Gap Structure of the Overdoped Iron-Pnictide Superconductor Ba(Fe_{0.942}Ni_{0.058})_{2}As_{2}: A Low-Temperature Specific-Heat Study

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Low-temperature specific heat (SH) is measured on the post-annealed Ba(Fe_{1-x}Ni_{x})_{2}As_{2} single crystal with x = 0.058 under different magnetic fields. The sample locates on the overdoped sides and the critical transition temperature \(T_{c}\) is determined to be 14.8 K by both the magnetization and SH measurements. A simple and reliable analysis shows that, besides the phonon and normal electronic contributions, a clear \(T^2\) term emerges in the low temperature SH data. Our observation is similar to that observed in the Co-doped system in our previous work and is consistent with the theoretical prediction for a superconductor with line nodes in the energy gap.

1. INTRODUCTION

The superconducting (SC) state of a superconductor is protected by an energy gap. The symmetry and structure of the energy gap can be very different in different SC materials. For the conventional superconductors (e.g. metallic superconductors), the gap is isotropic in the \(k\) space which is called the s-wave symmetry. In some materials (e.g. MgB_{2}), multiple gaps have been discovered on different Fermi surfaces. Highly anisotropic (the so-called d-wave) gap symmetry was confirmed in high-\(T_c\) cuprate superconductors. The situation is more complicated in the iron-pnictide superconductors, because there are typically four or five bands crossing the Fermi level. Theoretically several candidates symmetries of the SC gap(s) were proposed, among which the so-called S\(^{\pm}\) case seems to be accepted widely. On the experimental sides, the nodeless superconductivity has been confirmed in (K,Tl)\(_2\)Fe\(_{2-y}\)P\(_y\)Se\(_2\). However, the nodes (zero points) have been reported in the gap(s) of iron-pnictide superconductors. The symmetry and structure of the energy gap can be very different in different SC states (\(C_{sc}\) versus temperature can be rather different for different gap structures), where \(\Delta_0\) is the magnitude of the energy gap. In order to segregate the pure electron SH from the measured mixed contributions, many methods have been tried. In our previous work, we reported the clear presence of \(T^2\) term in \(C_{sc}\) of the overdoped Ba(Fe_{1-x}Co_{x})_{2}As\(_2\) from the raw data, giving a more solid evidence for the line-nodal gap structure. It is very important and necessary to investigate more systems with other dopants to check the universality of such a behavior.

In this paper, we studied the the low temperature SH of the Ni-doped BaFe\(_2\)As\(_2\) in the overdoped region. Here we also observed a clear \(T^2\) term in \(C_{sc}\), being consistent with the theoretical prediction for the line-nodal superconductors. Our result along with the previous work indicates that it is a universal feature of the electron doped 122 system.

2. MATERIALS AND METHODS

The Ba(Fe_{0.942}Ni_{0.058})\(_2\)As\(_2\) single crystal was grown by the self-flux method. The as-grown sample was annealed under high vacuum at 1073 K for 20 days, because it was reported that the annealing process can improve the sample quality significantly. The sample for the SH measurement have a mass of 2.9 mg. The actual Ni concentrations were checked and determined by the energy dispersive X-ray spectroscopy (EDS) measurements on a Bruker Quantax200 system. The dc magnetization measurements were done with a superconducting quantum interference device (Quantum Design, MPMS7). The specific heat were measured with a Helium-3 system based on the physical property measurement system (Quantum Design, PPMS). We employed the thermal relaxation technique to perform the specific heat measurements. The thermometers have been calibrated under different magnetic fields beforehand. The external field was applied perpendicular to the \(c\) axis of the single crystal.
The distribution of the Ni-dopant on a micro-scale was investigated by EDS measurements. The mapping image of Ni concentration and the chart of its distributions throughout an area of 38 $\mu$m $\times$ 28 $\mu$m for our sample are shown in Figures 1(a) and (b). The spatial resolution is 1.9 $\mu$m. The distribution shows a peak at about 0.058, which is very close to the average value. Consequently, this value is taken as the actual doping level. The SC transition of the obtained single crystal was checked by dc magnetization and specific heat measurements. As shown in Figure 2(a), the clear SC transition at about 14.8 K can be seen from both the $M$−$T$ and $C/T$−$T$ curves, indicating a high quality of the selected sample.

3. RESULTS AND DISCUSSION

We focus our attention on the SH data in the low temperature range to study the low-energy excitations. Generally speaking, in a system without magnetic order or magnetic impurities, the total SH is a simple integration of different components,

$$C(T) = \beta T^3 + C_{sc} + \gamma T. \quad (2)$$

The first term is the phonon SH, which is a very good approximation for the Debye model in the low temperature region. As mentioned in the introduction, the second term $C_{sc}$ is the electronic SH in the SC states excited by the thermal energy. This is the most important and concerned in our study, because its responding behavior to temperature supplies the information of the gap structure. The third term is quite complicated. Under zero field, it is a residual electronic term typically coming from small amounts of non-superconducting content in the sample or impurity scattering in some unconventional superconductors [3, 33]. With a field higher than the lower critical field, it reflects the contribution of the vortex states. Here we plot the raw data of SH as $C/T$.
of s-wave, the value of $C_{sc}$ is negligibly small in the low temperature region due to the exponential relation. For systems with point nodes, the contribution of $C_{sc}$ have the same $T^3$-dependence as the phonon term. In both cases, the $C/T \cdot T^2$ curves should show a linear behavior in the present low temperature region. Intuitively, the case of gap with line nodes is the best candidate. Consequently, we fitted our data using Eq. (2) based on the line nodal situation ($C_{sc} = \alpha T^2$). As represented by the solid lines, the fitting results are shown in Figure 3. One can see that the fitting curves coincide the experimental data very well. This gives a direct evidence for the presence of line nodes in the energy gap.

To further confirm the reliability of the analysis, we checked the obtained fitting parameters carefully. We show the field dependence of the parameters $\beta$, $\alpha$, and $\gamma$ in Figure 4 (a), (b), and (c), respectively. The value of $\beta$ is almost independent of field, which is reasonable because magnetic field can’t affect the phonon SH. Moreover, $\alpha(H)$ decreases monotonously with the increase of magnetic field up to 9 T. This is similar to that observed in overdoped Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$, and has been attributed to the combined effects imposed by the three-dimension dispersion of the line nodes on the Fermi surface and the destruction of V-shape of the density of states (DOS) at the nodes by the field. The residual value of $\gamma$ under zero field (denoted as $\gamma_0$) is estimated to be 0.75 mJ/mol K$^2$, which is also comparable to the reports in overdoped Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ and suggests a high sample quality. A clear increase of $\gamma$ with the field is observed. It is difficult to describe the field dependence of $\gamma$ using a simple formula due to the multi-band effect in the present system. Qualitatively, $\gamma$ increases more quickly in the system with a highly anisotropic gap. At the present stage, we could not evaluate the information supplied by the field dependent data, since the upper critical field $H_{c2}$ and the normal state electronic SH coefficient $\gamma_n$ are not clear.

The clear data and reasonable fitting parameters give us the confidence about the credibility of the present analysis process. More importantly, very few fitting parameters involve in this approach. However, we can’t obtain the precise location of the line nodes, since SH measurements integrate the information from different directions of the Fermi surface. Most likely, the magnitude and structure of the gaps on different Fermi surfaces are rather different. We must emphasize that such a multi-band does not destroy the validity of our analysis results because the electronic SH from the Fermi pockets with line nodes will prevail that from fully gapped pockets in the low temperature limit.

![FIG. 3](image_url) (color online) The raw data of the SH under different fields in the low temperature region. The data are shown in $C/T$ vs $T^2$ plot. The solid lines display the theoretical fitting (see text). The dashed straight line is the guide for the eyes.

![FIG. 4](image_url) (color online) Field dependence of the fitting parameters $\beta$ and $\alpha$ and $\gamma$. 
In summary, we studied the low-temperature specific heat on the Ba$_2$(Fe$_{1-x}$Ni$_{x}$)$_2$As$_2$ single crystal with $x = 0.058$. Before measurements, the single crystals were carefully annealed to improve the sample quality. We found a clear evidence for the presence of $T^2$ term from the raw SH data, which is consistent with the theoretical prediction for the superconductors with line nodes. Our result is very similar to the previous reports on the Co-doped system. Future investigations on other systems of the iron-pnictide superconductors are needed to check whether it’s a common feature for the presence of line nodes on the overdoped sides of the electron doped 122 system.

This work is supported by the Natural Science Foundation of China (No. 11204338) and the “Strategic Priority Research Program (B)” of the Chinese Academy of Sciences (No. XDB04040300 and XDB04030000). Gang Mu expresses special thanks to Grants-in-Aid for Scientific Research from the Japan Society for the Promotion of Science (JSPS) (Grant No. P10026).

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\[ K_{\text{FeAs Probed by Microwave}} \]

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