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Fluorescence EXAFS analysis of half-metallic ferromagnet "zinc-blende CrAs" grown on GaAs by molecular beam epitaxy

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Introduction

The thermal-equilibrium Cr-As compounds possess MnP- and Cu_2Sb-type crystal structure. Very recently, it is predicted by full-potential linearized augmented-plane wave (FLAPW) method that the band structure of zb-CrAs in the ferromagnetic state becomes half-metallic [1]. We have successfully fabricated thin zb-CrAs film epitaxially grown on GaAs by MBE, which shows ferromagnetic behavior above room temperature [2]. However, the geometrical structure of the CrAs thin film is not yet clear, because it is difficult to evaluate the geometrical structure of the CrAs film as thin as 3nm grown on GaAs by conventional method such as an x-ray diffraction measurement. The EXAFS measurement is a powerful technique to investigate the geometric structure around a specific element in ultra thin film in this work.

In this work, geometric structures for half-metallic ferromagnet "zinc-blende CrAs", which showed ferromagnetic behavior beyond room temperature, were investigated using fluorescence EXAFS measurement.

Experimental

The zb-CrAs thin film was grown on a GaAs(001) substrate by MBE. The CrAs thin film was grown at about 200 °C. Thickness of the CrAs film is 2nm. The CrAs thin film was capped by a 10 nm GaAs layer to prevent the oxidation. The EXAFS measurements were performed at the beam line BL12C at KEK-PF.

Results and discussion

Figure 1 represents the Fourier transform of Cr K-edge EXAFS oscillation function $k^3\chi(k)$ spectra for CrAs film MnP-type CrAs powder. In the radial distance range of 1.7 – 2.7 Å, main peak due to the first coordination shell around the Cr atoms were observed clearly. Position of the main peak in the CrAs thin film shifts toward the shorter radial distance side than that in the MnP-type CrAs, indicating that local structure between the CrAs thin film and the MnP-type CrAs are different.

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 [3]. From the curve-fitting result, It is found that in the CrAs thin film central Cr atoms are merely coordinated by As atoms, and the coordination number was 4. We also conducted the curve fitting for models coexisting Cr-As and Cr-Cr bonds such as the MnP- and Cu_2Sb-type structures, but reliable parameters for such models were not obtained. Thus, it is considered that CrAs thin film forms zb-type structure. The Cr-As bond length is 2.49Å, which is close to that which was estimated from lattice constant (5.82 Å) of ferromagnetic zb-CrAs calculated by full-potential linearized augmented-plane wave (FLAPW) method [4]. The XAFS analyses show that the theoretically-predicted zb-CrAs can be fabricated on GaAs(001) substrate by

References

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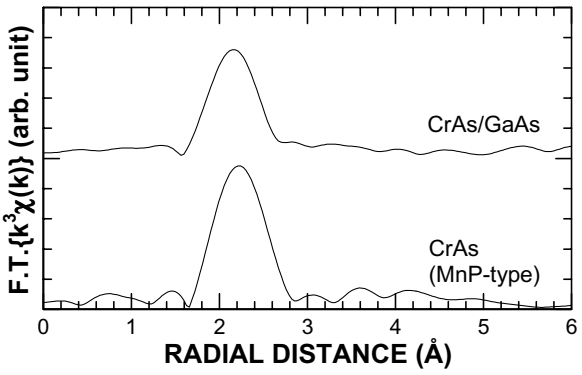

Fig. 1: Fourier transform of Cr K-edge EXAFS oscillation function $k^3\chi(k)$ spectra for CrAs film MnP-type CrAs powder. The Fourier transiformation was performed in the k range of 3.0 – 12.0 $Å^{-1}$.

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