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Pressure-induced Lifshitz transition in $FeSe_{0.88}S_{0.12}$ probed via ^{77}Se-NMR

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Recently, $FeSe_{1-x}S_x$ systems have received much attention because of the unique pressure–temperature phase diagram. We performed ^{77}Se-NMR measurements on a single crystal of $FeSe_{0.88}S_{0.12}$ to investigate its microscopic properties. The shift of ^{77}Se spectra exhibits anomalous enhancement at 1.0 GPa, suggesting a topological change in the Fermi surfaces, the so-called Lifshitz transition, occurs at 1.0 GPa. The magnetic fluctuation simultaneously changes its properties, which implies a change in the dominant nesting vector.

I. Introduction

In contrast to most iron pnictides, FeSe undergoes nematic and superconducting (SC) transitions without any magnetism: in iron pnictides, such as the $BaFe_2As_2$ family, a SC phase emerges near an antiferromagnetic (AFM) phase, which accompanies a tetragonal-to-orthorhombic transition so called a nematic transition [1]. The electronic state of FeSe dramatically changes under pressure [2]. The nematic transition temperature T_{s} is suppressed with increasing pressure and the AFM order is induced instead. These phases overlap each other in the pressure range of 1.2 GPa $< P <$ 2.0 GPa. The SC transition temperature T_{c} exhibits double-dome structure and it reaches $\sim$ 37 K at 6.0 GPa. Such complicated pressure-temperature ($P-T$) phase diagram makes it difficult to understand the origin of the high T_{c}.

Recently, the detailed $P-T$ phase diagram for S-substituted FeSe, $FeSe_{1-x}S_x$ ($0 < x < 0.17$), has been obtained from the resistivity measurements [3]. Intriguingly, the nematic and AFM phases are completely separated in the intermediate S concentration ($0.04 < x < 0.12$). In these compositions, the SC dome appears in a moderate pressure region. Therefore, a bare SC phase is more easily attainable than pure FeSe. To understand the pairing mechanism of FeSe systems, the 12%-S doped sample is preffered over the pure sample, because a high T_{c} over 25 K is attainable at low pressures ($\sim$ 3 GPa), and it is free from complicated overlapping of the nematic, SC, and AFM states.

II. Experimental Methods

We performed ^{77}Se-NMR measurements on a 12%-S doped single crystal, $FeSe_{0.88}S_{0.12}$, up to 3.0 GPa with a fixed field of 6.02 T applied parallel to the a axis. A single crystal with dimensions of about $1.0 \times 1.0 \times 0.5$ mm^3 was used for the measurements. We used a NiCrAl pressure cell [4] and Daphne oil

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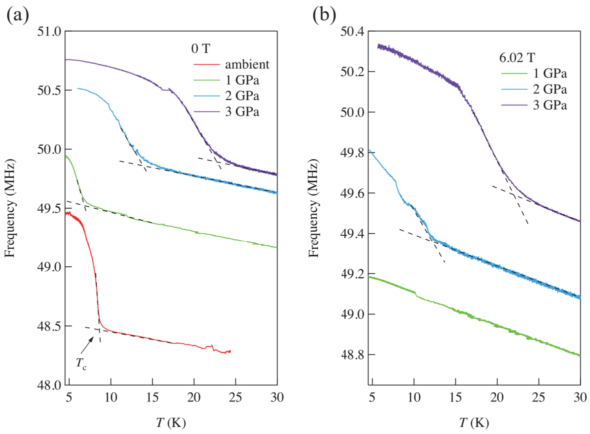

Figure 1: The T dependence of the AC susceptibility at several pressures. (a) and (b) show the AC susceptibilities at zero field and 6.02 T, respectively. The dashed lines correspond to the linear fittings, and the intersection points represent the superconducting transition points, T_cs.

as pressure transmitting medium. The pressure was determined by Ruby fluorescence measurements [4]. We placed the crystal in the pressure cell so that the FeSe plane was parallel to the applied field.

III. Experimental Results

i. Determination of T_c

Figure 1 shows the T dependence of the AC susceptibility at several pressures measured by the tank circuit of a NMR probe. To clarify the influence of the magnetic field on T_c, we measured the susceptibilities not only at zero field, but also at 6.02 T. A resonant frequency of the circuit f is expressed as follows:

$$f = \frac{1}{2\pi\sqrt{L(1+4\pi\chi)C}} \tag{1}$$

where L, C, and χ are the coil inductance, the capacitance of the variable capacitor, and the AC susceptibility, respectively. When a sample undergoes a SC transition, f diverges due to the Meissner effect ($\chi = -1/4\pi$). We determined T_c from the intersection point of linear fittings (Fig.1). T_c increases up to $\sim$ 27 K at 3.0 GPa from $T_c \sim$ 9 K at ambient pressure. We found that T_c at 1.0 GPa was anomalously suppressed at 6.02 T, and the system has not undergone the SC transition above 4.2 K. In contrast, T_cs at 2.0 and 3.0 GPa are slightly decreased by the field, as shown in Fig. 1.

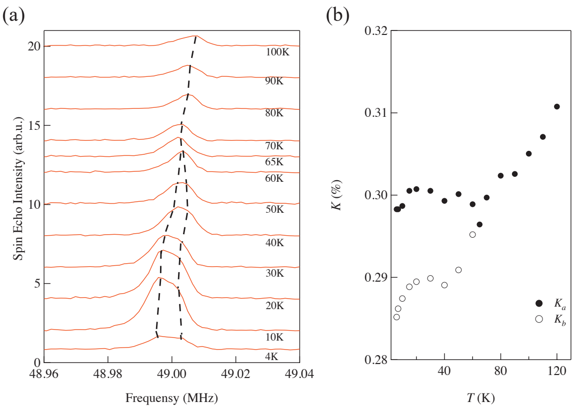

Figure 2: (a) The T evolution of ^{77}Se spectrum at ambient pressure. The black dashed line shows peak frequencies. (b) The ^{77}Se shift at ambient pressure determined from a single Gaussian fit. K_a and K_b reflect the high and low frequency peak, respectively.

ii. ^{77}Se-NMR spectra and ^{77}Se shift

We measured ^{77}Se-NMR ($I = 1/2$, $\gamma/2\pi = 8.118$ MHz/T) spectra on FeSe$_{0.88}$S$_{0.12}$ with a fixed field of 6.02 T. Figure 2(a) shows the T evolution of the spectra at ambient pressure. A single ^{77}Se signal in a tetragonal state ($T > 60$ K) becomes a double-peak structure below $T_s \sim 60$ K, which is in good agreement with the structural transition temperature observed by the resistivity measurements [3]. Figures 2(b) and 3 show the T dependence of the ^{77}Se shift at ambient pressure and the shift at several pressures, respectively. The average of the peaks below T_s is plotted for the data at ambient pressure in Fig. 3. The shift K is proportional to the density of states (DOS). In general, the DOS changes monotonically with increasing pressure due to a change in the bandwidth. In our sample, however, the DOS is enhanced at 1.0 GPa, and then it reduces with increasing pressure. As discussed below, the origin of this anomalous P dependence of the DOS could be interpreted as a topological change in the Fermi surfaces, the so-called Lifshitz transition.

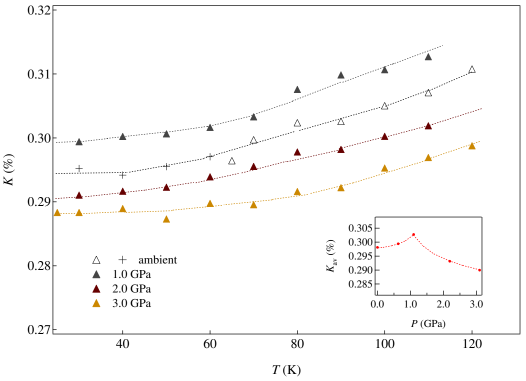

Figure 3: The ^{77}Se shift in the non-SC state at several pressures. The average of K_a and K_b is plotted below 60 K. The inset shows the ^{77}Se shift at 70 K, reflecting the pressure dependence of the DOS.

iii. The relaxation rate divided by temperature, $1/T_1T$

Figure 4 shows the relaxation rate divided by temperature, $1/T_1T$. We measured the relaxation time T_1 with the inversion-recovery method for ^{77}Se. The relaxation rate provides a measure for the low-energy spin fluctuations. In general, an AFM fluctuation is enhanced when a system comes near an AFM phase. By contrast, the AFM fluctuation of FeSe$_{0.88}$S$_{0.12}$ is strongly suppressed at 1.0 GPa and is slightly enhanced above 2.0 GPa, although the AFM phase is induced above 3.0GPa.

IV. Discussion

From the results mentioned above, we suggest that the Lifshitz transition at around 1.0 GPa is crucial to understand the anomalies of FeSe$_{0.88}$S$_{0.12}$. Firstly, the DOS suggested from the ^{77}Se shift shows that some kind of anomaly occurs at 1.0 GPa as mentioned above (see the inset of Fig. 3). According to a recent theoretical investigation in FeSe, a Lifshitz transition may occur with reducing the lattice constants [5]. S-substitution is isovalent and S-substituted FeSe has smaller lattice constants than pure FeSe [6]. Furthermore, applying pressure also causes the lattice compression. In our sample, FeSe$_{0.88}$S$_{0.12}$, therefore, the Lifshitz transition may account for the anomaly in the DOS.

Assuming that the Lifshitz transition occurs at around 1.0 GPa, the Fermi surfaces are reconstructed, and the reconstruction of the Fermi surfaces could induce a change in the dominant nesting vector. When the dominant nesting vector changes, it is possible that the AFM fluctuation at 3.0 GPa become weaker than that at ambient pressure, even though the AFM phase appears in a high pressure region. To clarify this scenario, it is necessary to determine the spin configuration of the pressure-induced AFM phase from the measurements in the higher pressure region.

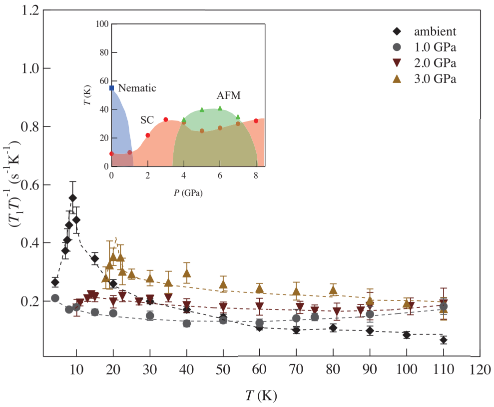

Figure 4: The T dependence of the relaxation rate divided by T, $1/T_1T$. The dashed lines are a guide to the eye. The inset shows the phase diagram of FeSe$_{0.88}$S$_{0.12}$ determined from the resistivity measurements [3].

V. Conclusions

We carried out ^{77}Se-NMR measurements on FeSe$_{0.88}$S$_{0.12}$, and the ^{77}Se shift suggests that the DOS exhibits an anomalous enhancement at 1.0 GPa. The Lifshitz transition, the change in topology of Fermi surface, could account for this anomaly. The Fermi surfaces are reconstructed due to the Lifshitz transition, resulting in a change of the dominant nesting vector. This is the reason why the AFM fluctuation at ambient pressure is stronger than that at 3.0 GPa despite the AFM order being induced above 3.0 GPa.

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