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Crystallographic and magnetic structure of the novel compound $ErGe_{1.83}$

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Abstract

The crystal structure and the magnetic ordering of the novel orthorhombic compound $ErGe_{2-x}$ has been studied by neutron powder diffraction and magnetic measurements. The crystal structure belongs to the $DyGe_{1.85}$-type (space group $Cmc2_1$)·$ErGe_{2-x}$ ($x = 0.17$ (2)) orders antiferromagnetically below $T_N = 6$ K and displays a metamagnetic behaviour. The magnetic cell has the same size as the chemical unit cell ($\boldsymbol{q} = 0$). The magnetic space group is $Cmc2_1$ (Sh_{36}^{173}). At $T = 1.5$ K the magnetic moments of the two erbium sites have the same ordered magnetic moment value of 7.63 (6)μ_B/Er and are antiferromagnetically coupled leading to an uniaxial structure along the a direction.

Keywords: Rare-earth metals; Crystal structures; Phase transitions; Antiferromagnetism

According to Ref. [1] the compound of nominal composition $ErGe_2$ undergoes two polymorphic transitions at 1080 K and 1205 K. The crystal structure of all modifications was unknown. The present investigation deals with the determination of the crystal structure and magnetic properties of the low temperature modification of the $ErGe_2$ phase. The 80 K data collected well above the Néel temperature ($T_N = 6$ K) (D2B, ILL, Grenoble) are indexed in the C- centred orthorhombic lattice ($a = 4.05263$ (7), $b = 29.4964$ (5), $c = 3.88712$ (6) Å). The structure was found to be isomorphic with the $DyGe_{1.85}$ structure type [2] (space group $Cmc2_1$) with refined composition $ErGe_{1.83(2)}$ (occup. = 0.67(2) for Ge4). The data were evaluated by the Fullprof program [3] (Fig. 1 bottom, $R_n = 5.8\%$ and $R_{wp} = 15.8\%$, $R_{exp} = 12.5\%$, $\chi^2 = 1.61$). The 1.5 K neutron data are indexed with the same C-centred unit cell as found for the nuclear reflections ($\boldsymbol{q} = 0$). The refinement of magnetic intensities showed that the Er-moments are oriented along the a axis and that Er atoms (Fig. 2) related by the screw axis 2_1 operation and neighbouring Er atoms occupying different symmetry sites have their moments oppositely aligned. This arrangement remains invariant under the assumption of the trivial magnetic space group $Cmc2_1$ (Sh_{36}^{173}). The final model (all atoms in 4(a) : 0yz) Er1 : $y = 0.0609$ (1), $z = 0.750$, $B_{iso} = 0.32$ (9) Å^2, Er2: $y = 0.1710$ (1), $z = 0.249$ (4), $B_{iso} = 0.16$ (8) Å^2, Ge1: $y = 0.3529$ (2), $z = 0.268$ (4), $B_{iso} = 0.6$ (1) Å^2, Ge2: $y = 0.4074$ (2), $z = 0.744$ (4), $B_{iso} = 0.72$ (9) Å^2, Ge3: $y = 0.2499$ (2), $z = 0.765$ (4), $B_{iso} = 0.54$ (9) Å^2, Ge4: $y = 0.5101$ (5), $z = 0.347$ (4), $B_{iso} = 1.7$ (3) Å^2, occup. = 0.64 (2) corresponds to the reliability factors $R_n = 3.8\%$,

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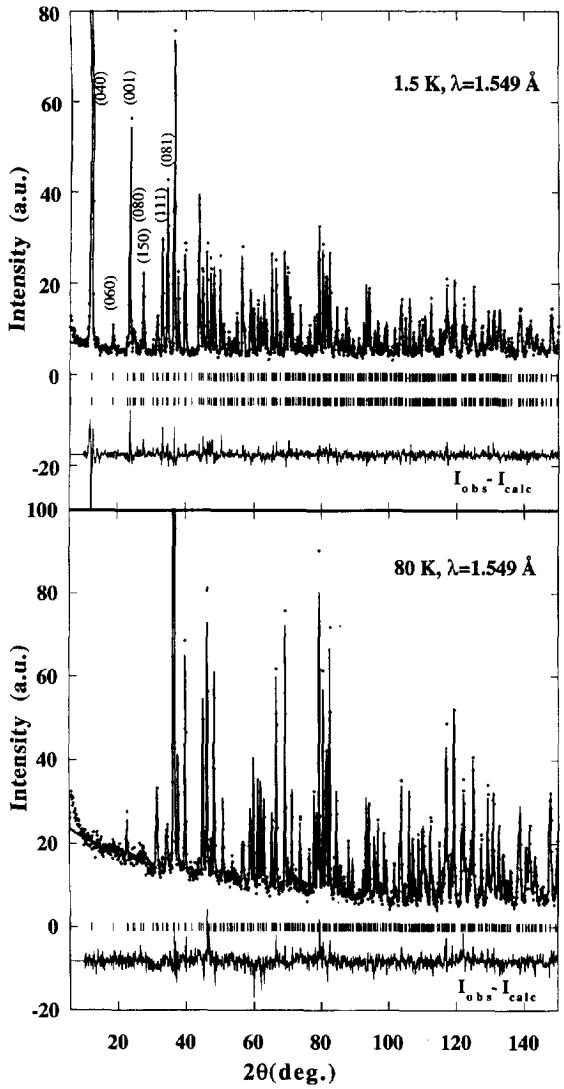

$R_m = 7.3\%$, $R_{wp} = 18.2\%$, $R_{exp} = 13.0\%$, $\chi^2 = 1.96$ (Fig. 1 top). Within the standard deviation the refined composition values at 1.5 and 80 K correspond to the off stoichiometric formula $ErGe_{1.83(2)}$. The ordered moment value 7.63(1) μ_B/Er at 1.5 K is lower than the free-ion value of Er^{3+} ($gJ\mu_B = 9\mu_B$). The resulted uniaxial antiferromagnetic structure has an alternating + − + − stacking of ferromagnetic layers along the longest orthorhombic axis *b* as shown in Fig. 2. The interlayer interaction for both Er sublattices for layers at $z = \frac{1}{4}$ or $\frac{3}{4}$ is ferromagnetic while the intralayer interaction is antiferromagnetic. However, the antiferromagnetic interlayer interaction along the *b* direction is substantially weakened because the magnetic measurements show that the antiferromagnetic structure can be broken already in comparatively small external magnetic fields.

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References

[1] V.N. Eremenko and I.M. Obushenko, Non-ferrous Met. Res. 9 (1981) 216.
[2] I.R. Mokra, V.K. Pecharsky, Z.M. Shpyrka, O.I. Bodak, V.K. Belsky and I.E. Pats, Dop. AN Ukr SSR, Ser. B, 3 (1989) 48.
[3] J. Rodriguez-Carvajal, Physica B 192 (1993) 55.

Fig. 1 Observed, calculated and difference neutron diagrams of $ErGe_{1.83}$ germanide (top part) measured at 1.5 K, (bottom part) measured at 80 K.

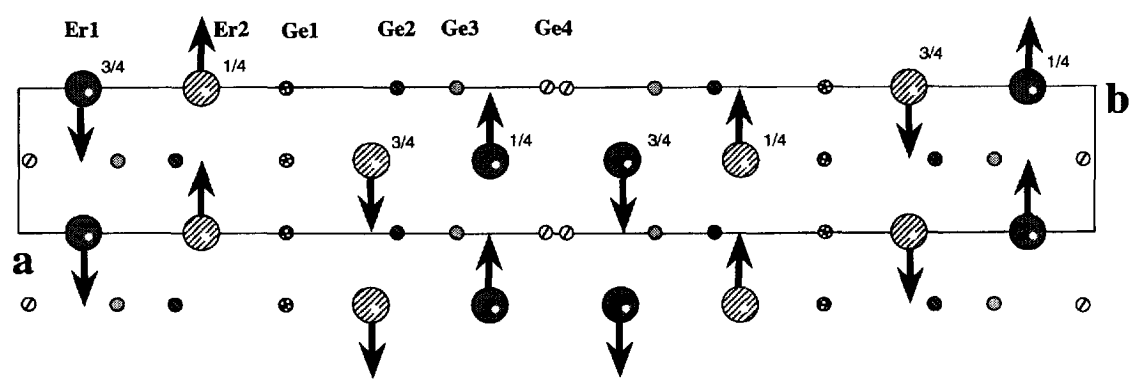

Fig. 2. Schematic representation of the collinear antiferromagnetic ordering in $ErGe_{1.83}$ when viewed along the [0 0 1] direction.