Cd$_{1-x}$Fe$_x$Se/Fe INTERFACE FORMATION
OBSERVED BY MEANS OF PHOTOEMISSION SPECTROSCOPY*

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We present a new outlook at the study of metal-semiconductor interface formation. A resonant photoemission spectroscopy tuned to the Fe 3p-3d transition (56 eV) was used to investigate the changes after sequential deposition of Fe atoms on freshly cleaved Cd$_{0.86}$Fe$_{0.14}$Se crystal surface. In the first stages (0.6-4 ML) of Fe deposition the contribution of Fe 3d electrons to the valence band grows up markedly indicating the increase in Fe content in the Cd$_{0.86}$Fe$_{0.14}$Se crystal surface region. When the amount of Fe exceed 40 ML the resonant photoemission spectra became similar to the Fe metal with some contribution of the ternary crystal substrate.

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1. Introduction

The dominant sources of interesting magneto-optical properties of diluted magnetic semiconductors (DMS) are: (1) the random distribution of transition metal (TM) atoms substituting for cation sites, and (2) the exchange interaction of the TM 3d electronic states with the electronic states of the parent semiconductor. A very important effect is the hybridization between the TM 3d states and the parent semiconductor $sp$ valence band states [1, 2]. Resonant photoemission spectroscopy with the use of synchrotron radiation is a powerful tool for distinguishing the partial contribution of TM 3d electrons to the valence band [3].

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The Fano-like resonance is the result of interference between the direct photoemission process of TM 3d electrons and the discrete TM 3p-3d transition followed by a super-Coster-Kronig decay. In the resonant photoemission process the photon energy is tuned to the absorption edge region of the TM 3p-3d transition in order to excite TM ions selectively and locally.

We used Fano-like resonance to follow the changes in the Fe 3d electron contributions to the valence band of the Cd$_{0.86}$Fe$_{0.14}$Se crystal during sequential deposition of a small number of Fe atoms. We were able to distinguish the differences in the energy distribution curve (EDC) spectra caused by both bulk and surface Fe derived states and to investigate the process of Cd$_{0.86}$Fe$_{0.14}$Se/Fe metal-semiconductor interface formation.

2. Experimental conditions and results

The experiment was carried out in a spectrometer attached to the line SA71 (TGM 2.5 m) of the storage ring SUPER-ACO in LURE, Orsay, France. The synchrotron radiation was used in the photon energy range of 20–130 eV with the resolution kept between 150 and 300 meV. The Cd$_{0.86}$Fe$_{0.14}$Se samples were grown by the modified Bridgman method at the Institute of Physics, Polish Academy of Sciences, Warsaw, Poland. The clean surface of the sample was obtained by cleavage using a knife-anvil technique under UHV conditions ($p = 1 \times 10^{-10}$ torr). The Fe flux was obtained from a Joule-heated pure Fe wire. The amount of Fe atoms deposited on the surface was measured by means of the quartz resonator.

Energy distribution curves (EDCs) were acquired at the photon energy range including the intra-atomic Fe 3p-3d transition (56 eV). Figure 1 presents the set of EDCs taken for different amounts (0–4 ML) of Fe atoms deposited on the Cd$_{0.86}$Fe$_{0.14}$Se crystal. The EDCs were obtained for Fe 3p-3d resonant energy equal to 56 eV. In the EDC acquired for the clean crystal surface one can observe the valence band of ternary compound extending to the 6 eV below the valence band edge. At 0.5 eV a small maximum is visible. This structure, as well as that observed at about 2.25 and 3.8 eV below the valence band edge, are believed to be fingerprints of the Fe 3d electrons [4]. The maximum at 0.5 eV arises due to the contribution of the Fe 3d spin down electron whereas the maxima at 2.25 and 3.8 eV correspond to the contribution of five Fe 3d spin up electrons [4]. The positions of these maxima are consistent with those obtained by Denecke et al. [5] for Cd$_{1-x}$Fe$_x$Se crystals. Even a deposition of small amounts of iron atoms changes considerably the spectra shown in Fig. 1. At every point of energy the intensity of EDC consists of the photoemission from the bulk Cd$_{1-x}$Fe$_x$Se crystal and from the Fe atoms deposited on the crystal surface. However, the uniform increase of 3d$^2\uparrow$, 3d$^3\uparrow$ and 3d$^4\downarrow$ peaks, connected with Fe bulk states, may be treated as a sign of the creation of the Cd$_{1-x}$Fe$_x$Se ternary crystal with a higher $x$ value. Such an interpretation is supported by the previous investigations of the Cd$_{1-x}$Fe$_x$Se/Fe Schottky barrier formation [6]. The 3d$^2\uparrow$, 3d$^3\uparrow$ and 3d$^4\downarrow$ rise proportionally only for 0.6 ML of the iron deposition. For the next steps of deposition the photoemission at 0.5 eV below the valence band edge rises more clearly, because it is enriched by photoemission from Fe islands. These islands start to grow at the surface of the crystal. For the next steps of Fe deposition we can observe at the edge of EDC
For the deposition of 40 ML of Fe, the edge of EDC corresponds well to the Fe crystal spectra [7]. Figure 2 presents the set of EDCs spectra containing Cd 4d band taken for Fe resonant energy equal to 56 eV. The spectra were acquired from 0 to 4 ML of deposited Fe atoms. The Cd 4d level obtained for the clean Cd$_{0.86}$Fe$_{0.14}$Se crystal surface does not show the spin–orbit splitting typically observed in Cd metal and CdSe crystal compound [8]. The reason seems to be in the presence of the local structure created by the Fe atoms located at the site of the Cd atom.

After the first step of Fe deposition the position of Cd 4d maximum increases by about 0.3 eV. This effect can be explained as a result of band bending, which accompanies a Schottky barrier formation process. After the next steps of iron deposition the binding energy of Cd 4d level is still located at -10.8 eV, though its shape changes a little as a consequence of the change of the Cd next nearest neighbours from Cd to Fe.

3. Summary

A resonant photoemission technique was applied for the investigation of the Cd$_{0.86}$Fe$_{0.14}$Se/Fe interface formation. In the first stages of Fe deposition the con-
tribution of Fe 3d electrons to the valence band well corresponds to the increase in $x$ in the ternary crystal. When the amount of Fe exceeds 40 ML, the photoemission spectra become similar to those of the Fe metal, with a small contribution of the ternary crystal substrate. A Schottky barrier formation manifests itself in 0.3 eV shift of Cd 4d level towards a higher binding energy.

References