Magnetization and specific heat of a UIrGe single crystal in high magnetic fields

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Abstract. The temperature and field dependence of the magnetization were measured on a single crystal of the antiferromagnet UIrGe in pulsed fields up to 51 T, and the specific heat in steady fields up to 18 T. At low temperatures, metamagnetic transitions are observed at critical fields \(B_c\) of 21 T and 14 T, applied along the \(b\)- and the \(c\)-axis, respectively. At 2 K, the magnetization jumps at \(B_c\) are 0.36 \(\mu_B/U\) along the \(b\)-axis and 0.28 \(\mu_B/U\) along the \(c\)-axis. The \(a\)-axis is the hardest magnetization direction with a weak linear magnetic response. Both along the \(b\)- and the \(c\)-axis, \(B_c\) decreases with increasing temperature. Consistent with the magnetization, the sharp anomalies observed in the specific-heat obey the same dependence.

1. Introduction
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 \(Pnma\)). The results of studies performed on polycrystalline UIrGe all point to the existence of antiferromagnetic (AF) order below \(T_N = 16-18\) K [1]. Magnetic measurements on single crystals of UIrGe reveal a large magnetic anisotropy with the hard magnetization direction along the \(a\) axis. For magnetic fields applied along the \(b\) and the \(c\) axis, metamagnetic transitions are observed [2]. Antiferromagnetism has been confirmed by neutron-diffraction experiments on this single crystal [3]. The magnetic structure of UIrGe is non-collinear and commensurate with the crystallographic unit cell. The ordered U magnetic moment is strongly reduced (0.36 \(\mu_B/U\) at 1.8 K) compared with U\(^{3+}\) or U\(^{4+}\) single ions. The single-crystal results on electrical resistivity and specific heat were, however, in some disagreement with polycrystalline data. In order to establish the intrinsic properties of UIrGe, a new single crystal has been grown of better quality and the magnetization, specific heat, electrical resistivity and neutron scattering have been investigated.
In this paper, we present the results of high-field magnetization, specific-heat and neutron-diffraction studies.

2. Experimental
A single crystal of UIrGe was grown in a tri-arc furnace by the Czochralski method from a stoichiometric mixture of the pure elements (99.9% U, 99.99% Ir and 99.999% Ge) which according to Laue pictures is of better quality than previously grown crystals. The lattice parameters determined by X-ray powder diffraction $a = 686.4$ pm, $b = 429.8$ pm, $c = 757.2$ pm are in good agreement with literature. No secondary phase was detected by microprobe analysis. The composition was found to correspond within experimental error (1%) to the 1:1:1 stoichiometry. The magnetization was measured by the extraction method in a PPMS-14 magnetometer (Quantum Design) in steady fields up to 14 T (Prague) and by the induction method in pulsed fields up to 51 T (Osaka). The specific-heat measurements in fields up to 14 T (PPMS-14) were extended to 18 T in Amsterdam. Neutron-diffraction experiments were performed in the double-axis diffractometer E4, installed at HMI with either the $a$- or the $c$-axis aligned along the rotational axis of the diffractometer that was parallel to the applied field of 14.5 T. The incident-neutron wavelength was 2.44 Å. Also the neutron-diffraction patterns indicate the quality to be better than that of the previous crystals.

3. Results and discussion
The magnetization curves along the principal axes, measured at 4.2 K (Fig. 1a), show that UIrGe has huge magnetic anisotropy. Along the hardest axis, the $a$-axis, a linear magnetic response is observed up to the highest applied field of 51 T. The magnetic-susceptibility value of $2.2 \times 10^{-8}$ m$^3$ mol$^{-1}$ corresponds well to the typical response of uranium compounds that do not exhibit magnetic ordering. Along the $b$- and the $c$-axis, the initial susceptibility is considerably higher than along the $a$-axis and metamagnetic transitions are observed at 21 T and 14 T, respectively. The magnetization jumps of 0.36 and 0.28 $\mu_B$ are found to be larger than reported in Ref. 2 and are compatible with the uranium magnetic moment $\mu_U = 0.36 \mu_B$ found in neutron-diffraction experiments (done, however, on another crystal [3]).

![Figure 1](image_url)

**Figure 1.** a). Magnetization curves of a UIrGe single crystal, measured in pulsed fields along the principal axes at 4.2 K. b). Temperature evolution of the $c$-axis magnetization curve in steady magnetic fields. The curve at 4.2 K (dashed line) was measured in pulsed field.

The magnetic isotherms strongly suggest that the anisotropy type of UIrGe is of easy-plane type or very similar to it. This is supported by the following consideration which is based on the crystallographic structure. The orthorhombic TiNiSi-type of structure is a derivative of the hexagonal AlB$_2$-type of structure. The $a$-axis of the TiNiSi lattice corresponds to the hexagonal $c$-axis of the AlB$_2$.
lattice and therefore may be expected to be more special with respect to the anisotropic properties than the \(b\)- and the \(c\)-axis.

Figure 1b shows the temperature dependence of the metamagnetic transition determined down to 6 K in steady fields applied along the \(c\)-axis and at 4.2 K in pulsed field. At the lowest temperatures, the transition occurs in a narrow field interval, suggesting the transition to be first order, and exhibits an hysteresis of 0.1-0.2 T. With increasing temperature, the transition shifts towards low fields and the jump of the magnetization \(\Delta M\) gradually decreases.

Figure 2 shows the temperature dependence of the specific heat, in \(C/T\) vs \(T\) representation, obtained in various fields applied along the \(b\)- and the \(c\)-axis. (The almost negligible influence on the \(C/T(T)\) dependence of the magnetic field applied along the \(a\)-axis confirms that this is the hard magnetization axis). The anomaly in the specific heat is related to the magnetic-order transition at \(T_N\). With increasing field, the anomaly shifts to lower temperatures; the effect being considerably stronger in fields applied along the \(c\)-axis. The lower \(B_c\) value for the field along the \(c\)-axis allows us to follow completely the evolution of the specific heat between the AF ground state and the paramagnetic state. In zero field, the magnetic ordering is represented by a \(\lambda\)-type anomaly which gradually becomes sharper with increasing magnetic field up to 7 T. For \(B\) larger than 7 T, the anomaly becomes symmetric and gradually broadens. The start of a similar trend along this axis is seen as well when we extended our measurements along the \(b\)-axis above 14 T, the maximum field available in PPMS-14.

In Fig. 3, the relationship is shown between the temperature at which the maximum of the specific heat occurs and the applied magnetic field. This dependence coincides well with the temperature dependence of the field of metamagnetic transition as derived from the magnetization measurements, showing that in UIrGe the AF state only exists up to the metamagnetic transition.

As for the determination of the AF structure of the present sample we have collected for the two orientations three sets of data consisting of total 29 inequivalent reflections: at 25 K in zero field; at 2 K in zero field and at 2 K in 14.5 T. The magnetic signal has been obtained by subtracting the paramagnetic set obtained at 25 K and fitted to all allowed models described in Ref. 3. The magnetic structure of the crystal was clearly in accord with the magnetic structure reported in Ref. 3. Merely slightly different magnetic-moment components were determined. The AF \(a\)- and the \(c\)-axis components amount to 0.18(8) \(\mu_B\) and 0.27(2) \(\mu_B\) respectively, with \(\chi^' = 5.2\). Compared with the results found in Ref. 3, we have found for the present crystal a much smaller \(a\)-axis component and a larger \(c\)-axis component. The found components along the \(a\)- and \(c\)-axis are seemingly in contradiction with
the equivalent magnetization behavior found along the $b$- and $c$-axis. This apparent inconsistency is not yet understood and will be subject of further study.

**Figure 3.** Temperature dependence of $B_c$ along the $c$-axis and the $b$-axis, determined from magnetization and from specific-heat measurements. The lines are guides to the eye.

**Figure 4.** Field dependence of the integrated intensity of the AF (010) reflection. The small intensity above the transition is due to $\sqrt{2}$ contamination from the (020) reflection.

While there is, in agreement with the magnetization data, no effect on the AF structure of UIrGe of 14.5 T applied along the $a$-axis, application of a field along the $c$-axis causes a metamagnetic transition to a field-induced ferromagnetic (FIF) state (Fig. 4). Above the transition, the ferromagnetic $c$-axis component amounts to 0.45(9) $\mu_B$, in agreement with the magnetization data. Whether the AF $a$-axis component prevails in the FIF state, as it is in the case of the isostructural compound UNiGe [4], is still unclear at present and needs further study.

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