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The Crystal and Magnetic Structure of $CeMn_2Si_2$

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Compounds presented by the formula RB_2X_2, where R is rare earth, alkaline earth, or actinide metal, B is a transition metal, and X germanium or silicon, have been extensively studied /1 to 15/. These compounds crystallize in the $ThCr_2Si_2$ type structure, space group D_{4h}^{17}-I4/mm. The lattice constants are approximately $a \approx 4$ Å and $c \approx 10$ Å. The ions R, B, and X occupy the 2(a), 4(d), and 4(e) positions in this space group. Magnetic measurements /5, 6, 9 to 15/ show that the RB_2X_2 compounds are ferromagnets or antiferromagnets. Basing on magnetic measurements, Narasimhan et al. /13/ concluded that $CeMn_2Ge_2$ is ferromagnetic with Curie temperature 316 K.

In the present paper we report the results of X-ray diffraction, neutron diffraction, and magnetometric measurements on a powder sample of $CeMn_2Si_2$ undertaken in order to determine its crystal and magnetic structure.

The sample was prepared by melting cerium, manganese (4N), and silicon (5N purity) in an induction furnace. The sample was then annealed in a quartz tube at 950 °C for 100 h, and cooled to room temperature.

The single-phase nature of the compound was established by X-ray analysis using FeK_α radiation. The powder pattern of the sample could be indexed on the basis of the body-centred tetragonal structure. A least-squares fit to the observed 2Θ values was used to obtain the lattice parameters (see Table 1).

Magnetic susceptibility measurements were carried out between 100 and 600 K, in a magnetic field of 2 to 11 kOe using an electronic balance. The temperature dependence of the magnetic susceptibility is shown in Fig. 1. At low temperatures the $CeMn_2Si_2$ compound exhibits antiferromagnetic properties,

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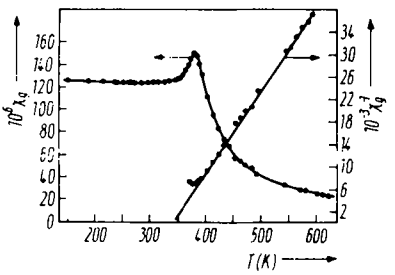

Fig. 1. Magnetic gram susceptibility and inverse susceptibility versus temperature for $CeMn_2Si_2$

apparent from its susceptibility maximum at the Néel temperature of 379 K. Above the Néel temperature the magnetic susceptibility satisfies the Curie-Weiss law with the paramagnetic Curie temperature Θ_p and the effective magnetic moment μ_{eff} equal to 330 K and $(3.0 \pm 0.1)\,\mu_B$, respectively.

Table 1

Magnetic and structural parameters in $CeMn_2Si_2$

temperature (K)	78	293	373
a_o (Å)	3.986 ± 0.005	4.026 ± 0.005	4.054 ± 0.005
c_o (Å)	10.491 ± 0.005	10.568 ± 0.005	10.611 ± 0.005
c_o/a_o	2.632	2.625	2.617
z	0.372 ± 0.001	$0.372 \pm 0\ 001$	0.372 ± 0.001
R (%)	6.1	6.0	6.7
B (Å^2)	0.25	0.55	0.65
μ (μ_B)	2.30 ± 0.05	-	-
T_N(K)	379 ± 2		
Θ_p(K)	$+ 330 \pm 5$		
μ_{eff} (μ_B)	3.0 ± 0.1		

Neutron diffraction patterns at 78, 293, and 373 K were taken at the EWA reactor in Świerk using neutrons of wavelength (1.324 ± 0.003) Å. Nuclear intensities were calculated for the structure shown in Fig. 2 with Ce, Mn, and Si at the positions 2(a), 4(d), and 4(e) of the space group I4/mm, respectively, see Table 2.

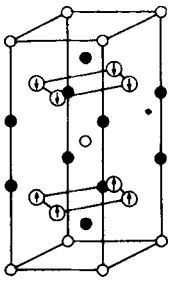

Fig. 2. The crystal and magnetic structure of $CeMn_2Si_2$; ○ Mn, o Ce, ● Si

The parameter z and the Debye-Waller factor were refined to give the best least-squares fit of the calculated to the observed integrated intensities. The refined z parameter with the corresponding weighted R factor is given in Table 1. The mixing of Mn and Si atoms among 4(d) and 4(e) positions /10/ was not confirmed by our experiment.

Table 2

Atomic positions in $CeMn_2Si_2$, space group I4/mm

position	coordinates
Ce in 2(a)	$0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
Mn in 4(d)	$0, \frac{1}{2}, \frac{1}{4}; \frac{1}{2}, 0, \frac{1}{4}; 0, \frac{1}{2}, \frac{3}{4}; \frac{1}{2}, 0, \frac{3}{4}$
Si in 4(e)	$0, 0, z; 0, 0, \bar{z}; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}+z; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}-z$

In the second step the magnetic structure was determined. At LN and RT two superlattice lines of magnetic origin are observed. These lines are indexed as (111) and (113) on the basis of the crystallographic unit cell which contains four manganese ions, at the following positions: S_1 (0, 0.5, 0.25), S_2 (0.5, 0, 0.25), S_3 S_3 (0, 0.5, 0.75), S_4 (0.5, 0, 0.75).

According to Bertaud /16/ the following collinear antiferromagnetic structures are possible in such a case:

$$G = S_1 - S_2 + S_3 - S_4,$$
$$C = S_1 + S_2 - S_3 - S_4,$$
$$A = S_1 - S_2 - S_3 + S_4.$$

Only for model C the possible magnetic reflections coincide with the observed ones. The absence of (001) magnetic peaks indicates that magnetic moments are parallel to the c-axis. This fact implies a simple ordering scheme with + - + - sequence of ferromagnetic layers built of Mn atoms, stacked in the c direction. The magnetic moment of Mn atoms is $(2.3 \pm 0.05)\,\mu_B$ at 78 K, taking the Mn^{2+} form factor after Watson and Freeman /17/. The magnetic space group of this structure is $I_p 4/m'm'm'$ in the western notation /18/ and Sb_{130}^{434} in the eastern notation /19/. In $CeMn_2Si_2$ Ce ions are in Ce^{4+} state with zero magnetic moment.

The determined magnetic structure of $CeMn_2Si_2$ is similar to that one of $ThMn_2Si_2$ /6, 15/. The layer structure of this compound suggests a strongly anisotropic character of magnetic interactions. Because of the short Mn-Mn distance (2.85 Å) the ferromagnetic interactions should be predominant. This is consistent with a positive paramagnetic Curie temperature. However, rather high magnetic transition temperatures and the fulfillment of the Curie-Weiss law indicate that interlayer interactions are not very weak. It seems therefore that conduction electrons are probably responsible for the magnetic interactions since similar compounds RFe_2Si_2 (R = Nd, Eu, Dy) and $GdMn_2Ge_2$ /7, 13/ are all electrical conductors.

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