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PHOTOELECTRON SPECTROSCOPY IN STUDIES OF THE BAND STRUCTURE OF IV-VI SPINTRONIC MATERIALS

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Among several groups of chemical compounds exploited in the quest for materials suitable for spintronic application diluted magnetic semiconductors have particular set of properties. Although the ferromagnetic transition temperatures observed in such systems are still markedly below the room temperature, their electronic characteristics, similar to those of the host semiconducting system, and the compatibility with electronic device technology are obvious advantages. $Ge_{1-x}Mn_xTe$, a member of the IV-VI semiconductor family, attracts considerable interest due to the relatively high Curie temperature-it can be as high as 190 K [1]. This inspired extensive investigations of this solid solution and development of technological methods in view of increase of the ferromagnetic transition temperature. The magnetic properties of systems based on IV-VI semiconductors depend on the interaction between the magnetic ions mediated by charge carriers of the host semiconductor. The interaction is successfully described by the RKKY model. As a consequence, knowledge of electronic band structure of such materials is important for understanding their transport, optical, and also magnetic properties. We present a set of experimental results, acquired by photoelectron spectroscopy, showing the electronic structure of $Ge_{1-x}Mn_xTe$ in comparison with GeTe and results of ab initio pseudopotential calculations.

Photoelectron spectroscopy with use of synchrotron radiation is the experimental technique particularly suitable for studying electronic structure of semiconductors. We used an angle-resolved photoemission spectroscopy to investigate samples of GeTe and $Ge_{0.85}Mn_{0.15}Te$. The epilayers of these two systems were grown by MBE on BaF_2 substrates. The rhombohedral structure of the layers was determined by X-ray diffraction measurements. The clean and ordered sample surface was prepared for photoemission experiments by cycles of Ar^+ ion sputtering and annealing under UHV conditions. The surface quality was assessed by LEED. In the experiments performed with use of the photoelectron spectrometer at the beamline 41 in the MAXlab synchrotron radiation laboratory of Lund University (Sweden) we acquired the data revealing the valence band structure of GeTe and $Ge_{0.85}Mn_{0.15}Te$ along the Γ-L (in the normal-emission mode) and T-W-L (under off-normal emission conditions) (Fig. 1) directions in the Brillouin zone. The Mn related features could be identified by comparison of the results acquired for these two systems.

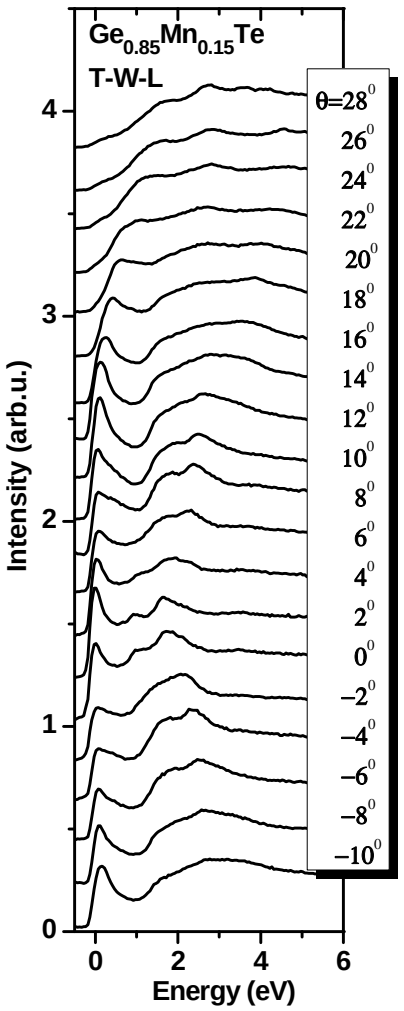

Figure 1. The set of photoemission spectra taken for $Ge_{0.85}Mn_{0.15}Te$ and corresponding to the scan of the valence band along the T-W-L direction in the Brillouin zone. The spectrum taken for normal emission corresponds to the T point.

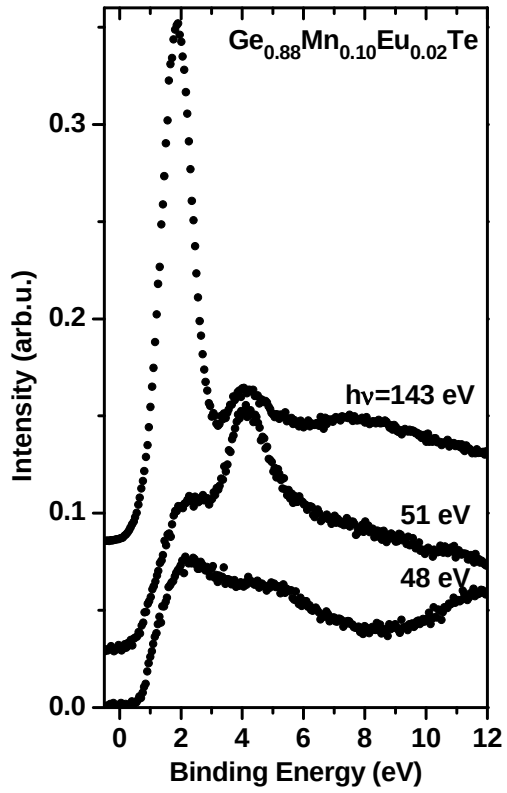

Figure 2. The resonant photoemission spectra of $Ge_{0.88}Mn_{0.10}Eu_{0.02}Te$ taken for photon energies of 48, 51, and 143 eV.

The experimental data were also compared with the results of fully relativistic LDA pseudopotential calculations of the band structure of GeTe. The primitive cell of GeTe was characterized by experimental values [2] of three parameters: lattice constant, a_0, angle between neighbouring bonds, α, and the position of Ge atom on the diagonal of the cell, τ. Best agreement between experimental $E(k)$ diagrams and the results of calculation was obtained for the highest valence band. Additional calculations for several different sets of the parameters a_0, α, τ showed that the shape of highest valence band depended mainly on α. The agreement between thecalculations and the experiment was achieved for $\alpha <$ 90°. This proved that rhombohedral distortion of the layers corresponded to that expected for bulk GeTe. Thus, we concluded that the 1μm GeTe/BaF_2 layer was relaxed and could be treated as a bulk crystal.

The electronic structure of $Ge_{1-x-y}Mn_xEu_yTe$ was investigated by resonant photoemission spectroscopy (Fig. 2). This system is supposed to exhibit particular magnetic properties, with increased T_C, due to co-doping with Mn and Eu [3]. The spectra were taken for an epitaxial layer (grown on BaF_2 by MBE) of $Ge_{0.88}Mn_{0.10}Eu_{0.02}Te$ for the photon energies close to the intra-ion transitions Mn 3*p*-3*d* and Eu 4*d*-4*f*. Thus, the Fano resonances and enhancement of emission from Mn 3*d* and Eu 4*f* states were observed at photon energies 51 and 143 eV, respectively. A comparison of the spectra taken at the resonances and anti- resonances allowed us to reveal the Mn 3*d* and Eu 4*f* contributions to the emission from the valence band of the system. The advantages of photoelectron spectroscopy with application of synchrotron radiation are emphasized with an example of investigation of $Ge_{1-x-y}Mn_xEu_yTe$ - a system containing both a transition metal and a rare earth element.

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