X-ray diffraction study of filled skutterudite SrFe₄As₁₂ under pressure

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1 Introduction

SrFe₄As₁₂ is a new skutterudite compound, which was synthesized as a reference compound of EuFe₄As₁₂. EuFe₄As₁₂ shows ferromagnetic transition at Curie temperature $(T_c) \sim 152$ K [1]. The purpose of this study is to clarify the mechanism of this high $T_{\rm C}$. Because the $T_{\rm C}$ rapidly increases with pressure, applying pressure is one of the key to understand the mechanism of the high $T_{\rm C}$. In order to understand systematically, we are investigating pressure dependence of physical properties and that of lattice properties as well as the relationship between the two. In order to distinguish what is attributed to Eu, we need to investigate the reference compounds. SrFe₄As₁₂ is an appropriate one. Sr of SrFe₄As₁₂ is divalent while Eu of EuFe₄As₁₂ is considered to be almost divalent. In addition, the lattice parameters of both compounds with 8.33 Å are almost the same. In our previous study, we investigated the pressure dependence of lattice parameter of EuFe₄As₁₂. We investigate the lattice parameter of SrFe₄As₁₂ under pressure in this study.

2 Experiment

SrFe₄As₁₂ was synthesized with high-pressure hightemperature method. The sample was grinded in a mortar into a fine powder. The uniform grain was obtained by using sedimentation method. The pressure was applied by diamond anvil pressure cell (DAC). The sample was exposed by the beam with a size of Φ 100 μ m and with a wave length $\lambda \sim 0.62$ Å. Imaging plate was used as a detector. In order to eliminate remaining spot of the Debye-ring, the stage of the DAC was oscillated during synchrotron x-ray exposure. The mixture of methanol and ethanol with 4:1 ratio was used as pressure transmission. The pressure was evaluated by ruby fluorescence method.

3 <u>Results and Discussion</u>

Figure 1 shows the X-ray diffraction pattern of SrFe₄As₁₂ at 0.92 GPa. The peaks that have strong intensity can be indexed by the pattern of skutterudite structure. Some peaks, which does not due to skutterudite structure, are observed mainly at $2 \theta \sim 13^{\circ}$ and 18° . This means some secondary phase still exists. Because this secondary phase was not observed before grinding in fine, these peaks are attributed to the oxidation among grinding procedure or following sedimentation procedure.

Because this is powder X-ray diffraction X-ray with fine powder, secondary phase affect little to pressure dependence of lattice parameter. Figure 2 shows the pressure dependence of lattice parameter of $SrFe_4As_{12}$. The lattice parameter monotonically decreases with pressure, which indicates no structural change or modification up to 10 GPa in this experimental accuracy. From Birch-Murnaghan equation of state, we evaluated the bulk modulus B_0 . B_0 of SrFe₄As₁₂ was calculated as 96 GPa, which can be comparable to EuFe₄As₁₂ with $B_0 \sim 97$ GPa.



Fig. 1: X-ray diffraction pattern of $SrFe_4As_{12}$ at 0.92 GPa (red) and that of calculated (black).



Fig. 2: Pressure dependence of lattice parameter of $SrFe_4As_{12}$.

References

[1] C. Sekine et al., J. Phys. Soc. Jpn. 78, 093707 (2009).

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