

Neutron Diffraction Study of $5f$ Itinerant Antiferromagnet UPtGa₅ and UNiGa₅

Koji Kaneko ^{a,1} Naoto Metoki ^{a,b}, Gerard H. Lander ^{a,c}, Nicholas Bernhoeft ^d, Yoshihumi Tokiwa ^{a,e}, Yoshinori Haga ^a, Yoshichika Ōnuki ^{a,e}, Yoshinobu Ishii ^a

^a Advanced Science Research Center, Japan Atomic Energy Research Institute, Tokai, Naka, Ibaraki 319-1195, Japan

^b Department of Physics, Tohoku University, Aoba, Sendai 980-8578, Japan

^c European Comission, JRC, Institute for Transuranium Elements, Postfach 2340, D-76125, Karlsruhe, Germany

^d DRFMC, CEN-Grenoble, F-38054, Grenoble, France

^e Graduate School of Science, Osaka University, Toyonaka, Osaka 560-0043, Japan

Abstract

Magneto-striction and magnetic form factors in $5f$ itinerant antiferromagnet UNiGa₅ and UPtGa₅ are studied by means of neutron scattering. Remarkable magneto-striction was observed around T_N , indicating large spin-orbit coupling in the itinerant system. The orbital magnetic moment is found to be strongly suppressed due to the hybridization of uranium $5f$ with Ga-4p electron.

Key words: UTGa₅, magnetic form factor, magneto-striction, itinerant antiferromagnetism

The f electron systems attract much interest because of the unconventional superconductivity and the coexistence with the magnetic ordering around the quantum critical point. Recent studies reported a new series of heavy fermion superconductor CeTIn₅ (T:Rh, Co, Ir)[1–3], which is followed by the discovery of high- T_C heavy fermion superconductor PuCoGa₅[4]. On the other hand, the iso-structural compounds UT'Ga₅ exhibit strong itinerant character of $5f$ electrons, UT'Ga₅ with T'=Fe, Co, Ru, Rh, Os, Ir exhibit Pauli paramagnetic behavior, while UNiGa₅, UPdGa₅, and UPtGa₅ are itinerant $5f$ antiferromagnet which show the characteristic weak magnetic susceptibility and a small ordered moment.[5] Our recent neutron scattering study revealed the magnetic structures in UNiGa₅ and UPtGa₅. The difference in the magnetic structure of these iso-electronic compounds were discussed in terms of the orbital ordering. In the present study we report the existence of magneto-striction and suppres-

sion of the orbital magnetic moment in UNiGa₅ and UPtGa₅ to shed light on the nature of the itinerant antiferromagnetism with uranium $5f$ electrons.

The neutron powder diffraction data were measured on HRPD at the research reactor JRR-3 in Japan Atomic Energy Research Institute. The magnetic form factors were measured by the triple-axis spectrometers TAS-1 and TAS-2. The details of sample preparation were published elsewhere.[6,8]

The lattice constants a and c are plotted as a function of temperature in Figs. 1 and 2 for UNiGa₅ and UPtGa₅, respectively. The lattice constants were obtained by Rietveld analysis using RIETAN-2000[9]. Small reliable factors typically $R_{wp}=5.48$, $R_e=4.82$, $R_F=1.59$ and $S=1.16$ for UPtGa₅ indicate the correctness of our analysis with the accuracy of lattice constants in the order of 10^{-4} Å. UNiGa₅ showed lattice expansion/contraction in the antiferromagnetic state ($T_N=86$ K) along the a - and c -axis, respectively. In contrast, the lattice expands both in the a and c directions below $T_N=26$ K in UPtGa₅. The existence of the remarkable magneto-striction is indicative of

¹ Corresponding author.
E-mail: kanekok@neutrons.tokai.jaeri.go.jp

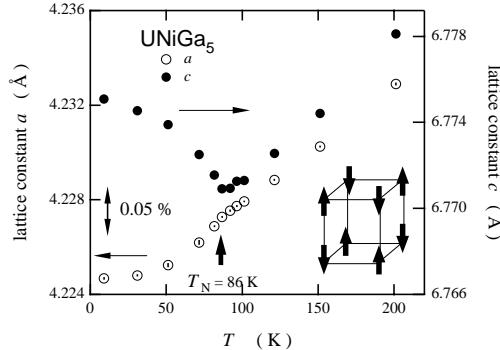


Fig. 1. Temperature dependence of lattice constants, a (open circle) and c (closed circle) in UNiGa_5 . The arrow indicates the transition temperature of $T_N=86\text{ K}$.

the large spin-orbit coupling. The opposite sign of the magneto-striction in the direction can be reasonably understood from the magnetic structure as shown in the inset of Figs. 1 and 2. The in-plane nearest-neighbor coupling is antiferromagnetic in UNiGa_5 , while that coupling is ferromagnetic in UPtGa_5 .

Figure 3 shows the magnetic form factor observed in UNiGa_5 . $\mu f(\mathbf{Q})$ can be described by the sum of Bessel's function within the dipole approximation,

$$\mu f(\mathbf{Q}) = \mu(\langle j_0 \rangle + C_2 \langle j_2 \rangle + \dots) \quad (1)$$

where μ is the total magnetic moment and \mathbf{Q} is the momentum transfer. The observed form factor clearly deviates from the one for U^{3+} free ion shown as dotted line. The fitted result using Eq. 1 is shown by the solid lines with $\mu=0.87(4)\mu_B$ and $C_2=2.57(21)$. It means that the contribution of the orbital moment $\mu_L/\mu_S = -1.64$ is suppressed from the value for free ion of $\mu_L/\mu_S = -2.56$. This suppression is most probably due to the hybridization of $5f$ electrons with $\text{Ga-}4p$ electrons. Nevertheless, it is noteworthy that a large orbital moment exists in the itinerant antiferromagnet based on uranium $5f$ electrons, which is consistent with the existence of magneto-strictions. A smaller suppression of $\mu_L/\mu_S = -2.1$ was also observed in UPtGa_5 .

The suppression of the orbital moment was reported in an itinerant $5f$ antiferromagnet UGa_3 as well. The orbital contribution $\mu_L/\mu_S = -1.66$ is very close to that obtained for UNiGa_5 . Note that UNiGa_5 and UGa_3 show a very flat magnetic susceptibility for $T > T_N$, while a weak Currie-Weiss behavior with a small effective moment $\mu_{\text{eff}} = 1.8\mu_B$ was observed in UPtGa_5 . It roughly means that the strength of the hybridization in UNiGa_5 might be comparable with UGa_3 but stronger than that in UPtGa_5 . Therefore, we conclude that the quenching of the orbital moment is correlated with the itinerancy of $5f$ electrons.

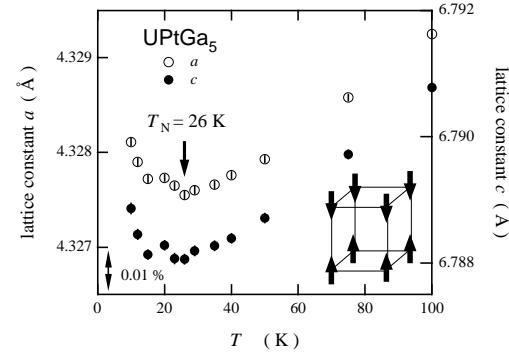


Fig. 2. Temperature dependence of lattice constants, a (open circle) and c (closed circle) in UPtGa_5 . The arrow indicates $T_N=26\text{ K}$.

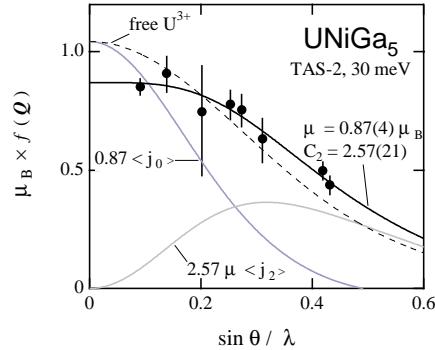


Fig. 3. Magnetic form factor of UNiGa_5 at 4 K .

References

- [1] R. Movshovich, M. Jaime, J. D. Thompson, C. Petrovic, Z. Fisk, P. G. Pagliuso, J. L. Sarrao, Phys. Rev. Lett. **86** (2001) 5152.
- [2] H. Heggar, C. Petrovic, E. G. Moshopoulou, M. F. Hendley, J. L. Sarrao, Z. Fisk, J. D. Thompson, Phys. Rev. Lett. **84** (2000) 4986.
- [3] C. Petrovic, R. Movshovich, M. Jaime, P. G. Pagliuso, M. F. Hundley, J. L. Sarrao, Z. Fisk and J. D. Thompson, Europhys. Lett. **53** (2001) 354.
- [4] J. L. Sarrao, L. A. Morales, J. D. Thompson, N. J. Curro, Bull. Am. Phys. Soc. **47** (2002) 164.
- [5] Yu. N. Grin, P. Rogl, K. Hiebl, J. Less-Common Met. **121** (1986) 497.
- [6] Y. Tokiwa, Y. Haga, E. Yamamoto, D. Aoki, N. Watanabe, R. Settai, T. Inoue, K. Kindo, H. Harima, Y. Ōnuki, J. Phys. Soc. Jpn. **70** (2001) 1744.
- [7] Y. Tokiwa, Y. Haga, N. Metoki, Y. Ishii, Y. Ōnuki, J. Phys. Soc. Jpn. **71** (2002) 725.
- [8] Y. Tokiwa, S. Ikeda, Y. Haga, T. Okubo, T. Iizuka, K. Sugiyama, A. Nakamura, Y. Ōnuki, J. Phys. Soc. Jpn. **71** (2002) 845.
- [9] F. Izumi and T. Ikeda, Mater. Sci. Forum **321-324** (2001) 538.
- [10] A. Hiess, F. Boudarot, S. Coad, P. J. Brown, P. Burlet, G. H. Lander, M. S. S. Brooks, D. Kaczorowski, A. Czopnik, R. Troc, Europhys. Lett. **55** (2001) 267.