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Opinion

The Jahn-Teller Effect of Magnetic Center With $3d^9$ Ion - Cu^{2+} in $ZnAl_2O_4$ Spinel

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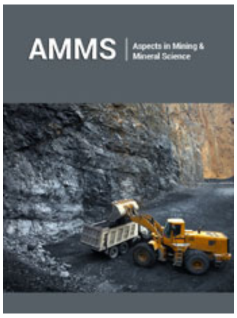

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Opinion

$ZnAl_2O_4$ crystals with 0.1% Cu^{2+} ions were grown by spontaneous crystallization from a solution of oxides in molten salts. The size of the optically homogeneous crystals was 2·2·2mm. The EPR spectrum at helium temperature was a superposition of three axial spectra of Cu^{2+} ions, the axes of symmetry of which are mutually orthogonal and directed along three axes of the fourth order of the oxygen octahedron forming the first coordination sphere of the magnetic ion. The EPR spectrum is shown in Figure 1. The EPR spectrum of Cu^{2+} ion in the crystal of $ZnAl_2O_4$ has been investigated with ν=9.23GHz in the temperature range T=4.2÷295K.. It is shown that Cu^{2+} EPR spectrum in $ZnAl_2O_4$ can be represented as a superposition of two spectra: the Low-Temperature spectrum (LT) and High-Temperature (HT) spectrum. Figure 2 shows the spectra for T=20K and T=100K. The LT spectrum is typical of Cu^{2+} ions in the octahedral environment with strong Jahn-Teller effect. It is a superposition of three axial spectra with the axes of symmetry orthogonal one to another. The spin Hamiltonian of one of the magnetic centers is of the form

$$H = g_{//}\beta H_Z S_Z + g_{\perp}\beta(H_X S_X + H_Y S_Y) + AS_Z I_Z + B(S_X I_X + S_Y I_Y),$$

where β is the Bohr magneton, S=1/2 is the electronic spin, I=3/2 is the nuclear spin, $g_{//}$=2.321±0.001, $g_{\perp}$=2.075±0.001, A=(153±7) $10^{-4}cm^{-1}$, B=(9±2) $10^{-4}cm^{-1}$.

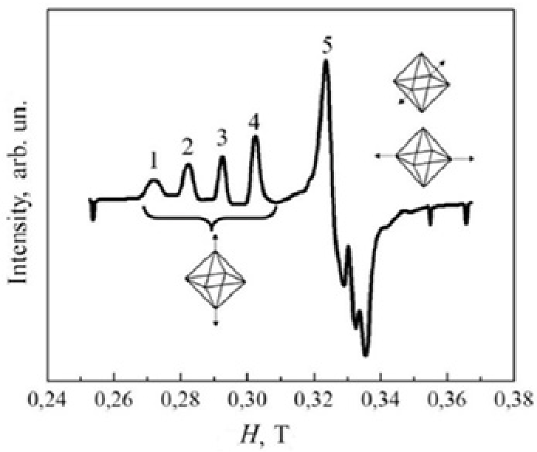

Figure 1: Experimental EPR spectrum in $ZnAl_2O_4$+0.1% Cu^{2+} single crystals in the H//C_4 field at ν =9.24GHz. T=4.2K.

The hyperfine structure of the EPR spectrum (Figure 2, lines 1,2,3,4, LT spectrum) corresponds to the magnetic center in the parallel orientation. The line width ΔH=33Oe. The intensive narrow peak (Figure 2, line 5, LT spectrum) is the EPR spectrum of the magnetic centers whose axes are normal to the magnetic field. The HT spectrum of Figure 2 is a relatively broad asymmetric line with the effective g-factor g=2.1±0.01. The line width varies from 0.45 to 0.6 kOe. The investigation of the temperature dependence of EPR spectrum shows that the temperature transformation of the spectrum are determined by a change in the integral intensities of the low- and high-temperature spectra. According to Figure 3, the integral intensity of the HT spectrum grows with temperature and that of the LT spectrum exponentially decreases. The parameter E_0=12cm^{-1} stands for the effective energy of activation. For the Jahn-Teller magnetic center of the Cu^{2+} ion in $ZnAl_2O_4$ the value of this parameter is defined by the height of the potential barrier between the potential wells [1].

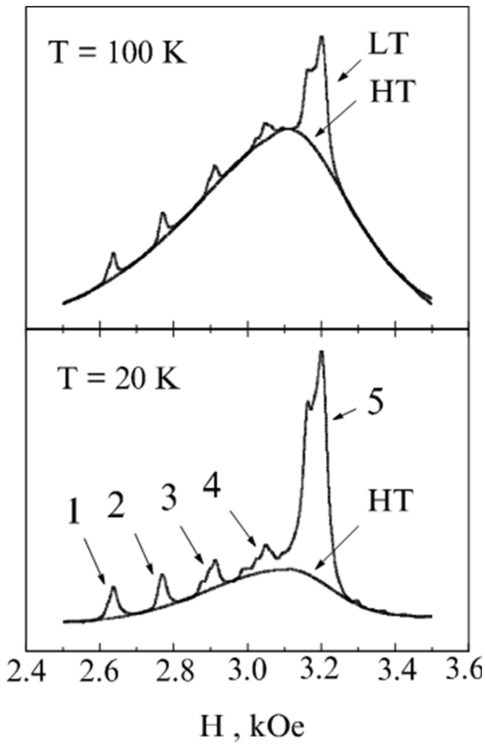

Figure 2: The temperature transformation of the spectrum is determined by a change in the integral intensities of the low- and high-temperature spectra.

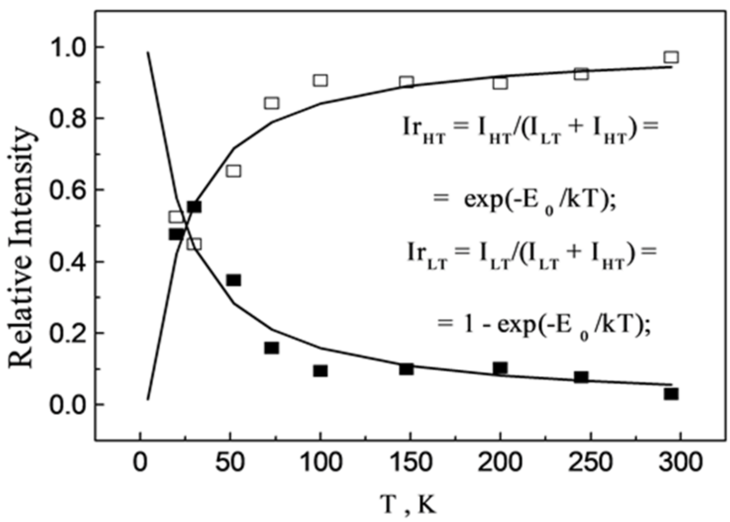

Figure 3: The integral intensity of the HT spectrum grows with temperature and that of the LT spectrum exponentially decreases.

References

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