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Three-dimensional atomic images of GeSbTe phase-change materials

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1 Introduction

GeTe is one of the laser-induced crystalline-amorphous phase change materials. Although its phase change speed is much slower than e.g., $Ge_2Sb_2Te_5$ (GST) used as the raw material for the commercially available DVD-RAM disks, GeTe is considered as a useful material for investigating the fundamental mechanism of the phase change.

X-ray fluorescence holography (XFH) is a powerful method that provides three-dimensional (3D) atomic images around a specified element which has a large spacial range of up to a few nm [1]. We utilized this technique to investigate the local structure around the Ge atoms in GST single-crystal thin film [2], and the results seem to support the umbrella flip model for the phase change mechanism proposed by Kolobov *et al.* [3]

In order to precisely investigate the mechanism of the phase change, we have measured Ge $K\alpha$ XFH on GeTe single-crystal thin film at room temperature. In this paper, we report the spacial fluctuations of each neighboring atom in the GeTe single crystal.

2 Experiment

GeTe single-crystal thin film sample was grown on a BaF_2 (111) substrate using a molecular beam epitaxy technique. The XFH experiments were performed at BL6C and BL15B of the PF-KEK. Incident x-rays were irradiated onto the (111) surface of the sample. The hologram patterns were collected in inverse mode at room temperature at seven different incident x-ray energies of 11.2–14.2 keV in steps of 0.5 keV. The Ge $K\alpha$ (9.885 keV) fluorescent x-rays were collected by an avalanche photodiode via a cylindrical graphite energy-analyzer [1]. Using Barton's algorithm [4], the three-dimensional (3D) atomic images were reconstructed by imposing holograms at different incident x-ray energies.

3 Results and Discussion

Crystal structure of GeTe is shown in Fig. 1, and the obtained 3D atomic image of GeTe around the central Ge atoms is given in Fig. 2. The images of the nearest-neighboring Te atoms are clearly seen in the obtained 3D image. The Te images are, however, not a normal spherical shape, but ellipsoid with angular directions. The second neighboring Ge atoms are hardly visible. Thus it can be concluded that the distortion of lattice is mainly occur at the central Ge sites, and the fluctuation of the Ge sites has the angular directions of the $GeTe_3$ pyramid. This conclusion may support the umbrella flip motion of the Ge atoms in the dynamical sense.

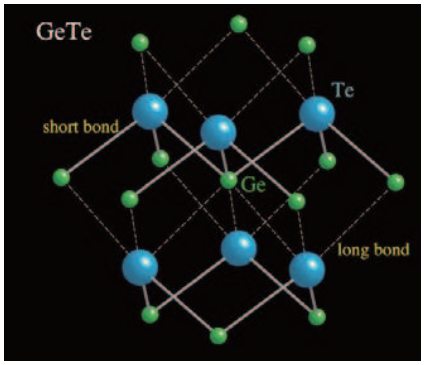

Fig. 1: Crystal structure of GeTe.

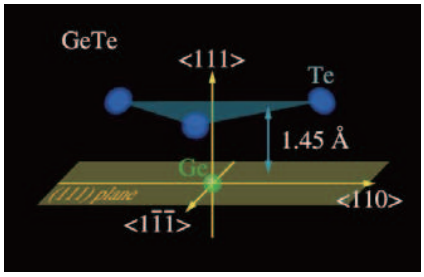

Fig. 2: 3D atomic image obtained from Ge $K\alpha$ XFH of GeTe.

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References

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