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Magnetic order of UGa_3 investigated by means of neutron scattering under uniaxial pressure

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Abstract

The magnetic moment orientation of UGa_3 has been revealed by means of both polarized and unpolarized neutron beam experiments under uniaxial pressure. The uniaxial pressure induces a anisotropic domain structure whose populations are quantitatively obtained by polarized beam experiments. We have concluded that the magnetic moment of UGa_3 is along the [011] direction.

1. Introduction

The uranium intermetallic compounds UX_3 demonstrate a wide variety of magnetic properties [1], which depend on the strength of the effect of hybridization between the 5f-electron state of the U atom and the s-, p-, d-electronic states of the X atom. There are many uncertainties as regards the origin of these phenomena. Among the UX_3 compounds, special attention has been paid to UGa_3 because experiments and band structure calculations strongly suggested an itinerant nature for the magnetism of UGa_3. UGa_3 orders below $T_N = 67$ K with a type-II antiferromagnetic structure in which alternate (111) ferromagnetic planes of U moments are coupled antiferromagnetically [2, 3]. The ordered moment is $\sim 0.6\ \mu_B$/U atom. UX_3 systems crystallize in a highly symmetric structure, of cubic $AuCu_3$ type. Therefore, the neutron diffraction measurement usually gives no conclusive information on the total magnetic moment orientation for UX_3 compounds because of their multidomain structures.

In this study, we apply weak uniaxial pressure to single-crystalline UGa_3 so as to induce anisotropic domain structure, which should provide clues as to the magnetic moment orientation of UGa_3. We demonstrate that the combination of uniaxial pressure and polarization analysis enables us to quantitatively estimate the domain population.

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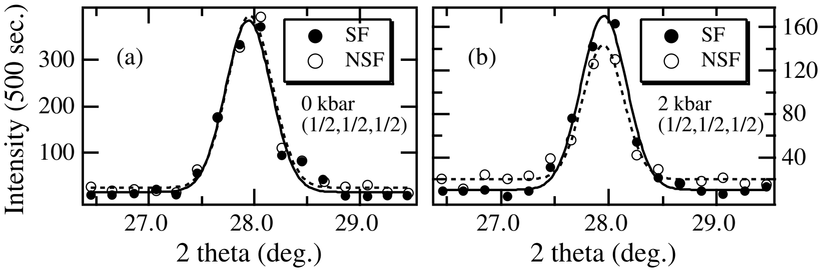

Figure 1. Polarization analysis of the (1/2, 1/2, 1/2) magnetic reflection at (a) 0 kbar and (b) 2 kbar. Measurements were performed at 8 K.

2. Experimental procedures

Experiments were carried out on the triple-axis spectrometer TAS-1 installed at the research reactor JRR-3M in Japan Atomic Energy Research Institute. The scans were performed in the (h, l, l) plane, and the uniaxial pressure was applied along the $[01\bar{1}]$ axis up to 2 kbar. The sample was shaped to a thin disc with parallel surfaces which are perpendicular to the $[01\bar{1}]$ axis, and put between the Cu–Be piston cylinders mounted in a clamp-type pressure cell. The surface area of the sample was 3×3 mm^2 and the thickness was 1 mm. Both polarized and unpolarized beam experiments were performed with an incident energy $E_i = 14.7$ meV. In the polarized beam experiments the neutron beam was polarized by a Heusler crystal. The incident neutron beam polarization was perpendicular to the scattering plane—that is, in vertical field (VF) geometry. In this configuration all the magnetic components in the scattering plane (hereafter referred to as in-plane components) are detected in the spin-flip (SF) channel, and the magnetic component perpendicular to the scattering plane (the out-of-plane component) is probed in the non-spin-flip (NSF) channel. In the unpolarized beam experiments the beam was monochromated and analysed using pyrolytic graphite (PG) crystals. A PG filter was used to remove higher-order contamination for both polarized and unpolarized measurements.

3. Results and discussion

Uniaxial pressure dependences of the polarization analysis for the (1/2, 1/2, 1/2) magnetic reflection are shown in figure 1. At 0 kbar the NSF intensity is almost equal to the SF intensity. At ambient pressure the ratio of in-plane and out-of-plane components is expected to be unity due to the isotropic domain distribution. On the other hand, the difference in integrated intensity between the NSF and SF cases becomes obvious at 2 kbar. The NSF/SF intensity ratio is estimated to be 0.61 ± 0.07 and indicates the deviation from the isotropic distribution. We now show that the determination of the in-plane and out-of-plane components by means of polarized neutrons as described above can be used to actually determine the domain population. Previously, we reported a method of estimating the magnetic moment orientation of UGa_3 from the pressure-dependent behaviours of several magnetic reflections [4]. The same method is also applied to the magnetic intensities measured by unpolarized experiments under the 2 kbar uniaxial pressure as plotted in figure 2. The y-axis represents the *angle factors* normalized to the value for (1/2, 1/2, 1/2). The angle factor is related to the angle between the magnetic moment vector and the scattering vector. If the multidomain structure remains under uniaxial pressure, the values for each magnetic reflection must be unity in this figure. Therefore, the non-flat behaviour in figure 2 confirms the induction of anisotropic domain structure by

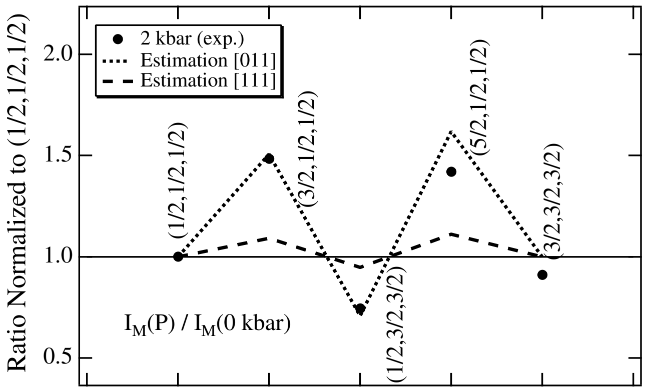

Figure 2. The ratio of intensities at 2 kbar to those at 0 kbar obtained by unpolarized measurements at 8 K. The estimated angle factors are also plotted for $\mu \parallel [011]$ (dotted line) and $\mu \parallel [111]$ (dashed line). All of the data are normalized to the intensity at (1/2, 1/2, 1/2).

Table 1. Values of $\sin^2\theta$, $\sin^2\alpha$, and W for [111]-equivalent axes.

	[111]	$[\bar{1}11]$	$[1\bar{1}1]$	$[11\bar{1}]$
$\sin^2\theta$	0	0	2/3	2/3
$\sin^2\alpha$	0	8/9	8/9	8/9
W	a	a	b	b

Table 2. Values of $\sin^2\theta$, $\sin^2\alpha$, and W for [011]-equivalent axes.

	[011]	$[01\bar{1}]$	[110]	[101]	$[10\bar{1}]$	$[1\bar{1}0]$
$\sin^2\theta$	0	1	1/4	1/4	1/4	1/4
$\sin^2\alpha$	1/3	1	1/3	1/3	1	1
W	a	b	c	c	c	c

uniaxial pressure. In addition, this behaviour tells us that an easy axis of the ordered magnetic moment in UGa$_3$ is definitely not along the [100] axis, because the calculated results for the [100] axis [4] show opposite behaviours to the results for the present experiment.

Therefore, we discuss the possibility that the total magnetic moment of UGa$_3$ is along the [011] or [111] axis. We define θ_n as the angles between the equivalent axes and the scattering plane (h, l, l), and α_n as the angles between the equivalent axes and the scattering vector (1/2, 1/2, 1/2). The NSF intensity for (1/2, 1/2, 1/2) magnetic reflection is described as

$$\mathrm{NSF} \propto \mu^2 \sum_n W_n \sin^2\theta_n, \tag{1}$$

where W_n are weighted factors. Similarly, the SF intensity for (1/2, 1/2, 1/2) magnetic reflection is written as

$$\mathrm{SF} \propto \mu^2 \sum_n W_n (\sin^2\alpha_n - \sin^2\theta_n). \tag{2}$$

Summaries of $\sin^2\theta_n$, $\sin^2\alpha_n$, and W_n for axes equivalent to [111] are listed in table 1 and for ones equivalent to [011] in table 2. The assignment of the weighted factors in tables 1 and 2 is determined from angles between the equivalent axes and the direction of uniaxial stress. The substitution of $a = b = c = 1/6$ for [011]-equivalent axes or $a = b = 1/4$ for

[111]-equivalent axes, which means the multidomain structure, certainly leads to the result for NSF = SF which is shown in figure 1(a). If an easy axis of UGa_3 is along the [111] direction, the NSF/SF intensity ratio is given by

$$\frac{\mathrm{NSF}}{\mathrm{SF}} = \frac{\frac{4}{3}b}{\frac{8}{9}a + \frac{16}{9}b - \frac{4}{3}b} = 0.6. \tag{3}$$

Equation (3) and the condition $2(a+b) = 1$ yield the results $a = 1/3$ and $b = 1/6$. The normalized angle factors calculated from this domain population are presented in figure 2, which is inconsistent with the experimental result. Next, we consider the possibility that the moment orientation is to along the [011] direction. The condition for the weighted factors is $a + b + 4c = 1$. In this case, the NSF/SF ratio is written as

$$\frac{\mathrm{NSF}}{\mathrm{SF}} = \frac{b+c}{\frac{1}{3}a + b + \frac{8}{3}c - (b+c)} = 0.6. \tag{4}$$

From the values at both the (3/2, 1/2, 1/2) and (1/2, 1/2, 1/2) magnetic reflections shown in figure 2, the following equation is obtained:

$$\frac{(3/2, 1/2, 1/2)}{(1/2, 1/2, 1/2)} = \frac{\frac{18}{22}a + b + \frac{48}{22}c}{\frac{1}{3}a + b + \frac{8}{3}c} = 1.5. \tag{5}$$

Therefore, the weighted factors are quantitatively obtained: $a = 25/42$ ($\sim$60%), $b = 5/42$ ($\sim$12%), and $c = 3/42$ ($\sim$7%). The normalized angle factors calculated from this domain population are also plotted in figure 2, which successfully reproduces the experimental result. The finding of the [011] direction is consistent with the report from investigation under hydrostatic pressure [4].

In summary, we have succeeded in determining the magnetic moment orientation of UGa_3 by means of polarized and unpolarized neutron beam experiments under uniaxial pressure. We found that the magnetic moment of UGa_3 is parallel to [011]. We consider that the determination of the domain population by means of VF polarized beam experiments should serve to provide the *correct* form factor under hydrostatic pressure, which includes information on the orbital moment quenching [5], because hydrostatic pressure contains a residual uniaxial component and may cause the development of anisotropic domain structure [4].

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