NMR studies in the half-Heusler type compound YbPtSb

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Abstract. 121Sb and 195Pt nuclear magnetic resonance (NMR) has been studied in the half-Heusler type compound YbPtSb to obtain information on local magnetic behavior. The characteristics of the localized 4f spins are observed in the Curie-Weiss type behavior of the Knight shifts $K$ for both $^{121}$Sb and $^{195}$Pt. From the slope of $K$-$\chi$ plots we estimated hyperfine coupling constants of -3.8 and -4.6 kOe/$\mu_B$ at Sb and Pt sites, respectively. It was found that the spin-echo decay rate $1/T_2$ of $^{121}$Sb shows a clear peaks at 10 K. Similar tendency was also observed in case of $^{195}$Pt. However, static properties do not show any anomalies near 10 K.

1. Introduction

The study of Yb-based compounds is an active area of research in strongly correlated electron systems. The 4f shell of trivalent Yb ion is one electron short of full occupation and it is often considered as the hole analog of trivalent Ce ion in which a lone electron resides in the 4f shell.

The huge linear-temperature specific heat coefficient, $\gamma$, in Yb-based compounds is one of the important issues in strongly correlated f electron systems. The extremely large $\gamma$ was first discovered in YbPtBi with $\gamma=8$ J/mol K$^2$ [1]. This value is an order magnitude more than in typical heavy-fermion materials. YbCo$_2$Zn$_{20}$ is also known to have a huge $\gamma=8$ J/mol K$^2$ [2] and the pressure-induced magnetic transition was suggested [3]. The important question is whether the massive electronic state observed in these Yb-base compounds can be associated with the existence of very heavy electrons or not.

YbPtSb forms the half-Heusler MgAgAs structure (space group F$\bar{4}3m$), which is isostructural to YbPtBi. The magnetic susceptibility of YbPtSb obeys the Curie-Weiss law with the effective magnetic moment, $\mu_{\text{eff}}=4.4\mu_B$, which is close to the free Yb$^+$ value (Yb$^{3+}:\mu_{\text{eff}}=4.54\mu_B$). The Weiss temperature, $\Theta$, derived from between 5 and 300 K is estimated to be $\Theta=-5.3$ K [4]. The electrical resistivity shows the metallic behavior. The value of $C_\Omega/T$ exceeds 6 J/mol K$^2$ at low temperatures [4, 5]. Here $C_\Omega$ is the electronic part of the specific heat. Low temperature specific heat and resistivity measurements suggested the magnetic ordering at 0.4 K [6]. It was also reported that an elastic softening of the longitudinal elastic constant $C_{11}$ below around 20 K and its strong field dependence [7].

2. Experimental

Single crystals of YbPtSb were grown from Sb-flux method. For performing the nuclear magnetic resonance (NMR) experiment, several single crystals were crushed into powder. NMR
measurements were carried out using a conventional phase-coherent pulse spectrometer in the temperature range between 1.5 and 250 K. The magnetic susceptibility was measured using a superconducting quantum interference device magnetometer (Quantum Design, MPMS-5) at applied magnetic field of 4.5 T.

3. Results and discussion

Figure 1 and 2 show the temperature dependence of the $^{121}\text{Sb}$ (nuclear spin $I=5/2$) and $^{195}\text{Pt}$ ($I=1/2$) NMR spectra obtained by sweeping external field at a fixed frequency of 42.5 MHz. At high temperatures $^{195}\text{Pt}$ NMR spectrum is a single Gaussian-type. On the other hand we observed two spectra overlap with a narrow peak and a broad one for $^{121}\text{Sb}$. These results are clearly seen in the inset of Fig. 1 and 2. We measured the magnetic field, $H$, dependence of $^{121}\text{Sb}$ NMR spectra (not shown). The line width of the narrow peak is proportional to $H$, whereas that of the broad one is independent of $H$. These results suggest that former is due to the inhomogeneous distribution of the Knight shift and latter is due to the inhomogeneous distribution of the electric field gradient (EFG). We suppose that two spectra overlap for $^{121}\text{Sb}$ originates from the local off-stoichiometry of Pt, as reported in other half-Heusler compounds [8].

The half-Heusler compound YbPtSb crystallizes in the face-centered cubic structure. Yb and Sb atoms are located at $4a(0, 0, 0)$ and $4b(1/2, 1/2, 1/2)$ positions forming rock salt structure arrangement and Pt atoms are located at one of the cube center positions $4c(1/4, 1/4, 1/4)$ leaving the other $4d(3/4, 3/4, 3/4)$ empty. However, it is likely that there are some voids at $4c$ positions or interstitial occupancies at $4d$ position in the present sample. The narrow NMR
spectrum of $^{121}\text{Sb}$ originates from $4b$ sites where the neighboring $4c$ position is occupied by Pt atom. Consequently the line width of $^{121}\text{Sb}$ should be narrow reflecting the cubic local symmetry of Sb site. On the other hand, there is local EFG experienced by those nuclei in the vicinity of crystalline defects (such as vacancies or interstitial occupancies), which break the local cubic symmetry of the Sb atoms. As a result, Sb NMR spectra become broad. $^{195}\text{Pt}$ spectra are not affected by local EFG owing to the lack of the nuclear quadrupole moment.

The NMR resonance lines of $^{121}\text{Sb}$ and $^{195}\text{Pt}$ shift to higher field side and broaden on cooling. We determined the $^{121}\text{Sb}$ and $^{195}\text{Pt}$ Knight shift ($^{121}K$ and $^{195}K$, respectively) from the peak position of the spectrum. Figure 3 displays the temperature dependence of $^{121}K$ and $^{195}K$. Both $^{121}K$ and $^{195}K$ are large, negative and follow the Curie-Weiss behavior of the bulk susceptibility, $\chi$. The inset of Fig. 3 displays the Knight shift vs $\chi$ plot with the temperature as an implicit parameter. $^{121}K$ and $^{195}K$ are proportional to $\chi$, indicating that the Knight shift is mainly due to a transferred hyperfine field from localized Yb 4f-moments. Note that we used $M/H$ as $\chi$ measured at 4.5 T, which is close value of magnetic field $H$ to the present NMR measurement. In fact $H$ dependence of the magnetization, $M$, does not show the linear relation at low temperatures. The slopes of the Knight shift vs $\chi$ yield hyperfine coupling constants of $^{121}A=-3.8$ kOe/$\mu_B$ and $^{195}A=-4.6$ kOe/$\mu_B$ for $^{121}\text{Sb}$ and $^{195}\text{Pt}$, respectively.

As temperature approaching $T^* \equiv 10$ K the $^{121}\text{Sb}$ NMR lines lose intensity (Fig. 1) due to highly enhanced spin-echo decay rate $1/T_2$. Figure 4 shows the temperature dependence of $1/T_2$. $T_2$ was determined by fitting the single exponential function to the spin-echo decay curve. Although $1/T_2$ of $^{121}\text{Sb}$ is almost independent of temperature above 50 K, it exhibits a strong peak at 10 K. Unfortunately reliable $1/T_2$ values of $^{195}\text{Pt}$ could not be obtained near 10 K due to the poor signal-to-noise ratio. Each value of $1/T_2$ and $T^*$ is unaffected by $H$. In order to obtain more information about this anomaly at 10 K, we have checked the static physical properties
in YbPtSb. In spite of careful measurement of $M$, any anomalies were not detected around $T^*$ in our experimental accuracy. Moreover, specific heat and resistivity measurements under $H$ do not show anomalous behavior [5]. The charge glass-like state is suggested by an elastic softening of the longitudinal elastic constant and its logarithmic temperature dependence below around 20 K [7]. However, the NMR Knight shift, following the Curie-Weiss law, indicates the trivalent Yb ions. The relevance of the elastic softening to the anomalous $1/T_2$ behavior is not clear now.

$^{121}$Sb has both a quadrupole and magnetic moments while $^{195}$Pt has only magnetic moment. Thus anomalous $1/T_2$ behavior observed in both nuclei can be understood to be the magnetic origin. In this case, $1/T_2$ is affected by the magnetic field fluctuation both parallel and perpendicular to the static magnetic field direction around observed nuclei. On the other hand, the spin-lattice relaxation rate $1/T_1$ is affected by the fluctuation only perpendicular to the static magnetic field. $1/T_1$ measurement is in progress to clarify an anisotropy of the fluctuations.

The isostructural compound YbPtBi exhibit the drastic enhancement of $1/T_2$ at low temperatures, accompanying the similar behavior of the spin-lattice relaxation rate $1/T_1$, but the peak of $1/T_2$ was not reported down to 35 K [9]. It is a open question whether the rapid increase of $1/T_2$ at low temperatures is inherent in the formation of the massive electron state in the Yb-based half-Heusler type compound or not.

4. Conclusion

We have presented a NMR investigation of YbPtSb which exhibits a sharp upturn of $C_{el}/T$ at low temperatures. $^{121}K$ and $^{195}K$ decrease with temperature. The Knight shifts show the linear relation with $\chi$, indicating that the $K$ is mainly due to a transferred hyperfine field from localized Yb 4f-moments. It appears that, in contrast to the temperature independent behavior above 50 K, $1/T_2$ of $^{121}$Sb shows the divergent increase around 10 K and decreases at low temperatures. However, no anomalies were detected in the temperature dependence of the NMR line width, $\chi$ and $C_{el}$ at present. To clarify the origin of the $1/T_2$, further experiment will be needed.

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