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Local-Orbital Ordering on Cr^{3+} Ions Doped in GaN

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Introduction

Some of the diluted magnetic semiconductors show ferromagnetic behavior at room temperature [1,2]. GaN carrying a small amount of Cr^{+3} ions is one of them [3], and several unique features, especially concentration quenching of the ferromagnetic nature, are found. However, the mechanism of its ferromagnetism is still not clear.

Here, we will examine the local coordinate alignment at Cr site to try to elucidate the origin of ferromagnetism of GaCrN through X-ray linear dichroism (XLD) observations and through the analysis of X-ray absorption fine structure (XAFS). The observed results are briefly discussed in terms of electron – phonon interaction.

Experimental

X-ray absorption spectra in Cr *K*-edge energy region detected in fluorescence mode were measured at a bending magnet beam-line BL9A. The spectra were detected with a solid-state detector (Ge:Li) with 19 elements because the specimens studied here are dilute (~1 atomic % or less) and so thin, (corresponding to a few mono layers when converted into CrN). The synchrotron radiation from a bending magnet port is horizontally polarized. The specimen orientation to the photon polarization was changed to observe the XLD.

Results

Through the analysis of the XAFS spectra around the Cr *K*-edge in GaCrN, we confirm at first if the doped Cr^{+3} ions occupy the substitutional sites or not. With a concentration of Cr^{+3} ions higher than about 3% under our deposition conditions described in experimental [4], the segregation of CrN is found. Specimens with a rather low concentration studied here do not have any segregation but the Cr^{+3} ions are completely substituted to Ga ions.

Figure 1 shows the XLD spectra around the pre-peak and *K*-edge absorption shoulder for cubic-GaCrN. We can see double peaks named Aα and Aβ, a weak hump named B, and shoulder C in the order of increasing photon energy. Shoulder C in cubic GaCrN is buried under the pre-edge of the *K*-absorption edge. Tentatively, we assign these structures as follows: A from the core 1s state to the 3d state, B to 4s, and C to 4p of Cr^{+3} ions, respectively. The transition to 3d state splits into $\boldsymbol{e}$ symmetry state and $\boldsymbol{t_2}$ symmetry state in the cubic ligand field. For convenience, we name the growth direction c-axis in cubic GaN, and the principal axis (c-axis) in hexagonal GaN is along the growth direction. The dichoism is observed at the Aα peak of both structures. Other parts in the spectrum show no explicit polarization effect in the cubic phase.

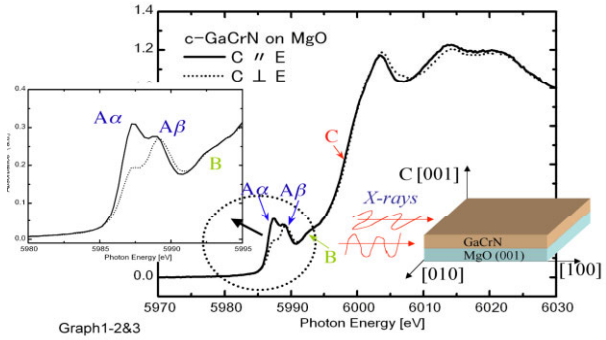

Fig.1 X-ray absorption spectrum at pre-peak and edge shoulder of K-edge of Cr in a direction different from that of electric field of photons.

Discussion

GaCrN shows unique ferromagnetic behavior as indicated below, which cannot be explained by any theoretical model proposed previously. Concentration quenching, which is frequently observed in luminescent centers, is recognized in GaCrN. This fact means that such atomic configurations or alignments as Ga-N-*Cr-N-Cr-N-* and/or Ga-N-*Cr-N-Ga-N-Cr-*N- hinder the occurrence of the ferromagnetism.

From the XAFS analysis, we have found splitting of the first peak corresponding to the Cr-N alignment into two peaks, suggesting the shift of Cr^{+3} ion along the <111> axis. The observation of XLD strongly supports this phenomenon. The shift of Cr^{+3} ions may be caused by pseudo Jahn- Teller effect (local-orbital ordering) [5]. The applied magnetic field may rigidly order them along itself when the potential barrier among the four equivalent valleys is very shallow, or in other words, stands in fine balance. Thus, the applied magnetic field forces to order the magnetic moment. This model could explain the unique behavior.

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References

1. Teraguchi *et* al., *Solid State Comm.* **122** (2002) 65.
2. M. Hashimoto, *et* al., *Solid State Comm.* **122** (2002) 37.
3. J. J. Kim, *et* al., *Phys. Rev.* B**70** (2004) 161315(R).
4. At the lower (e.g. 600K) substrate temperature, the Cr ions in the higher concentration can substitutionaly be incorporated into GaN matrix.
5. submitted to *Phys. Rev. Lett.*.

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