International Journal of Research in Engineering and Science (IJRES)
ISSN (Online): 2320-9364, ISSN (Print): 2320-9356
www.ijres.org Volume 5 Issue 7 ǁ Jul. 2017 ǁ PP.88-91

Lifshitz transition: Fe by intuition of Se

Bikash Mohapatra, Samareshmishra, Bhabesh Kumar Dadhichi, Nilambaripanda

Department of Physics, NM Institute of Engineering and Technology,Bhubaneswar , Odisha
Department of Physics, Raajdhani Engineering College,Bhubaneswar,Odisha
Department of Physics,Aryan Institute of Engineering and Technology Bhubnaeswar , Odisha
Department of Basic Science &Humanities ,Capital Engineering College,Bhubaneswar,Odisha

ABSTRACT: *As of late, FeSe1−xSx frameworks have gotten a lot of consideration as a result of the special pressing factor temperature stage graph. We performed 77Se-NMR estimations on a solitary gem of FeSe0.88S0.12 to examine its infinitesimal properties. The move of 77Se spectra ex-hibits strange upgrade at 1.0 GPa, recommending a topological change in the Fermi surfaces, the purported Lifshitz progress, happens at 1.0 GPa. The attractive variance all the while changes its properties, which suggests an adjustment in the predominant settling vector.*

I. INTRODUCTION

In contrast to most iron pnictides, FeSeunder- goes 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 accom- panies a tetragonal-to-orthorhombic transition so called a nematic transition [1]. The electronic state of FeSedramatically changes under pres- sure [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 $T_c$exhibitsdouble-domestructureanditreaches∼ 37 K at 6.0 GPa. Such complicated pressure-temperature(P−T)phasediagrammakesitdiffi- cult to understand the origin of the highT_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 completelyseparatedintheintermediateSconcen- tration (0.04 < x <0.12). In these compositions, theSCdomeappearsinamoderatepressureregion. Therefore,abareSCphaseismoreeasilyattainable than pure FeSe. To understand the pairing mech-anismofFeSesystems,the12%-Sdopedsampleis prefferedover the pure sample, because a high $T_c$over 25 K is attainable at low pressures (3 GPa), and it is free from complicated overlapping of the nematic, SC, and AFMstates.

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 aaxis.Asinglecrystalwithdimensionsofabout 1.0 1.0 0.5 mm^{3}was used for the measurements. WeusedaNiCrAlpressurecell[4]andDaphneoil

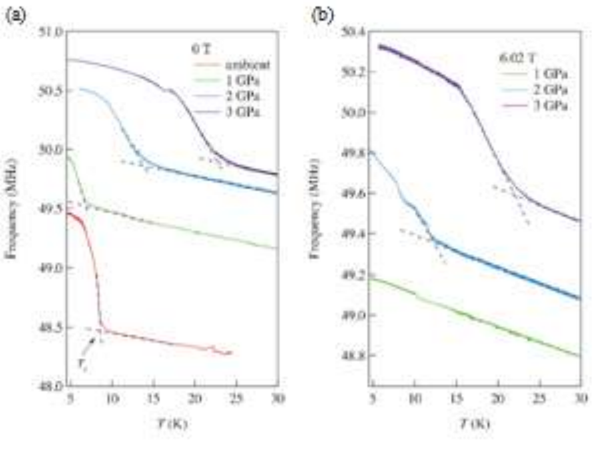

Figure1: TheTdependenceoftheACsusceptibilityat severalpressures.(a)and(b)showtheACsusceptibil-itiesatzerofieldand6.02T,respectively.Thedashed linescorrespondtothelinearfittings,andtheinter- section points

represent the superconductingtransition points,T_cs.

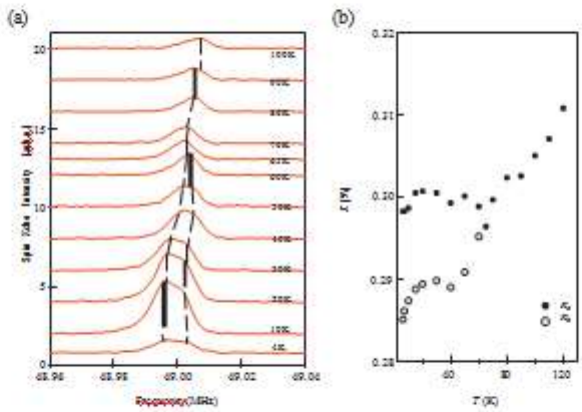

Figure2:(a)TheTevolutionof77Sespectrumatam- bientpressure.Theblackdashedlineshowspeakfre- quencies.(b)The77Seshiftatambientpressuredeter- mined from a single Gaussian fit. Kaand Kbreflect thehighandlowfrequencypeak,respectively.

aspressuretransmittingmedium.ThepressurewasdeterminedbyRubyfluorescencemeasurements[4]. We placed the crystal in the pressure cell so that the FeSeplane was parallel to the appliedfield.

III. EXPERIMENTAL RESULTS

i. Determination ofT_c

Figure1showstheTdependenceoftheACsuscep- tibility at several pressures measured by thetankcircuitofaNMRprobe.ToclarifytheinfluenceofthemagneticfieldonT_c,wemeasuredthesus cep- tibilitiesnotonlyatzerofield,butalsoat6.02T. Aresonantfrequencyofthecircuitfisexpressed asfollows:

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

whereL,C,andχarethecoilinductance,theca- pacitanceofthevariablecapacitor,andtheACsus- ceptibility, respectively. When a sampleundergoes aSCtransition,fdivergesduetotheMeissneref- fect ($\chi = -1/4\pi$). We determined $T_c$from the intersection point of linear fittings (Fig.1). $T_c$in- creasesupto$\sim$27Kat3.0GPafrom$T_c \sim$9Kat ambientpressure.Wefoundthat$T_c$at1.0GPawas Figure2:(a)TheTevolutionof^{77}Sespectrumatam- bientpressure.Theblackdashedlineshowspeakfre- quencies.(b)The^{77}Seshiftatambientpressuredeter- mined from a single Gaussian fit. $K_a$and $K_b$reflect thehighandlowfrequencypeak,respectively.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 de- creased by the field, as shown in Fig. 1.

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

We measured ^{77}Se-NMR ($I = 1/2$, $\gamma/2\pi=$ 8.118MHz/T)spectraon$FeSe_{0.88}S_{0.12}$withafixed 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_s60 K, which is in good agreement with the structural transition tem- perature 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 changesmonotonicallywithincreasingpressuredue to a change in the bandwidth. In our sample, how- ever, 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-calledLifshitz transition.

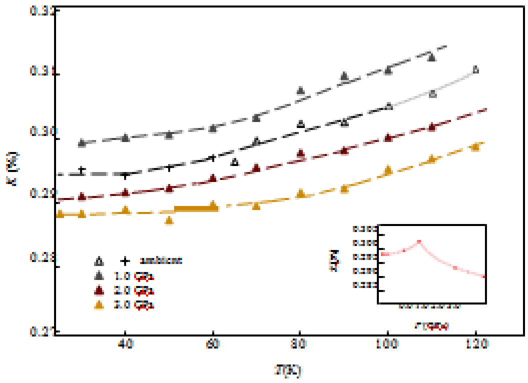

Figure3: The[77]Seshiftinthenon-SCstateatseveral pressures.TheaverageofK$_a$andK$_b$isplottedbelow 60K.Theinsetshowsthe[77]Seshiftat70K,reflecting the pressure dependence of theDOS.

iii. The relaxation rate divided bytemper- ature,$1/T_1T$

Figure 4 shows the relaxation rate divided by tem- perature, $1/T_1T$ .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 fluc-tuation 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 above3.0GPa.

IV. DISCUSSION

From the results mentioned above, we suggest that the Lifshitz transition at around 1.0 GPa is cru- cial to understand the anomalies of $FeSe_{0.88}S_{0.12}$. Firstly, the DOS suggested from the [77]Se shift showsthatsomekindofanomalyoccursat1.0GPa as mentioned above (see the inset of Fig. 3). Ac- cordingtoarecenttheoreticalinvestigationinFeSe, a Lifshitz transition may occur with reducing the lattice constants [5]. S-substitution is isovalentand S-substituted FeSehas smaller lattice constants than pure FeSe[6]. Furthermore, applyingpressure also causes the lattice compression. In our sample, $FeSe_{0.88}S_{0.12}$,therefore,theLifshitztransitionmay account for the anomaly in theDOS.

Assuming that the Lifshitz transition occurs at around 1.0 GPa, the Fermi surfaces are recon- structed, and the reconstruction of the Fermi sur- facescouldinduceachangeinthedominantnesting vector.Whenthedominantnestingvectorchanges, it is possible that the AFM fluctuation at 3.0 GPa becomeweakerthanthatatambientpressure,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 pressureregion.

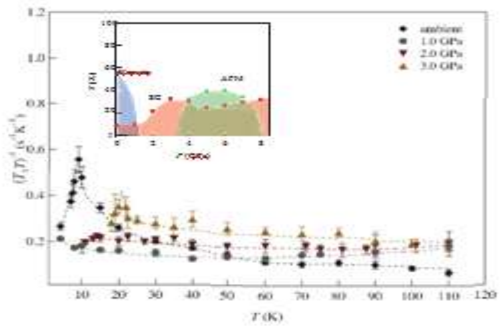

Figure4: TheTdependenceoftherelaxationratedi-videdbyT,1/T1T.Thedashedlinesareaguidetothe eye.TheinsetshowsthephasediagramofFeSe0.88S0.12 determinedfromtheresistivitymeasurements[3].

V. CONCLUSIONS

We carried out ^{77}Se-NMR measurements on $FeSe_{0.88}S_{0.12}$, and the ^{77}Se shift suggests that theDOSexhibitsananomalousenhancementat 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 3.0GPa.

REFERENCES :

[1] R M Fernandes, A V Chubukov, J Schmalian, What drives nematic order in iron-based superconductor?, Nat. Phys. **10**, 97(2014).

[2] JPSun,KMatsuura,GZYe,YMizukami,M Shimozawa, K Matsubayashi, M Yamashita, T Watashige, S Kasahara, Y Matsuda, J Q Yan, B C Sales, Y Uwatoko, J G Cheng, T Shibauchi, Dome-shaped magnetic order com- petingwithhigh-temperaturesuperconductivity at high pressures in FeSe, Nat. Commun. **7**, 12146(2016).

[3] K Matsuura, Y Mizukami, Y Arai, Y Sug-imura, N Maejima, A Machida, T Watanuki, T Fukuda, T Yajima, Z Hiroi, K Y Yip, Y C Chan,QNiu,SHosoi,KIshida,KMukasa,S Kasahara, J G Cheng, S K Goh, Y Mat- suda, Y Uwatoko, T Shibauchi, Maximizing $T_c$by tuning nematicity and magnetism in $FeSe_{1-x}S_x$superconductors, Nat. Commun. **8**, 1143(2017).

[4] N Fujiwara,T Matsumoto, K Nakazawa, AHisada, Y Uwatoko, Fabrication and efficiency evaluation of a hybrid NiCrAlpressure cell up to 4 GPa, Rev. Sci. Instrum. **78**, 073905 (2007).

[5] S L Skornyakov, V I Anisimov, D Vollhardt, I Leonov, Correlation strength, Lifshitztransi- tion, and the emergence of a two-dimensional to three-dimensional crossover in FeSeunder pressure, Phys. Rev. B **97**, 115165(2018).

[6] J N Millican, D Phelan, E L Thomas, J B Leão,ECarpenter,Pressure-inducedeffectson thestructureoftheFeSesuperconductor,Solid State Commun. **149**, 707(2009).