Multiband Superconductivity in CePt$_3$Si without Inversion Symmetry: $^{195}$Pt-NMR Study

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Abstract. We report on novel superconducting characteristics of the heavy fermion (HF) superconductor CePt$_3$Si without inversion symmetry through $^{195}$Pt-NMR study on a high quality single crystal with $T_c = 0.46$ K that is lower than $T_c \sim 0.75$ K for polycrystals. The observation of short and long components in a nuclear relaxation time $T_1$ has revealed the presence of inhomogeneities of superconducting characteristics even in a single crystal. By discriminating the clean domain from the disordered domains, we show that the intrinsic superconducting characteristics inherent to CePt$_3$Si can be understood in terms of the unconventional strong-coupling state with a line-node gap below $T_c = 0.46$ K. Furthermore, it was found that in some disordered domains that are inevitably contained in regardless of polycrystals or single crystals a conventional BCS $s$-wave superconducting state is realized below $T_c \sim 0.75$ K. We propose that these unusual superconducting and magnetic characteristics of CePt$_3$Si can be described by a multiband model on the basis of the experimental facts.

1. Introduction

CePt$_3$Si is the first heavy fermion (HF) superconductor without inversion symmetry along the c-axis, which exhibits superconductivity (SC) at $T_c = 0.75$ K in an antiferromagnetically ordered state below a Néel temperature of $T_N = 2.2$ K[1]. Although CePt$_3$Si has attracted considerable attention as the first superconductor without inversion symmetry theoretically[2], the $T_c$ value still remains a mystery experimentally[3, 4, 5]. Takeuchi and coworkers reported that a bulk SC at $T_c$ of a high-quality single crystal of CePt$_3$Si is 0.46 K from specific-heat measurements [6], which is remarkably lower than $T_c = 0.75$ K for a polycrystal [1]. Despite the lower $T_c$ of the sample, its quality is guaranteed by the extremely small value of a residual $\gamma$ term, i.e., the $T$-linear coefficient of the electronic specific heat well below $T_c$ is smaller than that for polycrystals [6]. In this high-quality single crystal, however, the resistivity drops to zero below 0.75 K, similar to the case of polycrystals. There still remains an underlying mystery, namely, the sample dependence of $T_c$ that prevents us from identifying any intrinsic SC properties of CePt$_3$Si.

2. Experimental

A high-quality single crystal (♯4) of CePt$_3$Si was grown by the Bridgman method in a Mo crucible, as described elsewhere [6]. The quality of this sample was guaranteed by a sharp jump
in the specific heat at $T_c = 0.46$ K, and by the small value of the residual $\gamma$ term, which was less than 34 mJ/K$^2$mol well below $T_c$. The resistivity of the sample began to decrease below 0.8 K; at 0.75 K, the resistivity became zero, as reported in literature [6]. In order to examine the possible disorder effects arising from lattice distortion, the NMR study was carried out by crushing coarse powder of polycrystal ($\# 3a$) into well-ground powder ($\# 3b$).

**Figure 1.** (Color online) (a) $^{195}$Pt-NMR spectra and (b) the recovery curves of $^{195}$Pt(2) nuclear magnetization $m(t)$ for the single crystal $\# 4$ and polycrystal $\# 1$ [1]. The fraction of long components in $T_1$ is larger for the polycrystal $\# 1$ than for the single crystal $\# 4$. (c)(d) It was also confirmed in the another polycrystal sample $\# 3a$ at both the Pt(2) and Si sites. Interestingly, the fraction of the long components becomes larger in the well-ground powder sample $\# 3b$ that is obtained by crushing the sample $\# 3a$. These facts reveal that the longer $T_1$ components arise from the domains affected by some disorders.

3. Results and discussions

We present the field-swept $^{195}$Pt-NMR spectra for the single crystal (4) and polycrystal (1) in Fig.1(a). Two inequivalent crystallographic Pt sites denoted by Pt(1) and Pt(2) [7] are distinguished by the difference in their Knight shifts. The NMR spectral widths for the single
crystals $\sharp 4$ is narrower than those for the polycrystal $\sharp 1$; from these spectral widths we can observe that the single crystal $\sharp 4$ has better quality on a microscopic level.

A recovery curve $m(t)$ of $^{195}$Pt nuclear magnetization ($I = 1/2$) is generally determined by a simple exponential function as $m(t) \equiv (M(\infty) - M(t))/M(\infty) = \exp(-t/T_1)$, when an electronic state is homogeneous over a sample. However, the $m(t)$ cannot be fitted by a single exponential function even in the high-quality sample $\sharp 4$ over the entire temperature ($T$) range, as shown in Fig. 1(b). Such behavior was also observed in the recovery curves at both the Pt(1) and Si sites, indicating the presence of some inhomogeneity in the electronic states over the sample, which are spatially distributed over a macroscopic scale. It is noteworthy that the fraction of long components in $T_1$ is larger for the polycrystal $\sharp 1$ than for the single crystal $\sharp 4$. In order to examine the possible disorder effects arising from lattice distortion, we compare the coarse powder polycrystal ($\sharp 3a$) with the well-ground powder ($\sharp 3b$), as shown in Figs. 1(c) and 1(d). The Pt and Si-NMR spectra of sample $\sharp 3b$ become broad, as indicated in the insets of the figures. Interestingly, the fraction of the long $T_1$ components of the well-ground powder sample $\sharp 3b$ becomes larger than that for the coarse powder $\sharp 3a$. These facts reveal that the longer components arise from the domains affected by some disorders such as impurities, crystal defects, local-lattice distortions, and so on. The recovery curve of the single crystal $\sharp 4$ is tentatively fitted by $m(t) = A_S \exp(-t/T_{1S}) + A_L \exp(-t/T_{1L})$, where $T_{1S}$ and $T_{1L}$ are short and long components in $T_1$, $A_S$ and $A_L$ are their fractions of the short and long components, respectively. It should be noted that $A_S \approx 0.7$ and $A_L \approx 0.3$ for the single crystal $\sharp 4$ correspond to the respective volume fractions of the homogeneous and disordered domains in the sample.

First we deal with a short component $T_{1S}$ that is more dominant for the high-quality single crystal($\sharp 4$), which represents an intrinsic property inherent to CePt$_3$Si. Figure 2 shows the $T$ dependence of $1/T_{1S}T$ at $H \sim 0.96$ T along the c-axis. The $T$ dependence decreases below $T_N = 2.2$ K and drops steeply below $T_c(H) \approx 0.35$ K at $H \sim 0.96$ T, which corresponds to the $T_c = 0.46$ K at $H = 0$ for the single crystal [6]. In the SC state, the $1/T_{1S}$ shows a $T^3$ dependence without a coherence peak just below $T_c$, followed by a $T_1T = const$-like behavior well below $T_c$. These facts are evidence of the unconventional superconducting nature of the intrinsic domain of CePt$_3$Si. As shown by the solid line in Fig. 2, the experimental result is well fitted by assuming a line-node gap model with $2\Delta_0/k_BT_c \approx 6$ and $N_{res}/N_0 \approx 0.41$, suggesting that strong-coupling SC emerges with line-node gap. It is expected that the large RDOS in the SC state is caused due to the impurity effect and/or the Doppler effect within the vortex core.

The long component $1/T_{1L}T$ for the single crystal $\sharp 4$ decreases below $T_N = 2.2$ K, and there is a marked decrease in $1/T_{1L}T$ with a tiny peak just below $T_c(H) \sim 0.6$ K that corresponds to the $T_c$ value in the field of $H \sim 0.96$ T for the polycrystal [1]. The result resembles that reported previously for the single crystal $\sharp 2$ [7], as shown by the dotted line in Fig. 2. Nevertheless, it is puzzling that $T_c = 0.75$ K for the disordered domains is higher than that for the homogeneous domains, namely, $T_c = 0.46$ K, despite the fact that disorders generally decrease $T_c$ in unconventional HF superconductors. In order to shed light on the SC characteristics of disordered domains, we examined a well-ground powder sample $\sharp 3b$ into which disorders were intentionally introduced. In the normal state, the $1/T_{1L}T$ of the disordered domain of the sample $\sharp 3b$ decreases below $T_N \sim 2.2$ K and stays a constant just above 0.8 K, as shown in Fig. 2. Remarkably, a distinct coherence peak appears just below $T_c \approx 0.8$ K, followed by an exponential-like decrease in $1/T_{1L}$ well below $T_c$. Unexpectedly, this result resembles that of $1/T_1T$ of the isostructural compound LaPt$_3$Si with $T_c = 0.6$ K, in which the $1/T_1T$ data are reproduced by an isotropic gap model with $2\Delta_0/k_BT_c \approx 2.9$ in a weak coupling regime of a BCS-type s-wave superconductor mediated by the electron-phonon interaction. Indeed, the increase of bulk $T_c$ is also corroborated by the specific heat measurement for the well-ground powder sample $\sharp 3b$. The effects of the disorders on thoroughly crushing the LaPt$_3$Si sample is not observed from the recovery curve and the $1/T_1$ data, which suggests that a conduction band
inherent to LaPt$_3$Si is not affected by the disorders.

In contrast with the SC characteristics that differ according to the quality of the samples, the antiferromagnetic (AFM) order with $T_N \sim 2.2$ K is robust against the disorders. These results suggest that the Fermi surfaces relevant with the onset of SC differs from that with the AFM order, and that the disorders suppress the unconventional SC emerging in the 4$f$-electrons-derived HF bands inherent to CePt$_3$Si. These facts allow us to account for by using a multiband model, that is, there exist three characteristic bands at least; the first one is a localized $f$-electron band far below the Fermi level that causes the long-range AFM order below 2.2 K. It should be noted that the large reduction in $1/T_1$ points to a possible opening of the gap at the Fermi level below $T_N$. The second one is the $f$-electrons-derived coherent HF bands that are derived from the formation of a periodic lattice of Ce atoms. The third one is a weakly correlated conduction band which leads to the onset of $s$-wave SC in LaPt$_3$Si. In the homogeneous domains in samples, the coherent HF bands, which are formed through the hybridization between $f$ electrons and conduction electrons, are responsible for the unconventional SC. Since the disorders break up the coherence of the periodicity of Ce atoms to suppress the unconventional SC inherent to the HF bands, eventually, the conduction bands in the inhomogeneous domains commonly found in LaPt$_3$Si may be responsible for the conventional $s$-wave SC possibly mediated by the electron-phonon interaction. In this model, if the sample were ideally homogeneous being free from any disorders, the conventional BCS $s$-wave SC taking place on the conduction bands may be unfavorable due to the pair-breaking originating from the strong electron correlation effect through an interband coupling with the HF bands. This is a possible explanation to settle several underlying issues reported thus far, for instance, the sample dependence of $T_c$.

4. Conclusion

$^{195}$Pt-NMR studies on CePt$_3$Si have revealed the presence of homogeneous and disordered domains even in a high-quality single crystal. Homogeneous domains inherent to CePt$_3$Si exhibit unconventional SC with a line-node gap below $T_c = 0.46$ K. In these domains, the coherent HF bands, which are formed through the hybridization between $f$-electrons and conduction electrons, are responsible for the unconventional SC. In contrast, the disordered domains reveal the conventional BCS $s$-wave SC with a high $T_c$ of 0.8 K, which is analogous to the SC state of LaPt$_3$Si. On the basis of these results, we propose that these unusual SC and magnetic characteristics of CePt$_3$Si can be described by a multiband model in which it is considered that the impurity scattering is caused by the disorders break up the 4$f$-electrons-derived coherent HF bands, but not others.

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