Solid State Communications 180 (2014) 35–38

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Positron probing of electron momentum re-distribution at the superconducting transition in $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals

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ARTICLE INFO

Article history:
Received 13 October 2013
Received in revised form
15 November 2013
Accepted 16 November 2013
by Hideo Hosono
Available online 23 November 2013

Keywords:
A. Pnictide
D. Superconductivity
E. Positron annihilation spectroscopy

ABSTRACT

Superconducting $Ba(Fe_{0.943}Co_{0.057})_2As_2$ single crystals with T_c $(R=0)=19.5$ K, and non-superconducting $BaFe_2As_2$ single crystals have been studied by coincidence Doppler broadening of positron annihilation radiation line-shape (coincidence DBPARL) down to ~ 14 K. This appears to be the first reporting of positron probing of any Fe-based superconductor. The superconducting sample shows, on cooling below ~ 40 K and towards T_c, a sharp decrease of S, the line-shape parameter, which gives the fraction of suitably defined low momentum electrons as probed by the positrons. No such decrease of S for the non-superconducting sample indicates the effect to be induced by superconductivity. The ratio curve analysis of the coincidence DBPARL spectra suggests that in the superconducting state the positrons are annihilating less with the 3d electrons of Fe and Co and more with the 5s and 4d electrons of Ba. In addition, a novel double measurement of coincidence DBPARL for the *a–b* plane and planes normal to the *a–b* plane of the single crystalline sample shows a nearly isotropic distribution of the lower electron momentum in this Fe-based superconductor.

1. Introduction

Thousands of superconductivity experiments, primarily on metallic systems, and excellent theoretical investigations since 1911 [1], had basically accepted, up to around 1986 [2], that superconductivity arises from phonon-mediated electron pairing [3]. Consequently, a theoretical upper limit for superconducting critical temperature (T_c) was calculated, and largely believed on finding no material superconducting above 23 K till the discovery [2] of the first High Temperature Superconductor (HTSC). The discovery of these Cu–O based HTSCs and 2008 [4] to 2013 discoveries of various Fe-based superconductors (with T_c up to 55 K) have been triggering interesting refinement and up-gradation of the understanding of superconductivity, more experiments and some applications [5–10]. The exciting HTSC findings included our and other Positron Annihilation Spectroscopy (PAS) results [11–20] on Bi-2212, (Bi,Pb)-2223, Y-123 and Y-124 HTSCs either in ceramic pellet or in single crystal form. Doppler broadened positron annihilation radiation lineshape (DBPARL) measurements showed an abrupt change of electron momentum distribution on cooling or heating across T_c in all the HTSCs studied. Electron or hole transfer between reservoir layers and conducting layers in any HTSC structure at the onset of superconductivity, implying abrupt change of carrier concentration at the annihilation sites has been held [10,13] responsible for the observed fall or rise of measured S parameter, representing the fraction of suitably defined low momentum electrons, as one cooled the sample towards T_c. This electron momentum re-distribution is linked to the mechanism of superconductivity, which is not fully understood either for HTSCs or for the Fe-based superconductors. So, it is high time that possible electron momentum re-distribution at T_c be examined by DBPARL technique in suitable Fe-based superconductors. It will also be the first positron probing of charge carriers for superconductivity intimately involving magnetic ions. Fermi surface topology of optimally doped iron arsenide superconductor has been probed both theoretically [21,22] and experimentally [23] by employing high-resolution Compton scattering spectroscopy. Muon spin rotation study of $Ba(Fe_{1-x}Co_x)_2As_2$ and $Pr_{(1-x)}Sr_xFeAsO$ has been reported [24], but not a single DBPARL or other positron investigation on any Fe-based superconductor.

Present measurements on single crystal samples of superconducting $Ba(Fe_{0.943}Co_{0.057})_2As_2$, to be called Co-doped 122, and non-superconducting $BaFe_2As_2$ have been done by employing coincidence DBPARL technique. This takes care of two possible difficulties. First is the elimination, through our use of single crystals, of likely contribution of grain boundaries and other trapping defects in polycrystals to the temperature dependent positron Doppler broadening. Second

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0038-1098/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.ssc.2013.11.021

difficulty of high background in DBPARL data [11] on N(E) vs. E, seriously affecting the high energy (E) wing portions, is effectively removed in the coincidence DBPARL technique. HTSC discovery added the possibility of superconductivity in Cu–O planes to the well developed concept of so-called conventional superconductivity in metallic systems with conduction electrons. Since the common building block of all the four homologous series of new Fe-based superconductors (e.g., LaFeAsO and RFe_2As_2 structures) is the square-lattice Fe sheets hybridized with As layers [25], these FeAs composite layers need to be considered as the third type of atomic structure hosting superconductivity. There is a special interest in such superconducting units with magnetic ions, traditionally believed to destroy superconductivity [26]. Superconductivity can be generated in $BaFe_2As_2$ structure either by electron doping, as in $Ba(Fe,Co)_2As_2$, or by hole doping, as in $Ba_{(1-x)}K_xFe_2As_2$.

2. Experimental outline

Positron measurement with a radioactive positron source needs a pair of large and identical plate-like sample pieces. The source (here, a ^{22}NaCl source of strength 10 μCi), often enclosed in a suitable cover (here, a mylar foil of 1.5 μm thickness), is sandwiched between the plate-like samples. Success in preparing such large single crystals of good quality for Co-doped 122 led us to select two pieces of 8 mm × 8 mm × 2 mm crystals of above-mentioned composition for this study. The single crystals were grown from self-flux using a glassy carbon crucible. After heating the Ba:(Fe, Co)As = 1:5 mixture to 1160 °C the crucible was cooled down very slowly at rates of 0.22–0.30 °C/h. At the end of the growth the crucible was tilted to decant the remaining flux.

The source–sample sandwich has been placed in the cold figure of a closed cycle He-cryogenerator (ARS, USA) with the Lakeshore (model 335) temperature-controller (temperature stability of ± 0.1 K). The sample temperature has been measured in the temperature range 14–300 K, with a cernox sensor, placed very close to the source–sample sandwich, and calibrated by comparing it with another thermometer that replaced the sample in the calibration run. In the present work four HPGe detectors (Efficiency: 12%; Type: PGC 1216sp of DSG, Germany) having energy resolution of ~1.1 keV at 514 keV of ^{85}Sr have been used for the two-fold (perpendicular to each other) coincidence Doppler broadening (CDB) measurement. Simultaneous measurement of the CDB spectra of the a–b plane and perpendicular to a–b plane of the single crystal have been recorded in two different dual ADC based multiparameter data acquisition systems (MPA-3 of FAST ComTec., Germany). Both the data acquisition systems have been calibrated identically with the energy per channel of 142 eV. The peak to background ratio of both the CDB measurement system with $\pm\Delta E$ selection is ~10^5:1. At each temperature, ~10^7 coincidence counts have been recorded. The CDB spectrum has been analyzed by evaluating the conventional S-parameter and also by the ratio curve analysis [18,27].

3. Results and discussion

Fig. 1 represents the a–b plane electrical resistivity of the Co-doped Ba-122 sample. A sharp superconducting transition with T_c (R=0) at 19.5 K, has been observed for the Co-doped Ba-122 sample, while the undoped one is non-superconducting.

The coincidence Doppler broadening spectra have been analyzed by evaluating the S-parameter defined by the ratio of the counts in the central area of the 511 keV photo-peak ($|511\text{ keV}-E_\gamma| \leq 0.85$ keV) and the total area of the photo peak ($|511\text{ keV}-E_\gamma| \leq 4.25$ keV).

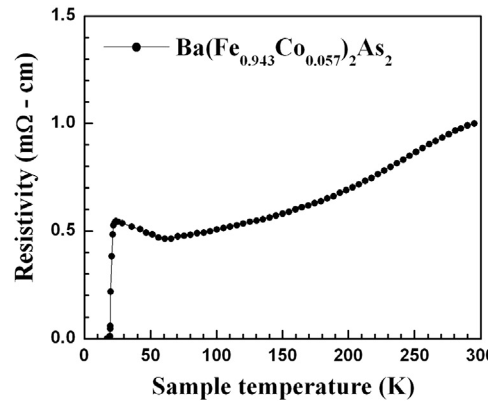

Fig. 1. Temperature dependence of a–b plane electrical resistivity of single crystalline samples of $Ba(Fe_{0.943}Co_{0.057})_2As_2$.

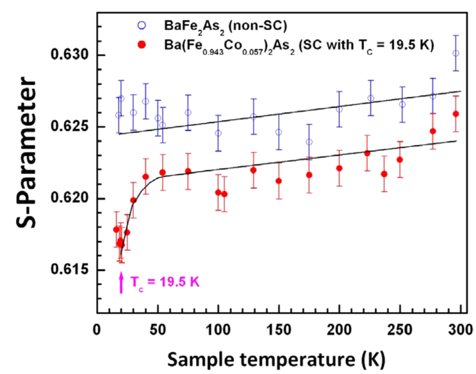

Fig. 2. (Colour online) Temperature dependent variation of positron annihilation S-parameter (i.e. the fraction of low momentum electrons, as detailed in the text) for the non-superconducting $BaFe_2As_2$ and superconducting $Ba(Fe_{0.943}Co_{0.057})_2As_2$ single crystalline samples. A polynomial fit is shown, as a guide to the eye, for the portion from 50 K to 19.5 K, of the graph for the superconducting sample, depicting a large decrease of S on cooling to T_c. Linear fits to the rest of this graph and to the graph for non-superconducting Ba-122, drawn as guides to the eye, approximately represent increase of S with increasing T due to lattice expansion.

The S-parameter represents the fraction of positrons annihilating with the lower momentum electrons, as defined by the above-mentioned energy window of 0.85 keV. Fig. 2 represents our experimental data on the variation of S with temperature (T) for superconducting Co-doped 122 crystals and non-superconducting undoped 122 crystals. Since the lattice expansion induced increase of S with increase of T, which can be approximately taken as linear, dominates the temperature variation of S for the non-superconducting part of the data for the superconducting sample and for the data for the non-superconducting sample, linear fits are shown to these two data sets as guides to the eye. Other possible contributions to the variation of S in these regions will not be explored in this work. In contrast to the small scattering of the data points from the mean linear fits, the decrease of S of the superconducting sample between 50 K and 19.5 K is large and steep, needing special attention.

There is no such significant change for the non-superconducting $BaFe_2As_2$ samples. This indicates that in this Fe-based superconductor, S-parameter or the fraction of lower momentum electrons as probed by positrons, decreases on cooling the sample to the superconducting state. Such a decrease of S has also been observed in various HTSC [11,13], where the S-parameter passes through a minimum at T_c and increases again on further cooling. In many Cu-based HTSCs, positrons are mainly probing the charge reservoir planes, with very low positron density distribution in the superconducting CuO planes. Unlike in these Cu-based HTSCs, positron wave functions are uniformly mapping the whole unit cell of various Fe based superconductors [28].