

Spin - spin and spin - lattice interactions of Er³⁺ ions in KY_{0.99}Er_{0.01}(WO₄)₂ single crystal

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The single ion EPR spectrum of 1%Er³⁺ : KY (WO₄)₂ (the spatial group of symmetry C_{6h}²=C₂/c) described by spin Hamiltonian $\hat{H} = \mu (\mathbf{B}\mathbf{g}\hat{S}) + \hat{S}\mathbf{A}\hat{I}$ consists from singlet corresponding to even isotopes of Er³⁺ (S = 1/2, I = 0) located in the center of the septet of odd isotopes (S = 1/2, I = 7/2). The EPR spectrum is characterized by a strong anisotropy of both the g-factors (g_x = 0, g_y = 3.37, g_z = 13.25) and the hyperfine interaction parameters (A_x = 0, A_y = -120.75*10⁻⁴ cm⁻¹, A_z = -462.1*10⁻⁴ cm⁻¹). The y axis coincides with the crystallographic **b** (C₂) axis, the z axis is directed at angle of 54° to the a axis [1]. The temperature dependence of the g-factors is caused by anharmonic part of the spin-phonon Hamiltonian as well as by a rotational contribution to this Hamiltonian. A spin-lattice relaxation is shown to result from two Orbach processes through the first and second excited levels of an electronic spectrum.

The spectrum of Er³⁺ ions pairs found is described by Hamiltonian : $\hat{H} = \hat{H}1 + \hat{H}2 + \hat{S}1(\mathbf{K}^{\text{MDD}} + \mathbf{K}^{\text{Ex}} + \mathbf{K}^{\text{As}})\hat{S}2$, where $K_{ij}^{\text{MDD}} = \mu^2/r^3(\delta_{ij} - 3n_i^2)g_i g_j$ is the magnetic dipole - dipole (MDD) interaction; $K_i^{\text{Ex}} = (g_i/g_J)^2(g_J-1)2j$ the isotropic exchange; \mathbf{K}^{As} the antisymmetric exchange ($K_{ij}^{\text{As}} = -K_{ji}^{\text{As}}$; $K_{ii}^{\text{As}} = 0$). In last three expressions i, j = x, y, z; $\delta_{ij} = 1$ at i = j and $\delta_{ij} = 0$ at i ≠ j; g_J is the factor Lande (6/5); j the isotropic exchange constant, r the interionic distance, n_i the directing cosinus of bond lines on the i axis.

The greatest interaction is observed for the nearest (ln) pair along the a axis of crystal. Calculated values of contribution MDD are following : $K_{yy}^{\text{MDD}} = (707 \pm 7) * 10^{-4} \text{cm}^{-1}$, $K_{zz}^{\text{MDD}} = (-12995 \pm 117) * 10^{-4} \text{cm}^{-1}$, $K_{yz}^{\text{MD}} = (802 \pm 9) * 10^{-4} \text{cm}^{-1}$. If $j_{ln} = -145 * 10^{-4} \text{cm}^{-1}$, $K_{xy}^{\text{As}} = 480 * 10^{-4} \text{cm}^{-1}$, $K_{yz}^{\text{As}} = 2500 * 10^{-4} \text{cm}^{-1}$, so the calculated positions of lines and their relative intensity coincide with experimental.

It is shown that for the others 27 configuration spheres, which pairs can be observed in an experimental spectrum, MDD makes a basic contribution to interaction energy. However, the contributions of isotropic and antisymmetric exchanges also take place.

[1] M.T. Borowiec, A.A. Prochorov, A.D. Prochorov, V.P. Dyakonov, and H. Szymczak. J.Phys.: Condens. Matter. 15 (2003), 5113-5120