

MAGNETIC PROPERTIES AND MAGNETIC STRUCTURE OF CeLiGe₂ COMPOUND

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ABSTRACT

X-ray and neutron diffraction as well as magnetic measurements have been performed on CeLiGe₂ compound. This compound crystallizes in the orthorhombic CaLiSi₂ structure type (Pnma space group). Crystal structure parameters have been refined on the basis of the X-ray data at 293 K and neutron diffraction data at 20 and 1.5 K. Below T_C=9.8(2) K Ce-magnetic moment equal 2.32(6) μ_B and form ferromagnetic structure with the moments parallel to the b-axis.

INTRODUCTION

CeLiGe₂ is one of 6 the ternary intermetallic compounds which are found in the Ce-Li-Ge system at 470 K [1]. This compound crystallizes in the CaLiSi₂ structure type (Pnma space group) [2]. Some magnetic properties for compounds of this system were measured earlier. CeLi₂Ge₆, CeLi₂Ge₅ and CeLiGe₂ are paramagnetics from 10 up to ~250 K. Magnetic susceptibility χ⁻¹ strongly increased above 250 K. In this paper we presented continuation of studies of magnetic properties and magnetic structure of the CeLiGe₂ compound.

EXPERIMENTAL

Alloy CeLiGe₂ was prepared from the pure metals. Purity of the elements were: Li and Ce ~98 wt.%, Ge 99.999 wt.%. The samples were arc melted in the Ti-gettered argon atmosphere.

Testing of the CeLiGe₂ crystal structure was carried out using the PHILIPS ANALYTICAL X-ray powder diffractometer with the Cu-K_α radiation. The measurement were carried out at room temperature between 30 and 70 degree in 2θ. Diffraction data were collected with 2θ steps of 0.02 degree and step time 2 s. The XPD data were analyzed with the Rietveld profile refinement method using the DBWS-9006PC program [3].

Magnetometric data were collected using a SQUID magnetometer operating in the magnetic fields up to 50 kOe.

Neutron diffraction pattern of CeLiGe_2 was recorded using the E6 diffractometer at the BER II reactor at the Hahn-Meitner Institute, Berlin. Neutron diffraction data were processed using the FULLPROF program [4].

RESULTS

3.1. Crystal structure

The X-ray diffraction at 293 K was measured. Testing of the CeLiGe_2 crystal structure confirmed that it crystallized in the CaLiSi_2 structure type (Pnma space group, $R_{\text{Bragg}}=0.063$, $R_{\text{prof}}=0.051$). The experimental X-ray diffraction pattern and the calculated and difference diffraction profiles after the Rietveld refinement are shown in Fig. 1.

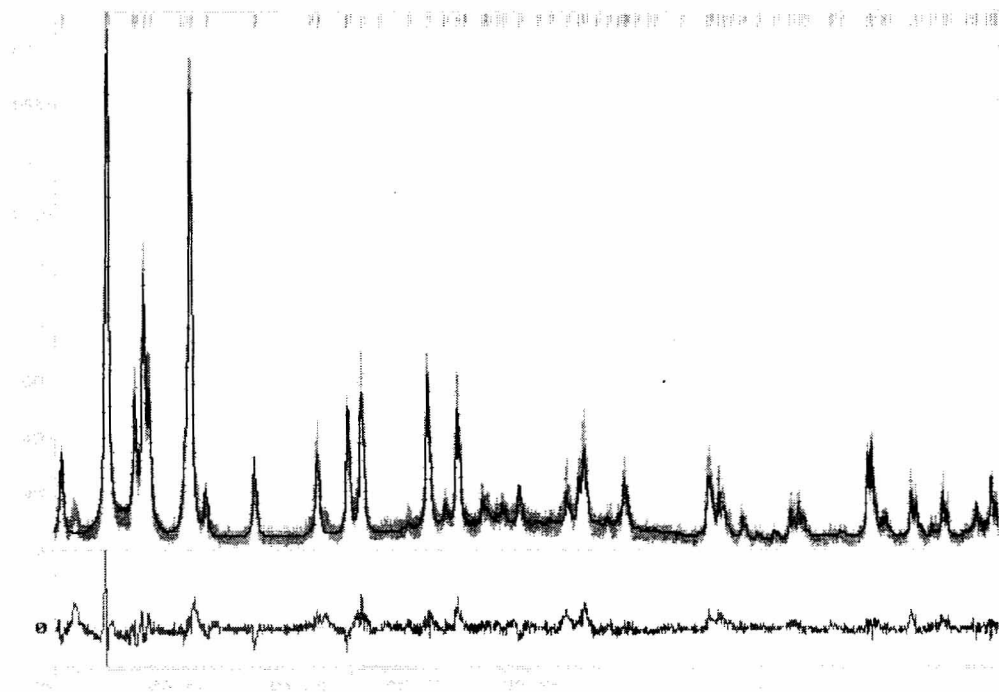


Figure 1. The experimental X-ray diffraction pattern and the calculated and difference diffraction profiles after the Rietveld refinement

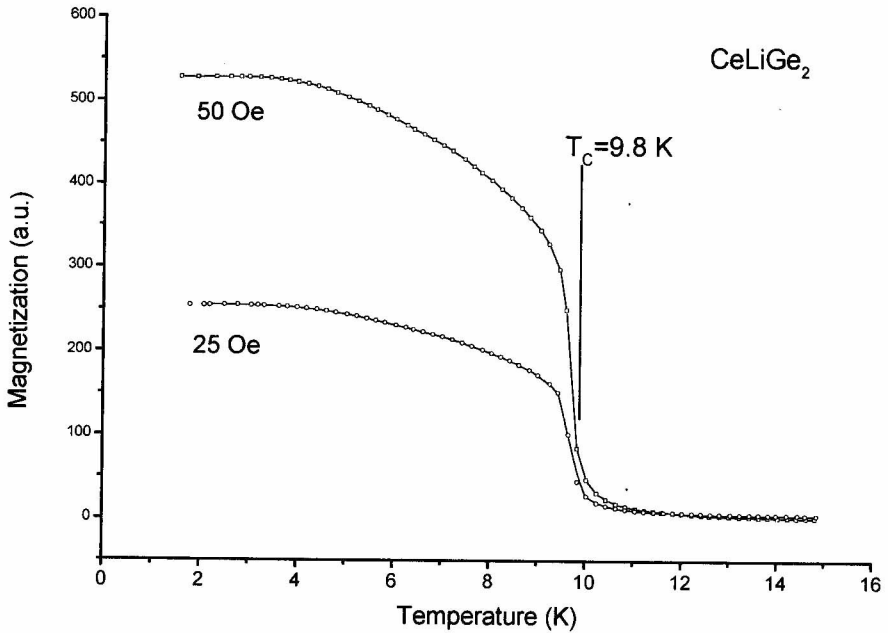
All atoms in the crystal structure of this compound occupied Wyckoff position 4(c) (x , $1/2$, z). The determined values of the lattice parameters a , b , c and the atomic coordinates x , z for the X-ray diffraction at 293 K and neutron diffraction at 20 and 1.5 K measurement are listed in the Table 1.

Table 1. Lattice parameters a , b , c and the atomic coordinates x , z for the CeLiGe_2 at the different temperatures.

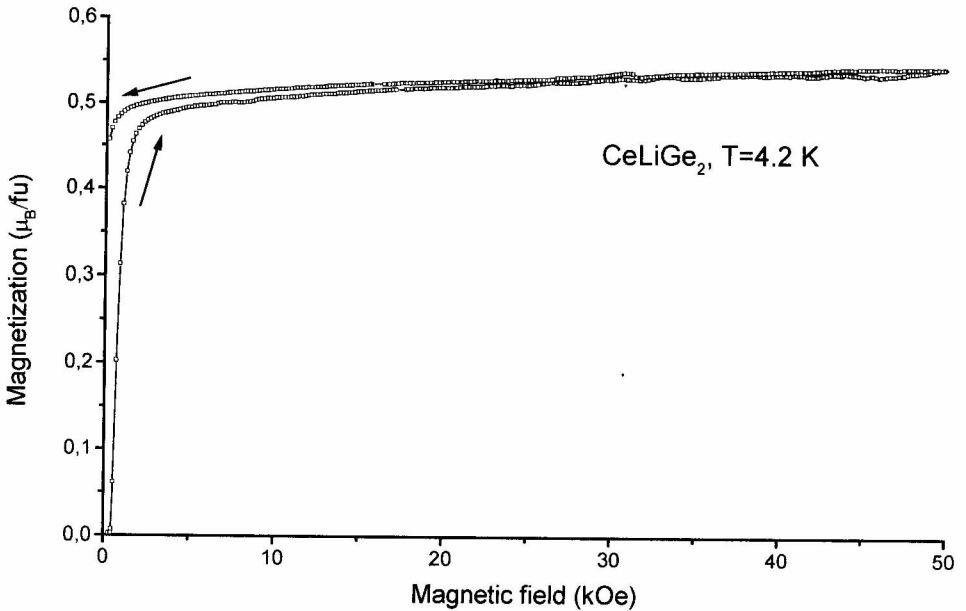
T (K)	293	20	1.5
a (Å)	7.8228(7)	7.785(17)	7.780(16)
b (Å)	3.9715(4)	3.954(6)	3.950(5)
c (Å)	10.7576(9)	10.730(19)	10.721(19)
x (Ce)	0.6419(7)	0.663(9)	0.660(8)
z (Ce)	0.1320(6)	0.145(5)	0.146(5)
x (Li)	0.995(2)	0.952(24)	0.967(22)
z (Li)	0.858(2)	0.869(16)	0.875(16)
x (Ge1)	0.611(1)	0.658(6)	0.656(5)
z (Ge1)	0.8200(9)	0.809(4)	0.814(3)
x (Ge2)	0.719(1)	0.736(5)	0.737(5)
z (Ge2)	0.441(1)	0.433(3)	0.430(3)

3.2. Magnetic Properties

Temperature dependence of the magnetization in low magnetic fields (25 and 50 Oe) give the Curie temperature for the CeLiGe_2 compound equal 9.8(2) K (Fig. 2a). Magnetization curve at 4.2 K and external magnetic field up to 50 kOe indicate the ferromagnetic properties with the Ce magnetic moment equal $0.55 \mu_B$ (Fig. 2b).



a



b

Figure 2. a) The temperature dependence of the magnetization of the CeLiGe_2 at low magnetic fields; b) The field dependency of the magnetization at 4.2 K. The arrows show the directions of the changes of the external field during the measurement.

3.3. Magnetic structure

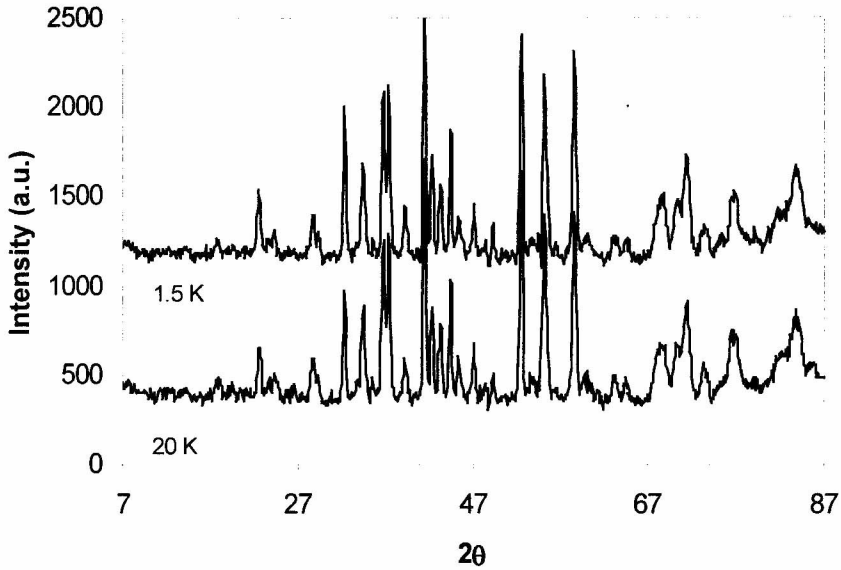


Figure 3. Neutron diffractograms of the CeLiGe_2 compound obtained at 1.5 and 20 K.

Comparison neutron diffractograms for the CeLiGe_2 compound recorded at 20 and 1.5 K (Fig. 3) indicate the very small contribution of the magnetic scattering. For this reason magnetic structure of the CeLiGe_2 compound was calculated from difference neutron diffractogram (Fig. 4).

LiCeGe_2

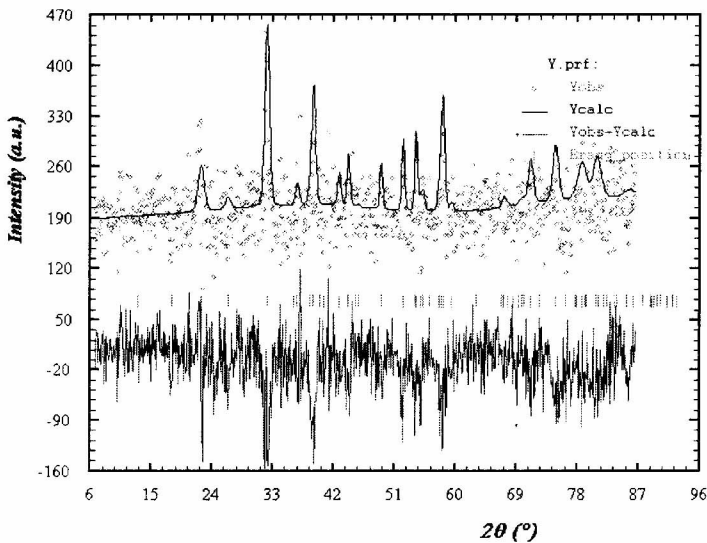


Figure 4. Difference neutron diffractogram of the CeLiGe_2 compound ($T=1.5-20$ K)

The observed peaks of magnetic origin were indexed as those originating from the crystal unit cell. The best refinement has been obtained for the ferromagnetic structure with the Ce magnetic moment equal $2.32(6) \mu_B$ and parallel to the b-axis. This structure is schematically shown in Fig. 5.

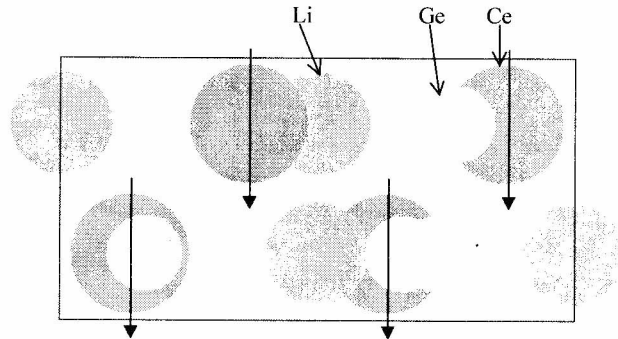


Figure 5. The ferromagnetic structure of the $CeLiGe_2$ compound projected on the a-b plane.

CONCLUSIONS

X-ray and neutron diffraction and magnetometric data indicate that the ternary cerium $CeLiGe_2$ compound crystallize in the $CaLiSi_2$ structure type. Below T_C equal $9.8(2)$ K the Ce magnetic moment equal $2.32(6) \mu_B$ forms the ferromagnetic structure with the moments parallel to the b-axis. The determined value of the Ce-moment is slightly larger than the value for the free Ce^{3+} ion ($2.14 \mu_B$).

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