Size quantization in thin cadmium telluride films

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Fine structure due to exciton transitions between size-quantized bands was observed in transmission spectra of thin cadmium telluride films at helium temperatures. The bulk values of the effective masses of light and heavy holes were determined from an analysis of the experimental data.

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We studied the transmission of thin mosaic single-crystalline cadmium telluride films near the characteristic absorption edge. Since the main experiments were performed at helium temperatures, absorption in CdTe in this range is determined by exciton effects.

To obtain cadmium telluride films, we used the method of laser deposition[1] on single-crystalline KBr substrates heated to $T \sim 300\,^\circ\mathrm{C}$. The structure obtained was then annealed in the same evacuated volume and held at 275 °C for three hours.

Electron-diffraction studies of the specimens obtained showed that we are dealing with single-crystalline films with the structure of sphalerite. In addition, preliminary measurements of film thickneses were performed on all specimens investigated by the method of ellipsometry, after which they were transferred onto a MgF_2 substrate, i.e., onto a material whose thermal-expansion coefficients were close to those of CdTe.

The transmission measurements were performed using a dual-beam-set-up, based on a chopper wheel with two rows of slots situated on opposite sides of the center of the disk.[2] With the help of this wheel and a SPM-2 grating monochromator, two identical monochromatic beams of light, modulated with frequency $\omega = 200$ Hz and shifted in phase relative to each other by $\pi/2$, were obtained. One of these beams was transmitted through a CdTe (MgF_2) film, which was immersed into a helium cryostat, while the other beam (comparison channel) was passed through a CdTe (MgF_2) film with approximately identical thickness, but at room temperature. The two beams were then focused on a detector (FÉU-83 photomultiplier) and their difference was recorded by a narrow-band amplifier with a synchronous detector (PAR 186A). By selecting the thickness of the film at $T = 300$ K (comparison channel), it is possible to achieve a minimum measurement signal in the spectral region $\hbar\omega \gtrsim E_g(d)$ at $T = 2$ K. Since any features in the absorption spectrum are strongly washed out at room temperature, it was possible to identify a weak fine structure in the transmission of the film at $T = 2$ K by increasing the sensitivity of the measuring setup.

Figure 1 shows the spectra ΔT (change in transmission) obtained in this manner for three films with different thicknesses. It is evident from the figure that the structure observed in the spectrum ΔT shifts with decreasing thickness toward shorter wavelengths with a simultaneous increase in the energy difference between neighbor-

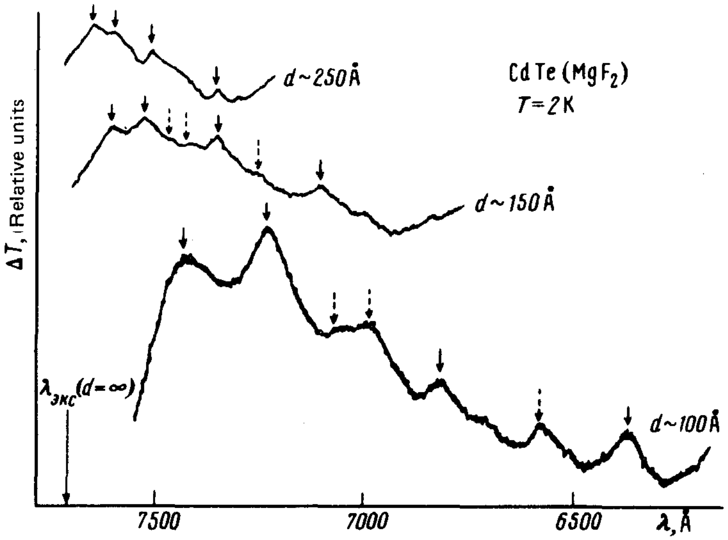

FIG. 1.

ing (identical) maxima. This behavior of the spectra as a function of film thickness can be viewed as a qualitative proof of the existence of size quantization.

In making a quantitative interpretation of the experimental data obtained, it is first necessary to take into account the fact that in thin films, size quantization should remove the degeneracy of the valence bands. In this case, the light and heavy hole bands are quantized with $K = 0$ independent of each other,[3] and there should be two types of excitonic optical transitions, whose intensity is determined by the symmetry of the corresponding wave functions, i.e., essentially by the numbers "n" of the size-quantized bands in the initial and final states and whether the excitons belong to the light- or the heavy-hole band.

Taking into account the fact that the perturbation removing the degeneracy of the valence band in thin films is analogous, from the point of view of the change in symmetry of the crystal, to uniaxial compression, quantized heavy-hole bands must have symmetry Γ_9, while quantized light-hole bands must have symmetry Γ_7.[4] For this reason, the main selection rules for interband optical transitions can be written as follows: $\Delta n = 0$, while the transitions $\Gamma_9 \to \Gamma_7$ (conduction band) are allowed for light polarization $\varkappa \perp z$, where the z axis is perpendicular to the plane of the film.

Figure 2 shows the results of polarization measurements, can be identified from some optical transitions. The breakdown of selection rules is attributed to the fact that the excitonic states are strongly affected by the region of K space $\sim 1/a_0$ (a_0 is the Bohr radius of the exciton), where the interaction of the quantized light- and heavy-hole bands must be taken into account.[3]

In order to provide a quantitative description of the energy state of any of the excitonic transitions, it was necessary to take into account the finite depth of the potential well, which was assumed to be equal to the work function of CdTe $\varphi_0 \sim 4.5$ eV, as well as the renormalization of the effective mass of electrons m_e and light holes m_{hl} the framework of Kane's theory for the three-band model.[5]

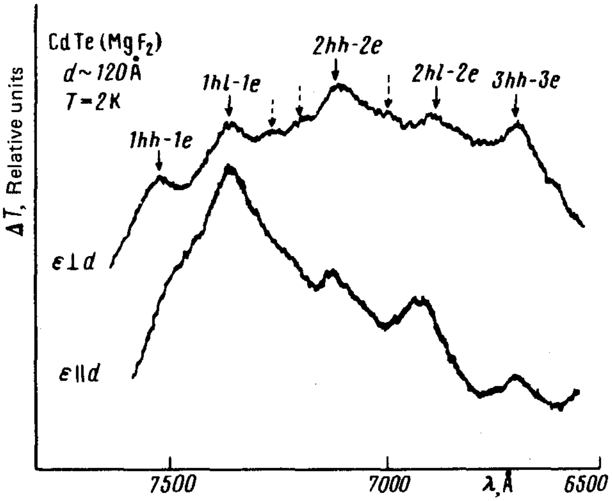

FIG. 2.

The following expressions were obtained for $m_e(d)$ and $m_{hl}(d)$:

$$\frac{m_e(d)}{m_0} = \frac{1}{2}\frac{m_e}{m_0}\left[1 + \sqrt{1 + 4\,\frac{2E_{g0} + \Delta_{so}}{E_{g0} + \Delta_{so}}\,\frac{\pi^2\hbar^2 n^2}{2m_e d^2 E_{g0}}}\right],$$

$$\frac{m_{hl}(d)}{m_0} = \frac{1}{2}\frac{m_{hl}}{m_0}\left[1 + \sqrt{1 + 4\,\frac{\pi^2\hbar^2 n^2}{2m_{hl} d^2 E_{g0}}}\right],$$

where $m_{e(hl)}$ are the bulk values of the effective masses of electrons and light holes, respectively. In deriving these relations, the terms proportional to $(\pi^2\hbar^2 n^2/2m_e(hl)\, d^2 E_{g0})^2$, were dropped and the fact that $m_0/m_{e(hl)} \gg 1$ was taken into account.

The analysis of the experimental data made it necessary, first, to improve the estimates of the thickness of the starting specimens and, second, to determine the effective masses of the light and heavy holes, which were estimated only theoretically in Ref. 6 and which are $m_{hl} = 0.103\, m_0$ and $m_{hh} = 1.38\, m_0$. The bulk value of the effective mass of electrons in CdTe was assumed to be known $m_e = 0.096\, m_0$.

The experimental data were analyzed as follows. For not very thin specimens ($d \simeq 250$ Å and $d \simeq 150$ Å), the difference $E^{2e}_{2hh} - E^{1e}_{1hh}$, which was equated to the computed magnitude of the energy interval between the first and second electron bands, was determined from the spectra ΔT (Fig. 1). In this approximation, i.e., ignoring the quantization of the heavy-hole band, it is possible to make a better estimate of the thickness of these films. Then, in the same approximation, knowing the thickness, the effective mass of light holes $m_{hl}(d)$ and its bulk value m_{hl} were determined from the energy difference, $E^{1e}_{1hl} - E^{1e}_{1hh}$. If it is now assumed that the quantity m_{hl} is known, then we can estimate the effective mass of the heavy holes m_{hh} from the spectra ΔT of the film with $d \simeq 100$ Å. However, the quantization of the heavy-hole band turned out to be of the order of the experimental error (~ 5 meV). For this reason, only a lower bound $m_{hh} > 1.5\, m_0$ can be obtained for m_{hh}. The proposed method for analyzing the experimental data, in which the difference between the exci-

TABLE I.

d (Å)	$E^{1e}_{1hh} - E_0$ meV	$E^{1e}_{1hl} - E_0$ meV	$E^{2e}_{2hh} - E^{1e}_{1hh}$ meV	$E^{1e}_{1hl} - E^{1e}_{1hh}$ meV	d^* (Å)	$\frac{m_{hl}}{m_0}$	$\frac{m_{hh}}{m_0}$
250	10	19	29	9	196	0,136	–
150	20	38	55	18	132	0,135	–
120	36	63	90	27	95	0,14	–
100	70	117	154	47	70	0,135	1,5

ton energies is compared with theory, greatly decreases the effect of size quantization of the energy spectrum of the exciton.[8] The basic experimental data and results of their theoretical analysis are presented in Table I.

In conclusion, we should note that the investigation of size quantization with the help of a detailed theory is one of the most effective methods for studying the band structure of semiconductors, permitting determination of effective masses of free carriers even when other methods are of little use.

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[1] S. V. Gaponov and N. N. Slashchenko, Élektronnaya promyshlennost' No. 1, 11 (1976).
[2] L. F. Mollenauer and D. H. Olson, Rev. Sci. Instrum. **46**, 677 (1975).
[3] M. I. D'yakonov and A. V. Khaetskiĭ, Zh. Eksp. Teor. Fiz. **82**, 1584 (1982) [Sov. Phys. JETP **55**, 917 (1982)].
[4] G. L. Bir and G. E. Pikus, Simmetriya i deformatsionnye éffekty v poluprovodnikakh (Symmetry and Deformational Effects in Semiconductors), Nauka, Moscow, 1972.
[5] O. Madelung, Physics of Semiconductors of Group III and V Elements [Russian translation], Mir, Moscow, 1967, p. 402.
[6] P. Lawaetz, Phys. Rev. B **4**, 3460 (1971).
[7] K. K. Kanazawa and F. C. Brown, Phys. Rev. A **135**, 1757 (1964).
[8] L. V. Keldysh, Pis'ma Zh. Eksp. Teor. Fiz. **29**, 716 (1979) [JETP Lett. **29**, 658 (1979)].

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