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OPTICAL PROPERTIES OF LEAD TELLURIDE FILMS

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Abstract: Room temperature transmission and reflection measurements over the photon energy range 1.2—3 eV have been made on Pb Te films of different thicknesses. The absorption coefficient is calculated and compared with values obtained for epitaxial single crystal films. The observed structure of reflectivity could be analyzed by comparison with a recent augmented plane wave band structure calculation.

1. *Introduction*

Lead telluride is a well known polar semiconductor with many useful properties. For many years, Pb Te has been of technological interest because Pb Te films can be used as highly sensitive infrared detectors$^{1)}$. In recent years, further work was motivated by the possible use of Pb Te films in thin film transistors$^{2)}$. More recently, Pb Te was found to be a suitable semiconductor for producing laser action$^{3)}$. Extensive studies on the electrical and optical properties of Pb Te have been made$^{4-8)}$, however the fundamental problems regarding the energy band structure of Pb Te are still not completely solved. Related to the optical constants of Pb Te, Cardona$^{9)}$ and Scanlon$^{11)}$ reported the absorption and reflectivity measurements of epitaxial films of lead salts and assigned the observed structure, however, no detailed studies on the variation of the absorption coefficient with film thickness and the effect of the substrate were reported. A first-principles calculation of the absorption coefficient of Pb Te crystals has been reported[10]. In this calculation a parabolic-band approximation has been made for the bands in the vicinity of the L point. The calculated absorption is in agreement with experiment[9] best near the fundamental edge. Recently Buss and Parada[12], used an improvement of the augmented-plane-wave (APW) calculation to obtain the optical constants of Pb Te and they identified the different transitions occuring.

The present contribution is aimed to investigate the optical properties of Pb Te films, deposited onto quartz substrates, in the energy range 1.2—3 eV. The optical absorption is measured for different thicknesses. The structures obtained in the reflectivity measurements are given and the effect of the quality of the films is considered.

2. *Experimental*

Lead telluride films were prepared by thermal evaporation in a vacuum of $\sim 10^{-5}$ torr at an evaporation rate of $\sim$ 15 Å per second from a tungsten foil onto quartz plates. The starting material was Pb Te having electron conductivity, the concentration of free electrons is equal to $3 \cdot 10^{19}$ cm^{-1}. Film thickness was determined by Tolansky interference method[13]. Photographs of the step fringes produced at layer edges enabled the thickness to be estimated with an accuracy ± 8%. Electrical measurements show, that all thin films (less than 500 Å) have hole conductivity. This difference between the behaviour of thin and thick samples may be accounted for by oxidation of the thin films due to the diffusion of oxygen atoms[14].

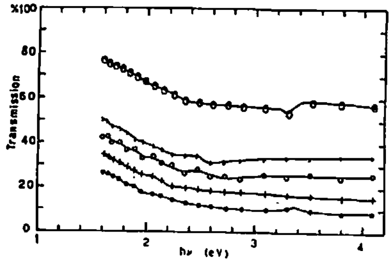

Fig. 1. The dependence of the optical transmission on the photon energy.

Room temperature optical transmission measurements were carried out using a Beckmann UV Spectrophotometer D.U. Reflectivity measurements were obtained using nearly normally incident monochromatic light and a special optical arrangement.

3. *Results and discussions*

Fig. 1 shows the variation of the transmission with photon energy for Pb Te films of different thicknesses deposited on quartz. The room-temperature reflectivity (R) of Pb Te films is shown in Fig. 2. compared with the theoretical curve of reflectivity for bulk single crystal[12] and other measurements[9]. The experimental curves, for different thicknesses, have no sharp E_1 and E_2 peaks as the theoretical curve, but the reflectivity exhibits a fine structure. The difference between the measured and calculated reflectivities could be attributed to the large amounts of mosaic structure of the thin films deposited on quartz (amorphous substrate). Reflectivity calculations [12] were done for single crystal, and Cardona's measurements[9] were obtained for single crystal epitaxial films of Pb Te evaporated onto single crystal K Br substrate. Electron microscopy investigation shows that the deposited Pb Te films are not single crystals, the individual spots on the electron diffraction patterns show that the samples have a fairly large amount of mosaic structure. Cardona[9], observed that the reflectivity maxima from etched surfaces of Pb Te occurs at lower energies than peaks obtained from cleaved single crystal surface. Therefore, the fine structure observed of the reflectivity could be attributed to the mosaic structure of the films investigated.

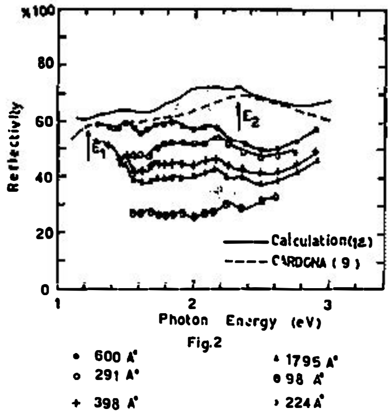

Fig. 2. The dependence of the measured reflectivity on photon energy.

Simultaneous transmission and reflection measurements on an absorbent layer permit one to obtain the absorption and reflection coefficients. The Drude theory[15] relates the refractive index n and the extinction coefficient k to the absorption coefficient a for a given wavelength, and the reflection coefficient r on the surface of an absorbent material by the equations

$$r = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}, \qquad a = \frac{4\pi k}{\lambda}. \tag{1}$$

For an absorbent material it is convenient to make the measurements by means of a homogeneous layer with plane parallel faces illuminated by parallel light under normal incidence. Under these conditions, multiple reflections are produced in the interior of the sample. The resultant intensity due to the contributions of all these reflections must be computed. Czerny et al.[16, 17] have shown that the measured transmittance T and the reflectance R can be obtained by the formulas

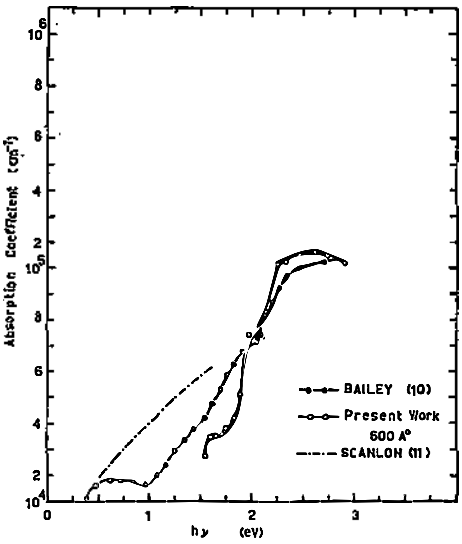

Fig. 3. Optical absorption coefficient versus photon energy for $d = 600$ Å compared with the results of others.

$$T = \frac{(1-r)^2 + 4r\sin^2\psi -}{e^{\alpha d/2} - r\,e^{-\alpha d/2})^2 + 4r\sin^2\left[\left(\frac{2\pi nd}{\lambda}\right) + \psi\right]}$$

and

$$R = r\,\frac{(e^{\alpha d/2} - e^{-\alpha d/2})^2 + 4\sin^2\left(\frac{2\pi nd}{\lambda}\right)}{(e^{\alpha d/2} - r\,e^{-\alpha d/2})^2 + 4r\sin^2\left[\left(\frac{2\pi nd}{\lambda}\right) + \psi\right]},$$

where $\tan\psi = \frac{2k}{n^2 + k^2 - 1}$ and d is the layer thickness. By summing up the intensities due to the contributions of all the multiple reflections on the faces of the layer the above equations reduced to

$$T = \frac{(1-r)^2 + 4r\sin^2\psi}{e^{\alpha d} - r^2 \cdot e^{-\alpha d}}; \quad R = r(1 + T e^{-\alpha d}). \tag{2}$$

Calculation of the optical constants requires the solution of Equ. 2. Replacing r by its value one can solve the resultant equation graphically18). The calculated absorption coefficient α is shown in Figs. 3,4. The behaviour of the absorption coefficient with photon energy, for a 600 Å sample (Fig. 4), is shown sesides the theoretical absorption curve of Bailey et al.10), and the results of experimental measurements of Scanlon11).

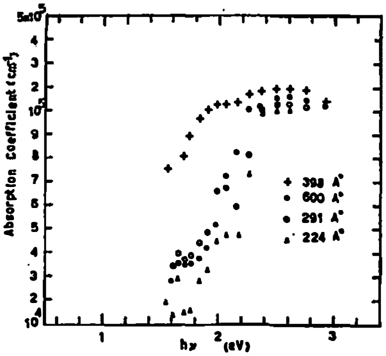

Fig. 4. Optical absorption coefficient versus photon energy for Pb Te films of different thicknesses.

Internal stresses may appear in films because of the difference between the thermal expansion coefficients of the film and the substrate. Deformation due to such internal stresses alters the absorption and the forbiden band structure19) and could give rise to a decrease in the absorption. Moreover, the structure of Pb Te at the interface with quartz is not the same as the bulk material. Strains at the interface may alter the atomic spacings in the layer and, therefore, affect the optical propeperties. This could explain the decrease of the absorbtion coefficient at lower energies.

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