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The magnetic structure of $CePd_2Ge_2$ and $Ce_2Pd_3Ge_5$

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Abstract

The magnetic structures of $CePd_2Ge_2$ and $Ce_2Pd_3Ge_5$ are determined by neutron powder diffraction. Both compounds show antiferromagnetic stacking of ferromagnetic planes of Ce moments, with moment values of $0.85\mu_B$ (parallel to the stacking vector $\boldsymbol{k}$) and $1.25\mu_B$ (perpendicular to $\boldsymbol{k}$), respectively.

Keywords: $CePd_2Ge_2$; $Ce_2Pd_3Ge_5$; Antiferromagnetic ordering; Kondo lattice

The behavior of the series CeT_2M_2 (T = transition metal, M = Si,Ge) is governed by the competition of magnetic exchange and the Kondo interaction [1]. This series can be mapped onto the Kondo-lattice phase diagram, assuming f–d hybridization to be the dominant parameter [2]. Only a few studies have been carried out on the structurally related series $Ce_2T_3M_5$. Recently, a new compound, $Ce_2Pd_3Ge_5$, has been shown to exhibit an antiferromagnetic (AFM) transition at $T_N = 3.8$ K [3]. Studies of the related compound $CePd_2Ge_2$ ($T_N = 5.1$ K) have been reported previously [4]. Here, we report the ordered magnetic structures of both these compounds as determined by neutron powder diffraction.

A polycrystalline $Ce_2Pd_3Ge_5$ sample has been prepared and characterized as described previously [3] and $CePd_2Ge_2$ was prepared by a similar procedure. The neutron diffraction studies have been carried out at the Chalk River Laboratories, Canada. Analysis of the data was carried out using GSAS [5]. $CePd_2Ge_2$ crystallizes in the tetragonal $ThCr_2Si_2$-type structure, space group I4/mmm, with $a = 4.316(1)$ Å and $c = 10.041(1)$ Å at $T = 1.8$ K. $Ce_2Pd_3Ge_5$ crystallizes in the orthorhombic $U_2Co_3Si_5$-type structure, space group Ibam. At $T = 40$ K, we find the lattice constants $a = 10.145(1)$ Å, $b = 12.080(1)$ Å, $c = 6.1460(5)$ Å. The atom coordinates are close to those reported for the prototype compound.

Fig. 1 shows the difference of the diffraction patterns measured at $T = 1.8\,\text{K} < T_N$ and $T = 5.6\,\text{K} > T_N$ for both compounds. On the basis of

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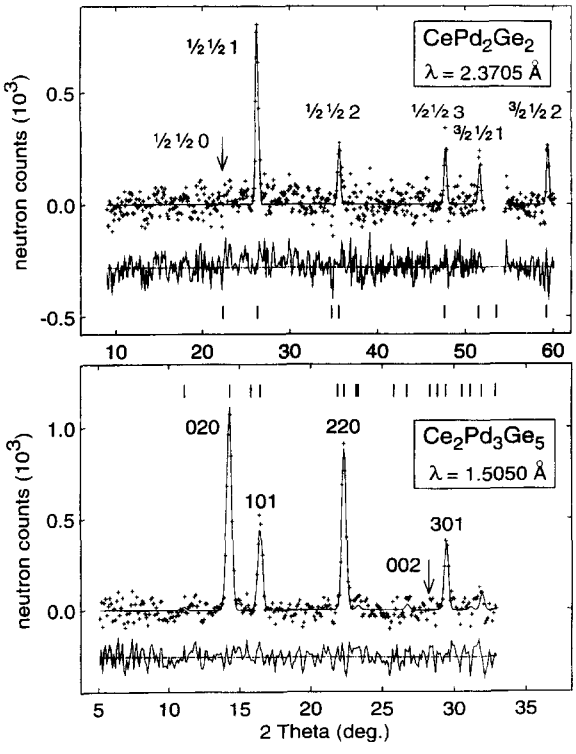

Fig. 1. Difference of the diffraction patterns measured at $T = 1.8\,\mathrm{K} < T_N$ and $T = 5.6\,\mathrm{K} > T_N$; top: for $CePd_2Ge_2$, bottom: for $Ce_2Pd_3Ge_5$. Some Bragg reflections are indexed on the basis of the crystallographic unit cells.

the tetragonal unit cell, the observed magnetic Bragg reflections $(h\,k\,l)$ in $CePd_2Ge_2$ can be indexed with half-integers h and k and integer l, indicating a doubling of the unit cell in the basal plane. The resulting magnetic structure (see Fig. 2) is characterized by an AFM stacking of (1 1 0) ferromagnetic (FM) planes. The absence of the $(\frac{1}{2}\,\frac{1}{2}\,0)$ reflection shows that the magnetic moments are oriented perpendicular to these planes. We find the ordered moment $\mu = 0.85(5)\mu_B$ at $T = 1.8\,\mathrm{K}$. The same structure has been observed in $CePd_2Si_2$ ($\mu = 0.62\mu_B$) [6].

The observed magnetic reflections in $Ce_2Pd_3Ge_5$ can be indexed with integers h, k, l, indicating that the magnetic and the crystallographic unit cells are identical. The magnetic Bragg pattern is consistent only with an AFM stacking of (0 1 0) FM planes (see Fig. 2). The absence of the (0 0 2) reflection

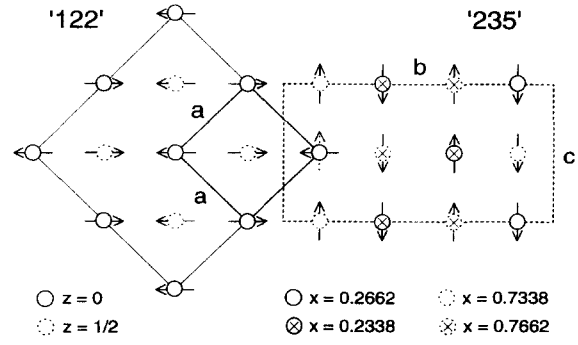

Fig. 2. The magnetic structures of $CePd_2Ge_2$ ('1 2 2') and $Ce_2Pd_3Ge_5$ ('2 3 5'), projected onto the basal plane of the '1 2 2' and the bc-plane of the '2 3 5' structure, respectively.

shows that the magnetic moments are oriented parallel to these planes. The ordered moment is $\mu = 1.25(5)\mu_B$ at $T = 1.8\,\mathrm{K}$. The very similar arrangement of Ce atoms in both germanides as well as the relationship of the magnetic structures is vizualized in Fig. 2. Notably, the stacking of the magnetic moments is equivalent, but their orientation differs by 90°.

Usually, the orientation of the magnetic moments in the ordered state is determined by the easy direction produced by the crystal electric field (CEF). In the case of $CePd_2Si_2$ and $CePd_2Ge_2$, however, the reported CEF level schemes correspond to a magnetically easy c-axis [4,7]. The actual orientation of the moments perpendicular to this direction has been discussed in terms of a hybridization-induced anisotropic exchange mechanism, which favors for Ce^{3+} ions the formation of FM coupled planes with the moments perpendicular to these planes [6]. Therefore, the small values of the ordered moments appear not to be due to Kondo screening but to the interplay of the CEF and the anisotropic exchange interaction. In $Ce_2Pd_3Ge_5$ – as a result of the smaller number of T ions per Ce and an correspondingly reduced hybridization – the ordered moment is of ordinary size. In this case, the moment orientation appears to be solely determined by the CEF.

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