Concentration dependence of the electron paramagnetic resonance line shape: The Cr^{3+} ion in $ZnWO_4$

A. A. Bugaĭ, B. K. Krulikovskiĭ, V. M. Maksimenko, and A. B. Roĭtsin

Semiconductors Institute, Ukrainain Academy of Sciences

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A new mechanism of the concentration dependence of the EPR linewidth and line shape is proposed. It consists of an interaction between the paramagnetic center and the electric field of the dipole formed by a similar paramagnetic center and an impurity that cancels its charge. The mechanism explains satisfactorily the experimental data on the Cr^{3+} ion (at all chromium concentrations) in $ZnWO_4$ crystals with a compensating lithium impurity. The Cr^{3+} and Li^+ ions produce pairs with a characteristic distance of 30 Å. These pairs are electric dipoles whose electric field shifts the energy levels of other, neighboring paramagnetic ions. The concentration dependence of the linewidth and line shape is also studied for external-magnetic-field directions such that the electric field does not affect the energy levels of the Cr^{3+} ions. The linewidth is several times smaller in this case, and its temperature dependence can be ascribed to magnetic dipole-dipole interaction. The role of dipole-quadrupole interaction is discussed, and the paramagnetic-center model is considered for the case when no compensating impurity is specially introduced.

1. INTRODUCTION

An investigation of the concentration dependence of the shape, and particularly the width of the EPR line, makes it possible to study the mechanisms of interaction between paramagnetic centers (PC), the character of their distribution in the sample, and the degree of perfection of the crystal. These data are important for the clarification or confirmation of the PC model, for a correct interpretation of the experimental data on the spin-lattice relaxation, for the clarification of the nature of the so-called residual broadening of the EPR line, the clarification of the mechanism of energy transfer over the crystal, the study of production of pairs and clusters of PC, and the solution of many other problems. The concentration dependence of the EPR spectrum was investigated in a number of studies[1-4]. These studies involved in most cases magnetic dipole-dipole and exchange interaction between the PC. In the present study we have observed and investigated the electric dipole interaction between the PC, which determines the concentration dependence of the EPR shape.

It is customary to introduce into chromium-doped $ZnWO_4$ crystals, during the crystal growth, also lithium ions that compensate for the excess charge of the Cr^{3+} ion. It was previously established[5] that the Li^+ ion is located at a distance of approximately 30 Å from the Cr^{3+} ion. We have paid attention to the fact that each pair consisting of a Cr^{3+} and a nearby Li^+ ion is an electric dipole with an arm $R \approx 30$ Å. The electric field of this dipole can shift the transition frequency of the neighboring Cr^{3+} ions (provided that the electric field in this crystal has a strong enough influence on the EPR spectrum[6]) and lead to an inhomogeneous broadening of the EPR line. The influence of the external electric field on the EPR spectrum of the Cr^{3+} ion in $ZnWO_4$ was investigated in[7]. The same study revealed a correlation between the angular dependences of the line width and the magnitude of its splitting in the electric field, thus pointing to an "electric" mechanism of the EPR line broadening (the interaction of the paramagnetic center with the electric fields of the charged defects).

The existence of electric dipoles can be the source of a new mechanism of the concentration dependence of the shape and width of the EPR line. To check on this premise, to assess the role of different compensating impurities, to establish the mechanism of broadening in those cases when the electric mechanism is not effective (in certain orientations of **H**), and to refine certain experimental data used in a preceding study[5], we have investigated the concentration dependence of the width and shape of the EPR line of the Cr^{3+} ion in $ZnWO_4$ in a wide range of concentrations for different types of specially introduced compensating impurities (including in the absence of the compensating impurities) and at different magnetic-field orientations.

2. EXPERIMENT

The $ZnWO_4$ single crystals were grown by the Czochralski method. The chromium impurity was introduced into the initial charge in the form of Cr_2O_3, in an amount corresponding to a chromium concentration from 0.001 to 1 at.%. Some of the single crystals were grown from a melt containing also lithium, sodium, or potassium impurities to compensate for the excess charge of the chromium in the lattice. The alkali-metal impurity was introduced into the initial charge in the form of the tungstate. The alkali-metal ion concentration in the melt exceeded the concentration of the chromium ion by several times.

The EPR lines were observed with a 3-cm-band EPR spectrometer with high-frequency modulation of the magnetic field. The measurements were performed at liquid-nitrogen temperature. At this temperature, the spin-phonon interaction does not influence the width of the Cr^{3+} line in the $ZnWO_4$[8]. The EPR signal was recorded with an automatic recorder in the form of the first derivative of the absorption line.

At all the chromium concentrations, with and without compensating impurity, the line width ΔH was anisotropic and the correlation effect took place[7]. The maximum value of ΔH was reached at $\theta = 25°$ and the minimum at $\theta = 4.5°$ (θ is the angle between the direction of the magnetic field **H** and the z axis of the magnetic susceptibility). At $\theta = 25°$, the influence of the electric field on the spectrum is maximal, and at $\theta = 4.5°$ there is no electric effect and the line-broadening mechanism should be different. For a more distinct separation of the different sources of the broadening, the concentration dependence was investigated at these two orientations of **H**.

Figure 1 shows the concentration dependence of ΔH (the solid curves were drawn through the experimental values) in samples without a compensating impurity for $\theta = 45^\circ$ (curve 1) and $\theta = 25^\circ$ (curve 2), in samples with Li for $\theta = 4.5^\circ$ (curve 3) and $\theta = 25^\circ$ (curve 4), and in samples with Na for $\theta = 4.5^\circ$ (curve 5) and $\theta = 25^\circ$ (curve 6). The experimental values of ΔH in the samples with K did not differ, within the limits of experimental error, from the values of ΔH in samples without a compensating impurity. The abscissas in Fig. 1 represent the concentration of the chromium ions in the batch, in atomic percent. When this concentration is $\leq 0.05\%$, it coincides with the concentration of the chromium in the crystal. At higher chromium concentrations in the batch, the segregation coefficient becomes less than unity and the maximum concentration of the chromium ions participating in the EPR in the crystal does not exceed 0.12 at.% when the concentration in the batch is increased to 1% or even more[9,10]. Figure 2 shows the concentration dependence of ΔH, where the abscissas represent the "real" concentration of the Cr^{3+} ions, calculated with the aid of graph 4 of[9] and measured with the aid of EPR.

Figure 3 shows the experimental data on the change of the EPR line shape at $\theta = 25^\circ$ as functions of the Cr^{3+} ion concentration in samples doped with lithium. The experiment reveals a change in the line wings, whereas the central part of the line (within $2\Delta H$) remains practically unchanged. Figure 3 shows therefore part of the wing of the EPR line. In the upper right corner of Fig. 3 is shown the schematic form of the EPR line and of that part (enclosed in the rectangle) which is shown in the figure. Similar results were obtained for $\theta = 25^\circ$ in samples without lithium. At $\theta = 4.5^\circ$, in samples with and without lithium, the line has a Lorentz shape. Only at the maximum chromium concentration 1% (in the charge), in the samples with lithium, does the line shape lie "higher" than the Lorentz line (in the samples without lithium the shape remains Lorentzian).

3. CALCULATION OF LINE WIDTH

It is seen from the experimental data that in the Cr^{3+} ion concentration region where the concentration dependence of the line width comes into play, the line shape is close to Lorentzian. According to the presently known line-broadening mechanisms, a Lorentzian shape results[11] from electric or magnetic dipoles randomly distributed around the PC, or else from spin-phonon interaction. Our measurements and the measurements performed earlier[8] have shown that at temperatures close to 78°K the spin-phonon mechanism makes no contribution to the line width, and will therefore be disregarded. On the other hand, the correlation effect is observed at all the investigated concentrations and temperatures. This indicates that an important role is played by the electric line-broadening mechanism. We have assumed that the paramagnetic ions interact with the electric fields of the dipoles ($Cr^{3+} - Li^+$ pairs), and this should lead to a Lorentzian line shape[1)]. This interaction can be called electric dipole-dipole, but it must be recognized here that we are considering dipoles of different types: the electric dipole moment of the paramagnetic ion Cr^{3+} (which causes the influence of the external electric field on the EPR) spectrum on the one hand, and the dipole moment of the $Cr^{3+} - Li^+$ pair on the other hand. Whereever there is no electric broadening mechanism ($\theta = 4.5^\circ$). The concentration dependence might be assumed to be determined by the magnetic dipole-dipole interaction of the chromium ions.

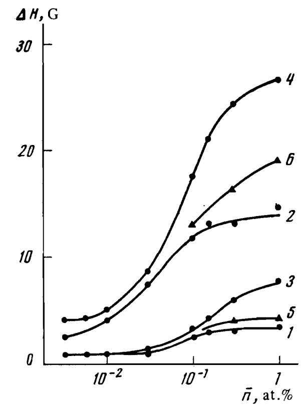

FIG. 1

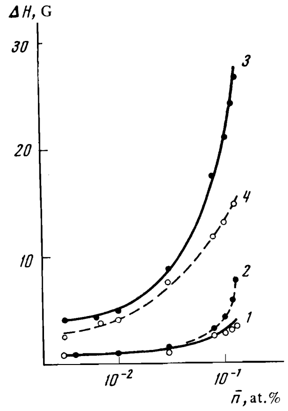

FIG. 2

FIG. 1. Concentration dependence of the EPR line width (at the maximum-slope points) of the Cr^{3+} ion in $ZnWO_4$. The absicissas represent the chromium concentration in the batch: 1, 2—samples without compensating impurities, the angle θ is equal to 4.5 and 25°, respectively; 3 and 4— samples with lithium, θ = 4.5 and 25°, respectively; 5 and 6— samples with sodium, θ = 4.5 and 25°, respectively. The curves were drawn through the experimental points.

FIG. 2. Concentration dependence of the EPR line width of the Cr^{3+} ion in $ZnWO_4$. The abscissas represent the chromium concentration in the crystal as obtained from EPR data: 1—theoretical curve corresponding to magnetic dipole-dipole interaction; the experimental values for θ = 45° in samples without compensating impurities are represented by circles; 2—curve drawn through the experimental values in samples with lithium at θ = 4.5°; 3—theoretical curve corresponding to the electric dipole-dipole interaction; dark points—experimental values in samples with lithium at θ = 25°; 4—curve drawn through the experimental values in samples without compensating impurity at θ = 25°.

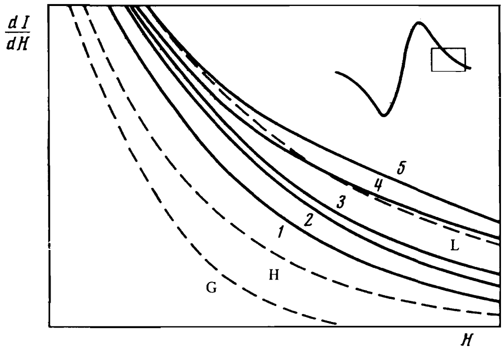

FIG. 3. EPR line shape in samples with lithium at θ = 25°: 1—concentration 10^{-3} at.%; 2—10^{-2} at.%; 3—10^{-1} at.%; 4—0.3 at.%; 5—1 at.%; for comparison, the dashed curves show the Gaussian (G), Holtsmark (H), and Lorentz (L) distributions.

a) The influence of randomly distributed electric dipoles on the EPR shape was considered in[11-13] on the basis of the statistical theory. We shall use formula (10) of[11] as the initial expression for the calculation of the line width (at the points of maximum slope). For the case of variation of the magnetic field in the xz plane, which is considered by us, this formula can be represented in the form

$$\delta=1{,}6neRca(\theta)\varepsilon^{-1}\ [\mathrm{G}], \qquad (1)$$

where n is the concentration of the Cr^{3+} ions per cm^3, e is the unit charge, R is the distance between the Cr^{3+} and Li^+ ions, c is a numerical coefficient, $a(\theta)$ is the coefficient of proportionality between the shift of the resonant value of the magnetic field and the intensity E of the external electric field that causes this shift, and ϵ is the dielectric constant. We note that in place of d_{max}, which enters in formula (7) of[11], we have substituted 4R/3, inasmuch as in the case considered by us the dipoles are fixed2). For the particular calculations we used the following values of the parameters: a) $(25^\circ) = 6 \times 10^{-5}\ V^{-1}\ cm\text{-}G$[7]; R = 30 Å[5]; $\epsilon = 16$, c = 3.4; $e = 4.8 \cdot 10^{-10}$ CGSE; $n = 0.01\,\bar{n}n_0$, where $\bar{n}$ is the concentration of the Cr^{3+} in at.%, and $n_0 = 1.5 \times 10^{22}\ cm^{-3}$ is the concentration of the Zn atoms. Substituting the values of the parameters in (1), we obtain the contribution of the electric dipole-dipole interaction to the EPR line width when the external magnetic field H is oriented at an angle $\theta = 25^\circ$ to the z axis:

$$\delta_e(25^\circ)=132\,\bar{n}[\mathrm{G}]. \qquad (2)$$

b) To calculate the line broadening due to the magnetic dipole-dipole interaction, we used formula (58) of[2], which can be represented in the form

$$\delta=1.16\frac{8\pi^2}{9\sqrt{3}}qg\beta n\quad [\mathrm{G}]. \qquad (3)$$

We have introduced the factor 1.16, since we are interested in the distance between the maximum-slope points, g is the spectroscopic-splitting factor, β is the Bohr magneton, and q is a characteristic proportionality coefficient which enters in the correction that must be introduced into the transition frequency to compensate for the spin interaction. To find this coefficient, we calculated the energy corrections connected with the dipole-dipole interaction operator

$$\hat{W}=\frac{g^2\beta^2}{r^3}\left(\mathbf{S}_1\mathbf{S}_2-3\frac{(\mathbf{r}\mathbf{S}_1)(\mathbf{r}\mathbf{S}_2)}{r^2}\right),$$

where $S = 3/2$. As the initial zeroth-approximation wave functions we chose the products of the spin functions of two PC corresponding to sublevels of lower Kramers doublets ($D > g\beta H$,[14]). To simplify the calculations we have put $\theta = 0^\circ$ in place of $\theta = 4.5^\circ$. As a result, we obtained a value $3/2$ for the parameter q. Substituting in (3) the values g = 1.97[14], $\beta = 9.3 \times 10^{-21}$ erg/g, $q = 3/2$, and $n = 0.01\,\bar{n}n_0$, we obtain the contribution of the magnetic dipole-dipole interaction to the EPR line width at θ close to zero degrees:

$$\delta_M(0^\circ)=24\,\bar{n}[\mathrm{G}]. \qquad (4)$$

c) When expressions (2) and (4) are to be compared with the experimental data, the contribution made to the line width by other mechanisms must be taken into account. Thus, at $\theta = 4.5^\circ$ part of the line broadening, as seen from Figs. 1 and 2, does not depend on the concentration. The nature of this "residual" broadening for the Cr^{3+} ion is not yet clear. It has been established, however[15], that in the case of the Fe^{3+} ion the line shape at low concentrations is determined by the ligand fine structure. Therefore, comparing with the experimental data at $\theta = 4.5^\circ$ it is necessary to add to expression (4) the residual width 0.8 G. Figure 2 (curve 1) shows the corresponding plot. The theoretical curve passes close to the experimental points obtained with uncompensated crystals. The experimental points corresponding to crystals with lithium added lie above this theoretical curve (the dashed curve 2 of Fig. 2 is drawn through these points). This indicates that in crystals with lithium there is at $\theta = 4.5^\circ$, another mechanism, besides the magnetic dipole-dipole broadening mechanism, which leads to an additional concentration dependence. Its nature will be discussed in the next section.

To describe the experimental data at $\theta = 25^\circ$ it is necessary to add to expression (2) the residual width 4 G, at $\theta = 25^\circ$, and the concentration broadening due to all other mechanisms. The contribution of these mechanisms should correspond to the experimentally measured concentration broadening at $\theta = 4.5^\circ$ in samples with lithium increment. The theoretical concentration dependence obtained in this manner is shown in Fig. 2 (curve 3). The agreement with experiment (points) is good.

4. DISCUSSION OF RESULTS. DIPOLE-QUADRUPOLE INTERACTION

a) It is seen from Fig. 2 that for the entire concentration region there is good agreement between theory and experiment at $\theta = 25^\circ$. This is evidence of the correctness of the initial model, according to which the broadening is due to electric dipoles that are randomly distributed in the crystal and consist of Cr^{3+} and Li^+ ions spaced ~30 Å apart. (It is of interest in this connection to note the following correlation: at the maximum possible concentration of Cr^{3+} in $ZnWO_4$, namely 0.12 at.%[9,10], the average distance between the chromium ions is 38 Å; this is close to the dipole arm R ≈ 30 Å.)

b) According to the experimental data (Fig. 1), the concentration dependence of the line width depends on the type of the compensation of the charge of the Cr^{3+}. The largest difference is observed between the case of compensation with lithium ions and the case when no special compensating impurities is introduced. In spite of the fact that at the present time there are no concrete data on the model of the compensator in the second case (the corresponding discussion will be given below), the fact mentioned above, namely the difference between the concentration dependences for $\theta = 25^\circ$, is qualitatively understandable, namely, the compensators together with the Cr^{3+} ion constitute sources of electric fields characterized by different parameters (for example, different effective dipole arms). What we did not expect was the difference between the EPR line width at $\theta = 4.5^\circ$ for crystals with different compensators, when there are no electric effects, and the only possible broadening mechanism might be assumed to be the magnetic dipole-dipole interaction, which does not depend on the type of compensator.

It is seen from Fig. 2 (curve 1), that the concentration dependence calculated under the assumption of magnetic dipole-dipole broadening fits satisfactorily the experimental points corresponding to the case when there is no specially introduced compensating impurity. The experimental curve 2 for samples containing lithium ions lies above the theoretical curve, indicating the appearance in this case of a certain additional mechanism of interaction between the PC at $\theta = 4.5^\circ$.

c) An additional mechanism that explains the difference between the line widths at $\theta = 4.5^\circ$, in our opinion, is the electric dipole-quadrupole interaction between the PC, which is next in order of magnitude to the electric dipole-dipole interaction that determines the broadening at $\theta = 25^\circ$.

For a more detailed analysis of this question, we represent the PC in the form of a particle with pointlike charges q_i that are distributed over a certain volume. If the distance $\mathbf{r}$ between the PC exceeds the characteristic dimensions ρ_i of the PC, then the energy of interaction between two PC can be represented in the form of a series in the small parameter ρ_i. The terms containing ρ_i raised to the zeroth and first power will not shift the EPR line, since the PC are neutral on the whole, and the "resonant" PC does not depend on the coordinates ρ_i (for details see below). From along the terms quadratic in ρ_i, only the dipole-dipole interaction is effective in the EPR. The terms of interest to us, which are cubic in ρ_i, can be represented in the form

$$V = \frac{1}{2r^7} \sum_{klm} [r^2(\delta_{kl}x_m + \delta_{km}x_l + \delta_{ml}x_k) - 5x_k x_l x_m] \times (Q_1 L_{2lkm} - 3P_{1m}T_{2kl} + 3T_{1lm}P_{2k} - Q_2 L_{1lkm}), \tag{5}$$

x_k, x_l, and x_m are the components of the vector $\mathbf{r}$ ($k, l, m = 1, 2, 3$); Q_i, P_k, T_{kl}, and L_{klm} are the summary charge and the components of the dipole, quadrupole, and octupole moments of the PC. The subscripts 1 and 2 distinguish two interacting PC. Let PC 1 be "resonant," and let PC 2 be the one that shifts its EPR line. The first term in the curly brackets of (5) characterizes the influence of the field of the octupole PC 2. This term makes no contribution to the shift of the EPR line, since it contains no dependence of the coordinates ρ_{1i} of the electron of the PC 1, over which it is necessary to carry out the quantum-mechanical averaging. (This term will lead to a constant shift of all the levels of the Cr^{3+} ion.) The second term describes the energy of the interaction of the dipole moment of PC 1 with the electric quadrupole field of PC 2. This term does not contribute to the shift of the EPR line of PC 1 at $\theta = 4.5^\circ$, since there is no electric effect at $\theta = 4.5^\circ$. The third term describes the energy of the interaction of the quadrupole moment of PC 1 with the electric field gradient of the dipole of PC 2. This is the only one that can make a contribution to the shift of the EPR line, since the fourth term vanishes because $Q_2 = 0$.[3)]

The following facts point to the effectiveness of the considered mechanism:

1) The decrease like r^{-4}, which is typical of the dipole-quadrupole interaction, should lead to a stronger concentration dependence than the r^{-3} law typical of the dipole-dipole interaction. An analysis of the observed concentration dependence for the proposed mechanism confirms this conclusion.

2) The decrease like r^{-4} should lead to a line shape that attenuates less steeply than the Lorentzian typical of the dipole-dipole interaction. It is seen from Fig. 3 that for concentrations where the difference between the line widths for samples with and without lithium is appreciable (see Fig. 2), the line "goes outside" the limits of the Lorentzian. At the same time, as indicated in Sec. 2, the line shape is Lorentzian for the samples without lithium.

3) The dipole-quadrupole interaction mechanism, as seen from (5) and from the analogous formula for the dipole-dipole interaction, is smaller in order of magnitude than the dipole-dipole interaction by as many times as the characteristic dimensions ρ_1 of the PC 1 are smaller than the average distance between the PC. For the Cr^{3+} ion in $ZnWO_4$, as seen from the experimental data (Fig. 2), this relation is approximately satisfied if one puts $\rho_1 \approx 5$ Å.

We note that the interaction next in order of magnitude to the dipole-quadrupole interaction is the quadrupole-quadrupole interaction, which decreases like r^{-5} and which is considered in[3].

d) The EPR line shape and the angular dependence of its width did not depend on the presence of special compensators in the crystal. This indicates that the compensation of the excess charge of the Cr^{3+} has common features, regardless of whether a special compensator is or is not added to the crystal.

It can be assumed that the compensator is the vacancy of the Zn^{2+} ion[16,17]. In order for the complex to be neutral as a whole, one must admit of the existence of the "tripole" $2Cr^{3+}$ + Zn^{2+}-ion vacancy. If the ions are in the immediate vicinity of the vacancy, then an additional EPR spectrum can be produced. At large distances between the "tripole" components, a broadening of the fundamental line of the spectrum will be observed. With increasing chromium concentration, the line broadening will be determined by the electric field of the randomly distributed "tripoles."

e) We note in conclusion that the considered mechanism of the interaction between the PC and the dipoles can determine the concentration dependence of the spin-lattice relaxation time. We point out in this connection a paper[18] dealing with the influence of thermal modulation of the electric fields of point charges on the spin-lattice relaxation of PC.

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[1)] The interaction with the electric fields of randomly distributed point charges leads to a "Holtsmark" shape [5].

[2)] The authors are grateful to M. D. Glinchuk for a discussion of the question of the value of d_{max} and of the coefficient c in the case when the dipole arm is fixed.

[3)] To prevent misunderstandings, we emphasize that $Q_1 \neq 0$, inasmuch as in our case Q_1 is the total charge of only the Cr^{3+} ion.

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