, slope 2.3; O E = 2.121 eV, slope 2.0; △ E = 2.126 eV, slope 2.3. F-scale only valid for E = 2.084 eV

density of states $N = 2x10^{20}$ cm^{-3}. This result is in agreement with thermoelectric measurements by Ziegler et al. (11).

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