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Resonant photoemission study of $Ga_{1-x}Mn_xN$

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Introduction

Diluted magnetic semiconductors (DMS) have attracted much attention because of the combination of magnetic and semiconducting properties and hence high potential for new device applications in the field of spintronics. In recent years, DMS based on III-V compounds have been extensively studied since doping high concentrations of transition-metal ions was realized by molecular beam epitaxy (MBE) [1]. In a recent theoretical study, on the other hand, ferromagnetism with very high T_c has been predicted to occur in wide-band gap DMS such as *p*-type $Ga_{1-x}Mn_xN$ [2]. However, the occurrence of the ferromagnetism is still controversial. Also, the electronic structure of $Ga_{1-x}Mn_xN$ has not been studied experimentally so far.

Experimental

Resonance photoemission measurements (RPES and XPS) were performed at BL-18A. The RPES and XPS experiments were made in an ultrahigh vacuum of 5×10^{-10} Torr at room temperature. For sample surface cleaning, we made Ar-ion sputtering at 1.0 kV and annealing up to 500 K. The cleanliness of the surface was checked by low-energy electron diffraction (LEED) and X-ray photoemission spectroscopy (XPS).

The Mn 3*p*-to-3*d* core absorption occurs at photon energies above 50 eV. Interference between the normal photoemission and the Mn 3*p*-to-3*d* transition followed by a 3*p*-3*d*-3*d* super-Coster-Kronig decay generates a resonance enhancement of the Mn 3*d*-derived photoemission. From such measurements, we could obtain a resonantly enhanced Mn 3*d* PDOS in the valence- band spectra.

The valence-band spectra taken at various photon energies are shown in Fig. 1(a). Here, the intensities have been normalized by the photon flux. All binding energies are referenced to the Fermi energy (E_F). One can see that in going from $h\nu$ = 46.5 to 50.5 eV, the peak at the binding energies (E_B) of 2.5 and 5.5 eV grow in intensity. By subtracting the anti-resonant ($h\nu$ = 48.5 eV) spectrum from the on-resonant ($h\nu$ = 50.5 eV) one, we obtained the Mn 3*d* paratial density of states (PDOS) as shown in the bottom panel of Fig. 1(a).

We have analyzed the spectrum of the Mn 3*d* PDOS thus obtained using the configuration-interaction (CI) cluster model. The calculation treats several electronic configurations with different *d*-electron numbers both in the initial and final states of photoemission. We considered the MnN_4 cluster as a model to analyze the Mn 3*d* PDOS.

The best fit result is shown in Fig. 1(b) with parameter values Δ = 5.3±1.0 eV, U = 5.0±1.0 eV and ($pd\sigma$) = -1.5±0.1 eV. The values of Δ and U are larger than the other DMS compounds. The absolute value of ($pd\sigma$) is also larger than the other DMS (e.g. Δ, U and ($pd\sigma$) are 1.5, 3.5, -1.0 eV for $Ga_{1-x}Mn_xAs$ respectively [3]). These parameters are close to the value of the II-VI oxide DMS $Zn_{1-x}Mn_xO$ for which Δ, U and ($pd\sigma$) are 6.5, 5.2, -1.6 eV respectively [4].

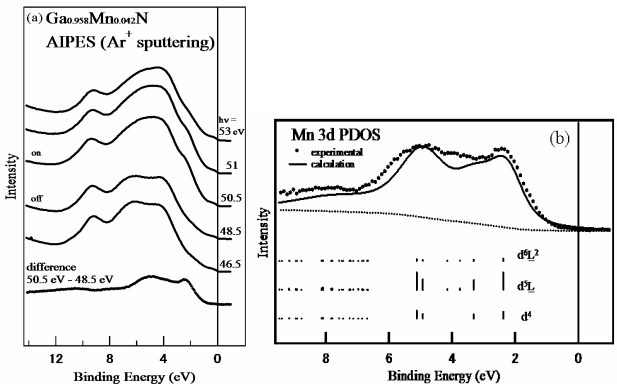

FIG.1 (a) A series of photoemission spectra of $Ga_{1-x}Mn_xN$ for various photon energies near the Mn 3*p*-to-3*d* core excitation threshold (a). The difference between the on-resonance ($h\nu$ = 50.5 eV) and the off-resonance ($h\nu$ = 48.5 eV) spectra, which is a measure of the Mn 3*d* PDOS, is shown at the bottom. (b) Cluster-model analysis of the Mn 3d partial density of states (PDOS) of $Ga_{1-x}Mn_xN$ assuming the Mn^{2+} valence state. The calculated spectrum is shown by a solid curve. The vertical bars are unbroadend spectra. The background is shown by a dotted curve.

References

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