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The field-induced magnetic structure in UIrGe

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Abstract
We have investigated the field-induced ferromagnetic phase in UIrGe by means of neutron diffraction in fields up to 14.5 T applied along the *c*-axis. At 2 K, the ground-state antiferromagnetic structure of UIrGe (non-collinear with a non-zero hard-axis antiferromagnetic component) transforms into a simple ferromagnetic structure above a critical field of 14.2 T applied along the *c*-axis. The value of the U moment amounts to 0.36(8) μ_B, in good agreement with the zero-field value. This result shows that the anisotropic interactions along the *a*-axis are weaker than the isotropic ones.

1. Introduction

Systems with 5f electrons display a rich variety of cooperative phenomena, which are very often sensitive to variations of external variables such as pressure and magnetic field. The description of the magnetic properties of 5f intermetallic compounds is traditionally based on a scenario in which the 5f electrons are more or less delocalized due to the hybridization with other electron states. The hybridization is strongly geometry dependent (causing a huge magnetocrystalline anisotropy) and affects both the degree of the 5f electron delocalization and the intersite magnetic coupling effects. Whereas in the strong hybridization limit no magnetic ordering is found, intermediate and low hybridization allows for magnetic ordering with steadily increasing magnetic moment magnitudes. The type of the magnetic order is very sensitive to external variables although the critical fields needed for the destruction of the antiferromagnetic order (if it exists) are usually larger than those for the 4f counterpart materials. Moreover, the very high magnetocrystalline anisotropy implies very different values of these critical fields depending on the applied field direction. In this contribution, we describe a field-induced magnetic structure in a single crystal of UIrGe studied by means of neutron diffraction experiments performed in magnetic fields up to 14.5 T.

UIrGe belongs to the large family of UTX compounds (T = transition metal and X = Si or Ge) and crystallizes in the orthorhombic TiNiSi type of structure (space group *Pnma*). Magnetic measurements on single crystals of UIrGe reveal a magnetic phase transition to antiferromagnetic (AF) state around 16 K and a large magnetic anisotropy with the hard magnetization direction along the *a*-axis [1, 2]. The AF structure of the U magnetic moments in UIrGe is non-collinear and commensurate with the crystallographic unit cell [3]. The four ordered U moments in the crystallographic unit cell are strongly reduced (0.36 μ_B/U at 1.8 K) compared to the U^{3+} or the U^{4+} single-ion moment although it has to be mentioned that the U moment values in UIrGe are dependent on the sample preparation conditions. For magnetic fields applied along the *b*- and the *c*-axis, a metamagnetic transition (MT) towards a field-induced ferromagnetic (FIF) phase is observed. The critical-field B_c value for the MT along the *b*-axis is about 50% higher than that along the *c*-axis (B_c = 14.2 T at 2 K). In this contribution, we report on the field-induced phase for the field applied along the *c*-axis as studied using neutron diffraction. We compare the findings with results obtained on the antiferromagnet UNiGe that exhibits in elevated magnetic fields a canted FIF phase with a non-negligible AF *a*-axis component [4] which is the hard magnetization direction in both compounds. The present question is whether there is such an AF *a*-axis component in the high-field phase of UIrGe as well.

2. Experimental details

The single crystal of UIrGe studied in the present experiment originates from the same batch as that used previously for magnetic measurements [1, 2] and in the previous neutron diffraction experiment [3]. The sample preparation details are given in [1].

The integrated intensities were measured on the E4 diffractometer installed at the BER-II reactor at the Hahn–Meitner Institute, Berlin. The crystal was mounted with the c-axis parallel to the rotational axis of the diffractometer, which was also the direction of the applied magnetic field. The magnetic fields up to 14.5 T were produced using a superconducting split-pair cryomagnet manufactured by Oxford Instruments. The fact that the split has only 20 mm and an additional $\pm 2^\circ$ opening restricted us to the $(hk0)$ diffraction planes. The crystal was wrapped in aluminum foil and measured with an incident-neutron wavelength of 2.44 Å implying that only a very limited number of reflections could be reached. The E4 diffractometer is currently equipped with a 20 cm $\times$ 20 cm position-sensitive detector. Two $\lambda/2$ filters imply a residual $\lambda/2$ contamination at a level of less than 0.1%.

The single crystal was oriented using the two strongest nuclear reflections. The individual scan profiles were analyzed by fitting to Gaussian profiles. The crystallographic and magnetic structures were determined by fitting to given models using the computer code WinPLOTR [5]. The appropriate scattering lengths and the standard U^{3+} magnetic form factor were used in the refinement. We have also followed the intensities of a few reflections as a function of temperature and magnetic field. During the experiment we have collected three identical sets of reflections, so-called rocking curves, at 25 K and zero field, at 2 K and zero field, and at 2 K and at 14.5 T. Each of the 12 inequivalent reflections was measured for about 75 min.

3. Results and discussion

The refinement of the data set taken at 25 K to the UIrGe crystal structure (described in [2]) provided us with the scaling and extinction parameters needed for the magnetic structure refinement. During the fit to the structural model, we had to fix the z-position numbers for all three atoms because of the limited set of reflections of the $(hk0)$ type. At temperatures below 16 K, which corresponds very well to the magnetic phase transition temperature, an additional scattering intensity is observed at the position of the (010) Bragg reflections, which are otherwise forbidden due to symmetry. In total, only four Bragg reflections showed a significant additional magnetic contribution and only two of them had a signal three times larger than the statistical error. However, even this is enough to rule out six of eight magnetic structures allowed by the symmetry analysis [6]. The remaining two can be clearly distinguished from the observed intensities. The results of the present refinement to data obtained by subtracting the intensities at 25 K from the low-temperature data set are similar to the results given in [2] and [3].

If the field applied along the c-axis is gradually increased, the intensity of the prominent (010) reflection stays nearly unaffected up to 14.1 T and then decreases steeply to zero. The disappearance of the (010) reflection marks the transition towards a FIF state. Among all the magnetic structure models allowed by the symmetry (the symmetry analysis and the list of all the compatible magnetic structures are given in [3]), there is only one with a ferromagnetic component along the c-axis, which at the same time allows a non-zero AF a-axis component. The existence or the non-existence is reflected in the appearance/disappearance of the additional magnetic signal on top of various Bragg reflections. In the case of UNiGe [4], it has been shown that the magnetic signal for the (120) reflection is directly proportional to the a-axis component. In the case of UIrGe, we have not observed any additional magnetic intensity at this reflection below T_N. At the same time, one would need to observe magnetic intensity at the position of the (100) reflection which is forbidden for the crystal structure. This is, however, not the case. Both observations rule out the existence of an AF a-axis component in the FIF state of UIrGe which conforms with the irreducible representation Γ_7 listed in [3]. For completeness, we have tried also other AF a-axis configurations, namely Γ_2 and Γ_4 combined with a ferromagnetic c-axis component (although we are aware of the fact that this would require mixing of IRs). Both models, however, also lead to a large magnetic contribution to the (010) or (110) reflections. Good agreement could be achieved only for the IR Γ_7 with the a-axis component equal to zero. The best fit yields U magnetic moments of 0.36(8) μ_B with a χ^2 value of 6.02. The moment value found in the present experiment is in very good agreement with the ground-state value [3] but is somewhat lower than the magnetization value at 14.5 T resulting from magnetic bulk experiments [2].

It is interesting to compare the magnetic structures of UIrGe, UNiGe and the isostructural ferromagnetic superconductor URhGe [7]. The former two exhibit a non-collinear AF ground-state structure with, respectively, two and all three principal-axis components. The latter compound is a simple ferromagnet. Although they have different magnetic structures, the types of magnetocrystalline anisotropy are the same for the three compounds. The a-axis is always the hard magnetization direction which is believed to be the consequence of a strong 5f–5f overlap along the buckled chains in this direction. In the b–c plane, one observes rather small magnetocrystalline anisotropy of the order of tens of kelvins and all three materials can thus be classified as having the easy-plane type of anisotropy. The anisotropy between the a-axis and the b–c plane is more than one order of magnitude larger. Upon application of a magnetic field that is larger than a certain critical value one can modify the ground-state arrangement of the magnetic moments and stabilize a new phase. In the case of URhGe along the c-axis direction, there is of course no phase transition possible and the moments remain oriented along the c-axis. However, if the field is applied along the b-axis, one induces a spin-reorientation transition at 12 T which is accompanied by a second region of unconventional superconductivity [8]. The type of ordering remains ferromagnetic. In the cases of UNiGe and UIrGe

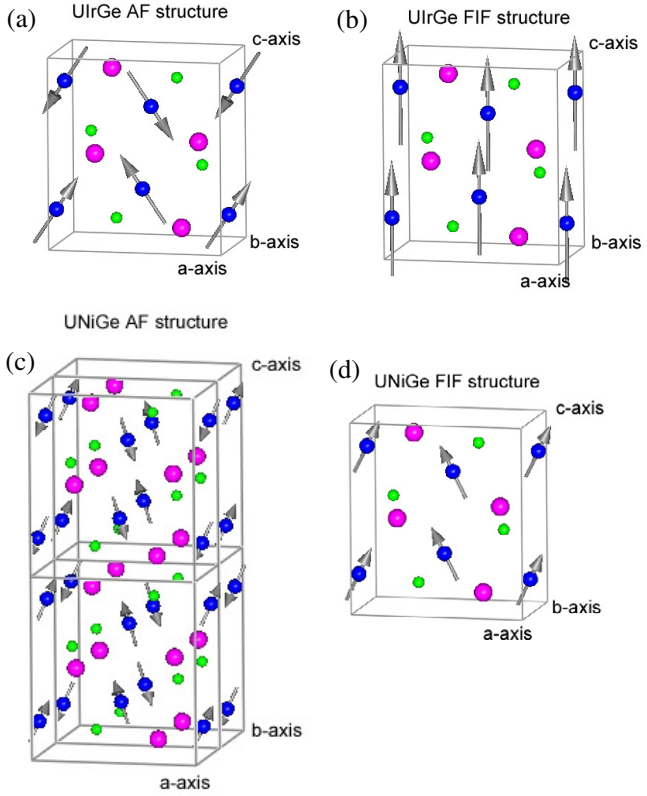

Figure 1. Schematic representation of the magnetic structures of the UTGe (T = Ni, Rh, Ir) group of compounds: the ground-state antiferromagnetic structure of UIrGe (a), the field-induced ferromagnetic state that is stable for fields applied along the *c*-axis above 14.2 T (b), the ground-state antiferromagnetic structure of UNiGe with all three principal axes components and propagation vector (0, 1/2, 1/2) (c) and the field-induced ferromagnetic structure of UNiGe that is established for fields applied along the *c*-axis above 10 T (d). The ground-state magnetic structure of URhGe is collinearly ferromagnetic and equal to that shown in (b). The U moments in UIrGe are magnified by a factor of five. The biggest spheres denote Ge atoms, spheres with arrows denote U atoms and their magnetic moments and the remaining spheres denote transition-metal atoms.

(This figure is in colour only in the electronic version)

along the *c*-axis direction, one observes, respectively, two magnetic phase transitions and one magnetic phase transition towards a FIF phase. Although both compounds order antiferromagnetically and also the critical-field values along the *c*-axis are quite comparable (10 T for UNiGe and 14 T for UIrGe), the FIF phase is different. The AF *a*-axis component survives in UNiGe but not in UIrGe. The comparison is schematically shown in figure 1. In [4] it has been shown that the existence of such a hard magnetization direction component can be explained as to be due to the presence of anisotropic exchange interactions. The fact that the *a*-axis component cannot be well aligned in high magnetic fields indicates that the AF interaction between the *a*-axis components is much stronger than those between the others. The absence of the *a*-axis component in the FIF phase of UIrGe indicates that the anisotropic interaction along the hard axis is weaker.

4. Conclusions

We have investigated the field-induced ferromagnetic phase in UIrGe by means of neutron diffraction in fields up to 14.5 T applied along the *c*-axis. The findings enable us to establish that the FIF structure in UIrGe is of simple ferromagnetic type, in contrast to a more complicated canted ferromagnetic structure in UNiGe [4]. This result shows that the hard magnetization axis, the AF component which is due to anisotropic interaction, is not a general feature in uranium compounds with the TiNiSi type of structure and that it has to be treated independently from case to case. In the case of UIrGe, the anisotropic interaction along the hard magnetization direction is of the same order of magnitude as or smaller than the isotropic one.

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