Materials Science

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Crystal structure of $La_2O_2Fe_2OSe_2$ under high pressure

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Introduction

Transition metal pnictides and chalcogenides have been the focus of intense research in recent years, mainly due to the discovery of superconductivity (SC). Although the mechanism of SC is still not fully understood, various experiments have shown that the As-Fe-As bond angle, the pnictogen height and an orthorhombic distortion are correlated with SC [1]. In order to understand the mechanism of SC, we need to research in the new iron-based systems. Recently, new layered iron-oxychalcogenide $La_2O_2Fe_2OSe_2$ was discovered. In this study, we try to clarify the crystal structure and phase transition of $La_2O_2Fe_2OSe_2$ by applying high pressure.

Experimental and Results

Experimental

Polycrystalline sample $La_2O_2Fe_2OSe_2$ (T_N~100K) 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-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

The all diffraction patterns at room temperature can be indexed a tetragonal crystal structure with space group *I4/mmm* (Fig.1). The lattice constants *a* and *c* were found slightly modified by pressure, as shown in Fig.2-(a). The reduction in lattice constant *a* is only about 1% while lattice constant *c* decreases almost 5% at 7GPa. We can not detect the clear phase transition from tetragonal to orthorhombic by applying the pressure.

In recent inelastic neutron scattering, we found that spin fluctuation of $La_2O_2Fe_2OSe_2$ still survive at room temperature. Interestingly, (200) peak broadening in FeSe was observed around the temperature that spin fluctuation start to enhance [2]. In order to understand the spin fluctuation under high pressure, we plot the pressure dependence of the FWHM of (200) and (006) peaks (Fig.2-(b)). The FWHM of (006) peak monotonically increases with pressure, while that of (200) peak shows maximum around 2GPa. This result suggests that application of pressure further enhances spin fluctuation in $La_2O_2Fe_2OSe_2$.

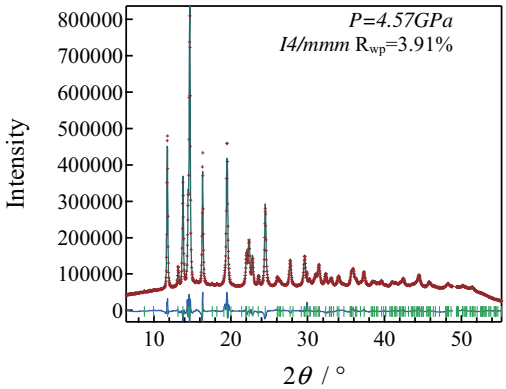

Fig.1: (a) Observed (crosses) and calculated (solid line) powder diffraction patterns of the $La_2O_2Fe_2OSe_2$ at 4.57GPa.

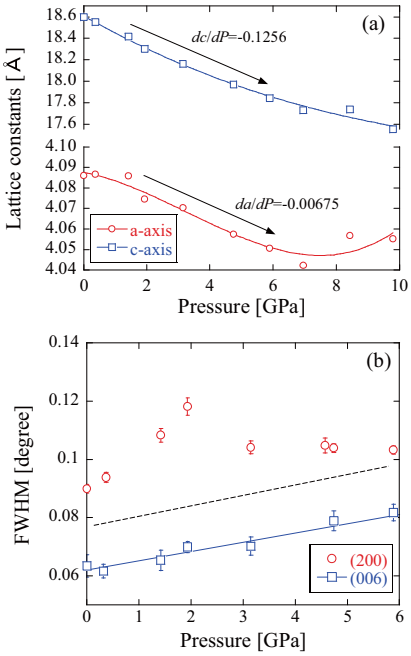

Fig.2: (a) Pressure dependence of lattice constant and (b) FWHM of (200) and (006) peaks in $La_2O_2Fe_2OSe_2$. Lines are guide to the eye.

References

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