NEUTRON DIFFRACTION STUDY OF THE MAGNETISM IN SINGLE-CRYSTALLINE $CeCu_2(Si_{1-x}Ge_x)_2$*

O. Stockert, M. Deppe, C. Geibel, F. Steglich

Max-Planck-Institute CPfS, Nöthnitzer Straße 40, 01187 Dresden, Germany

D. Hohlwein and R. Schneider

Hahn-Meitner-Institute, Glienicker Straße 100, 14109 Berlin, Germany

We have studied single-crystalline $CeCu_2(Si_{1-x}Ge_x)_2$ using neutron diffraction to determine the antiferromagnetic order in the regime with low Ge content, $x \leq 0.5$. The system orders in an incommensurate magnetic structure with a propagation vector close to $\tau = (0.25\ 0.25\ 0.5)$. Up to two additional phase transitions were observed below the Néel temperature characterized by a spin reorientation and a lock-in to a probably commensurate structure.

PACS numbers: 75.30.Mb, 71.27.+a, 71.10.Hf, 75.20.Hr

1. Introduction

Heavy-fermion systems show exciting low temperature phenomena and unusual ground states due to the competition between Kondo-screening, leading to a non-magnetic ground state, and RKKY interaction, resulting in long-range magnetic order. In particular, the heavy-fermion system $CeCu_2(Si_{1-x}Ge_x)_2$ (with tetragonal $ThCr_2Si_2$ structure) offers an unique possibility to tune the system via alloying from the local moment antiferromagnet $CeCu_2Ge_2$ to the first discovered heavy-fermion superconductor $CeCu_2Si_2$, which also exhibits an unconventional type of magnetic order (so-called A-phase) [1, 2]. While some information is available about the magnetic structure in heavily doped $CeCu_2(Si_{1-x}Ge_x)_2$, $x \geq 0.6$, and $CeCu_2Ge_2$ [1, 3–5], previous neutron diffraction studies did not succeed in

---

determining the magnetic order in the lowly doped regime ($x \leq 0.5$). Especially the nature of the so-called A-phase in $CeCu_2Si_2$ is still discussed controversially. To shed more light on to the interplay between magnetism and superconductivity in $CeCu_2Si_2$, it is essential to know the evolution of the magnetic order in $CeCu_2(Si_{1-x}Ge_x)_2$ at low Ge concentrations.

2. Sample characterization and experimental procedure

Large single crystals of $CeCu_2(Si_{1-x}Ge_x)_2$ were grown by a modified Bridgman technique using a melt with Cu excess which acts as flux. With this technique single crystals with masses up to $m \approx 2\,g$ were obtained. The lattice constants checked by X-ray powder diffraction agree with the reported values [1,2]. All single crystals were oriented with X-ray Laue backscattering. The neutron diffraction experiments were performed on $CeCu_2(Si_{1-x}Ge_x)_2$ single crystals with $x = 0.5; 0.23; 0.05$ on the flat-cone diffractometer E2 at the HMI Berlin using a wavelength $\lambda = 2.39\,\text{Å}$. The primary scattering plane was the $(h\,k\,0)$ plane (except for $x = 0.05$: $(h\,h\,l)$ scattering plane). Using the flat-cone geometry reciprocal $(h\,k\,l_0)$ planes could be accessed from $l_0 = 0$ to $l_0 = 1$. This permitted to record intensity maps of $(h\,k\,l_0)$ planes at various temperatures between $T = 50\,\text{mK}$ and $5\,\text{K}$.

3. Results and discussion

Maps of reciprocal $(h\,k\,l_0)$ planes were taken at different l_0 values with a step size adjusted to the vertical resolution along c^* such that two successive maps overlap and no intensity could be missed. Only for $l_0 \approx 0.5$ additional magnetic intensity was detected. Fig. 1 shows an intensity map of the reciprocal $(h\,k\,0.51)$ plane in $CeCu_2(Si_{0.5}Ge_{0.5})_2$ measured at $T = 70\,\text{mK}$. All observed peaks are of magnetic origin and disappear above T_N (except for two spurious nuclear peaks belonging to a small grain with different orientation). Scans across the magnetic peaks along the c^* direction reveal that the magnetic satellites do not occur at the commensurate $l = 1/2$ position but are slightly off. Due to a relaxed vertical resolution along c^* not only the magnetic satellites of $(h\,k\,0)$ nuclear peaks, appearing at $(h\,k\,0.51)$, are measured but also those at $(h\,k\,0.49)$ which are satellites of $(h\,k\,1)$ nuclear peaks. An analysis of the incommensurate magnetic order yields a wave vector $\tau \approx (0.277\ 0.277\ 0.51)$ at lowest temperature $T = 70\,\text{mK}$. The magnetic moments are mainly confined to the [001] plane and a rough estimation of the ordered moment at lowest temperature gives $\mu \approx 0.5\ \mu_B$ assuming a sinusoidal modulation of the moments which are aligned along $[1\bar{1}0]$.

The temperature dependence of two magnetic reflections is displayed in Fig. 2. The magnetic intensity saturates below $\approx 1\,\text{K}$ and vanishes at the
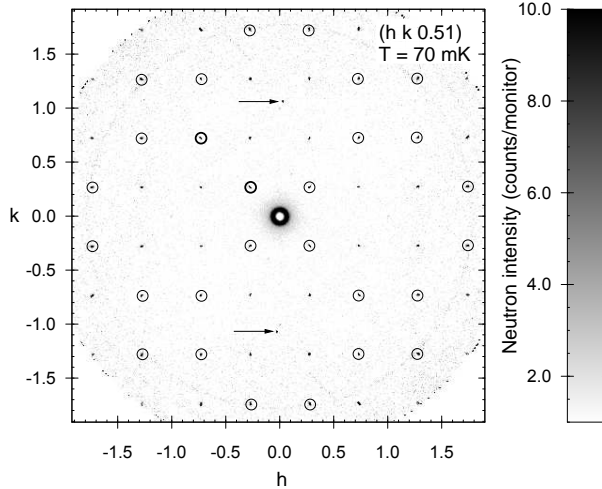
Fig. 1. Intensity map of the reciprocal (h k 0.51) plane in $CeCu_2(Si_{0.5}Ge_{0.5})_2$ at $T = 70\,mK$. The peaks surrounded by circles are magnetic satellites of (h k 0) nuclear peaks, while the other magnetic peaks originate from (h k 1) nuclear peaks. Two spurious nuclear peaks not connected to the magnetic structure are marked by arrows. The temperature dependence of the magnetic order was measured on the two magnetic peaks specially indicated by thick circles and they are referred to as $(000)^+$ and $(110)^+$.

Néel temperature $T_N = 3.1\,K$. The intensity of the $(000)^+$ peak exhibits a sharp maximum at $T \approx 2.23\,K$ associated with a hysteresis in the wave vector which characterizes a first order phase transition due to a spin re-orientation. However, this is not observed for the $(110)^+$ reflection, most likely because of the moment direction. The h component of the wave vector $\tau = (h\ h\ 0.51)$ decreases roughly linearly with temperature below T_N, but shows a distinct step at $T \approx 1.3$ K and remains constant at lower temperatures indicating a lock-in transition to a possibly commensurate value. These three phase transitions are confirmed by thermodynamic measurements on the same crystal [6].

Magnetic peaks were also found for the less heavily doped alloys ($x < 0.5$) below their Néel temperatures $T_N \approx 2\,K$ and $1\,K$ for $x = 0.23$ and 0.05, but no further transitions within the ordered state were observed. While the wave vector of the magnetic order changes only slightly with Ge concentration, the ordered moment decreases strongly from $\mu \approx 0.5\,\mu_B/Ce$ for $x = 0.5$ to only $\mu \approx 0.1\,\mu_B/Ce$ for $x = 0.05$.

Recent calculations of the Fermi surface of the heavy quasiparticles in $CeCu_2Si_2$ [7] reveal nesting properties for $q \approx (0.23\ 0.23\ 0.5)$. This value is very close to the observed ordering wave vector in $CeCu_2(Si_{1-x}Ge_x)_2$ suggesting that the magnetic order is due to nesting of the Fermi surface. Since
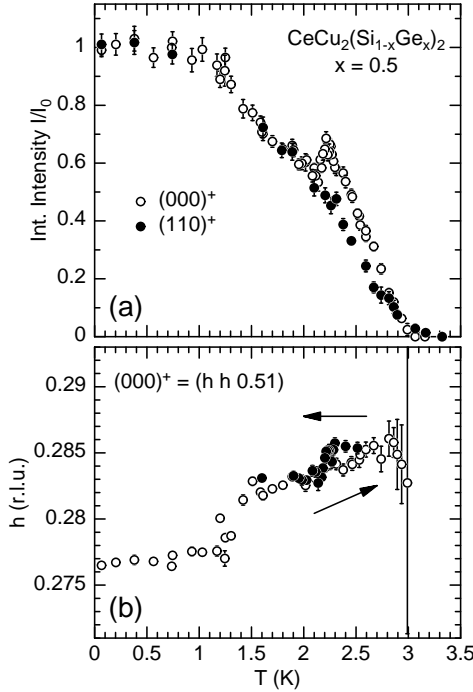
Fig. 2.　(a) Temperature dependence of the integrated intensity of the $(000)^+$ and $(110)^+$ magnetic Bragg peaks in $CeCu_2(Si_{0.5}Ge_{0.5})_2$.　(b) Wave vector $\tau = (h,\ h,\ 0.51)$ as a function of temperature T.

magnetic Bragg peaks are even observed for $x = 0.05$ which is considered to exhibit unconventional A-phase magnetism, a major step towards the understanding of the A-phase in pure $CeCu_2Si_2$ has been made.

REFERENCES

[1] G. Knebel *et al.*, *Phys. Rev.* **B53**, 11586 (1996).
[2] O. Trovarelli *et al.*, *Phys. Rev.* **B56**, 678 (1997).
[3] G. Knopp *et al.*, *Z. Phys.* **B77**, 95 (1989).
[4] A. Krimmel *et al.*, *Phys. Rev.* **B55**, 6416 (1997).
[5] A. Krimmel, A. Loidl, *Physica* **B234–236**, 877 (1997).
[6] N. Oeschler, E. Lengyel, R. Borth, M. Deppe, C. Geibel, unpublished results.
[7] G. Zwicknagl, private communication.