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Fluorescence EXAFS analysis of local structures around Fe atoms in heavily doped GaN by low-temperature molecular beam epitaxy

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Introduction

In the present work, highly Fe-doped GaN films grown by ECR microwave-assisted low-temperature molecular beam epitaxy (LT-MBE) were investigated by fluorescence x-ray absorption fine structure (XAFS) measurements using synchrotron radiation (SR) in order to elucidate the relationship between the local structures around the Fe atoms and the magnetic properties. We have successfully fabricated highly Fe-doped GaN films with Fe concentrations as high as 10^{19} cm^{-3} showing ferromagnetic behavior under 100K [1]. However, the origin of the ferromagnetic transition in highly Fe-doped GaN is not yet fully understood. It is expected that the Fe atoms in doped GaN play an essential role in the ferromagnetic transition. The fluorescence EXAFS measurement is a powerful technique for investigating local structures around a specific element and was suitable for evaluating the geometric and electronic structures around Fe atoms in the present study.

Experimental

The highly Fe-doped GaN samples were grown on sapphire(0001) substrates by ECR microwave-assisted LT-MBE. The EXAFS measurements were performed at the beam line BL12C at KEK-PF.

Results and discussion

Figure 1 represents the Fourier transformed Fe K-edge and Ga K-edge $k^3\chi(k)$ extended X-ray absorption fine structure (EXAFS) spectra for heavily Fe-doped GaN samples. Despite the high level of Fe doping in the GaN (N[Fe] = 3×10^{19} cm^{-3}), several peaks (marked by arrows) are clearly observable even at a longer radial distance, indicating that the local structures around Fe atoms were well-ordered with respect to short-range ordering. In addition, a great similarity between the spectra at the Fe and Ga K-edges can be observed. The similarity of spectra between the Fe and Ga K-edges can be identified based on theoretically calculated spectra for the substitutional Fe atom on the Ga-site in the cubic GaN lattice. We therefore conclude that Fe atoms in heavily doped GaN substitute the Ga-site in the GaN lattice.

In order to analyze the details of the measured spectra, curve-fitting for the EXAFS spectra was carried out with theoretically calculated spectra using FEFF6 [2]. For all the samples, species of neighboring atoms and coordination numbers show good agreement with those of the GaN film. Although we also carried out curve-fitting for models of various iron nitrides such as FeN and Fe_4N, reliable parameters for such models were not obtained. We therefore conclude that the majority of Fe atoms in all the samples substitute the Ga-site in GaN.

References

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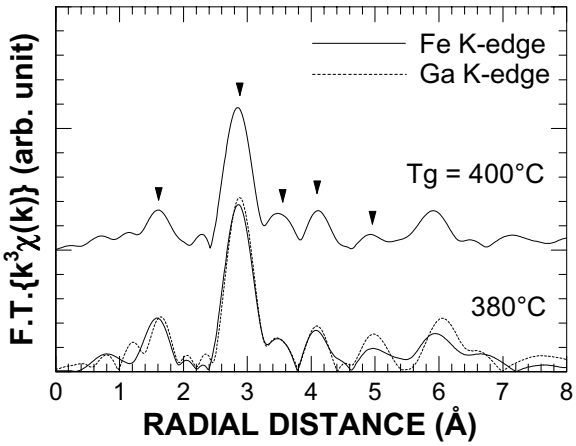

Fig. 1: Fourier transform of Fe K-edge (solid lines) and Ga K-edge (dotted lines) EXAFS oscillation functions $k^3\chi(k)$ spectra for highly Fe-doped GaN. The Fourier transformation was performed in the k range of 4.0-13.0 $Å^{-1}$.

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