

Magnetic structure of the heavy-fermion alloy $\text{CeCu}_2(\text{Si}_{0.5}\text{Ge}_{0.5})_2$

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Abstract

The heavy-fermion alloy $\text{CeCu}_2(\text{Si}_{0.5}\text{Ge}_{0.5})_2$ orders antiferromagnetically with a Néel temperature of $T_N \approx 3.1$ K. In an elastic neutron scattering experiment (performed at $T \geq 0.33$ K) antiferromagnetic satellite reflections were observed. A first interpretation of the observed intensities in terms of a magnetic structure is given.

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The heavy-fermion system $\text{CeCu}_2(\text{Si}_{1-x}\text{Ge}_x)_2$ (with tetragonal ThCr_2Si_2 structure, space group $I4/mmm$) shows unusual low-temperature phenomena and different ground states due to the competition between Kondo screening, leading to a nonmagnetic ground state, and the RKKY interaction, resulting in long-range magnetic order. It offers the unique possibility to tune the Néel temperature T_N of the system via alloying. While CeCu_2Ge_2 orders antiferromagnetically below $T_N = 4.15$ K, the Néel temperature decreases when substituting germanium by silicon. The other parent compound CeCu_2Ge_2 shows superconductivity in addition to a magnetic order of unknown type, the so called A-phase. In particular the $\text{CeCu}_2(\text{Si}_{0.5}\text{Ge}_{0.5})_2$ compound shows two ordered phases below the Néel temperature and might shed light on the magnetic order in CeCu_2Si_2 . The magnetic structure of $\text{CeCu}_2(\text{Si}_{1-x}\text{Ge}_x)_2$ is known from powder neutron diffraction only for $x \geq 0.6$ [1–3]. Here we report on the magnetic structure of $\text{CeCu}_2(\text{Si}_{0.5}\text{Ge}_{0.5})_2$ well below T_N .

Recent developments on crystal growth techniques allow the growth of large single crystals of $\text{CeCu}_2(\text{Si}_{1-x}\text{Ge}_x)_2$. Several experiments on a $4 \times 6 \times 4$ mm³ single crystal of $\text{CeCu}_2(\text{Si}_{1-x}\text{Ge}_x)_2$ with a nominal concentration $x = 0.5$ and a mass of 570 mg have been performed. Antiferromagnetic satellite reflections below T_N have been observed in a first neutron diffraction experiment at the HMI in Berlin [4]. Magnetic satellites occur at positions described by a propagation vector $\tau = (\tau_H \tau_H \tau_L)$. Due to experimental restrictions the τ_L component of τ could be determined only roughly ($\tau_L \approx 0.5$). Recently, we have performed an experiment on the same crystal at the diffractometer D23 at the ILL in Grenoble to study the antiferromagnetism in more detail. The sample was mounted inside a ³He cryostat to give access to the temperature range $T = 0.33$ K – 3.5 K. Unpolarized neutrons with a wavelength of $\lambda = 1.2805$ Å have been used to collect intensities of selected magnetic satellite reflections. Magnetic peaks were observed below $T_N \approx 3.1$ K in agreement with previous measurements [4].

The tetragonal crystal structure is confirmed with the lattice parameters $a = 4.117$ Å and $c = 10.023$ Å at $T = 0.33$ K. No nuclear superstructure has been found indicating a statistical distribution of the silicon and

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germanium atoms. The only free parameter left in the structure is the z -position of the silicon/germanium site. The refinement of the crystal structure yielded $z = 0.3784(1)$ in agreement with [1,2].

The magnetic propagation vector has been calculated from the position of several magnetic satellite reflections at the lowest temperature. The temperature-dependent shift of the propagation vector has been determined from rocking scans of the $(2\ 2\ 0)^- = (2 - \tau_H\ 2 - \tau_H - \tau_L)$ and $(0\ 0\ 6)^+ = (\tau_H\ \tau_H\ 6 + \tau_L)$ reflections for which the diffractometer is in the 2θ range of highest resolution. Both reflections have enough intensity to obtain good statistics. The rocking scan of the $(0\ 0\ 6)^+$ reflection is mostly sensitive to a change of τ_H , whereas the rocking scan of the $(2\ 2\ 0)^-$ reflection is sensitive to the difference $\tau_H - \tau_L$.

Fig. 1 shows the temperature dependence of the propagation vector. The results for τ_H agree with the previous experiment [4]. Furthermore, τ_L could be determined with nearly the same precision as τ_H . The propagation vector below τ_N is temperature dependent. Below the first-order transition at $T_L \approx (1.4 \pm 0.1)$ K the propagation vector τ locks into a constant value of $\tau = (0.272\ 0.272\ 0.505)$. Band structure calculations [5] indicate that the magnetic ordering is determined by a nesting of the Fermi surface.

The measured intensities of the magnetic reflections at the lowest temperature have been used to determine the magnetic structure. For this purpose the Cambridge Crystallographic Subroutine Library has been used [6]. Since no higher harmonic satellite peaks are observed, the magnetic structure is assumed to be a sinusoidal modulation of the magnetic moments. The analysis yields that the magnetic moments are aligned perpendicular to the propagation vector, i.e. they are transversally oriented, and confined mainly to the basal plane with a direction along $[2\ \bar{1}\ 0]$ ($(-30 \pm 4)^\circ$ to the a -axis). However, a small component of the magnetic moment perpendicular to the basal plane is still possible (moment

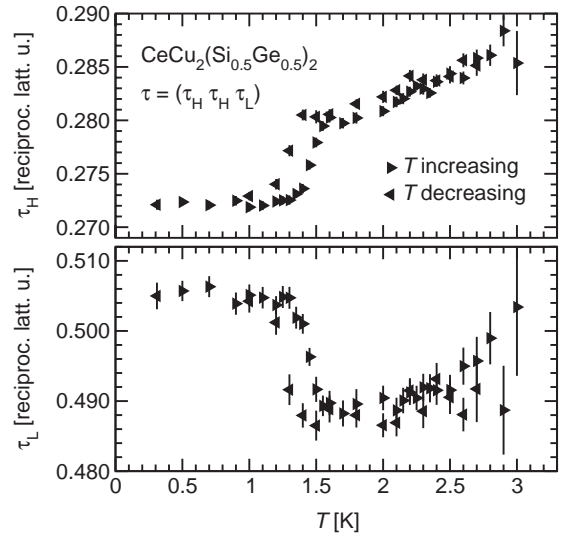


Fig. 1. Temperature dependence of the magnetic propagation vector $\tau = (\tau_H\ \tau_H\ \tau_L)$ as determined from the $(2 - \tau_H\ 2 - \tau_H - \tau_L)$ and the $(\tau_H\ \tau_H\ 6 + \tau_L)$ reflections, respectively.

tilted by $(3 \pm 3)^\circ$). A first refinement of the magnetic moment amplitude results in $m = 0.75\ \mu_B$. Further measurements are planned to investigate the magnetic structure of the ordered phases above T_L .

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