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Electronic property of $SrFe_2As_2$ under high pressure studied by ^{57}Fe Mössbauer spectroscopy

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Abstract We have studied the electronic state of Fe atoms in $SrFe_2As_2$ under pressure at room temperature by ^{57}Fe Mössbauer spectroscopy using a single crystalline sample. A center shift $\delta_{c.s.}$ and an electric quadrupole interaction parameter $e^2qQ/2$ show the discontinuous increase and decrease at around 7 GPa,respectively, implying the pressure-induced structural phase transition. Furthermore, $\delta_{c.s.}$ deviates from the linear pressure dependence above 4 GPa without any anomaly in the pressure dependence of $e^2qQ/2$. The anomaly corresponds to a change of the pressure dependence of lattice parameter ratio c/a, where volume of the unit cell decreases monotonously with increasing pressure.

Keywords $SrFe_2As_2$ · Mössbauer spectroscopy · High pressure

1 Introduction

After the discovery of superconductivity in F-doped LaFeAsO with FeAs layers [1], various Fe-based materials show superconductivity. $SrFe_2As_2$ has a $ThCr_2Si_2$-type tetragonal structure with FeAs layers and physical properties are similar to those in LaFeAsO [2–4]. With replacing LaO by Sr^{2+}, the crystal structure is much simpler

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than that of LaFeAsO. $SrFe_2As_2$ shows a spin density wave (SDW) transition at $T_{SDW} = 200$ K with a structure change [3, 4]. The SDW transition is suppressed by pressure and then superconductivity appears around 4∼7 GPa [2, 3]. There is a correlation between magnetism, structure and superconductivity in this system. The ^{57}Fe Mössbauer spectroscopy is a local probe that is extremely sensitive to the electronic state and the local structure of Fe atoms in a compound. Thus, the purpose of this study has been to investigate the electronic state of Fe atoms in $SrFe_2As_2$ under pressure by ^{57}Fe Mössbauer spectroscopy.

2 Experimental procedure

Single crystals of $SrFe_2As_2$ enriched with 97 at.% ^{57}Fe were grown by a Sn flux method. The T_{SDW} value was estimated to be 200.4 K by the temperature dependence of the magnetic susceptibility. This value is very good agreement with the previous results [3, 4].

In the previous ^{57}Fe Mössbauer experiments on powder samples, asymmetric Mössbauer spectra were observed in AFe_2As_2 (A : Ca, Sr, Ba, and Eu) below T_{SDW}. Recent our ^{57}Fe Mössbauer experiment using the single crystal samples indicates that the origin of the asymmetry in the spectra using powder samples comes from an imperfect powder condition [5]. Thus, we have measured the ^{57}Fe Mössbauer spectra using the single crystal sample under pressure at room temperature to obtain the center shift $\delta_{c.s.}$ and the electric quadrupole interaction parameter $e^2qQ/2$, precisely. A clamp-type diamond anvil cell (DAC) was used to apply pressure with Daphne7474 as a pressure-transmitting medium to be ensured the hydrostatic condition. The DAC was mounted on a translation stage with the sample at a distance of approximately 3 mm from a ^{57}Co(Rh) point source [6]. The direction of the incident γ-ray was parallel to the [001] axis in the samples. The velocity scale was calibrated with a standard α-Fe foil.

3 Results and discussion

Typical ^{57}Fe Mössbauer spectra at some selected pressures are shown in Fig. 1. As can been seen, a single like absorption peak is observed and the position of the absorption peak decreases with increasing pressure. Since the $FeAs_4$ tetrahedron is not regular in $SrFe_2As_2$ with the tetragonal structure [2], two absorption peaks should be observed in the spectrum. Thus, these results indicate that the electrical quadrupole interaction is small in $SrFe_2As_2$. The principle z-axis of the diagonalized electric-field-gradient (EFG) tensor is along the [001] axis and the asymmetrical parameter of EFG tensor is zero because of the $\bar{4}m2$ local symmetry at the Fe site in $SrFe_2As_2$ with the tetragonal structure. The intensity ratio of two absorption peaks depends on the angle between the direction of the incident γ-ray and the principle z-axis of EFG tensor using a single crystalline sample. In the present experimental condition where the incident γ-ray is parallel to the [001] direction, the intensity ratio is 3. The solid lines in Fig. 1 represent the best fitting curves by this analysis.

Figure 2 shows the pressure dependences of the refined $\delta_{c.s.}$ and $e^2qQ/2$. The value of $\delta_{c.s.}$ decreases up to about 6 GPa with increasing pressure and shows a distinct

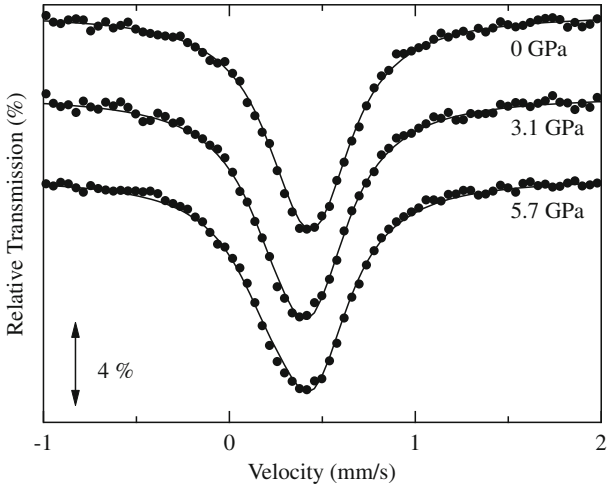

Fig. 1 Typical ^{57}Fe Mössbauer spectra at some selected pressures and room temperatures. The *solid lines* represent the results of fitting

anomaly at 6.8 GPa, as seen in Fig. 2a. Furthermore, $\delta_{\mathrm{c.s.}}$ decreases linearly above 7 GPa with increasing pressure. As shown in Fig. 2b, $e^2qQ/2$ increases monotonously up to about 6 GPa and has a lack of pressure dependence above 7 GPa within our experimental accuracy. These results strongly suggest that the electronic state of Fe atoms in $SrFe_2As_2$ changes discontinuously at around 7 GPa.

We obtain a good fit of the linear form below 3 GPa,

$$\delta_{\mathrm{c.s}} = 0.395(2) - 0.0159(9)\ P\ \ \mathrm{mm/s}. \tag{1}$$

In the pressure range between 4 and 6 GPa, $\delta_{\mathrm{c.s.}}$ deviates from (1) and shows the smaller pressure dependence than that below 3 GPa. Above 7 GPa, we also obtain a good fit of the linear form,

$$\delta_{\mathrm{c.s}} = 0.385(7) - 0.0045(8)\ P\ \ \mathrm{mm/s}. \tag{2}$$

The obtained coefficient of P above 7 GPa is 3.5 times smaller than that below 3 GPa. The anomalies in the pressure dependence of $\delta_{\mathrm{c.s}}$ reveal that the electronic state of Fe atoms in $SrFe_2As_2$ changes at around 4 and 7 GPa. Meanwhile, the pressure dependence of $e^2qQ/2$ indicates the anomaly only at around 7 GPa, as seen in Fig. 2b.

Recently it was found by the high-pressure x-ray diffraction measurements at room temperature [7] that the phase transition from the tetragonal to a collapsed tetragonal structure occurs at 10 GPa with large volume reduction. Below 10 GPa, the pressure dependence of lattice parameter ratio c/a changes at around 5 GPa, where volume of the unit cell decreases monotonously with increasing pressure. Accordingly, the anomalies in the pressure dependence of $\delta_{\mathrm{c.s}}$ and $e^2qQ/2$ at 7 GPa most likely correspond to the pressure-induced structural phase transition at 10 GPa. The difference of the critical pressure between both experiments is caused by non-hydrostatic pressure conditions in the high-pressure x-ray diffraction measurements because they did not used pressure-transmitted medium. The deviation from the

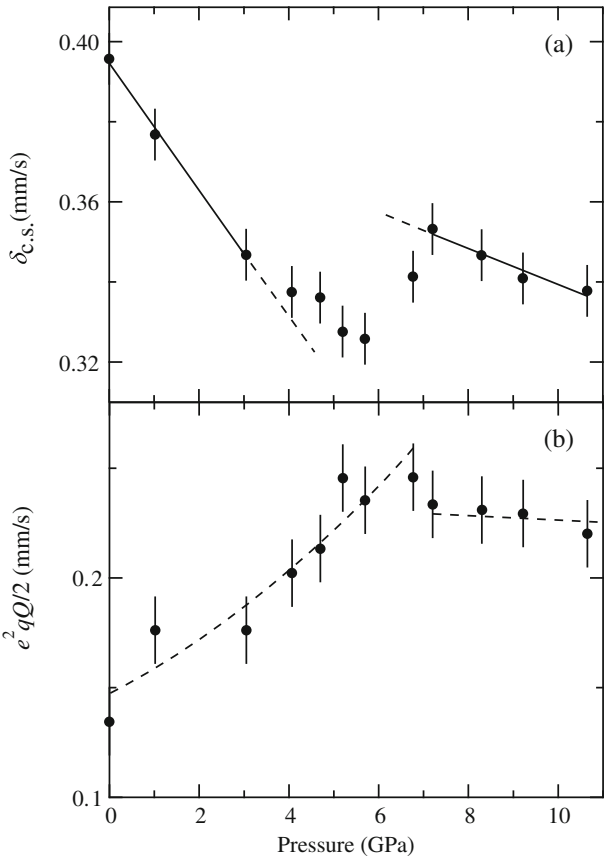

Fig. 2 Pressure dependences of the refined **a** center shift $\delta_{c.s.}$ and **b** electric quadrupole interaction parameter $e^2qQ/2$ in $SrFe_2As_2$ at room temperature. The *solid lines* represent the results of fitting. The *broken lines* are guides to the eye

linear relation between $\delta_{c.s}$ and P around 4 GPa correlates with the change of the pressure dependence of c/a. Since we did not observed any anomaly in the pressure dependence of $e^2qQ/2$ around 4 GPa, the volume of the $FeAs_4$ tetrahedron decreases monotonously around 4 GPa with increasing pressure.

4 Summary

We have measured the ^{57}Fe Mössbauer spectra of $SrFe_2As_2$ under high pressure at room temperature using the single crystalline sample. The pressure dependences of $\delta_{c.s}$ and $e^2qQ/2$ show the anomalies at 7 GPa, which correspond to the pressure-induced structural phase transition. The change of the pressure dependence of $\delta_{c.s}$ around 4 GPa correlates with that of the pressure dependence of c/a in the tetragonal structure. It is noted that the pressure range from 4 to 7 GPa almost coincides with that where the superconductivity appears in $SrFe_2As_2$ at low temperature [3, 4]. In order to investigate this relation, it is necessary to measure the temperature dependence of ^{57}Fe Mössbauer spectra in $SrFe_2As_2$ under high pressure.

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