8A, 8B/2009S2-008

High Pressure X-ray Crystal Structure Analysis of $FeSe_{0.5}Te_{0.5}$

Kazumasa HORIGANE*[1], Kazuhiko IKEUCHI[2], Akiko NAKAO[2], Hironori NAKAO[2], Haruhiro Hiraka[3], and Youichi MURAKAMI[2]
[1]Tohoku Univ., WPI-AIMR, Aoba-ku, Sendai, Miyagi 980-8577, Japan
[2]KEK-PF, Tsukuba, Ibaraki 305-0801, Japan
[3]Tohoku Univ., IMR, Aoba-ku, Sendai, Miyagi 980-8577, Japan

Introduction

The iron-based superconductors have been intensively studied with respect to the interplay between crystal structure and superconductivity. Recently, Lee at al. have reported that T_c becomes maximum when $FeAs_4$-lattices form a regular tetrahedron (As-Fe-As angle α=109.47°) [1]. On the other hand, theoretical calculation shows that T_c increased with increasing the pnictogen height [2]. These results indicated a relationship between crystal structure and superconductivity. In this study, high pressure x-ray diffraction experiments were carried out for $FeSe_{0.5}Te_{0.5}$ to get direct evidence between crystal structure and superconductivity.

Experimental and Results

Experimental

Polycrystalline sample $FeSe_{0.5}Te_{0.5}$ (T_c~14K) was prepared. All the x-ray diffraction data were collected with an imaging plate system by Si-doble-crystal monochromatized synchrotron radiation (λ=0.6888Å) at the beam line BL-8A,8B of photon Factory(PF), KEK. A diamond-anvil cell (DAC) with 0.8mm tip diamonds was used for the diffraction measurements under high pressure.

Results

Figure 1 shows the diffraction pattern of $FeSe_{0.5}Te_{0.5}$ at various pressure up to 9.58GPa. The all diffraction patterns can be indexed a tetragonal crystal structure with space group *P4/nmm*. The final reliable factors were in the range from 2.85% to 4.08%.

In order to compare the relationship between T_c and crystal structure, we were performed on high pressure x-ray crystal structure analysis. Figure 2 shows the pressure dependence of angle α and calcogen height in $FeSe_{0.5}Te_{0.5}$. In the T_c-α relation, it is expected that T_c will increase with increasing α. However, our result can not be explained this relation. On the other hand calcogen height tends to increase with increasing pressure. This result suggests that anion height is the important factor for the superconductivity

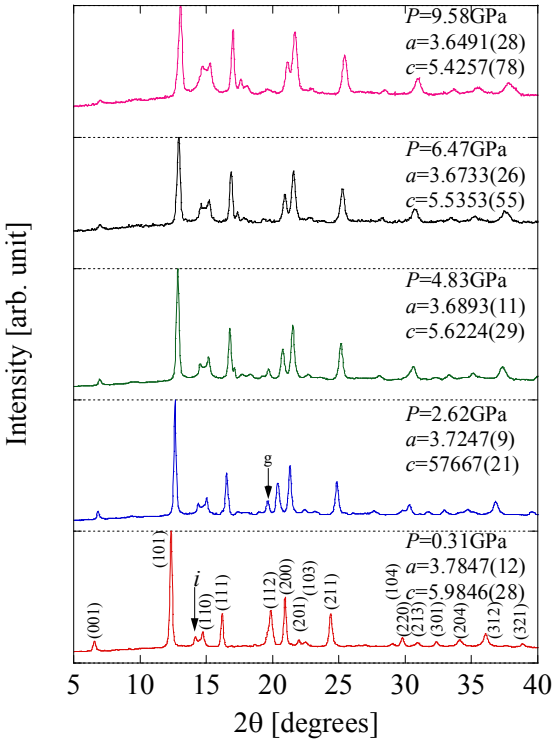

Fig.1: Pressure dependence of diffraction pattern of $FeSe_{0.5}Te_{0.5}$ at RT. *i* and *g* correspond to impurity phase (Fe_7Se_8) and gasket.

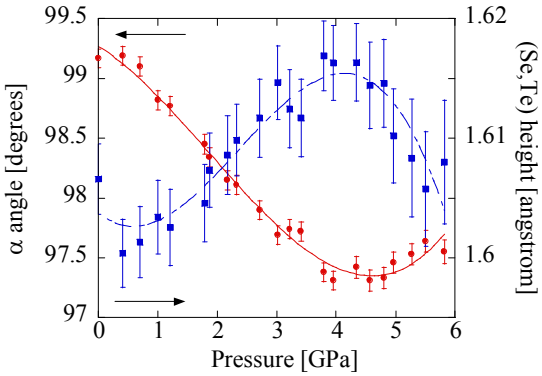

Fig.2: Pressure dependence of angle α and (Se,Te) height in $FeSe_{0.5}Te_{0.5}$

References

[1] C. H. Lee at al., J. Phys. Soc. Jpn. **77**, 083704 (2008)
[2] K. Kuroki et al., Phys. Rev. B **79**, 224511 (2009)

* khorigane@imr.tohoku.ac.jp