Electronic Structure of Condensed Matter

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Electronic structure of the core/shell-formed diluted magnetic semiconductor Fe-doped ZnO nano-particles

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Introduction

There is growing interest in diluted magnetic semiconductors (DMS), where magnetic ions are doped into the semiconductors, due to the possibility to utilize both charge and spin degrees of freedom in the same material, which allows us to design a new generation of spin electronic devices with enhanced functionalities. Theoretical studies on the basis of Zener's *p*-*d* exchange model have shown that transition-metal-doped wide-gap semiconductors such as ZnO are promising candidates for room temperature ferromagnetic DMS [1] and a number of experiments on the ZnO-based DMS have revealed ferromagnetic properties at room temperature [2].

Recently, Karmakar *et al.* [3] have reported room temperature ferromagnetism in Fe-doped ZnO nanoparticles and proposed that the ferromagnetism is originated from exchange interaction in the core/shell structure of the underlying nano-particle system. Based on magnetic measurements, they proposed that some randomized surface spins are superimposed on the coredominated ferromagnetism. It is indispensable to clarify the core/shell electronic structures of the system. In order to discuss the electronic states in the shell-layer region of the nano-particles, we have performed resonant photoemission spectroscopy (RPES) on the $Zn_{0.9}Fe_{0.1}O$ nano-particles.

Reslts and Discussions

Figure 1 (a) shows the valence-band photoemission spectra of the Zn_{0.9}Fe_{0.1}O nano-particles as a fuction of photon energies in the Fe 3p-3d core excitation region and Fig. 1 (c) shows the magnified view of the valencemaximum region. For the valence-band band photoemission spectra, all binding energies $(E_{\rm B})$ are referenced to the Fermi level $E_{\rm F}$. Figure 1 (b) shows the Fe 3p-3d absorption spectrum near the Fe 3p-3d core excitation threshold of the Zn_{0.9}Fe_{0.1}O nano-particles measured by the total electron yield method. In Fig. 1 (b), one can see that a peak appears at 58 eV, representing the Fe 3p-3d absorption. For α -Fe₂O₃ (Fe³⁺), the peak is found at 58 eV [4]. For FeO (Fe²⁺), on- and off-resonance energies are reported to be 57 and 53 eV, respectively [5].



Fig. 1. Valence-band photoemission spectra of $Zn_{0.9}Fe_{0.1}O$ nano-particles. (a) A series of photoemission spectra taken with photon energies in the Fe 3p-3d core excitation region. Difference curves at the bottom represent the Fe 3d PDOS. (b) Fe3p-3d absorption spectrum recorded in the total electron yield mode. (c) Magnified view of the valence-band maximum.

From this comparison, we conclude that 3p-3d absorption due to Fe³⁺ ions is mainly observed in this sample. In Fig. 1 (c), one can see that in going from hv=53 eV to 58 eV, the tale of the spectrum at $E_B \simeq 3-4$ eV grows in intensity. By subtracting the off-resonance spectrum (hv=53 eV) from the Fe³⁺ (hv=58 eV) and Fe²⁺ (hv=57 eV) onresonant ones, we have obtained the Fe 3d PDOS for Fe³⁺ and Fe²⁺ as shown in the bottom panels of Fig. 1 (a). The 58-53 eV difference spectrum which yields the Fe³⁺ 3d PDOS reveals a feature at $E_B=3-4$ eV. On the other hand, the 57-53 eV difference spectrum which yields the Fe²⁺ 3d PDOS reveals no clear feature. Taking these results into account, it is concluded that the Fe³⁺ ions are dominant on the surface region of the Zn_{0.9}Fe_{0.1}O nanoparticles.

References

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