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NUMERICAL STUDIES OF MAGNETIZATION RELAXATION OF Mn^{2+} IN ZINC BLENDE CRYSTALS

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The results of numerical simulation of magnetization relaxation of Mn^{2+} centers are presented. They show that the relaxation can be exponential in certain time intervals, with the relaxation rate related by a simple formula to the transition probabilities.

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Recently a number of papers [1] were devoted to experimental studies of magnetization relaxation in high magnetic fields. The investigated materials are diluted magnetic semiconductors based on CdTe, with Mn as a magnetic ion. In such a case the Mn^{2+} ground state is an orbital singlet with $S = 5/2$.

The temporal evolution of magnetization relaxing toward its thermal equilibrium is strictly exponential only in two level systems. For n-level systems the temporal behavior is described by the sum of $n-1$ exponents. An analytical solution for the parameters in such a sum exists for $n \leq 4$ [2]. Therefore, for Mn^{2+}, when the ground state is split by a magnetic field into 6 spin sublevels, only numerical solutions are possible.

In our model we assume that transitions (see Fig. 1) with a change of S_z of ± 1 ($W1$) and ± 2 ($W2$) are possible [3, 4]. Therefore, the system is described by the following six rate equations describing the occupancy n_i of the i-th level:

$$\frac{\mathrm{d}n_1}{\mathrm{d}t} = -(W1_{\mathrm{u}} + 0.5\, W2_{\mathrm{u}})n_1 + W1_{\mathrm{d}}n_2 + W2_{d}n_3,$$

$$\frac{\mathrm{d}n_2}{\mathrm{d}t} = W1_{\mathrm{u}}n_1 - (W1_{\mathrm{d}} + 0.4\, W1_{\mathrm{u}} + 0.9\, W2_{\mathrm{u}})n_2 + 0.4\, W1_{\mathrm{d}}n_3 + 0.9\, W2_{\mathrm{d}}n_4,$$

$$\frac{\mathrm{d}n_3}{\mathrm{d}t} = 0.5\, W2_{\mathrm{u}}n_1 + 0.4\, W1_{\mathrm{u}}n_2 - (0.4\, W1_{\mathrm{d}} + 0.5\, W2_{\mathrm{d}} + 0.9\, W2_{\mathrm{u}})n_3 + 0.9\, W2_{\mathrm{d}}n_5,$$

$$\frac{\mathrm{d}n_4}{\mathrm{d}t} = 0.9\, W2_{\mathrm{u}}n_2 - (0.4\, W1_{\mathrm{u}} + 0.5\, W2_{\mathrm{u}} + 0.9\, W2_{\mathrm{d}})n_4 + 0.4\, W1_{\mathrm{d}}n_5 + 0.5\, W2_{\mathrm{d}}n_6,$$

$$\frac{dn_5}{dt} = 0.9\,W2_{\rm u}n_3 + 0.4\,W1_{\rm u}n_4 - (W1_{\rm u} + 0.4\,W1_{\rm d} + 0.9\,W2_{\rm d})n_5 + W1_{\rm d}n_6,$$

$$\frac{dn_6}{dt} = 0.5\,W2_{\rm u}n_4 + W1_{\rm u}n_5 - (W1_{\rm d} + 0.5\,W2_{\rm d})n_6,$$

where subscripts u and d denote transitions up and down, respectively.

The relaxation process is assumed to be a direct process (with the emission or absorption of one phonon), and phonons are described by the Debye spectrum. Therefore, the transition probabilities can be written in the form (e.g. [2]):

$$W1_{\rm u} = A1\Delta E^3/[\exp(\Delta E/kT) - 1],$$

$$W1_{\rm d} = A1\Delta E^3\,\{1 + 1/[\exp(\Delta E/kT) - 1]\},$$

$$W2_{\rm u} = A2(2\Delta E)^3/[\exp(2\Delta E/kT) - 1],$$

$$W2_{\rm d} = A2(2\Delta E)^3\,\{1 + 1/[\exp(2\Delta E/kT) - 1]\},$$

where $A1$ and $A2$ are treated as parameters. The most important is the ratio $A2/A1$ showing the importance of $\Delta S_z = \pm 2$ transitions.

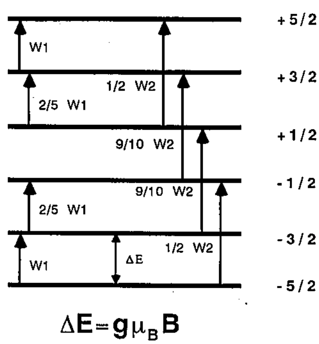

Fig. 1. The energy levels of the Mn^{2+} ground state in a magnetic field $\boldsymbol{B}$ and possible transitions between the levels.

The calculations were performed for different fields for $T = 2$ K and $A2/A1 = 0.01$. At low fields (below 10 T) the relaxation is mainly governed by transitions with $\Delta S_z = \pm 2$ (Fig. 2a) and after quite a short transition period the relaxation is exponential over many orders of magnitude (with a relaxation rate $RR2 = W2_{\rm u} + W2_{\rm d}$ (Fig. 2d)). At higher fields the relaxation whose rate is due to transitions with $\Delta S_z = \pm 1$ begins to be more important and the non-exponential behavior is more pronounced. First, for a few orders of magnitude the relaxation is described by the relaxation rate $RR1 = W1_{\rm u} + W1_{\rm d}$ and later, after a non-exponential transition period, by $RR2$ (Fig. 2b). At very high fields the basic part of the relaxation is exponential, with relaxation rate $RR1\,(\Delta S_z = \pm 1)$.

Our results strongly support the idea that studies of magnetization relaxation should be done at high magnetic fields and low temperatures, because only under such conditions the experimental results have a simple theoretical description.

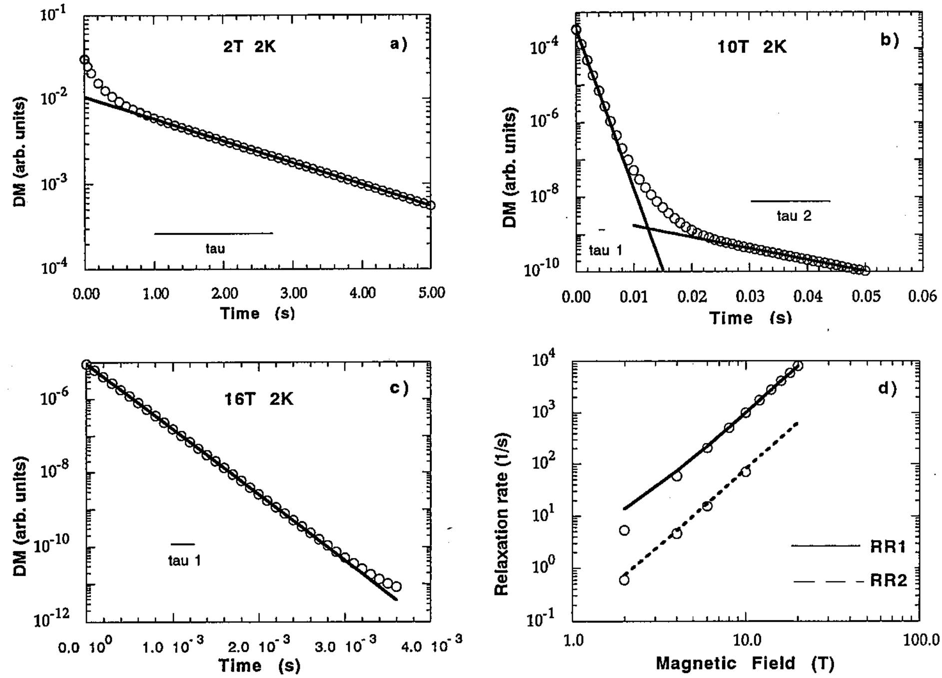

Fig. 2. Typical dependence of magnetization difference $\Delta M = M(t) - M_0$ on time after the heat pulse at different magnetic fields ($T = 2$ K). The lines show fits of exponential dependence (a, b, c). The fited relaxation rates compared with calculated $RR1$ and $RR2$ (d) (see the text).

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