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REFLECTIVITY STUDY OF $\text{HgSe}_{1-x}\text{Te}_x$ CRYSTALS

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The room temperature reflectivity spectra of $\text{HgSe}_{1-x}\text{Te}_x$ ($x = 0, 0.4, 0.5, 1.0$) crystals were measured in the visible and ultraviolet range from 1.5 to 12 eV. The maxima characteristic of the binary HgA^{IV} compounds can be revealed in the mixed crystals spectra, but their position depends on the crystal composition. There is no duplication of the spectral features in spite of the different energy position of the maxima for HgSe and HgTe . This suggests that the virtual crystal approximation could be used to describe basic optical properties of $\text{HgSe}_{1-x}\text{Te}_x$.

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Mixed crystals have attracted attention of physicists for many years. The thorough investigations gave insight into the band structure formation and showed many factors determining both optical and electric properties of the solids. The studies concerned covalent $\text{Si}_{1-x}\text{Ge}_x$ and III-V systems, on the one hand, and ionic crystals, on the other hand. Cation substituted II-VI mixed crystals are also well known and widely investigated for both their interesting physical properties (e.g. semimagnetic semiconductors) and useful applications (e.g. $\text{Cd}_{1-x}\text{Hg}_x\text{Te}$ based infrared detectors). However, this is not the case of the anion substituted II-VI materials.

The introduction into the anion sublattice of two elements of the sixth column of the periodic table should modify the electronic bands in a quite different way than it was observed for cation substituted crystals. The empty cation orbitals contribute strongly to the conduction band states but the partially filled d -states of transition metal ions (like Mn, Fe, Co) influence markedly the structure of the valence band, too. This leads to the complicated changes in the optical spectra that are usually used as a tool for the band structure investigations. The situation is clearer for anion substituted materials. The anion states dominate in the valence band and determine its structure. Thus, modification observed in the optical spectra can be ascribed mainly to the changes in the valence band structure.

Such an interpretation can be also supported by arguments derived from model calculations of the optical functions describing mixed crystals performed by Onodera and Toyozawa [1]. According to this approach, the ratio of the difference Δ of the energies of the bands in the components to the width T of the bands determines the characteristics of the mixed crystals. If Δ/T is bigger than

a critical value, features characteristic of the components survive in the bands of the mixed crystal. Otherwise, the features fuse into a new spectrum with maxima that shift between positions characteristic of the components. This theory (with further completions [2]) were successfully used to interpret the optical spectra of many different mixed crystals, but every new example is an argument for its universality.

In this paper we deal with the $\text{HgSe}_{1-x}\text{Te}_x$ system. The crystals were grown by the Bridgman method. The binary constituents are zero-gap materials with a zinc-blende structure. The similarity of the crystalline structures enables us to grow the mixed crystals with arbitrary chosen compositions within the range of $0 \leq x \leq 1$. The dependence of the energy gap on the crystal composition was determined for some of the similar systems (e.g. $\text{ZnSe}_{1-x}\text{Te}_x$, $\text{CdSe}_{1-x}\text{Te}_x$), but apart from that the scheme of the changes in their band structures is far from being complete. In particular, this concerns the $\text{HgSe}_{1-x}\text{Te}_x$ crystals.

Thus, the room temperature reflectivity spectra of $\text{HgSe}_{1-x}\text{Te}_x$ ($x = 0, 0.4, 0.5, 1.0$) crystals were measured in the visible and ultraviolet range from 1.5 to 12 eV. The results are shown in Fig. 1.

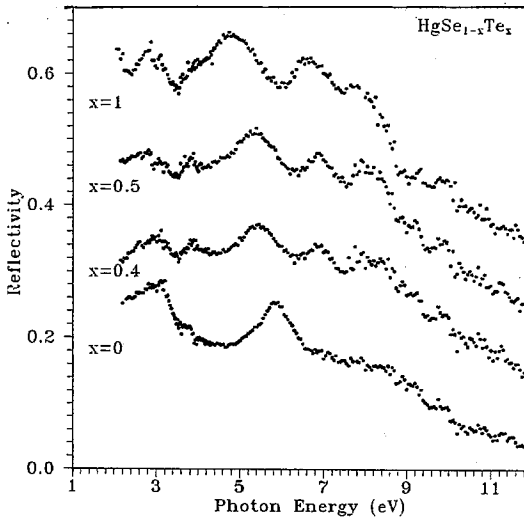


Fig. 1. The reflectivity spectra of $\text{HgSe}_{1-x}\text{Te}_x$ at 300 K.

The structure of the reflectivity data is interpreted in terms of the electronic band structure of the binary material. The structures of HgTe and HgSe are well known and the assignment of the optical spectra features to interband transitions have already been determined [3]. This enables us to interpret the maxima revealed in the spectra of the mixed crystals, too. The assignment is summarized in the Table.

An analysis of the reflectivity coefficient spectra (Fig. 1) and the $\text{Im } \epsilon(h\nu)$ curves (Fig. 2) shows that the maxima characteristic of the binary HgA^{IV}

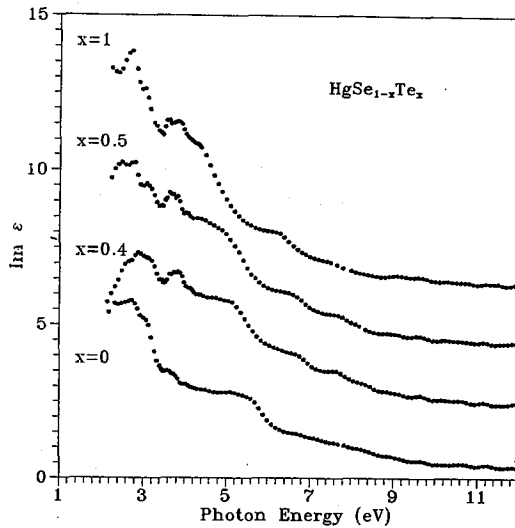


Fig. 2. The $\text{Im } \epsilon(h\nu)$ curves obtained by means of a Kramers-Kronig analysis of the reflectivity spectra.

TABLE
The energies and interband transitions associated with prominent optical structure in $\text{HgSe}_{1-x}\text{Te}_x$.

Energy [eV] of the peaks for the following crystal compositions					
$x = 0.0$	$x = 0.4$	$x = 0.5$	$x = 1.0$		Assignment
3.0	3.0	2.9	2.9	E_1	$L_{4,5} - L_6$
3.8	3.9	3.9	3.9		near Δ
5.8	5.5	5.4	4.8	E_2	at X, K, Δ
	6.9	6.9	6.6		volume (4-6)
plateau					(0.6, 0.5, 0.3)
7-8.6	8.0	8.0	7.8	E'_1	at L, W
					volume (3-7)
					(0.6, 0.3, 0.1)

compounds can be revealed in the mixed crystals spectra, but their position depends on the crystal composition. There is no duplication of the spectral features in spite of the different energy position of the maxima for HgSe and HgTe. Some broadening of the spectra can also be observed, however it is markedly weaker than that caused by the presence of transition metal ions in semimagnetic semiconductors. It is rather comparable with the very weak broadening of the optical spectra of the mixed crystals with two cations of the second column of the periodic table.

These observations correspond well to the conclusions of Onodera and Toyozawa [1]. The energy difference of the valence bands of HgSe and HgTe (according to the energy positions of p -states of Se and Te) is small with respect to the width of the bands. Thus, we can expect that the band structure and (as a consequence) the structure of the optical spectra are similar to a result of an interpolation of HgSe and HgTe spectra rather than to a summation weighted by the crystal composition. Moreover, this suggests that the virtual crystal approximation could be successfully used to describe basic optical properties of $\text{HgSe}_{1-x}\text{Te}_x$.

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