# NMR study of electronic state in $CePt_3Si$

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**Abstract**

$CePt_3Si$ is the first heavy fermion superconductor with a non-centrosymmetric structure center. In this article, we report the temperature dependence of spin-lattice relaxation rates at two Pt sites and one Si site in $CePt_3Si$. $1/T_1$ for both Pt sites between 2 K and 300 K and $1/T_1$ of Si between 3 K and 10 K($\sim T_{\mathrm{K}}$) are well explained by SCR theory for nearly antiferromagnet. $1/T_1$ for Si keeps nearly constant between 10 K and 100 K. Just below $T_{\mathrm{c}}$ no enhancement in $1/T_1$ was observed. The estimated value of superconducting gap is about $2\Delta = 3k_{\mathrm{B}}T_{\mathrm{c}}$.

*Key words:* NMR, superconductivity, $CePt_3Si$

Recently, Bauer *et al.* reported a new heavy fermion superconductor $CePt_3Si$ with Néel temperature ($T_{\mathrm{N}}$) and superconducting (SC) transition temperature ($T_{\mathrm{c}}$) of 2.2 K and 0.75 K, respectively.[1] The first feature of this compound is no spatial inversion center in the chemical unit cell, which favors spin singlet pairing in the superconductivity. The second feature is the large $\mathrm{d}H_{\mathrm{c2}}/\mathrm{d}T$ (= – 8.5 T/K) and $H_{\mathrm{c2}}$ (∼5 T), which suggest that Cooper pairs form out of the heavy quasiparticle state. The large $H_{\mathrm{c2}}$, which exceeds the estimated Pauli-Clogston limiting field, might be a signature for spin triplet pairing. A mixed spin singlet and triplet pairing state might be one of the candidate to answer this paradox.[2] To investigate the electronic state of this compound microscopically, we performed $^{29}$Si and $^{195}$Pt NMR experiments on non-annealed and annealed $CePt_3Si$ samples, hereafter referred to "as cast" and "annealed", respectively.

The starting materials of samples are Ce, Pt and Si with 99.9%(3N), 99.95%(3N5) and 6N purity, respectively. Polycrystalline samples were prepared from stoichiometric amounts of starting materials by arc melting in Ar atmosphere. The half of "as cast" sample was annealed successively at 950°C for 1 week. The powder X-ray diffraction measurement showed no extra phase in both "as cast" and "annealed" samples. A conventional pulsed spectrometer and a SC magnet were employed for the NMR measurements.

Shown in fig. 1 is the NMR spectrum of $^{195}$Pt for aligned powder of $CePt_3Si$. Under high magnetic field, powder of $CePt_3Si$ can be easily oriented to the magnetically easy-axis by some mechanical vibrations due to highly anisotropic susceptibilities. There exist two crystallographically inequivalent Pt sites in $CePt_3Si$: one is Pt(1) site which is located near face-centered position of *ac* plane in the unit cell, the other site Pt(2) is on *c*-axis together with Si site. The site occupancy-ratio for Pt(1) and Pt(2) is 2:1. As shown in this figure, two sharp peaks with an NMR intensity ratio of ∼2:1 were observed at 4.2 K. From the intensity ratio of them, the larger peak at higher field and the smaller peak at lower field are found to come from Pt(1) and Pt(2) sites, respectively. Below $T_{\mathrm{N}}$, however, their line widths for both Pt(1) and (2) sites become broader due to the internal field from antiferromagnetically ordered Ce magnetic moment. The bottom spectrum displays the overlapping NMR lineshape from both Pt sites at 1.4 K. Above 60 K, two peaks of Pt(1) and Pt(2) sites become closer each other, and then make a single peak above 80 K (not shown in the figures). On the other hand, $^{29}$Si NMR line shape stays sharp and symmetric above 4.2 K. No significant difference in the NMR spectra was observed between "as cast" and "annealed" samples in the whole $T$ range.

Fig. 2 shows the temperature ($T$) dependence of spin-lattice relaxation rate ($1/T_1$) for Si and Pt sites measured at peak positions in the NMR spectra. As shown in fig. 2, $1/T_1$ for both Pt sites between 2 K and 300 K and $1/T_1$ of Si between 3 K and 10 K($\sim T_K$) vary nearly as $T^{1/2}$, which is well explained by SCR theory for nearly antiferromagnet.[3] Above 80 K, two relaxation rates for both sites coincide each other, associated with the overlapping NMR line shapes. $1/T_1$ for Si keeps nearly constant between 10 K and 100 K, where the $T$-independence is governed by the low frequency fluctuations of Ce moments. An increase of $1/T_1$ above 100 K may be ascribed to the second excitation level ($\Delta$ =280 K) of CEF measured by the recent neutron scattering experiment.[4]

As shown in this figure, $1/T_1$ for Si in "as cast" is markedly enhanced with a distinct peak near the antiferromagnetic (AF) transition, reflecting a critical slowing down of the fluctuations of Ce moment. However, no peak in $1/T_1$ for "annealed" sample was observed, as displayed in the inset. This sample dependence is consistent with the result of susceptibility measurement: only "as cast" sample has a rapid increase of susceptibility just above $T_N$.[5] Below $T_N$, $1/T_1$ for both samples decrease rapidly probably due to the formation of AF gap at the Fermi surface. Since the overlapping for two peaks of Pt(1) and Pt(2) is seen in fig. 1, it is difficult to measure relaxation rates of Pt(1) and Pt(2) separately below $T_N$. So, the $T$ dependence of $1/T_1$ for Pt(1), where the AF fluctuations could be canceled crystallographically, was mainly measured at a peak position in the spectrum. In the normal state below $T_N$, $1/T_1$ decreases rapidly and then it becomes proportional to $T$, which means that the system is in the Fermi liquid state.

According to the published data[1], the SC transition $T$ is estimated as $T_c(H)$=0.6 K under a magnetic field of 1.4 T, where our NMR measurements were performed. Moreover, the coherence length in the present $T$ range and magnetic field is also estimated as 160 Å.[6] Considering the lattice parameters, the volume-ratio of vortex core in the total volume is estimated as ~50%. Thus, most of relaxation behaviors have the contributions from the normal fluxoid cores via the thermal fluctuation of fluxoids and the spin diffusion to vortex cores. In this case, $1/T_1$ decreases in proportion to $T$ through $T_c$. The long component is, of course, ascribed to the intrinsic relaxation in SC region. So, only the long component, which has a minor part in the nuclear recovery curve, was tentatively evaluated. As a result, no remarkable Hebel-Schrichter coherence peak was observed just below $T_c$, and $1/T_1$ decreases with decreasing $T$. Assuming the SC gap is isotropic, the value of SC gap is roughly estimated as about $2\Delta = 3k_BT_c$. The $T$ dependence of $1/T_1$ of Si for "annealed" sample is now in progress.

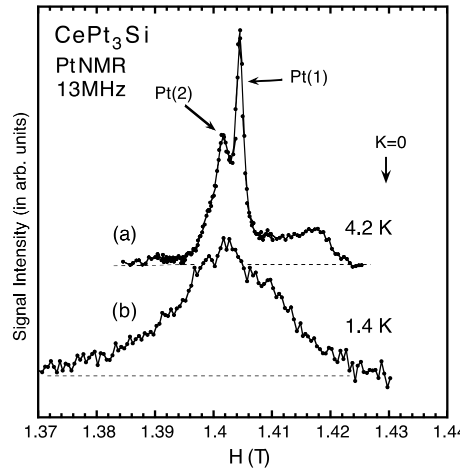


Fig. 1. Pt NMR spectrum of (a) magnetically oriented powder sample to magnetic field direction at 4.2 K, and (b) overlapping Pt spectra obtained in oriented powder sample at 1.4 K.

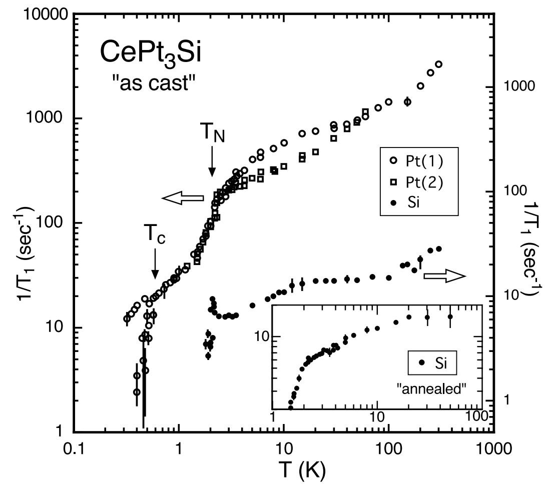


Fig. 2. Temperature dependence of spin-lattice relaxation rate ($1/T_1$) of Pt(1) site, Pt(2) site and Si site in "as cast" sample. Inset is that of Si site in "annealed" sample.

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