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INFLUENCE OF Yb ON VALENCE BAND DENSITY OF STATES OF CdYbTe AND PbYbTe — A RESONANT PHOTOEMISSION STUDY*

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Photoemission measurements using synchrotron radiation were performed on PbYbTe (bulk crystal) and CdYbTe (MBE thin film). The resonant enhancement of the photoemission was applied for investigation of the contribution of Yb 4f electrons to the valence band. The set of the energy distribution curves was collected for energies in the region close to the 4d-4fFano transition. The Yb $4f^{14}$ were observed at the binding energies close to the edge of the valence band while the $4f^{13}$ states were revealed deep in the valence band.

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1. Introduction

In this paper we will compare the contribution of 4f electrons to the valence bands of CdYbTe and PbYbTe — two tellurides with different crystallographic structures as well as band structures. PbTe is a narrow-gap semiconductor with a direct gap at the *L* point, it crystallizes in the rock-salt structure, whereas CdTe is a wide-gap semiconductor with a direct energy gap at the Γ point and with the zinc-blende structure.

Since the resonant behaviour of the photoemission from the 4f shell occurs only for the Yb³⁺($4f^{13}$) state [1], we were able to discriminate between the features connected with Yb³⁺($4f^{13}$) and Yb²⁺($4f^{14}$). Although the resonant photoemission for Yb²⁺($4f^{14}$) does not occur, some changes in the intensity of the structure ascribed to this charge state are clearly observed. These changes are in agreement with the results of a theoretical calculation of the Yb 4f photoemission cross-section [2].

2. Experimental conditions

In the resonant photoemission experiments we used synchrotron radiation of the photon energies ranging from 30 to 190 eV for PbYbTe and 90 to 200 eV for CdYbTe.

For PbYbTe the experiments were performed on the unique line Flipper II of DORIS II Storage Ring in HASYLAB, DESY in Hamburg, Germany. The spectra were normalised to the monochromator output and corrected for variations in photons flux.

The spectra of CdYbTe were acquired at the LURE synchrotron radiation laboratory in Orsay, France. The storage ring SUPER-ACO was the source of synchrotron radiation.

The bulk PbYbTe samples were obtained by a modified Bridgman method in the Institute of Physics, Polish Academy of Sciences in Warsaw. They contained 4% of Yb. Clean surfaces for the photoemission experiments were prepared *in situ* by scraping the sample with a diamond file or by cleavage.

The thin film (1.5 μ m thick) of CdYbTe was grown by MBE at the growth temperature of 320°C on the CdTe (100) buffer layer crystallized on a GaAs (100) substrate (2° off-oriented towards [011]). The surface of the sample was cleaned by the argon ion bombardment and annealing.

3. Experimental results and discussion

Figure 1 presents the energy distribution curves (EDCs) spectra obtained for PbYbTe (a) and CdYbTe (b). The binding energy is measured with respect to the valence band maximum. The A and C spectra were collected for energies close to the resonance energy, while B and D spectra were recorded for the energies near to the energy of antiresonance. In order to show the influence of Yb ions on the valence band structure, in both pictures the differences between the spectra were shown (the lowest spectrum in each figure). The dominant contribution of ytterbium to PbYbTe valence band was revealed as structures at -9.4 eV and -13.6 eV. The change in intensity of these peaks as a function of photon energy

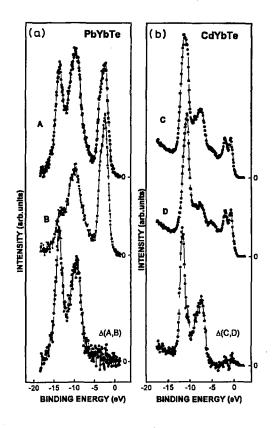


Fig. 1. The sets of EDC spectra of PbYbTe (a) and CdYbTe crystals (b). The photon energies are: A = 184.2; B = 181.2; C = 177.5; D = 174.5 eV. The lowest spectrum in each figure shows the differences between the A and B or C and D spectra, respectively. The zero of the energy scale corresponds to the edge of the valence band.

was clearly observed. In the A spectrum these two peaks become higher than in the B spectrum. Taking into account that the resonance occurs only for partly occupied states, we can connect these structures with presence of $4f^{13}$ state.

The shape of this structure corresponds quite well to the final-state multiplet splitting calculated by Gerken [3]. The energy separation between the peaks is also similar to that obtained for Yb_2O_3 [4].

The very similar effect was observed for the curves obtained for the CdYbTe sample. The contribution of Yb $4f^{13}$ was found at -7.7 eV and -12 eV. The distance between these peaks is very similar to that obtained for PbYbTe.

The set of the energy distribution curves for CdYbTe and CdTe presented in Fig. 2 allows us to compare structure of the valence bands. The spectra for CdYbTe were recorded for the same photon energies but for surfaces prepared by different procedures. The F spectrum was measured after 30 minutes of Ar⁺ ion sputtering and 35 minutes of heating at 275°C. The E spectrum was recorded after extra sputtering lasting 20 minutes. In the E curve two maxima appear

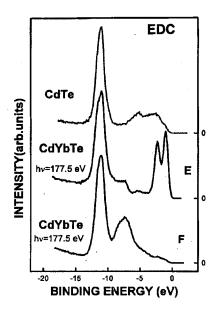


Fig. 2. The EDC spectra for CdTe and CdYbTe. The photon energy has been written above the spectra. The F spectrum was measured after 30 minutes of Ar^+ ion sputtering and 35 minutes of heating at 275°C. The E spectrum was recorded after extra sputtering lasting 20 minutes.

at -1.1 eV and -2.3 eV. The separation between them corresponds well to the spin-orbit splitting of two Yb $4f^{14}$ components $(4f_{7/2}, 4f_{5/2})$ [5]. Thus, the surface preparation procedure can change the charge state of ytterbium ions. More detailed studies show that strength of this feature depends on surface conditions.

4. Conclusion

The results of the resonant photoemission studies show that ytterbium introduced as an impurity to PbTe and CdTe crystals occurs as Yb^{3+} ions in both materials. This state was observed as two peaks separated by about 4 eV.

After surface treatments of the CdYbTe crystal two maxima characteristic of spin-orbit split components of Yb^{2+} state appear.

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