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Middle range local structure analysis of semiconductor $ZnSnAs_2$ thin film by X-ray fluorescence holography

Akiko SUZUKI[1], Keitaro YAMAGAMI[1], Naohisa HAPPO[*2], Kouichi HAYASHI[3], Shinya HOSOKAWA[4], Wen HU[5], Motohiro SUZUKI[6], Naotaka UCHITOMI[1]
[1]Department of Electrical Engineering, Nagaoka University of techonology, Niigata 940-2188, Japan
[2]Graduate School of Information Sciences, Hiroshima City University, Hiroshima 731-3194, Japan
[3]Tohoku University, Sendai 980-8577, Japan
[4] Kumamoto University, Kumamoto 860-8555, Japan
[5]Quantum Beam Science Directorate, JAEA, Sayo, Hyogo 679-5148, Japan
[6]SPring-8/JASRI, Sayo, Hyogo 679-5198, Japan

1 Introduction

The continued research into semiconductors exhibiting room-temperature ferromagnetic for spintronics application has led to the exploration of transition metal oxides and ternary compounds for preparing diluted magnetic semiconductors. The $ZnSnAs_2$:Mn thin film, which is grown by a molecular beam epitaxy, is a II-IV-V_2 compound semiconductor with the ferromagnetism at T_c = 333 K [1]. The film is lattice-matched to the InP substrate ,which is the III-V compound semiconductor. Thus, the $ZnSnAs_2$:Mn is one of the promising candidates for the next generation spintronics materials. Erwin and Žutić reported that the Mn atoms can substitute for both Zn and Sn atoms in the cation sites [2]. Figure 1 shows two possible crystal structural models of $ZnSnAs_2$. However, we have not known which of them is dominant in the film sample. In order to understand the true crystal structure of the $ZnSnAs_2$, we performed the X-ray fluorescence holography experiment, which is a powerful tool for the local structure analysis [3].

2 Experiment

We observed the holograms at synchrotron radiation facilities of Photon Factory and SPring-8. The obtained 3D atomic images around Mn and Zn within 3 nm in a radius. (This large analytical range is called the "middle range").

3 Results and discussion

Figure 2 shows the reconstructed atomic images around Zn in $ZnSnAs_2$. Moreover, we calculated holograms for the chalcopyrite model structure, and reconstructed the atomic images, as shown in Fig. 3. The cation plane atomic image at z = 0.0 Å of the theoretical holograms shows the chalcopyrite site pattern in Fig. 3 (a). However, such a pattern cannot be seen in the experimental atomic image in Fig. 2(a). Thus, it suggests that the sphalerite structure is dominat in the film sample. Moreover, in Fig.2 (b), the As images at z = 1.5 Å are rarely observed compared with the cation plane, revealing strong distortions at the As plane. The As plane plays an role of a buffer layer for relaxing the cation layer where Zn and Sn are randomly substituted for the cation sites.

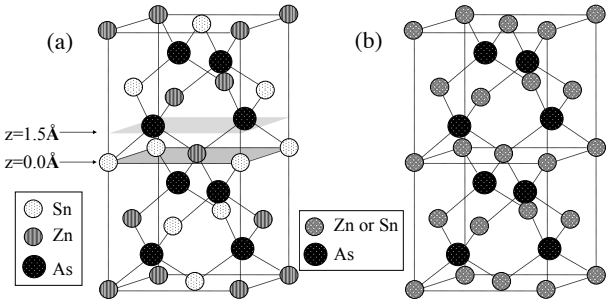

Fig. 1 Structural models of $ZnSnAs_2$.(a) Chalcopyrite model. (b) Sphalerite model.

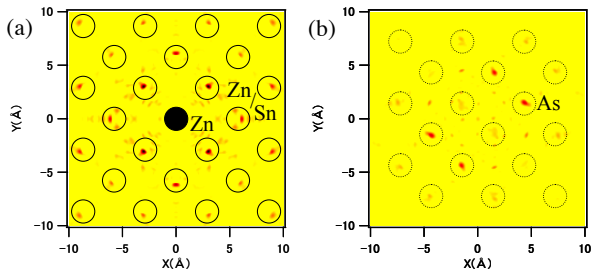

Fig. 2 Experimental atomic images around Zn in $ZnSnAs_2$. (a) z = 0.0Å. (b) z = 1.5 Å.

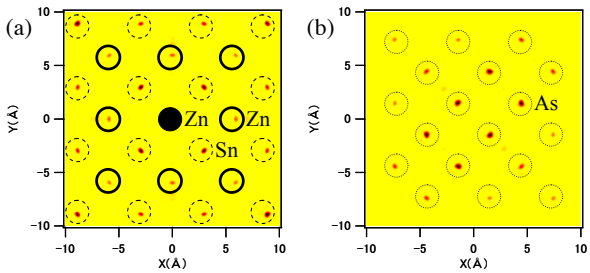

Fig. 3 Theoretical atomic images around Zn in $ZnSnAs_2$. (a) z = 0.0Å. (b) z = 1.5 Å.

References

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* happo@hiroshima-cu.ac.jp