$Cd_{1-x}Fe_xTe$ TERNARY CRYSTAL FORMATION STUDIED BY RESONANT PHOTOEMISSION

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A resonant photoemission was used to study the ternary crystal formation, when small amount of Fe atoms was deposited (in one monolayer range of thickness) on the clean CdTe(100) surface. The constant initial state spectra taken near the Fe $3p-3d$ transition after Fe deposition and then again after heating process show the existence of two Fano-like resonance. The differences of the energy distribution curves taken for both resonance and antiresonance, respectively, allow us to distinguish two kind of Fe $3d$ contributions to the valence band: one derived from the metallic Fe islands on the surface and the second — derived from the Fe atoms built into the $Cd_{1-x}Fe_xTe$ crystal.

PACS numbers: 79.60.–i, 68.35.Fx

In the very first stages of the metal atoms deposition on clean semiconductor surface the Shottky barrier can be formed if the deposited atoms create the islands of metal and then monolayer of it. If the deposited atoms react with the substrate the doping of semiconductor surface region appears and the ternary crystal layer can be created on the surface. The paper presents results of a unique experimental method very sensitive on surface electronic properties to distinguish between these two possible positions in a case of Fe atoms deposited on CdTe clean surface. Recently many of investigations are sacrificed to study the process of formation of semimagnetic semiconductors (SMSC) in the region near the surface, when transition metal (TM) atoms were deposited on the clean II–VI or III–V semiconductor's surface [1–3].

The experimental method of study of TM $3d$ contribution into the valence band density of states (DOS) is a resonant photoemission spectroscopy in which TM $3d$ electrons excited selectively and locally according to the equation

$$TM3p^6 3d^N \rightarrow TM3p^5 3d^{N+1} \rightarrow TM3p^6 3d^{N-1} + e.$$
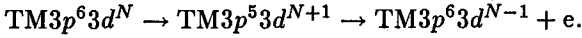
This additional contribution to the measured spectrum of photoemitted electrons appears only for resonant energy $h\nu$ corresponding to Fe $3p$–$3d$ transition. The effect is described as a Fano-type resonance [4]. The differences in energy distribution curves (EDC) taken for resonant and antiresonant energy show the contribution of TM $3d$ electrons to the SMSC valence band density of states.

The experiment was carried out in a very clean ultra high vacuum conditions using the synchrotron radiation obtained from the beam line Flipper II of the Storage Ring DORIS II in HASYLAB in Hamburg, Germany. The synchrotron radiation was used in the photon energy range of 50–130 eV.
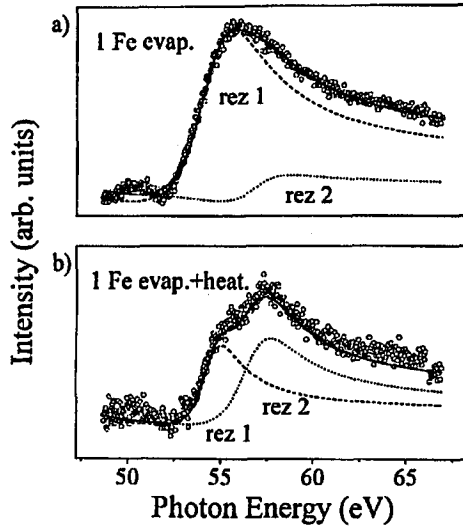

Fig. 1. Constant initial states spectra of CdTe(100) crystal measured for initial state 4.6 eV below the Fermi level: (a) after evaporation of Fe, (b) after heating of obtained CdTe(100)/Fe crystal.

The experiment consisted of two technological processes: (i) Fe atoms in the monolayer range were deposited on the clean CdTe(100) surface; (ii) after the Fe deposition the heating of the sample led to the diffusion of Fe atoms into the CdTe crystal and the layer of the semimagnetic semiconductor $Cd_{1-x}Fe_x Te$ was created in the region near the surface. In order to investigate the energy of Fe $3p$–$3d$ resonance the constant initial state (CIS) spectrum was taken after evaporation and heating processes. Figure 1 presents the CIS curves and result of the deconvolution of the spectra on two Fano-like curves. The CIS curve measured after the Fe evaporation process (Fig. 1a) shows the existence of mainly one Fano

resonance with the maximum at an energy 55.5 eV. After heating the shape of CIS curve changes (Fig. 1b), one can observe that the CIS curve consists of two contributions: apart from that with the maximum at an energy 55.5 eV appears the second one with the maximum at an energy 57.2 eV. Therefore we believe that the resonance at 55.5 eV is derived from the Fe atoms adsorbed on the crystal surface (Fe islands) whereas the resonance at 57.2 eV is derived from the Fe atoms built into the $Cd_{1-x}Fe_xTe$ crystal. Our conclusion is consistent with the results obtained by Lad and Henrich [5], where it was found out that the Fano resonance energy is lower for metallic Fe than for Fe^{2+} and Fe^{3+} ions.
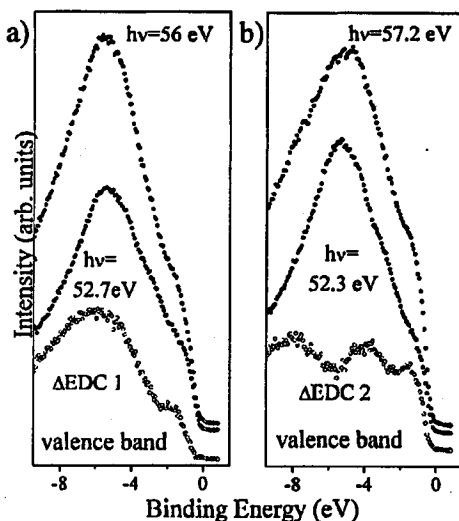

Fig. 2. Energy distribution curve of CdTe(100)/Fe crystal (solid circles) taken on resonance and antiresonance energy of both resonances (56 eV and 57.2 eV). The difference spectrum (ΔEDC) is a measure of the Fe 3d partial density of states (open circles): (a) resonance EDC ($h\nu = 56$ eV), antiresonance EDC ($h\nu = 52.7$ eV) and ΔEDC of the first resonance (Fe evaporated on the surface), (b) resonance EDC ($h\nu = 57.2$ eV), antiresonance EDC ($h\nu = 52.3$ eV) and ΔEDC of the second resonance (Fe from $Cd_{1-x}Fe_xTe$ layer).

Figures 2a and b present the photoemission measurements taken after heating of CdTe/Fe crystal. In Fig. 2a the EDC curves taken near resonant (56 eV) and antiresonant (52.7 eV) energies of the first resonance are shown. The result of the subtraction of the resonant and antiresonant EDCs (ΔEDC) is plotted below. We expect that ΔEDC in Fig. 2a (ΔEDC 1) represents Fe 3d-derived partial valence band spectrum of iron atoms absorbed on the surface. In the curve ΔEDC 1 two structures appear: the narrow one at 1.7 eV and the wide at 6 eV below the Fermi level. The former is a structure typical of Fe 3d states, whereas the latter is a satellite usually observed in transition metals like Fe, Co, Ni [6]. A resonant and antiresonant EDC of the second resonance (57.2 eV) are presented in Fig. 2b.

The curve ΔEDC 2 shows the Fe $3d$-derived partial valence band spectrum of $Cd_{1-x}Fe_xTe$ created in the region near the crystal surface. It reveals three contributions with maximum located at: 7.9, 4.0 and 1.75 eV below the Fermi level. The positions of the maxima are consistent with those obtained from the preliminary theoretical calculations obtained by means of tight binding method, which predicts that Fe $3d$-states in $Cd_{1-x}Fe_xTe$ crystal should give a triple contribution to the valence band density of states: near the edge of the valence band (narrow structure derived from $e_{g\downarrow}$ states), a wide structure with maximum about 2.0 eV below the first one (derived from $t_{2g\uparrow}$ states) and the third one, which is situated between 4.2 and 6.2 eV below the valence band edge (derived from $t_{2g\uparrow}$ and $e_{g\downarrow}$ states). The results are also consistent with these obtained for $Cd_{1-x}Fe_xSe$ bulk crystals [7, 8].

In the first stages of Fe atoms deposition on CdTe (100) surface the two states of Fe atoms were distinguished. One is ascribed to the metallic Fe islands and the other to the Fe atoms built into $Cd_{1-x}Fe_xTe$ alloy.

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