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Two-gap superconductivity in $R_2\text{Fe}_3\text{Si}_5$ ($R = \text{Lu and Sc}$)

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Abstract. High-quality single crystals of Lu$_2$Fe$_3$Si$_5$ and Sc$_2$Fe$_3$Si$_5$ are grown by the floating-zone method, and their temperature dependences of specific heat are measured down to 0.35 K. Both compounds show anomalously small jump in specific heat at the superconducting transition temperature, $T_c$, and large residual specific heat coefficient even at 0.2$T_c$, where BCS superconductor shows negligible electronic contribution. We also find drop in the specific heat coefficient below 0.2$T_c$. These characteristics are very similar to MgB$_2$, and temperature dependences of specific heat in both compounds are well reproduced by assuming two superconducting gaps. Upper critical field measurements confirm that both Lu$_2$Fe$_3$Si$_5$ and Sc$_2$Fe$_3$Si$_5$ are weakly one-dimensional superconductors.

1. Introduction

$R_2\text{Fe}_3\text{Si}_5$ ($R = \text{Sc, Y, Lu}$) contains nonmagnetic iron, and has one of the highest superconducting transition temperature, $T_c$, among iron-containing superconductors [1,2], except for the recently found iron-based oxypnictides [3]. The most remarkable properties of $R_2\text{Fe}_3\text{Si}_5$ is an anomalous temperature dependence of specific heat, $C(T)$, found in polycrystalline samples down to 1 K [4]. The jump of specific heat at $T_c$, $\Delta C/\gamma T_c$ ($\gamma_n$: electronic specific heat coefficient) is reduced from the BCS value, and there are apparent residual values of specific heat coefficients in the low-temperature limit. We have grown high-quality polycrystalline samples of Lu$_2$Fe$_3$Si$_5$ and confirmed these anomalies [5]. However, for more detailed discussion on the anomalous nature including anisotropy, high-quality single crystals are indispensable. In the present study, we have grown single crystals of Lu$_2$Fe$_3$Si$_5$ and Sc$_2$Fe$_3$Si$_5$, and measured temperature dependence of specific heat down to 0.35 K. All anomalous specific heat features are reproduced also in single crystals. In addition, we find the second drop of specific heat coefficient below 1 K. By assuming two energy gaps, we can reproduce $C(T)$ reasonably well. These facts strongly suggest that Lu$_2$Fe$_3$Si$_5$ and Sc$_2$Fe$_3$Si$_5$ are two-gap superconductors similar to MgB$_2$ [6]. Hall coefficient measurements and band structure calculation also support the multiband contributions to the normal state transport properties. We also discuss the anisotropic properties of $R_2\text{Fe}_3\text{Si}_5$, and significance of two-gap superconductivity in this system.

2. Experiments

Single crystals of Lu$_2$Fe$_3$Si$_5$ and Sc$_2$Fe$_3$Si$_5$ have been grown by the floating-zone technique using an image furnace. The starting rods for the single-crystal growth are prepared by melting stoichiometric ratio of constituent elements in an arc furnace. In some cases, transition temperatures of as-grown
crystals are lower and the transition widths are broad. Annealing at high temperature (~1250°C) for an extended period of time has improved the superconducting characteristics dramatically. Resistivity measurement is performed by the conventional four-probe technique under magnetic field up to 5 T, from which we estimate the anisotropic upper critical field. Hall coefficient is measured by the six-probe configuration. Magnetization measurements for the quality check of crystals are performed by using SQUID magnetometer (MPMS-XL5, Quantum Design). Specific heat is measured by the relaxation method with home-built electronics down to 0.35 K using 3He cryostat.

3. Results and Discussion

The inset of Fig. 1 shows the temperature dependences of \( \rho_{ab} \) (I//ab) and \( \rho_c \) (I//c) in \( \text{Lu}_2\text{Fe}_3\text{Si}_5 \). It is clear that \( \rho_c \) is lower than \( \rho_{ab} \), indicating that \( \text{Lu}_2\text{Fe}_3\text{Si}_5 \) is a weakly one-dimensional superconductor. This fact is further confirmed by measuring temperature dependence of upper critical field, \( H_{c2}(T) \), which is determined by the midpoint of resistive transition at a constant field. \( H_{c2}(T) \) for \( H//c \) and \( H//ab \) are plotted in Fig. 1. \( H_{c2}^{ab}(T) \) is larger than \( H_{c2}^{c}(T) \) with anisotropy parameter of \( \gamma \approx 2.0 \). This value of \( \gamma \) is consistent with the ratio of \( \rho_c \) and \( \rho_{ab} \), since \( \rho_{ab}/\rho_c=(H_{c2}^{c}(T)/H_{c2}^{ab}(T))^2 \). It should be noted that both \( H_{c2}(T) \)'s are linear in the measured temperature range. Recent measurement of \( H_{c2}(T) \) down to 0.4 K confirm this tendency \[7,8\]. Figures 2(a), (b) show temperature dependences of Hall coefficients for two configurations, \( I//c, H//ab \) and \( I//ab, H//c \). Hall coefficients for the two configurations are negative at room temperature. However, they show strong temperature dependences including sign change for \( I//ab, H//c \). Band structure calculations for \( \text{Lu}_2\text{Fe}_3\text{Si}_5 \) reveal the presence of three bands: two hole bands and one electron band. These facts strongly suggest that multiple carriers are responsible for the normal state properties in this system.
Figure 3 shows temperature dependence of specific heat in Lu$_2$Fe$_3$Si$_5$. Here, the electronic specific heat jump at $T_c$, $\Delta C_e$, is strongly reduced from the BCS value of $\Delta C_e/\gamma T_c=1.43$. At $0.2T_c$, where BCS superconductors show negligible electronic contribution, an appreciable $C_e/\gamma T_c$ is observed, which is followed by a second drop below $0.2T_c$. All these anomalous features of $C_e/\gamma T_c$ have been reported in MgB$_2$ with two distinct superconducting gaps originating from two-dimensional $\sigma$-band and three-dimensional $\pi$-band [6]. In a two-gap superconductor, electronic specific heat is given by the sum of two contributions with different gap values, $C_e(T) = x_1C_1(T) + x_2C_2(T)$. The solid line in Fig. 3 shows the best fit based on the two-gap model. The obtained two gap values for Lu$_2$Fe$_3$Si$_5$ are $2\Delta_1/k_B T_c=4.4$ and $2\Delta_2/k_B T_c=1.1$ with $x_1:x_2=47:53$. The Arrhenius plot of $C_e(T)$ shown in the inset of Fig. 3 shows the slope corresponding to the smaller gap. At the present state, which bands of the three are responsible for the large or the small gaps is not clear yet. From the analogy of MgB$_2$, however, we speculate that the existence of bands with different dimensionalities may play an important role in the two-gap superconductivity in Lu$_2$Fe$_3$Si$_5$.

Figure 4 shows the temperature dependence of upper critical field determined by the mid point of resistive transition for Sc$_2$Fe$_3$Si$_5$. Similar to the case of Lu$_2$Fe$_3$Si$_5$, $H_{c2}(T)$ is larger than $H_{c2}^{ab}(T)$, indicating that Sc$_2$Fe$_3$Si$_5$ is also a weakly one-dimensional superconductor. The anisotropy parameter $\gamma$ is 2.0, and it is weakly temperature dependent.
Figure 5 shows temperature dependence of specific heat in $\text{Sc}_2\text{Fe}_3\text{Si}_5$. The jump in specific heat is again reduced from the BCS value. The solid line in Fig. 5 shows the best fit based on the two-gap model similar to the case of $\text{Lu}_2\text{Fe}_3\text{Si}_5$. The obtained two gap values for $\text{Sc}_2\text{Fe}_3\text{Si}_5$ are $2\Delta_1/k_BT_C=3.53$ and $2\Delta_2/k_BT_C=1.7$ with $x_1:x_2=36:64$. It is natural to expect similar two-gap behavior in $\text{Sc}_2\text{Fe}_3\text{Si}_5$ since $\text{Sc}_2\text{Fe}_3\text{Si}_5$ keeps the same crystal structure as $\text{Lu}_2\text{Fe}_3\text{Si}_5$ with only slight difference in lattice constants.

Finally, we want to stress the uniqueness and importance of two-gap superconductivity in $R_2\text{Fe}_3\text{Si}_5$. In the case of MgB$_2$, well-established two-gap superconductor, the small size of single crystals is an obstacle for any detailed measurements of unconventional properties. In $R_2\text{Fe}_3\text{Si}_5$, crystals of mm size are readily available. The impurity effect is an important diagnosis to study the gap structure of unconventional superconductors. In $R_2\text{Fe}_3\text{Si}_5$, we can prepare the 100% solid solution of $\text{Lu}_2\text{Fe}_3\text{Si}_5$ and $\text{Sc}_2\text{Fe}_3\text{Si}_5$, where 3$d$ band of iron responsible for the superconductivity is intact. This would give us a unique opportunity for the study of the effect of inter-band scattering in two-gap superconductors, which is expected to suppress the larger gap and enhance the smaller gap until they merge together.

4. Summary

Temperature dependence of specific in $\text{Lu}_2\text{Fe}_3\text{Si}_5$ and $\text{Sc}_2\text{Fe}_3\text{Si}_5$ are investigated down to 0.35 K. Phenomenological two-gap model reproduces $C_e(T)$ reasonably well in both compounds. It is also found that both compounds are weakly one-dimensional superconductors.

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References