Resonant photoemission study of Ga$_{1-x}$Mn$_x$N

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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$_x$N [2]. However, the occurrence of the ferromagnetism is still controversial. Also, the electronic structure of Ga$_{1-x}$Mn$_x$N 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 $5 \times 10^{-10}$ 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 3p-to-3d core absorption occurs at photon energies above 50 eV. Interference between the normal photoemission and the Mn 3p-to-3d transition followed by a 3p-3d-3d super-Coster-Kronig decay generates a resonance enhancement of the Mn 3d-derived photoemission. From such measurements, we could obtain a resonantly enhanced Mn 3d 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 (EF). 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 3d partial density of states (PDOS) as shown in the bottom panel of Fig. 1(a).

We have analyzed the spectrum of the Mn 3d 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 Mn$_N$ cluster as a model to analyze the Mn 3d PDOS.

The best fit result is shown in Fig. 1(b) with parameter values $\Delta = 5.3 \pm 1.0$ eV, $U = 5.0 \pm 1.0$ eV and $(p|d\sigma) = -1.5 \pm 0.1$ eV. The values of $\Delta$ and $U$ are larger than the other DMS compounds. The absolute value of $(p|d\sigma)$ is also larger than the other DMS (e.g., $\Delta$, $U$, and $(p|d\sigma)$ are 1.5, 3.5, -1.0 eV for Ga$_{1-x}$Mn$_x$As respectively [3]). These parameters are close to the value of the II-VI oxide DMS Zn$_{1-x}$Mn$_x$O for which $\Delta$, $U$ and $(p|d\sigma)$ are 6.5, 5.2, -1.6 eV respectively [4].

**References**


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