

Proc. XIX International School of Semiconducting Compounds, Jaszowiec 1990

SURFACE PHOTOVOLTAGE SPECTROSCOPY OF $\text{Cd}_{0.97}\text{Fe}_{0.03}\text{Se}$ AND $\text{Cd}_{0.97}\text{Fe}_{0.03}\text{Te}$ CRYSTALS*

A. SAREM†, B.A. ORLOWSKI

Institute of Physics, Polish Academy of Sciences, Al.Lotników 32/46, 02-668 Warszawa,
Poland

AND S. KUŹMIŃSKI

Institute of Physics, Technical University of Wrocław, Wybrzeże Wyspiańskiego 27,
50-370 Wrocław, Poland

(Received August 8, 1990)

The surface electronic structure of the $\text{Cd}_{1-x}\text{Fe}_x\text{Se}$ and $\text{Cd}_{1-x}\text{Fe}_x\text{Te}$ crystals with $x = 0$ and $x = 0.03$ has been studied by Surface Photovoltage Spectroscopy (SPS). The change of surface photovoltage was observed due to photo-excitation of the electrons from the deep donor state Fe 3d to conduction band edge. This gave possibility to determine energy position of the Fe 3d state at 0.64 and 0.15 eV over the top of the valence band for CdSe and CdTe, respectively.

PACS numbers: 71.25.Tn

The $\text{Cd}_{1-x}\text{Fe}_x\text{Se}$ and $\text{Cd}_{1-x}\text{Fe}_x\text{Te}$ crystals belong to the group of semimagnetic semiconductors (SMSC). The SMSC crystals are obtained by substitution of cation in II-VI compounds by transition metals like Mn, Fe and recently Co. The electronic structure of those crystals is affected by the hybridization of *s-p* electrons with the localized 3d electrons and by created disorder — structural, chemical and magnetic [1-5]. The Fe impurity in the wide-gap semiconductors CdSe and CdTe acts as deep donor state, located in the forbidden energy gap [6-8]. The influence of the Fe 3d state on the density of states distribution in the valence band of these materials was a subject of several papers [2, 4, 5, 7, 8].

In this paper, we report the measurements of spectral dependence of contact potential difference — CPD (Surface Photovoltage Spectroscopy) of $\text{Cd}_{0.97}\text{Fe}_{0.03}\text{Se}$

*This work was supported in part by CPBP 01.04 and 01.08.

†permanent address: Department of Physics, Faculty of Science, Tishreen University, Latakia, Syria.

and $\text{Cd}_{0.97}\text{Fe}_{0.03}\text{Te}$ crystals surface. The experimental data are used to determine the energy position of the iron level relatively to the valence band edge.

Figure 1 (a and b) presents the spectral dependence of the CPD for $\text{Cd}_{1-x}\text{Fe}_x\text{Se}$ and $\text{Cd}_{1-x}\text{Fe}_x\text{Te}$ with $x = 0$ and $x = 0.03$. Insets to this figure present energetic scheme for $\text{Cd}_{0.97}\text{Fe}_{0.03}\text{Se}$ and $\text{Cd}_{0.97}\text{Fe}_{0.03}\text{Te}$ crystals. For all investigated samples two main edges were seen in the spectra. For $x = 0.03$ the edges corresponding to the energy of 1.16 and 1.36 eV were observed (see Fig. 1a and 1b), while this was not observed for CdSe and CdTe crystals without iron. Illumination of the surface causes an optical excitation of electrons from the Fe 3d band. This leads to the creation of the charge at the surface region, and consequently, to an increase of the CPD signal causing the appearance of these edges. Therefore, the values of the two photovoltaic thresholds 1.16 and 1.36 eV well correspond to the energies of the optical excitation of the electrons from Fe 3d to the conduction band edge. The position of the Fe level was found at 0.64 and 0.15 eV (see insets in Fig. 1a and 1b) over the top of the valence band edge for CdSe and CdTe respectively. This shows that the introduction of Fe 3d into crystal leads to an appearance of additional states in the band gap region, above the top of the valence band. Also it was found that the position of the $\text{Fe}^{+2} 3d^6$ state is independent of temperature and iron concentration. This effect agrees with the results reported previously [3, 6, 8].

The energy edge at 1.61 eV (see Fig. 1a) slightly visible above the edge obtained for $\text{Cd}_{0.97}\text{Fe}_{0.03}\text{Se}$ corresponds to transitions from the surface CdSe states to the conduction band edge.

The threshold at 0.96 eV, $\text{Cd}_{0.97}\text{Fe}_{0.03}\text{Te}$, corresponds to the transitions of the electrons from surface states of CdTe (see Fig. 1b). This transition is clearly visible for different temperatures, and was observed in pure CdTe spectrum reported in many papers [9, 10].

By illumination of the samples with white light the voltage barrier at the surface V_s was determined for different temperatures. It was found that due to the poor vacuum in the measuring chamber (10^{-5} Pa) and the adsorption of the oxygen at low temperatures, the adsorbed atoms interact with the electrons in states close to the surface, leading to the decrease of the voltage barrier at the surface.

Finally, the investigation of the surface structure of $\text{Cd}_{1-x}\text{Fe}_x\text{Se}$ and $\text{Cd}_{1-x}\text{Fe}_x\text{Te}$ leads to the following conclusions:

1. The position of the $\text{Fe}^{+2} 3d^6$ state is independent of temperature and iron concentration (up to $x = 0.03$ for $\text{Cd}_{1-x}\text{Fe}_x\text{Te}$ and $x = 0.03$ for $\text{Cd}_{1-x}\text{Fe}_x\text{Se}$).
2. The SPS spectra consist of main edges corresponding to optical excitation from the Fe 3d band, and a position of the band was found at 0.64 and 0.15 eV over the top of the valence band edge for CdSe and CdTe respectively.
3. The introduction of the Fe atoms into the crystal leads to an appearance of additional states in the band gap region, above the edge of the valence band.

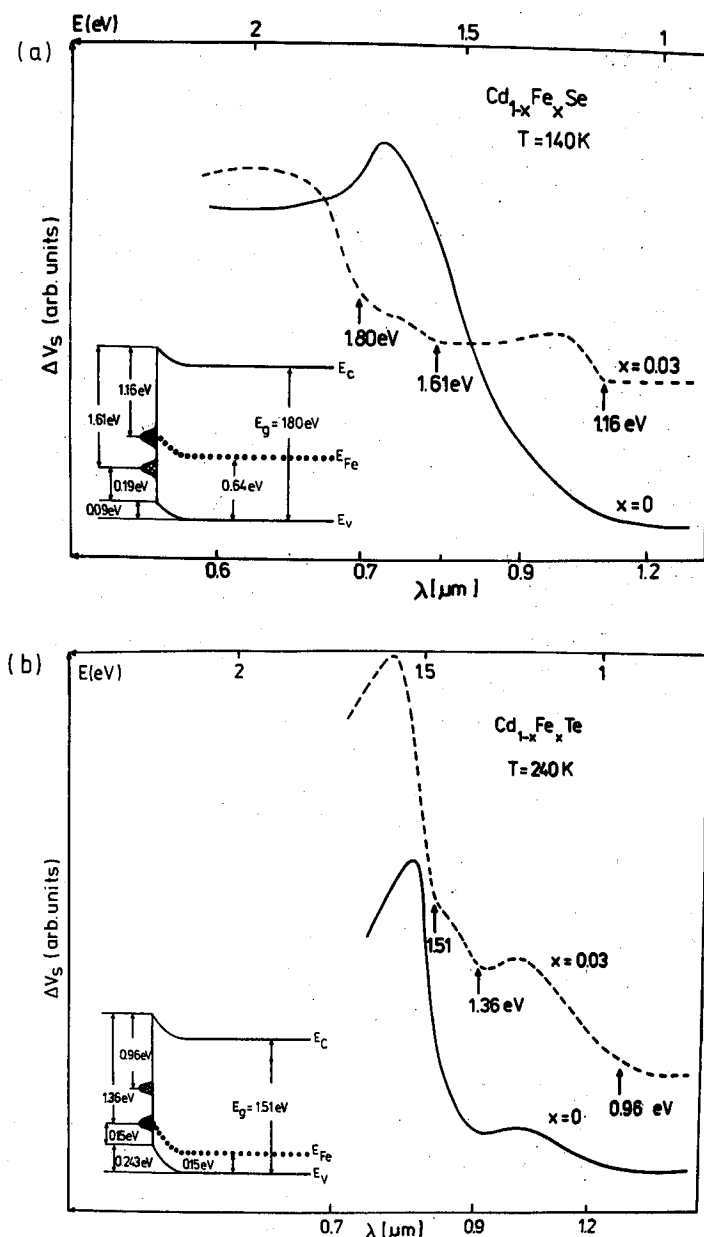


Fig. 1. Spectral dependence of Contact Potential Difference : a) measured at the temperature 140 K for CdSe and $\text{Cd}_{0.97}\text{Fe}_{0.03}\text{Se}$ crystals and b) measured at the temperature 240 K for CdTe and $\text{Cd}_{0.97}\text{Fe}_{0.03}\text{Te}$ crystals. Surfaces of these samples were mechanically and chemically polished. The spectral dependence of the contact potential difference between the sample and the reference gold coated vibrating string electrode was measured with the Kelvin method (SPS). As a monochromatic light source the SPM-2 monochromator ($0.6 \leq \lambda \leq 1.5 \mu\text{m}$) with G-60 prism was used.

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