Elastic Anomalies Associated with superconducting phase transitions in Iron-based Superconductor \( \text{Ba(Fe}_{1-x}\text{Co}_{x})_{2}\text{As}_{2} \)

A. Ismayil\textsuperscript{a,*}, R. Kamiya\textsuperscript{a}, R. Onodera\textsuperscript{a}, D. Kimura\textsuperscript{a}, T. Chiba\textsuperscript{a}, Y. Nakanishi\textsuperscript{a,d}, K. Kihou\textsuperscript{b,d}, M. Nakajima\textsuperscript{c,d}, C. H. Lee\textsuperscript{b,d}, A. Iyo\textsuperscript{b,d}, H. Eisaki\textsuperscript{b,d}, S. Uchida\textsuperscript{c,d}, and M. Yoshizawa\textsuperscript{a,d}

\textsuperscript{a} Graduate School of Engineering, Iwate University, Morioka 020-8551, Japan
\textsuperscript{b} National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba 305-8568, Japan
\textsuperscript{c} Graduate School of Science, The University of Tokyo, Tokyo 113-0033, Japan
\textsuperscript{d} Transformative Research-project on Iron Pnictides (TRIP), Japan Science and Technology Agency, Tokyo 102-0075, Japan

E-mail: t5510007@iwate-u.ac.jp

Abstract. We have measured the temperature dependence of elastic constants of iron pnictide superconductors \( \text{Ba(Fe}_{1-x}\text{Co}_{x})_{2}\text{As}_{2} \) with optimal doped \( x = 0.060 \) and over-doped 0.116, with different superconducting phase transition temperatures \( T_{sc} \). We have observed remarkable anomalies at \( T_{sc} \). The coupling between the superconducting order parameter and elastic strain was discussed based on the elastic anomaly at \( T_{sc} \). The elastic constant \( \frac{C_{11}+C_{12}+2C_{66}}{2} \) shows a large anomaly at \( T_{sc} \), which clearly indicates a large Grüneisen parameter of this system. The amount of Grüneisen parameter is 62 comparable to that of the strongly correlated electron system.

1. Introduction

Trailing behind the cuprates, iron-based superconductors are the second highest temperature superconducting materials known to date. In early 2008 the discovery of superconductivity with a high transition temperature of \( T_{sc} \) in F-doped LaFeAsO compound causes an outpouring of experimental and theoretical studies of the materials containing Fe-As layers as a structural unit [1]. Up to date the highest \( T_{sc} \) in iron-based superconductors have been raised to 55 K [2]. \( \text{Ba(Fe}_{1-x}\text{Co}_{x})_{2}\text{As}_{2} \) has the same structure with \(
\text{ThCr}_{2}\text{Si}_{2} \), at the FeAs layer by replacing of Co or Ni ion with Fe , and by replacing of K ion with Ba , the superconductivity comes out [3, 4]. Iron based superconductivity is very recent superconducting material family and a great many number of studies have been carried out, these studies opened new research field of high-temperature superconductivity, we have studied whether neighboring orders show any effect on the lattice coupling mechanism. \( \text{BaFe}_{2}\text{As}_{2} \) itself does not show superconducting properties, but undergoes structural transition from a tetragonal to orthorhombic at 140K, and exhibits an antiferromagnetic order at the same temperature with \( T_{s} \) through a weak first-order phase transition in which the antiferro-order appears discontinuously [5], [6]. The substitution of \( \text{Fe}^{2+} \) with \( 3d^{6} \) orbitals by \( \text{Co}^{2+} \) with \( 3d^{7} \) orbitals in \( \text{Ba(Fe}_{1-x}\text{Co}_{x})_{2}\text{As}_{2} \) separated both structural...
and magnetic phase transitions from each other and superconductivity comes out [7]. The temperature \((T)\) versus \(x (T - x)\) phase diagram indicates that above \(x = 0.035\) superconductivity is observed, apparently in the orthorhombic-ferromagnetic phase. Above \(x = 0.060\) the structural-magnetic transitions vanish [8]. Among many iron pnictides with different structures, the tetragonal compound \(\text{Ba(Fe}_{1-x}\text{Co}_x)\text{As}_2\) is suitable for the basic research, because large single crystals are available for the investigation of physical properties depending on crystal anisotropy [9].

The symmetry of superconducting states of iron pnictide superconductors have been discussed by theoretically and experimentally [10, 11]. Experiments on the nonmagnetic impurity effect indicate that the iron-based superconductors are robust against nonmagnetic impurities [12, 13, 14]. In iron-based compounds, As ions are located asymmetrically with respect to the Fe plane [15], therefore, there are many hopping between Fe 3d orbitals, which are not allowed without As ions, and which increases opportunity of superconducting states. It has been improved that antiferromagnetism plays an important role in the emergence of superconductivity. In iron-based superconductors the superconducting phase is located closely to a magnetic phase transition rather than structural phase transition. Such a mechanism often seen in many systems of oxide superconductors, these beg a question of whether the neighboring orders participate in the mechanism of the superconductivity of iron-based superconductors?

2. Experimental

Single crystalline \(\text{Ba(Fe}_{1-x}\text{Co}_x)\text{As}_2\) were grown by an As self-flux high temperature solution technique. The sample which Co concentrations are optimal 6%, over doped 11.6 % were prepared for this study. Detailed description of the crystal growth procedure for this series can be found elsewhere [16]. The Co concentration in the grown crystals was determined by EDX measurements. The Co concentration in the samples are different from the prepared one. The prepared concentration of 3.7% and 6.0% and 11.6 % are 0.050, 0.080 and 0.15, respectively. Elastic constants have been measured by an ultrasonic pulse-echo phase comparison method as a function of temperature between 5 K to 300 K by using a cryostat equipped on a GM cryocooler. Elastic polymer Thiokol LP-32 was used for bond the transducers on both sides to the sample with parallel end faces. To prevent from the damage of the sample, temperature rate was controlled by 10 K/h near superconducting transitions. The elastic constant was obtained by the formula of \(C = \rho v^2\) with the density of \(\rho = 6.485 \text{ g.cm}^{-3}\) and 6.493 g.cm\(^{-3}\) for 6 % and 11.6 % respectively. We have measured \(C_{44}, \frac{1}{2}(C_{11} - C_{12})\) and \(C_L = (C_{11} + C_{12} + 2C_{66})/2\). The temperature dependence of the shear elastic constants of a tetragonal \(\text{Ba(Fe}_{1-x}\text{Co}_x)\text{As}_2\) with \(x = 0.060\) and 0.116 were performed in this study. The propagation and displacement directions of the sound velocity are [110] and [100] for \(C_L\), [100] and [001] for \(C_{44}\), and [110] and [110] for \(\frac{1}{2}(C_{11} - C_{12})\). The corresponding elastic strains are \(\varepsilon_{xx}\) and \(\varepsilon_{xx} - \varepsilon_{yy}\) respectively. Here, the xyz coordinate was defined by the unit cell of \(I_{4/mmm}\) crystal structure [17].

3. Results and discussion

Figure 1 shows the temperature dependence of \(C_L = (C_{11} + C_{12} + 2C_{66})/2\) in the magnetic field. The magnetic field was applied parallel to the propagation direction of the sound [110]. It shows a rapid decrease with decreasing temperature above 25 K. The softening of the longitudinal CL mode in Fig. 1 originates from the softening of \(C_{66}\), because \(C_L\) involves \(C_{66}\) in part [18]. A remarkable step-like anomaly at 24.5K, which is associated with the superconducting transition \(T_{sc}\). The \(T_{sc}\) tends to decrease as applying the field, which confirms that this
anomaly is originated from the superconductivity. Figures 2 and 3 show the temperature dependence of the transverse elastic constants of $C_{44}$ and $\frac{1}{2}(C_{11} - C_{12})$, they commonly show a monotonous increase with decreasing temperature, and insets show a small dips observed around the superconducting phase transition temperatures. On the other hand, for 11.6% sample, the $C_{44}$ and $C_{E}$ show a slight softening toward $T_{sc}$. The elastic anomaly at $T_{sc}$ gives information on the coupling between the superconducting order parameter $\eta$ and the elastic strain $\varepsilon$. From the shape of the elastic constant anomalies, we consider the coupling to be $\eta^2\varepsilon$ both for $C_{44}$ and $\frac{1}{2}(C_{11} - C_{12})$ of the overdoped sample. In the case of $\frac{1}{2}(C_{11} - C_{12})$ of the underdoped sample, the shape of the anomaly at the $T_{sc}$ is very peculiar, which has been never seen so far. We infer the coupling to be either $\eta^2\varepsilon$ or $\eta^2\varepsilon^2$ for this sample. It would be considered to concern with the occurrence of orthorhombicity below $T_{sc}$. These would provide the information on the mechanism of superconductivity in the cooper pairing in the iron-based superconductivity. To investigate this point, the measurement of elastic constants in other modes about temperature dependence of ultrasonic measurements around $T_{sc}$ are currently in progress.

This study showed strong electron-lattice coupling with respect to the structural transition. Such strong correlation between lattice and electrons is also found at superconducting transition. Grüneisen parameter $\Omega_{sc}$ for $T_{sc}$, which is defined as $\Omega_{sc} \equiv -\frac{1}{\rho_{sc}} \frac{\partial \rho}{\partial T}$, where $\rho_{sc}$ is the elastic strain belonging to $\Gamma$ irreducible representation, can be estimated by using the formula of $\Delta C = -\Omega_{sc}^{2} \Delta C_{V} T_{sc}$. Here, $\Delta C$ and $\Delta C_{V}$ are jump of the elastic constant and the specific heat at $T_{sc}$, respectively. By using $\Delta C_{L} = 1$ GPa and $\Delta C_{V} = 0.67$ J/mol · K [19], we get $[\Omega_{sc}] = 62$. This value is comparable to $\Omega_{sc} = 15$ and -40 for a and c axes, respectively, which were evaluated from thermal expansion data [19] and Ehrenfest relation. Large $\Omega_{sc}$ has been reported in heavy fermion systems [20]. It may lead us to infer that this system is categorized into strongly correlated electron system [21]. Such a large Grüneisen parameter may be related to the fact that this system is located closely to the quantum critical point.

Acknowledgments

We wish to thank M. Nakamura and T. Kowata for their help in the experiments. This work was supported by a Grant-in-Aid for Scientific Research on Innovative Areas “Heavy Electrons” (No. 2010/2007) of The Ministry of Education, Culture, Sports, Science, and Technology, Japan, and Transformative Research-project on Iron Pnictides of Japan Science and Technology Agency.

References

[1] Kamihara Y 2008 et al., J. Am. Chem. Soc. 130 3296
[2] Ren Z A, Lu W, Yang J, Yi W, Shen X L, Li Z C, Che G C, Dong X L, Sun L L, Zhou F, and Zhao Z X, Chin 2008 Phys. Lett. 25 2215
[3] Sefat A S 2008 et al., Phys. Rev. Lett. 101 107007
[4] Rotter M 2008 et al., Phys. Rev. Lett. 101 107006
[5] Rotter M, Tegel M, Johrendt D, Schellenberg I, Hermes W, and Pöttgen R 2008 Phys. Rev. B 78 020503(R)
[6] Huang Q, Qiu Y, Bao W, Green M A, Lynn J W, Gasparovic Y C, Wu T, Wu G, and Chen X H 2008 Phys. Rev. Lett. 101 257003
[7] Nandi S, Kim M G, Kreyssig A, Fernandes R M, Pratt D K, Thaler A, Ni N, Bud’ko S L, Canfield P C, Schmalian J, McQueeney R J, and Goldman A I 2010 Phys. Rev. Lett. 104 057006
[8] Jiun-Haw Chu, James G. Analytis, Chris Kucharczyk, and Ian R. Fisher 2009 Phys. Rev. B 79 014506
[9] Canfield P C and Bud’ko S L 2010 Annu. Rev. Condens. Matter Phys. 1 27
[10] Ning F, Ahilan K, Imai T, Sefat A S, Jin R, McGuire M A, Sales B C, and Mandrus D 2009 J. Phys. Soc. Jpn. 78 013711
[11] Ding H, Richard P, Nakayama K, Sugawara K, Arakane T, Sekiba Y, Takayama A, Souma S, Sato T, Takahashi T, Wang Z, Dai X, Fang Z, Chen G F, Luo J L, and Wang N L 2008 Europhys. Lett. 83 47001
[12] Sato M, Kobayashi Y, Lee S C, Takahashi H, Satomi E, and Miura Y 2010 J. Phys. Soc. Jpn. 79 014710
[13] Lee S C, Satomi E, Kobayashi Y, and Sato M 2010 J. Phys. Soc. Jpn. 79 023702
[14] Cheng P, Shen B, Hu J, and Wen H H 2010 Phys. Rev. B 81 174529
[15] Mizuguchi Y and Takano Y 2010 J. Phys. Soc. Jpn. 79 102001
[16] Ni N, Tillman M E, Yan J Q, Kracher A, Hannahs S T, Bud’ko S L, and Canfield P C 2008 Phys. Rev. B 78 214515
[17] Rotter M, Tegel M and Johrendt D 2008 Phys. Rev. Lett. 101 107006
[18] Goto T 2011 et al., J. Phys. Soc. Jpn. 80 073702
[19] Hardy F 2009 et al., Phys. Rev. Lett. 102 187004
[20] Lüthi B and Yoshizawa M 1987 J. Mag. Mag. Mater 63 and 64 274
[21] Terashima T 2010 et al., J. Phys. Soc. Jpn. 79 053702

Figure 1. Temperature dependence of \((C_{11}+C_{12}+2C_{66})/2\) for 6.0 % sample in the magnetic field of 0, 3 and 5 T is displayed with an expanded scale near \(T_{sc}\).

Figure 2. Temperature dependence of \(C_{44}\) of 11.6 % sample. Inset shows the anomaly at around the superconducting transition.
Figure 3. Temperature dependence of \( \frac{1}{2} (C_{11} - C_{12}) \) of 6 % and 11.6 % samples. Inset shows the anomaly at around the superconducting transition.