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Hyperfine interactions in the itinerant system $UFeGa_5$

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ABSTRACT

We report ^{69}Ga NMR measurements on the itinerant compound $UFeGa_5$ using a single crystal sample. Hyperfine coupling constants at both the Ga(1) and Ga(2) sites are determined for $H\|a$ and c-axes based on Knight shift versus susceptibility plots. The T-dependence of the spin-lattice relaxation time (T_1) has been determined at both sites for $H\|a$ and *c-axes.* From these quantities, the magnetic fluctuations are estimated for both axes. The complex nature of the hyperfine interactions is discussed.

1. Introduction

Recently, new superconductors have been discovered in Pu-based, $HoCoGa_5$(1 1 5)-structure compounds: $PuCoGa_5$ (T_c = 18.5 K) [1] and $PuRhGa_5$ (T_c = 9 K) [2]. These discoveries have stimulated a great deal of interest in actinide compounds, since T_c for these compounds is quite high compared with Ce-based 115 superconducting compounds (e.g. $T_c = 2.1$ K in $CeRhIn_5$ under pressure [3]), indicating a possible non-phonon based pairing mechanism. In fact, d-wave superconductivity is suggested by spin-lattice relaxation time (T_1) measurements in both $PuCoGa_5$ [4] and $PuRhGa_5$ [5]. In contrast, magnetically ordered or paramagnetic states, but no superconductivity, has been found in U- and Np-based 115 compounds up to now [6].

In the 115 actinide compound family, various ground states have been found to occur, e.g. antiferromagnet (AFM) in $UPtGa_5$ ($T_N = 25$ K), $NpFeGa_5$ ($T_N = 117$ K), and $NpCoGa_5$ ($T_N = 47$ K); paramagnet (PM) in $UFeGa_5$ and $UCoGa_5$; and superconducting (SC) in $PuRhGa_5$ ($T_c = 9$ K). Among these, $UFeGa_5$ is considered to be a Pauli paramagnet with weak magnetic correlations [7]. In this report, NMR hyperfine coupling parameters and spin-relaxation rates ($1/T_1$) are reported for $UFeGa_5$. Since the magnetic correlations are weak in this compound, it is not necessary to consider the q-dependence of the dynamical susceptibility. Taking advantage of this simplification, a quantitative estimate for the magnetic fluctuations is derived here for $UFeGa_5$.

2. Experimental

High-quality single crystal samples were prepared by the Ga-flux method [6]. ^{69}Ga NMR measurements have been performed using a conventional pulsed spectrometer with a 12 T superconducting magnet. Both $\pi/2-\pi$ and $\pi/2-\pi/2$ pulse sequences were used to excite nuclear spin-echo signals. The NMR spectra which we analyse are field-sweep spectra taken at constant frequency, using periodic digital averaging of the nuclear spin-echo signals. Spin-lattice relaxation time (T_1) data were also obtained using digital averaging of spin-echo signals. These relaxation times have been determined using both the central ($m = \frac{1}{2} \leftrightarrow -\frac{1}{2}$) and the satellite ($m = -\frac{1}{2} \leftrightarrow -\frac{3}{2}$) transitions, yielding results which agree within expected errors.

3. Static susceptibility and Knight shift

Fig. 1 shows the T-dependence of the static susceptibility χ for $H\|$a and c-axes. The T-dependence of χ is weak for both axes, in agreement with a previous report [8], indicating that this compound is an itinerant Pauli paramagnet with weak magnetic exchange enhancement.

Fig. 2 shows field-sweep ^{69}Ga NMR spectra for the central transition of the Ga(1) and Ga(2) sites. The observed narrow peaks (resonance half-widths <0.1 kOe) attest to the high-quality of the sample. The Knight shift is determined from the central and satellite transition peaks in order to take account of nuclear quadrupolar effects. The Knight shifts at the Ga(1) (4c site) and the Ga(2) (4i site) show a T-dependence similar to that of χ, as shown in Fig. 3. As a result, Knight shift versus static susceptibility plots ($K-\chi$

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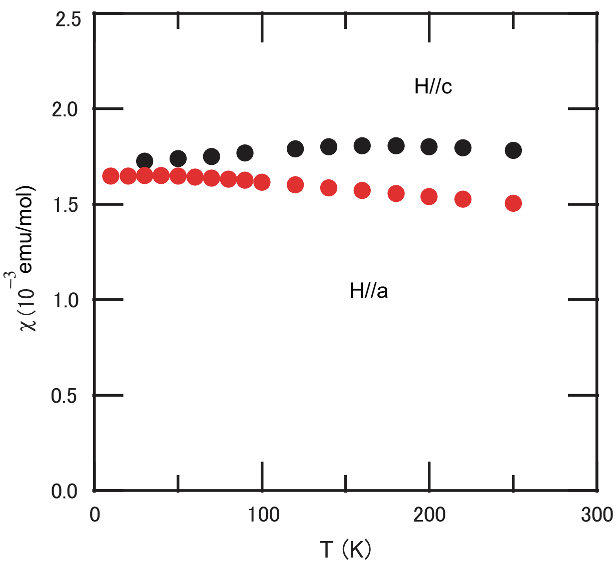

Fig. 1. *T*-dependence of the static susceptibility for $H\|a$-axis (χ_a) and $H\|c$-axis (χ_c).

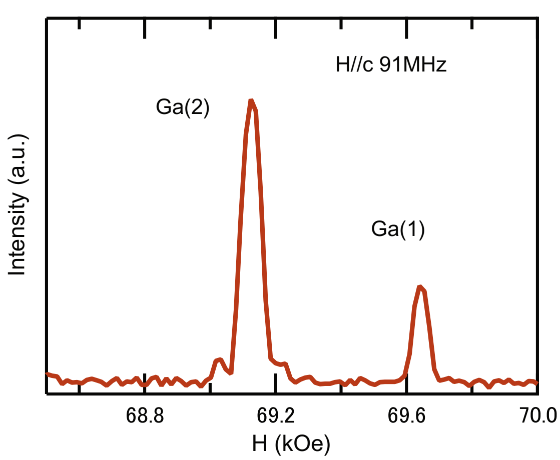

Fig. 2. Field-sweep [69]Ga NMR spectra at 91 MHz for the central transitions ($m = \frac{1}{2} \leftrightarrow -\frac{1}{2}$) of the Ga(1) and Ga(2) sites ($H\|c$-axis).

plots) are linear for all cases. For example, $K - \chi$ plots for $H\|c$-axis are presented in Fig. 4. From the slopes of such $K - \chi$ plots, the hyperfine coupling constants are obtained.

4. Hyperfine coupling constants and the spin-lattice relaxation time

Table 1 shows the hyperfine coupling constants A_α determined from static susceptibility versus Knight shift plots ($K - \chi$ plots). Here, A_α is determined from the slope of the K_α vs. χ_α plot (α: a, b, c-axes). The isotropic part of the hyperfine coupling constant $A_{\rm iso}$ is defined as $A_{\rm iso} \equiv (A_a + A_b + A_c)/3$. The magnitude of the hyperfine coupling constant is rather large, indicating that transferred spin polarization from U-5f to Ga-4s,p orbitals is the main origin of hyperfine coupling here.

Fig. 5 shows the *T*-dependence of $1/T_1T$ at the Ga(1) and Ga(2) sites for $H\|$a and *c-axes*. The observed $1/T_1T$ is only weakly *T*-dependent. This Korringa-like behaviour is consistent with the Pauli paramagnetic nature of this compound. In fact, the magnitude of $1/T_1T$ for $UFeGa_5$ is less than one-tenth that of the antiferromagnetic compound $NpCoGa_5$ [7], indicating that magnetic correlations are weak in $UFeGa_5$. In addition, $1/T_1T$ is nearly isotro-

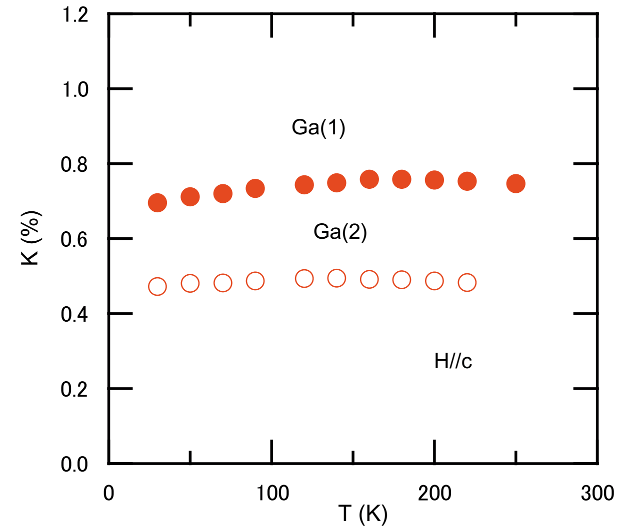

Fig. 3. *T*-dependence of the [69]Ga Knight shift at the Ga(1) and Ga(2) sites for $H\|c$-axis.

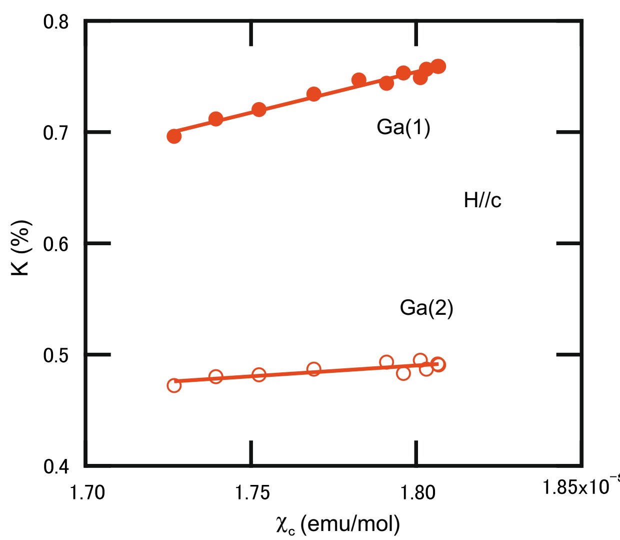

Fig. 4. [69]Ga Knight shift *K* versus static susceptibility χ ($K - \chi$) plot for the Ga(1) and Ga(2) sites with $H\|c$-axis. The solid lines are obtained from least-squares fits.

Table 1
Hyperfine coupling constants A_α in kOe/μ_B for the Ga(1) and Ga(2) sites in $UFeGa_5$ obtained from $K_\alpha - \chi_\alpha$ plots (α: a, b, c-axes). From their tetragonal local symmetry, $A_a = A_b$ at the Ga(1) sites.

	Ga(1)	Ga(2)
A_a	17	17
A_b	17	19
A_c	54	14
$A_{\rm iso}$	29	17

pic, implying that magnetic fluctuations are not strongly anisotropic in this compound. The dynamical susceptibility ${\rm Im}\,\chi(q, \omega_n)$ and $1/T_1T$ are related by

$$(1/T_1T)_\| = \frac{\gamma_n^2 k_B}{2} \sum_q A(q)_\perp^2 \frac{{\rm Im}\chi_\perp(q,\omega_n)}{\omega_n}, \quad (1)$$

where ω_n is the NMR frequency, the subscription $\|$ and $\perp$ indicate crystal axes which are orthogonal each other. In the present case,

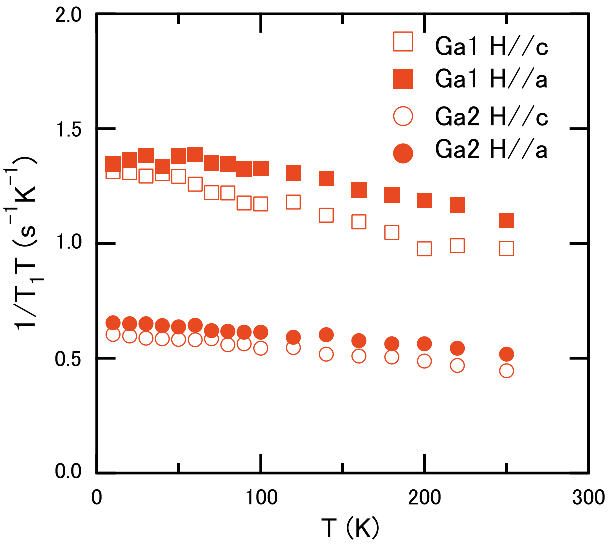

Fig. 5. *T*-dependence of $1/T_1T$ for $H\|a$ and $H\|c$-axes at the Ga(1) and Ga(2) sites.

the q-dependence of $\mathrm{Im}\,\chi(q,\omega_n)$ can be ignored, since magnetic correlations are not strong, then we find

$$(1/T_1T)_\parallel = \frac{\gamma_n^2 k_B}{2\omega_n} \mathrm{Im}\,\chi_\perp(q,\omega_n) \sum_q A(q)_\perp^2. \tag{2}$$

If q-dependence of $A(q)_\perp$ can be ignored, the following equation for $\mathrm{Im}\,\chi(q,\omega_n)$ is obtained using $A_\perp = A(0)_\perp$ which is presented in Table 1

$$\mathrm{Im}\,\chi_\perp(q,\omega_n) = \frac{2\omega_n}{\gamma_n^2 k_B} \frac{1}{T_1 T_\parallel A_\perp^2}. \tag{3}$$

The dynamical susceptibility $\mathrm{Im}\,\chi(q,\omega_n)$ estimated from the Ga(1) data should be same as that from the Ga(2) data, since the origin of $\mathrm{Im}\,\chi(q,\omega_n)$ is the U-5f magnetism. However, if we use the anisotropic hyperfine coupling constant A_α (α: a,b,c-axes), $\mathrm{Im}\,\chi_{\parallel,\perp}(q,\omega_n)$ estimated from the Ga(1) data is different from that from Ga(2) data. This deviation indicates that a q-dependence of $A(q)$ for the Ga(1) and G(2) sites should be considered, and/or q-dependence of $\mathrm{Im}\,\chi(q,\omega_n)$ may be rather large even in this Pauli paramagnetic like compound. Otherwise, it may be possible that orbital fluctuations are also important in addition to the spin-fluctuations. Further investigation is necessary to understand the hyperfine coupling and spin-lattice relaxation at the Ga(1) and Ga(2) sites in a consistent way.

5. Conclusion

The *T*-dependence of the Knight shift (K) and spin-lattice relaxation time (T_1) have been measured in a single crystal of $UFeGa_5$. The hyperfine coupling constants are determined from $K-\chi$ plots. Since K and $1/T_1T$ have a weak *T*-dependence, this compound is considered to be a Pauli paramagnet with weak magnetic interactions. In order to have a consistent picture for the observed hyperfine coupling constants and spin-lattice relaxation times, a q-dependence of hyperfine coupling constant and dynamical susceptibility may be considered here.

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