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Crystal structure of single crystal and electrical resistivity of UMn_5Al_7

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Abstract

The crystal structure of UMn_5Al_7 determined from single crystal refinement is tetragonal of the $ThMn_{12}$-type with space group *I4/mmm* and with the room temperature lattice parameters: $a = 8.7870(10)$ Å and $c = 5.0850(10)$ Å. The U atoms are located in the 2(a) sites, whereas the Mn atoms are in the 8(f) and 8(j) sites. Electrical resistivity increases weakly with increasing temperature and is strongly sample dependent.

Keywords: Crystal structure; Electrical resistivity; Single crystals

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1. Introduction

The structure and magnetic properties of the UMn_xAl_{12-x} system have been examined recently [1]. These investigations have shown that these alloys exist in the single phase form ($ThMn_{12}$-type) for $3 \leq x \leq 7$. Except for the alloy with $x = 3$, the remaining materials are paramagnetic throughout the investigated temperature range, however, the Curie–Weiss law is observed at $T > 100$ K with the effective magnetic moment, p_{eff}, and the paramagnetic Curie temperature, θ, varying linearly with composition, x. This behavior seems to suggest the importance of the Mn subsystem in the magnetism of the UMn_xAl_{12-x} alloys. In turn, UMn_3Al_9 exhibits an anomaly in the $\chi_{ac}(T)$ plot and a deviation from linearity in the $M(H)$ dependence at 4.2 K. The latter plot shows a ferromagnetic character, although the highest value of the magnetic moment amounts to 0.25 μ_B/f.u. at a magnetic field of 14 *T*. These findings put in doubt the possibility of elucidation of a magnetic order by neutron diffraction for this composition.

For the rare earth compounds with $x = 4$ and 6 a magnetic order is formed with magnetic moment on the rare earth atoms [2,3]. This finding is confirmed by the low value of the transition temperatures and scaling with the de Gennes factor. The compounds with $x = 5$ have not been reported, but it does not mean that they do not exist.

After prolonged attempts we have succeeded in obtaining small single crystals of UMn_5Al_7 and now we report on the crystal structure of this material. Also the results of the electrical resistivity for this compound as well as for UMn_4Al_8 are presented. One should note that among the uranium compounds with $ThMn_{12}$-type structure with a low concentration of the transition element the present paper reports only the second crystal structure determination after UFe_4Al_8 [4].

The crystals were obtained by mineralization, the stoichiometric UMn_5Al_7 alloy being earlier prereacted in an arc-furnace in an argon protective atmosphere. The polycrystalline samples used for electrical measurements after the arc-furnace melting were annealed at 900 °C for two weeks.

The X-ray examination was performed in a KUMA-Diffraction KM-4 four circle single crystal diffractometer using graphite-monochromatized Mo Kα radiation ($\lambda = 0.7103$ Å). The unit cell parameters were refined from settings of 15 reflections. The crystal data and measured parameters are collected in Tables 1–4. The intensities of the reflections were corrected for the Lorentz and polarization effects. The structure was refined by the full-matrix least-squares method using the SHFLXL-93 software system in a 486 IBM PC computer.

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Table 1
Summary of crystallographic data

Formula	UMn_5Al_7
Crystal system	Tetragonal
Space group	*I4/mmm*
Lattice parameters (A)	
a	8.787(1)
c	5.085(1)
Volume (A^3)	392.62(10)
Z	2
Calculated density	5.935 mg m^{-3}
Radiation	Graphite monochromated Mo Kα
Absorption coefficient	27.676 mm^{-1}
Scan mode	ω-2θ
2θ range	2.0 to 65.0°
Reflection collected	629
Number of unique data	215 ($R_{int}=8.96\%$)
Observed reflections	171 ($F>4.0\sigma(F)$)
$R=\Sigma(\lvert F_o\rvert-\lvert F_c\rvert)/\Sigma\lVert F_o\rvert$	4.38%
$R_w=\Sigma\omega(\lvert F_o\rvert-\lvert F_c\rvert)^2/\Sigma\omega\lvert F_o\rvert^2))^{1/2}$	7.25%
$\omega^{-1}=\sigma^2(F)$	
Extinction correction	$\chi=0.0021(6)$, where $F^*=F[1+0.002\chi F^2/\sin(2\theta)]^{-1/4}$

Table 2
Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement coefficients ($Å^2\times 10^3$)

Atom	Position	*x*	*y*	*z*	$U_{(eq)}$	Occupancy
U	2a	0	0	10	8(1)	1
Mn(1)	8f	2500	2500	2500	15(1)	1
Al(1)	8i	0	3450(9)	0	14(2)	1
Mn(2)	8j	5000	2802(9)	0	15(1)	0.25
Al(2)	8j	5000	2802	0	15(1)	0.75

Table 3
Bond lengths (Å)

U–Mn(1)	3.357(1)
U–Mn(2a)	3.193(5)
U–Al(1)	3.032(8)
Mn(1)–Mn(2)	2.552(1)
Mn(1)–Mn(1c)	2.543(1)
Mn(1)–Al(1)	2.672(3)
Mn(2)–Mn(2f)	2.731(11)
Al(1)–Mn(2c)	2.770(5)
Al(1)–Al(1b)	2.723(16)
Al(1)–Mn(2e)	2.814(8)

Table 4
Anisotropic displacement coefficients ($Å^2\times 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
U	6(1)	6(1)	12(1)	0	0	0
Mn(1)	15(2)	15(2)	15(2)	−1(1)	1(1)	1(1)
Al(1)	15(4)	10(4)	17(4)	0	0	0
Al(2)	15(2)	15(2)	15(2)	0	0	0

The present investigations confirm the tetragonal $ThMn_{12}$-type structure with space group *I4/mmm* (Fig. 1). The lattice parameters are $a=8.7870(10)$ Å and $c=5.0850(10)$ Å. The same parameters of the polycrystalline material are $a=8.803$ Å and $c=5.091$ Å [1], whereas the parameters determined for UMn_4Al_8 in a neutron diffraction experiment [5] are $a=8.845(3)$ Å and $c=5.096(1)$ Å. One can see that an increase in the Mn concentration decreases both the values of lattice parameters resulting from substitution of larger Al atoms (atomic radius = 1.43 Å) by smaller Mn atoms (atomic radius = 1.35 Å). The atomic coordinates are in fair agreement with those previously reported for UFe_4Al_8 [4], UMn_4Al_8 [5] and UCu_5Al_7 [6].

The electrical resistivity, ρ, of UMn_5Al_7 vs. temperature presented in Fig. 2 is one of few measurements of the uranium compounds with the $ThMn_{12}$-type structure in a broad composition range. There are systematic investigations of the electronic transport properties of the $UCu_{4+x}Al_{8-x}$ system [7] but because this system is partly antiferromagnetic and heavy-fermion-like the comparison of the present results and those published in Ref. [7] is not particularly informative. In Fig. 2 the temperature dependences of electrical resistivity are recorded for three different samples obtained in the same way but from three different batches. One can see that the results for samples #1 and #2 are relatively close to each other, whereas sample #3 exhibits under a microscope the presence of clear cracks and hence apparently higher resistivity is observed in materials. Therefore, we have to reject these results. Shown in the inset the resistivity of UMn_4Al_8 [8] vs. temperature exhibits considerably lower resistivity. This behavior is obviously related to larger crystallographic disorder in UMn_5Al_7 in which the Mn atoms also partly occupy the 8(j) position. Such an increase in the resistivity has been observed also in the $UCu_{4+x}Al_{8-x}$ system [7] with increasing Cu/Al ratio. Contrary to UMn_5Al_7, the resistivities of $UCu_{4.5}Al_{7.5}$ [9] and $U(Ni,Cu)_4Al_8$ [10] systems are lower and we cannot present any explanation

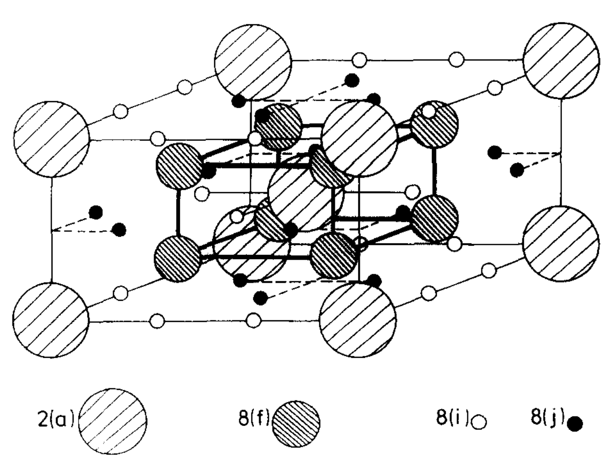

Fig. 1. Crystal structure of $ThMn_{12}$-type compounds.

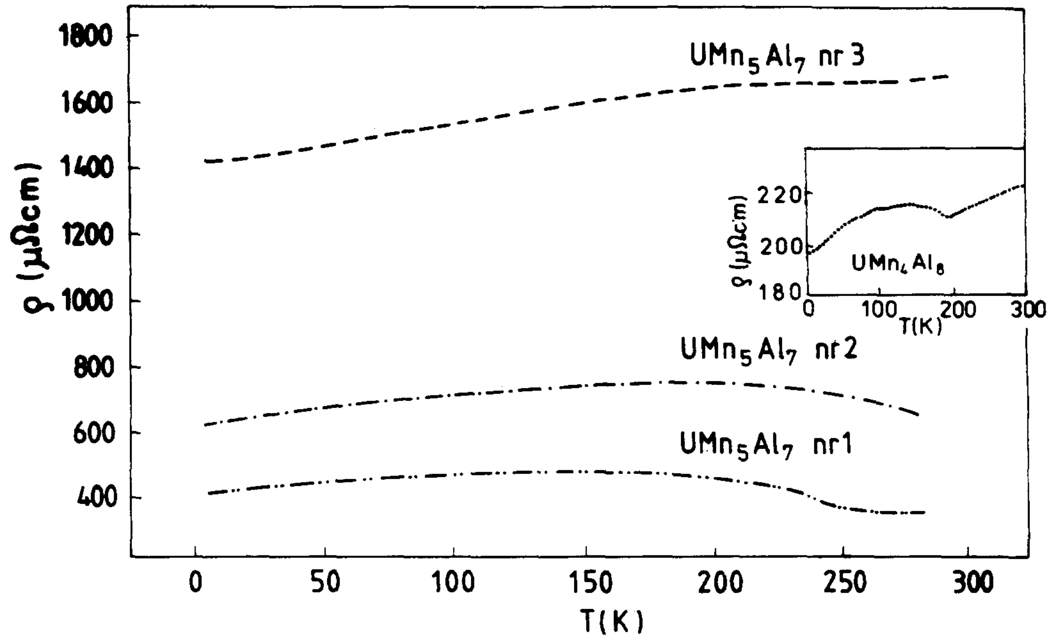

Fig. 2. Electrical resistivity, ρ, vs. temperature for three different samples of UMn_5Al_7. The inset shows the ρ(T) plot for UMn_4Al_8 [7].

of this phenomenon. Both the Mn containing samples exhibit a weak temperature dependence of resistivity with a diffuse maximum at about 200 K, the reason of which is obscure at present. A weak temperature dependence of ρ above T_N is also observed for $UCu_2Ni_2Al_8$ [10].

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