STRUCTURAL AND MAGNETIC ORDERING IN $UPd_{1.85}Sn$*

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(Received July 10, 2002)

Neutron diffraction experiments have been used to investigate the structural and magnetic ordering in the moderately disordered heavy fermion compound $UPd_{1.85}Sn$. The material crystallizes in the fully ordered cubic Heusler lattice of $Fm3m$ symmetry. Below the antiferromagnetic transition temperature $T_N = 25.7$ K magnetic Bragg scattering has been observed. The magnetic spectrum can be accounted for by an antiferromagnetic wave vector $\vec{k} = [0\ 0\ 0]$, *i.e.*, the magnetic and crystallographic unit cells are identical. The magnetic moment is evaluated to $\mu_{\rm ord} = 0.97(9)\ \mu_{\rm B}$.

PACS numbers: 75.25.+z, 75.30.Mb, 75.50.Ee

1. Introduction

Previously, it has been established that the physical and structural properties of the heavy fermion compound UPd_2Sn drastically depend on the Pd-stoichiometry. Initial studies [1, 2] carried out on UPd_2Sn reported the system to crystallize within an orthorhombic *Pnma* structure. Neither superconductivity nor magnetic ordering was detected. In contrast, in investigations on off-stoichiometric $UPd_{1.85}Sn$ antiferromagnetic order has been ob-

* Presented at the International Conference on Strongly Correlated Electron Systems, (SCES 02), Cracow, Poland, July 10–13, 2002.

served [3,4]. The transition from paramagnetic to antiferromagnetic ground state is probably triggered by a structural transition, as $UPd_{1.85}Sn$ crystallizes in a cubic Heusler ($Fm3m$) lattice.

In the structural investigation of UPd_2Sn there has been ambiguity about the occupation of inequivalent sites in the *Pnma* lattice, possibly giving rise to atomic site disorder [2]. Moreover, antiferromagnetism in $UPd_{1.85}Sn$ is affected by atomic site disorder [3]. In this context, it is important to establish the structural and magnetic properties of $UPd_{1.85}Sn$ on a microscopic scale. Therefore, we have performed a detailed neutron diffraction study on the structural and magnetic properties of $UPd_{1.85}Sn$, first results of which we present here.

2. Experimental details

A polycrystalline sample $UPd_{1.85}Sn$ was prepared by arc-melting the constituents in stoichiometric ratio under Argon atmosphere. No heat treatment was applied. Neutron powder diffraction data on $UPd_{1.85}Sn$ have been collected at temperatures ranging from 1.5 to 32 K on the E6 diffractometer at the Hahn–Meitner Institute in Berlin, using a neutron wave length $\lambda = 2.448$ Å . Full Rietveld structure refinements of the diffraction data were performed employing the program WinPlotr/FULLPROF [5].

3. Results and discussion

A typical neutron scattering spectrum for temperatures above the magnetic transition ($T_N = 25.7$ K) of $UPd_{1.85}Sn$ is displayed in Fig. 1. Note that the intensity of the main peak at 62° exceeds the scale by a factor 4.

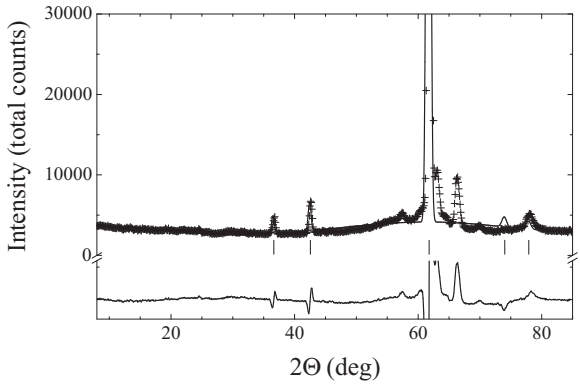

Fig. 1. The neutron diffraction spectrum of $UPd_{1.85}Sn$ at 32 K. We include Bragg peak positions (tics), the result of the refinement and the difference between refinement and data (solid lines).

A full Rietveld refinement of the diffraction spectrum is obtained by assuming a fully ordered cubic Heusler structure $Fm3m$, yielding a Bragg value $R_{\mathrm{Bragg}} = 7.8\,\%$. The lattice parameter $a = 6.742(4)$ Å is in good agreement with previously reported values [3, 4]. From the comparison of the refinement with the data we find four peaks from a minority phase. The peak positions correspond to those of the orthorhombic *Pnma* lattice. Therefore we attribute the peaks to regions in the matrix crystallizing in this superstructure of the Heusler lattice (about 5 % volume amount).

Neutron diffraction spectra taken in the antiferromagnetic state reveal the presence of additional magnetic Bragg peaks. By subtracting the spectra measured at $T = 32\,\mathrm{K}$ from the 1.5 K spectrum we obtain the magnetic difference spectrum $I_{1.5\mathrm{K}} - I_{32\mathrm{K}}$ plotted in Fig. 2.

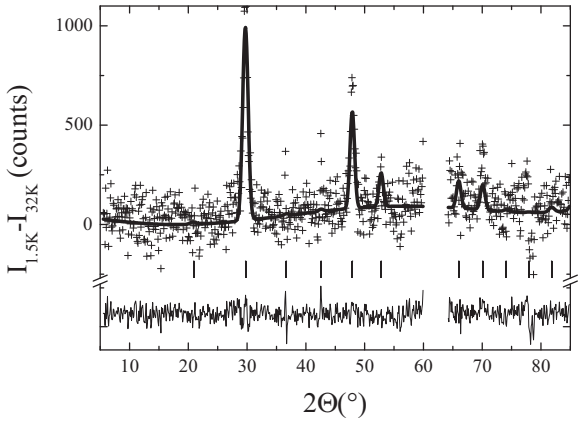

Fig. 2. The magnetic Bragg intensity $I_{1.5\ \mathrm{K}} - I_{32\ \mathrm{K}}$ of $UPd_{1.85}Sn$. The data (+) is refined (solid line) assuming the structure from Fig. 3. Bragg peak positions are indicated by tics, the solid line in the lower panel represents the difference between fit and data. The area of the main structural Bragg peak at 62° is omitted.

Assuming a simple antiferromagnetic arrangement of the spins as depicted in figure 3 we can fit the magnetic spectrum, with an ordered magnetic moment $\mu_{\mathrm{ord}} = 0.97(9)\ \mu_{\mathrm{B}}$. In the refinement we obtain a comparatively large value $R_{\mathrm{Bragg}} = 22\,\%$, which however mostly is due to the large scattering of the background. From our data we cannot determine the direction of the moment with respect to the unit cell axes. The moment is typical in size for moderate heavy fermion compounds, with partial reduction from Kondo screening (for comparison: U_2Pd_2Sn: $\mu_{\mathrm{ord}} = 2\ \mu_{\mathrm{B}}$ [6]; $U_2Rh_3Si_5$: $\mu_{\mathrm{ord}} = 2.4\ \mu_{\mathrm{B}}$ [7]; UPdSn: $\mu_{\mathrm{ord}} = 1.3\ \mu_{\mathrm{B}}$ [8]). The structure corresponds to an antiferromagnetic ordering vector $\vec{k} = [000]$, *i.e.*, structural and magnetic unit cells are identical.

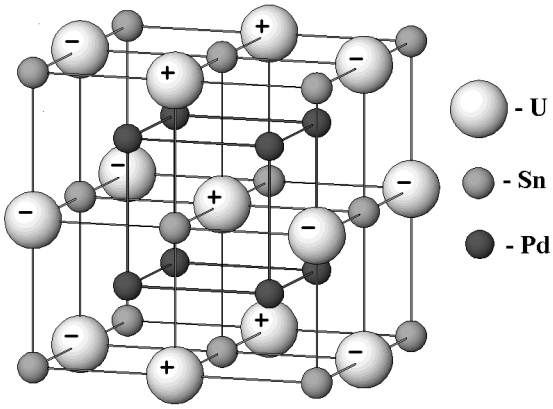

Fig. 3. The cubic Heusler $Fm3m$ and magnetic structure of $UPd_{1.85}Sn$, with the antiferromagnetic spin arrangement indicated by "+" and "−".

In summary, we have investigated the structural and magnetic properties of $UPd_{1.85}Sn$ by means of a neutron scattering study and established the structural and magnetic symmetry of the system.

We acknowledge financial support by the Deutsche Forschungsgemeinschaft DFG under grant no. SU 229/1-1/2 and the Hahn-Meitner Institut. The sample has been produced within FOM-ALMOS.

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