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Crystal-field interactions in $ErBa_2Cu_3O_7$

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Abstract

Magnetic and thermal properties of $ErBa_2Cu_3O_7$ have been analyzed within the crystalline-electric-field (CEF) approach. A full set of CEF parameters for the orthorhombic $ErBa_2Cu_3O_7$ is proposed reproducing the energy level scheme obtained by inelastic-neutron-scattering studies. Very weak exchange interactions of -0.05 T/μ_B, relevant to an internal field of 0.22 T, produce a magnetic singlet ground state below Néel temperature of 0.6 K, with the zero-field Er-ion magnetic moment of $4.38\mu_B$ lying along the *a*-direction. The critical field for destroying the antiferromagnetic order for the *c*-axis is estimated to be 0.44 T.

The electronic and magnetic properties of the $ErBa_2Cu_3O_7$ high-T_c superconductor are well described within the crystalline-electric-field (CEF) approach [1–3]. Recently, the CEF transitions of Er^{3+} in $ErBa_2Cu_3O_x$ have been studied by inelastic-neutron-scattering (INS) experiments [2,3] and the sets of the CEF parameters for the orthorhombic $ErBa_2Cu_3O_7$ have been evaluated. For low-dimentional anisotropic magnetic system $ErBa_2Cu_3O_7$, the specific-heat measurements on single crystalline sample have revealed the anisotropic ratio of 2.0 of the effective gyromagnetic factors [1]. In this paper, an improved set of CEF parameters of the Er^{3+} is evaluated taking into account the results of measurements on single crystalline sample. The calculations are compared with all known experimental results on $ErBa_2Cu_3O_7$.

Details of the growing of single crystal $ErBa_2Cu_3O_7$, and results of the specific-heat measurements on single crystalline sample in the temperature range 0.3–3 K and magnetic field 0–2 T have been reported in Ref. [1]. Below 0.6 K antiferromagnetic (AF) order with magnetic moments in the *ab* plane occurs. By applying an external field the phase transition is shifted to lower temperatures confirming the AF order. These experiments have revealed strong anisotropy of the influence of the magnetic field. Namely, the influence is larger for the field perpendicular to the *c*-direction with the anisotropic ratio of 2.0.

The CEF specific heat is calculated by considering the following Hamiltonian for the Er^{3+} ions:

$$H_R = \sum\sum B_n^m O_n^m + g\mu_B J(-ng\mu_B\langle J\rangle + B_{ext}).$$

The first term is the CEF Hamiltonian written for the lowest multiplet $^4I_{15/2}$ given by Hund's rules with $J = 15/2$, $S = 3/2$, $L = 6$ and the Landé factor $g = 6/5$. It contains 9 parameters B_n^m for the orthorhombic symmetry ($m = 0, 2, 4, 6$; $n = 2, 4, 6$). The second term represents the exchange interactions between the Er-moments and the interaction with the external magnetic field written in the mean-field approximation. For the analysis of the specific heat at low temperatures, the set of CEF parameters: $B_2^0 = 0.5$ K, $B_4^0 = -16.95$ mK, $B_6^0 = 85.5$ μK, $B_2^2 = 0.25$ K, $B_4^2 = 5.284$ mK, $B_4^4 = 87.76$ mK, $B_6^2 = -80$ μK, $B_6^4 = 2.5$ mK, $B_6^6 = 25.36$ μK, and the exchange interaction coefficient $n = -0.05$ T f.u./μ_B have been used. The calculated contribution of the Er^{3+} ion to the specific heat of $ErBa_2Cu_3O_7$ in a field applied along the *c*-axis, shown in Fig. 1, reproduces well the λ-type of peak at 0.6 K, as well as the Schottky anomalies in fields of 1 and 2 T. The field-splitting of the Kramers-doublet ground state of the Er^{3+} ion is very anisotropic. The effect of the external field is characterized by $g_{\parallel}^{eff} = \Delta/B_{\parallel} = 2.88$ and $g_{\perp}^{eff} = \Delta/B_{\perp} = 5.88$ (Δ is the energy separation of the doublet levels), giving the effective gyromagnetic ratio $g_{\perp}/g_{\parallel} = 2.0$, in excellent agreement with the experimental value. In Table 1, our set of CEF parameters is compared with previous sets. The sets [2] and [3] give much lower anisotropy ratio. The energy level scheme of the Er^{3+} ion resulting from our improved set of CEF parameters is shown in Fig. 2, in excellent agreement with the INS observations [2]. The eigen-function of the Kramers-doublet ground state is given by:

$$\Psi = +0.002|\mp\tfrac{15}{2}\rangle - 0.531|\pm\tfrac{13}{2}\rangle - 0.284|\mp\tfrac{11}{2}\rangle - 0.026|\pm\tfrac{9}{2}\rangle - 0.002|\mp\tfrac{7}{2}\rangle + 0.578|\pm\tfrac{5}{2}\rangle + 0.544|\mp\tfrac{3}{2}\rangle + 0.082|\pm\tfrac{1}{2}\rangle$$

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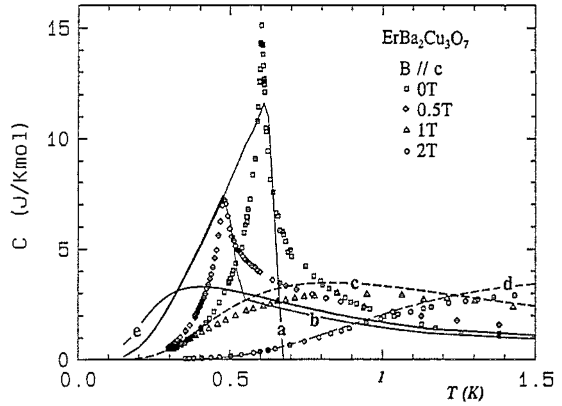

Fig. 1. Specific heat of $ErBa_2Cu_3O_7$ for different magnetic fields B_{ext} applied parallel to the c-direction. Lines represent the calculated curves at 0 (a), 0.4 (b), 0.8 (c) and 1.6 T (d) respectively, i.e. with $B_{cal} = 80\% B_{ext}$ (see text). The λ-type of peak is found to disappear at the field calculated-value of 0.44 T (e).

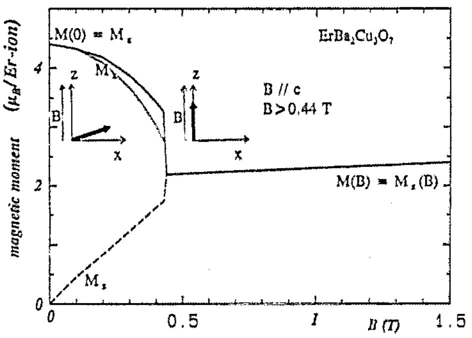

Fig. 3. The effect of the external field applied parallel to the c-axis on the magnetic moment. The critical field H_c for destroying the ab-plane antiferromagnetic order amounts to 0.44 T.

Table 1
Various sets of CEF parameters for $ErBa_2Cu_3O_7$

	Ref. [2]	Ref. [3]	This work
B_2^0 (K)	+0.41	+0.593	+0.50
B_4^0 (mK)	−16.61	−15.52	−16.95
B_6^0 (μK)	+88.12	+85.33	+85.50
B_2^2 (K)	+0.343	+0.672	+0.250
B_4^2 (mK)	+5.284	−0.202	+5.284
B_6^2 (μK)	−13.69	−107.0	−80.0
B_4^4 (mK)	+80.76	+89.47	+87.76
B_6^4 (mK)	+2.511	+2.503	+2.50
B_6^6 (μK)	+15.36	0	+25.36

yielding $M_x = 4.38\mu_B$ and $M_z = 2.15\mu_B$. Below 0.6 K, all the doublets are split by exchange interactions, that are relevant to an internal field of 0.22 T. The effect of the external field applied parallel to the c-axis on the magnetic moment is shown in Fig. 3. The zero-field ab-plane moments amount to $4.38\mu_B$, reproducing the Mössbauer value of $(4.2 \pm 0.1)\mu_B$ [4]. The in-plane moments are found to decrease with increasing magnetic field and disappear above the critical field H_c, whereas the out-of-plane component increases. Above H_c the moments are forced to lie along c-axis and next they increase linearly with increasing the magnetic field. The critical field H_c for destroying the ab-plane antiferromagnetic order is estimated to be 0.44 T for the field parallel to the c-axis. This effect is reflected by the disappearance of the λ-type of peak in the specific heat (see Fig. 1). However, we notice here that our specific-heat fits are much better if the calculated-values for the magnetic fields B_{cal} are taken by 20% smaller than the applied-values B_{ext} in the experiments (i.e. $B_{cal} = 80\% B_{ext}$), i.e. the data in 0.5, 1 and 2 T are well fitted with the calculated curves at 0.4, 0.8 and 1.6 T, respectively. The results suggest that only 80% of the applied field can penetrate into samples though fields were applied above the superconducting transition temperature.

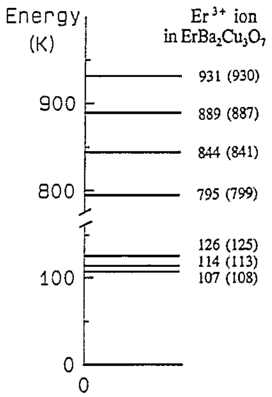

Fig. 2. The CEF level scheme of $ErBa_2Cu_3O_7$ resulting from our improved set of CEF parameters (see Table 1). The observed CEF transitions [2] are written in brackets.

In conclusion, the specific-heat measurements on single crystalline samples in applied fields provide the correct evaluation of CEF parameters. The improved set of CEF parameters of the Er^{3+} ion in $ErBa_2Cu_3O_7$ reproduces well all known experimental results on this compound.

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