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Anisotropic magnetic properties of $ErRu_2Si_2$ as a consequence of the tetragonal structure

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Abstract

Magnetic properties of $ErRu_2Si_2$ have been calculated as resulting from the fine electronic structure of the $4f^{11}$ configuration of the Er atom taking into account crystal-field and inter-site spin-dependent exchange interactions. Our calculations yield the zero-temperature moment value and its direction, single-crystalline magnetization curves, temperature dependence of the magnetic susceptibility and of the specific heat with the sharp peak at T_N in very good agreement with experiment. Magnetic properties have been found to be strongly anisotropic due to the tetragonal crystal symmetry. These studies reveal the importance of low-symmetry charge multipolar interactions in description of magnetic properties of real 4f systems.

Keywords: Crystal electric field; Magnetic anisotropy; $ErRu_2Si_2$

$ErRu_2Si_2$ crystallizes in the tetragonal structure $ThCr_2Si_2$-type and orders antiferromagnetically below $T_N = 6\,K$ with the easy axis [1 1 0] [1]. The magnetic ordering is marked in the temperature dependence of the specific heat as a large λ anomaly [2]. The magnetic structure of $ErRu_2Si_2$ deduced from neutron diffraction experiments [3,4] reveals antiferromagnetic interactions between ferromagnetic layers with the magnetic wave vector $q = (1/5, 0, 0)$. The experimentally observed ordered magnetic moment Er-ions is $m_{Er} = 7.3\mu_B$ [1–4]. The aim of this paper is to present results of the calculations of magnetic properties of $ErRu_2Si_2$. These properties have been related to the Er^{3+} ions possessing the configuration $4f^{11}$. The associated fine electronic structure is obtained by taking into account crystal-field (CEF) and inter-site spin-dependent exchange interactions. The general Hamiltonian contains the single-ion-like and the intersite terms

$$H = \sum\sum B_n^m \hat{O}_n^m(J, J_z) + n_{mol} g_J^2 \mu_B^2 \left(-J\langle J\rangle + \frac{1}{2}\langle J\rangle^2\right) + g_J \mu_B J \cdot B_{ext} \quad (1)$$

The first term is the CEF Hamiltonian written for the lowest multiplet ($^4I_{15/2}$, $g_J = 6/5$). The second term represents the exchange interactions between the Er moments written in the dynamical-mean-field approximation with the molecular-field coefficient n_{mol}. The third term describes the Zeeman effect. The energy level scheme of the $4f^{11}$ (Er^{3+} ion) in the tetragonal CEF Hamiltonian contains 8 Kramers doublets Fig. 1. A final set of the tetragonal CEF parameters, $B_2^0 = +1.6\,K$, $B_4^0 = -5.0\,mK$, $B_4^4 = -4.5\,mK$, $B_6^0 = -5\mu\,K$ and $B_6^4 = -0.52\,mK$, has been derived by our self-consistent analysis of experimental data with making use of parameters derived for $PrRu_2Si_2$ (direct single-ion recalculations from the $PrRu_2Si_2$ parameters give: $B_2^0 = +1.58\,K$, $B_4^0 = -4.97\,mK$, $B_4^4 = -4.52\,mK$, $B_6^0 = -105\mu\,K$ and $B_6^4 = -0.393\,mK$) [5,6]. The final set of CEF parameters describes well: (i) large anisotropy of the temperature dependence of the susceptibility in the paramagnetic region, (ii) the direction of the magnetic moment in the ordered state, (iii) the spontaneous

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moment of the Er ion of $m_{Er} = 7.2\mu_B$, (iv) the large anisotropy of the magnetization curves (with the observed in-plane anisotropy), (v) temperature dependence of the specific heat with the characteristic λ-type peak at T_N. The consistent description of so many physical properties provides the strong argument for our theoretical approach.

At T_N of 6 K the magnetic order starts to dominate the temperature disordering. In our calculations, it is accounted for by the effective exchange interaction parameter n_{mol} of $0.34\,T/\mu_B$. The magnetic ordering produces the abrupt change in the energy level scheme (the removal of the Kramers degeneracy), Fig. 1, that manifests as the λ peak at T_N (Fig. 3). The calculated moment of the Er ion is parallel to the [1 1 0] direction in agreement with experiment. It amounts to $7.2\mu_B$ at 0 K reproducing the experimental datum [1]. This moment consists of the spin and orbital part ($m_S = +2.4\mu_B$ and $m_L = +4.8\mu_B$). The magnetic moment of the Er^{3+} ion is tied to the [1 1 0] direction by the higher-order charge multipolar interactions. The full magnetization curves, at 2.0 K, calculated within our CEF-based approach are presented in Fig. 2. They are highly anisotropic. Our results in Fig. 2 have been shifted by the spin-flop field B_{sf} of 0.4 T in order to take into account the antiferromagnetic interactions. The way of taking into account the internal field has been discussed in Ref. [5].

The rare-earth specific heat of $ErRu_2Si_2$, calculated by making use of the general formula based on the free energy calculation (Eq. 2) in Ref. [7], is shown on Fig. 3. Our heat calculations reproduce well: (i) a λ-type peak at 6 K associated with the occurrence of the antiferromagnetic order (ii) a tail of the Schottky-like peak above T_N, (iii) the overall entropy. This good agreement indicates the substantial confidence to the presently derived fine electronic structure. The obtained values of the CEF parameters for $ErRu_2Si_2$ are close to parameters directly recalculated from the isostructural compound $PrRu_2Si_2$. It is a good confirmation of the found CEF parameters for both compounds $PrRu_2Si_2$ and $ErRu_2Si_2$.These studies reveal the importance of low-symmetry charge multipolar interactions in description of magnetic properties of real 4f systems.

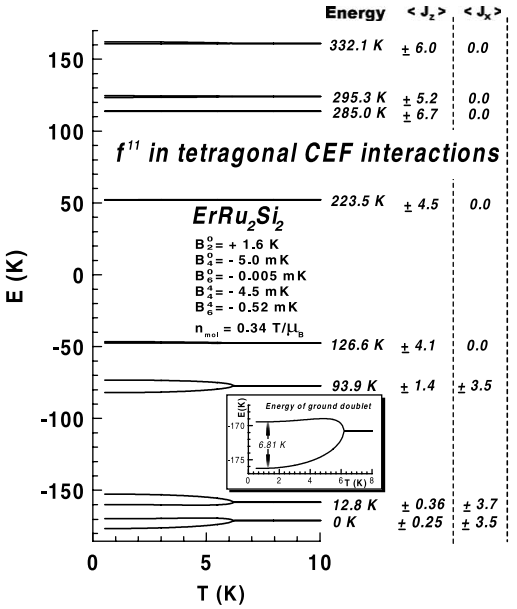

Fig. 1. The energy level scheme of the $ErRu_2Si_2$ with the expectation values of J_z and J_x in the paramagnetic state.

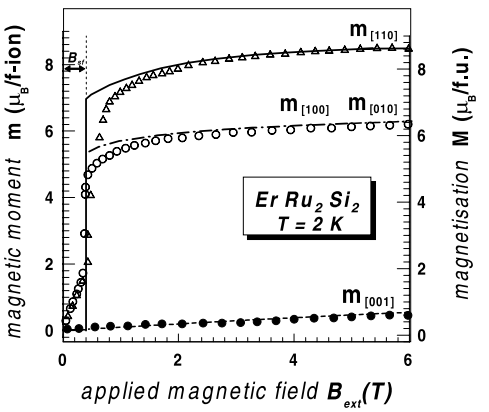

Fig. 2. The calculated magnetization curves at 2.0 K (lines) along the main crystallographic directions of the tetragonal unit cell. Points denote experimental data from Ref. [1].

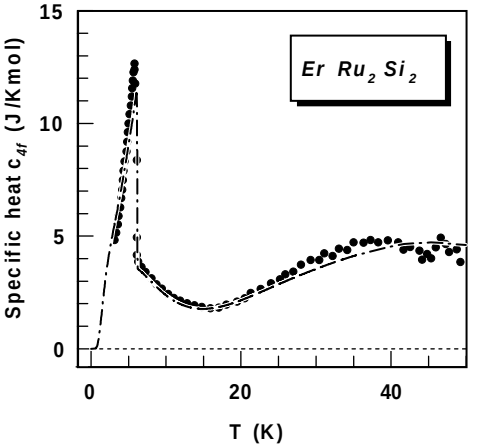

Fig. 3. The calculated temperature dependence of the 4f contribution to the specific heat of $ErRu_2Si_2$ (the dashed-point line). Points are experimental data from Ref. [2].

References

[1] T. Takeuchi, et al., J. Magn. Magn. Mater. 177–181 (1998) 1081.
[2] R. Hamada, et al., J. Magn. Magn. Mater. 140–144 (1995) 907.
[3] M. Slaski, et al., J. Magn. Magn. Mater. 46 (1984) 114.
[4] A. Szytula, et al., J. Magn. Magn. Mater. 80 (1989) 200.
[5] R. Michalski, et al., J. Phys.: Condens. Matter 12 (2000) 7609.
[6] R. Michalski, et al., Acta Phys. Pol. A 97 (2000) 767.
[7] R.J. Radwanski, et al., J. Phys.: Condens. Matter 4 (1992) 8853.