X-ray fluorescence holography of distorted rhombohedral GeTe

Naohisa HAPPO1, Yuki TAKEHARA1, Shinya SENBA2, Wen HU1, Shinya HOSOKAWA1, and Kouichi HAYASHI1
1Hiroshima City University, Hiroshima 731-3194, Japan
2Ube National College of Technology, Ube 755-8555, Japan
3SPring-8/JAEA, Sayo, Hyogo 679-5148, Japan
4Hiroshima Institute of Technology, Hiroshima 731-5193, Japan
5Tohoku University, Sendai 980-8577, Japan

Introduction
The magnetic ion doped IV-VI diluted magnetic semiconductor Ge1–xMnxTe is expected as a spintronics material, because it shows a ferromagnetic order below 140 K at x = 0.51 [1]. It is believed that the ferromagnetism largely relates to the arrangements of the Mn ions and the cation vacancies. Due to such vacancies, the crystal would distort, which may also influence the ferromagnetism of this material. X-ray fluorescence holography (XFH) is a powerful tool to investigate such atomic distortions by obtaining three-dimensional (3D) atomic images.

Recently, we performed the XFH experiments on the Ge0.6Mn0.4Te [2, 3] in order to investigate the local structures around the Ge and Mn atoms. The results suggest that the Ge positions are not stable at the exact positions of fcc cation sublattice, and reveal the fluctuations of Ge positions and/or the existence of cation vacancies. It seems that the fluctuation is due to the pure GeTe, which is a distorted rhombohedral structure with the short and long bonds, as seem in Fig.1. Thus, the pure GeTe is an important standard material for the study on Ge1–xMnxTe. In this study, the Ge Kα XFH measurement was carried out on the GeTe thin film.

Experimental procedure
The GeTe single crystal thin film sample was grown on a BaF2 (111) substrates by a molecular beam epitaxy technique. The Ge Kα XFH experiment was performed at BL6C and BL15B of the PF/KEK. Incident X-rays were irradiated onto the (111) sample surface. The hologram data were collected in inverse mode at room temperature at different incident X-ray energies of 11.2–14.2 keV in 0.5 keV steps. The Ge Kα (9.885 keV) fluorescent X-rays were detected by an avalanche photodiode via a cylindrical graphite energy-analyzer. From the hologram patterns obtained with 7 different incident X-ray energies, an atomic configuration image was reconstructed using Barton’s algorithm [4].

Results and discussion
The obtained 3D atomic image from the Ge Kα XFH of GeTe was depicted in Fig. 2. The central Ge atom locates at the center of the (111) plane. The images of the first-neighboring Te anions were clearly seen around the central Ge atom. The distance between the (111) plane on the first-neighboring Te and that on the central Ge is 1.45 Å. The value is shorter than the distance 1.60 Å of the Ge0.6Mn0.4Te, as seen in Fig.3. Detailed analysis of the present XFH data are now in progress.

References
* happo@hiroshima-cu.ac.jp

Fig. 1 Crystal structure of GeTe.
Fig. 2 3D atomic image from Ge Kα XFH of GeTe.
Fig. 3 3D atomic image of Ge0.6Mn0.4Te.