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Magnetic Structure of UCu_5

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Recently some data concerning the magnetic behaviour of UCu_5 have been published (1). It was reported that the magnetic susceptibility measured over the temperature range 4.2 to 900 K exhibits a sharp maximum at 15 K indicating an antiferromagnetic transition.

The aim of this neutron-diffraction study was: a) to verify that magnetic ordering in UCu_5 does occur and that it is not parasitic, b) to determine the corresponding magnetic structure, and c) to determine the magnetic moment of U ion in the ordered state.

UCu_5 crystallizes in a face-centered cubic structure of $F\bar{4}/3m$ space group with the following atomic positions: 4U in 4(a), 0,0,0; 4Cu in 4(c) 1/4,1/4,1/4; 16Cu in 16(e) x,x,x; + f.c. translation. For a perfect close-packed arrangement x = 5/8. The lattice constant of UCu_5 $a_o = 7.04$ Å (1).

Neutron-diffraction powder patterns were obtained with 2-axis diffractometer DN-500 located at the reactor EWA and using an incident neutron wavelength of 1.32 Å. The powder sample of UCu_5 (40 g) was sealed in a thin-walled vanadium container and held within a low temperature cryostat. Measurements were performed at 293 and 4.2 K. Also the temperature dependence of the height of the magnetic reflection was measured as the sample was warmed up slowly. The temperature of the sample was controlled by a gold-chromel thermocouple.

The neutron-diffraction diagrams recorded at 293 and 4.2 K showed the peaks which could be indexed on the basis of an $AuBe_5$-type crystal structure. Their integrated intensities were in good agreement (R = 0.04) with those calculated for x = 0.626.

Comparing liquid helium and room temperature diagrams we have noticed that the peak at 2θ position where the trace of $\lambda/2(311)$ occurs, shows an increase

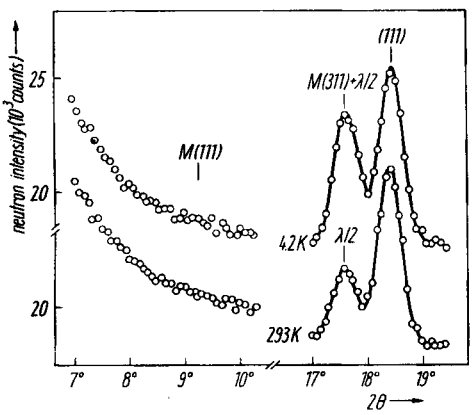

Fig. 1. Low angle fragments of neutron-diffraction patterns of UCu_5

in intensity with that observed at 293 K. A careful examination of its temperature dependence showed that it disappeared at 15 K (Fig. 2). On the basis of a cubic unit cell whose lattice constant was twice enlarged it was possible to index this magnetic peak as M(311). Subsequently we found also very weak traces of M(331) and M(333) + M(511) reflections. However, even in measurements with long counting time the M(111) peak was not detected (see Fig. 1).

The magnetic lattice of UCu_5 can be described as consisting of parallel sheets ((111) planes) within which all the U magnetic moments are coupled ferromagnetically but with antiferromagnetic coupling between neighbouring sheets (Fig. 3). The proposed model is then quite similar to those for MnO, MnS, and MnSe described by Shull et al. (2). In their original paper the authors discussed three cases of interest concerning the relative orientation of the moments and lattice axes.

a) The magnetic moments are parallel to arbitrary [100] direction.

b) The magnetic moments are perpendicular to the ferromagnetic sheets.

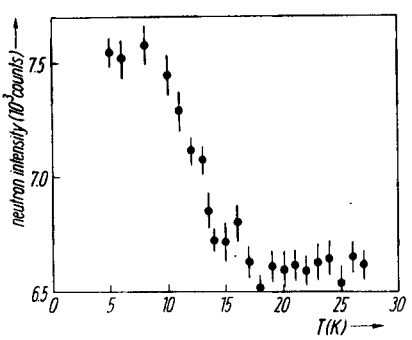

Fig. 2

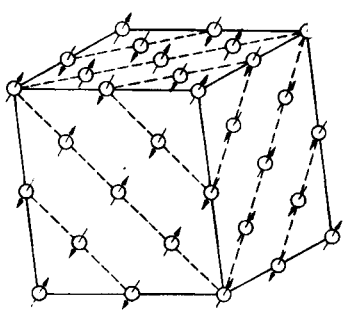

Fig. 3

Fig. 2. Temperature dependence of M(311) peak height

Fig. 3. Antiferromagnetic structure in UCu_5

c) The magnetic moments are aligned arbitrary in the ferromagnetic planes.

The lack of M(111) reflection in our diagram at 4.2 K clearly indicates that the case (b) is to be preferred. Moreover, in the model (b) M(311) peak appears as the strongest one and this fact explains why other magnetic reflections could not be easily detected. The magnetic moment at 4.2 K estimated from M(311) peak was found to be $(0.9 \pm 0.1)\mu_B$.

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