Local structure distortion and spin Hamiltonian parameters for Cr^{3+}–V_{Zn} tetragonal defect centre in Cr^{3+} doped $KZnF_3$ crystal*

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The quantitative relationship between the spin Hamiltonian parameters (D, $g_{\|}$, Δg) and the crystal structure parameters for the Cr^{3+}–V_{Zn} tetragonal defect centre in a Cr^{3+}:$KZnF_3$ crystal is established by using the superposition model. On the above basis, the local structure distortion and the spin Hamiltonian parameter for the Cr^{3+}–V_{Zn} tetragonal defect centre in the $KZnF_3$ crystal are systematically investigated using the complete diagonalization method. It is found that the V_{Zn} vacancy and the differences in mass, radius and charge between the Cr^{3+} and the Zn^{2+} ions induce the local lattice distortion of the Cr^{3+} centre ions in the $KZnF_3$ crystal. The local lattice distortion is shown to give rise to the tetragonal crystal field, which in turn results in the tetragonal zero-field splitting parameter D and the anisotropic g factor Δg. We find that the ligand F^- ion along [001] and the other five F^- ions move towards the central Cr^{3+} by distances of $\Delta_1 = 0.0121$ nm and $\Delta_2 = 0.0026$ nm, respectively. Our approach takes into account the spin–orbit interaction as well as the spin–spin, spin–other-orbit, and orbit–orbit interactions omitted in the previous studies. It is found that for the Cr^{3+} ions in the Cr^{3+}:$KZnF_3$ crystal, although the spin–orbit mechanism is the most important one, the contribution to the spin Hamiltonian parameters from the other three mechanisms, including spin–spin, spin–other-orbit, and orbit–orbit magnetic interactions, is appreciable and should not be omitted, especially for the zero-field splitting (ZFS) parameter D.

Keywords: spin-Hamiltonian parameter, charge-compensation effect, local structural distortion, complete diagonalization method

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1. Introduction

The perovskite crystals AMF_3 (A=Rb, Cs, K; M=Cd, Mg, Zn) doped with transition metal ions, such as Cr^{3+}, Fe^{3+}, Ni^{2+}, Co^{2+}, and Ti^{3+}, are of great interest due to their applications in solid-state lasers.[1−4] In particular, $KZnF_3$ doped with Cr^{3+} ions has attracted much attention due to its excellent optical properties even at room temperature, a large range of frequency tunability, and its potential use in high power lasers.[3−5] The impurity of Cr^{3+} ions in the materials plays a major role, as they can improve the optical properties. To understand the role of the impurities on a microscopic scale, it is necessary to know the defect nature and the local geometry of the impurity centres.

A perfect $KZnF_3$ crystal has a cubic structure, the Zn^{2+} ion is surrounded by six F^- ions in a regular octahedron. The trivalent Cr^{3+} ions replace the divalent Zn^{2+} ions when they are doped into the $KZnF_3$ crystals. Nevertheless, the electron paramagnetic resonance (EPR) experiment[6,7] shows that the Cr^{3+} ion is in the strong tetragonal axial symmetry environment. This result implies that the local structure of the Cr^{3+} ion presents a tetragonal lattice distortion and the local symmetry around the Cr^{3+} ion changes from O_h to C_{4v}. Takeuchi and Arakawa[6] reported the spin Hamiltonian (SH) parameters including the zero-field splitting (ZFS) parameter D and the Zeeman g factors ($g_{\|}$ & $g_{\perp}$) for the tetragonal Cr^{3+} centre defect site in the Cr^{3+}:$KZnF_3$ crystal and proposed that the most likely source of the tetragonal axial symmetry crystal field was the Zn^{2+} vacancy (V_{Zn}) in the [001]-axis direction (see Fig. 1). So far there has been no satisfactory theoretical work to explain of all of these experimental findings. The present paper attempts to provide a microscopic interpretation.

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2. Theoretical method and analysis

The free-ion ^{4}F ground term of $3d^3$ ions (e.g., Cr^{3+}) splits in the octahedral symmetry crystal field (CF) into $^4A_{2g}$, $^4T_{2g}$, and $^4T_{1g}$ states, and $^4A_{2g}$ is the ground state. The ground state $^4A_{2g}$ is not spilt by the tetragonal symmetry crystal field (CF) (C_{4v}, D_4, D_{4h}, D_{2d}), but its irreducible representation changes to $^4B_1$. Due to the combined action of the tetragonal CF and the magnetic interactions, $^4B_1$ will split further, which can be expressed by the group theory as[8]

$$B_1 \otimes D^{(3/2)} \to B_1 \otimes (E' \oplus E'') \to E'' \oplus E'. \quad (1)$$

We can see in the following that the value of splitting is twice as big as that of the ZFS parameter D.

For the Cr^{3+} ions at the tetragonal sites in $KZnF_3$, the effective spin Hamiltonian at the tetragonal symmetry sites taking into account the ZFS and the Zeeman terms can be written as

$$\begin{aligned} H_{\rm S} =& D\left[S_z^2 - \frac{1}{3}S(S+1)\right] + \mu_{\rm B} g_{\parallel} B_z S_z \\ &+ \mu_{\rm B} g_{\perp}(B_x S_x + B_y S_y), \end{aligned} \quad (2)$$

where S denotes the effective electron spin, μ_B denotes the Bohr magneton, B_x, B_y, and B_z denote the magnetic field in the x, y, and z directions, respectively, and the z axis is along the [001] direction for the tetragonal symmetry.

According to the spin Hamiltonian theory, the ZFS parameter D can be expressed as

$$D = \frac{1}{2}[E(\pm 3/2) - E(\pm 1/2)], \quad (3)$$

where E denotes the energy level. For a spin $S = 3/2$ system described by $H_{\rm S}$ with zero magnetic field, it is well established that the ground state $|\tilde{M}_{\rm S} \pm 1/2\rangle$ corresponds to $D > 0$, whereas $|\tilde{M}_{\rm S} = \pm 3/2\rangle$ corresponds to $D < 0$.[9]. Correspondingly, equation (3) yields positive and negative D for the ground states $|\tilde{M}_{\rm S} = \pm 1/2\rangle$ and $|\tilde{M}_{\rm S} = \pm 3/2\rangle$, respectively. The microscopic expressions for the g factors are obtained by means of the matrix element equivalence between the effective Zeeman term in Eq. (2) and the physical one as follows,[10–12] for the $|\tilde{M}_{\rm S} = \pm 1/2\rangle$ ground state,

$$\begin{aligned} g_{\parallel} =& 2(k\langle\psi_{+1/2}|L_0^{(1)}|\psi_{+1/2}\rangle \\ &+ g_{\rm e}\langle\psi_{+1/2}|S_0^{(1)}|\psi_{+1/2}\rangle), \end{aligned} \quad (4a)$$

$$\begin{aligned} g_{\perp} =& \frac{\sqrt{2}}{2}[k(\langle\psi_{+1/2}|L_{-1}^{(1)}|\psi_{-1/2}\rangle \\ &- \langle\psi_{+1/2}|L_{+1}^{(1)}|\psi_{-1/2}\rangle) \\ &+ g_{\rm e}(\langle\psi_{+1/2}|S_{-1}^{(1)}|\psi_{-1/2}\rangle \\ &- \langle\psi_{+1/2}|S_{+1}^{(1)}|\psi_{-1/2}\rangle)]; \end{aligned} \quad (4b)$$

for the $|\tilde{M}_{\rm S} = \pm 3/2\rangle$ ground state,

$$\begin{aligned} g_{\parallel} =& \frac{2}{3}(k\langle\psi_{+3/2}|L_0^{(1)}|\psi_{+3/2}\rangle \\ &+ g_{\rm e}\langle\psi_{+3/2}|S_0^{(1)}|\psi_{+3/2}\rangle), \end{aligned} \quad (5a)$$

$$\begin{aligned} g_{\perp} =& \frac{\sqrt{2}}{\sqrt{3}}[k(\langle\psi_{+3/2}|L_{-1}^{(1)}|\psi_{+1/2}\rangle \\ &- \langle\psi_{+3/2}|L_{+1}^{(1)}|\psi_{+1/2}\rangle) \\ &+ g_{\rm e}(\langle\psi_{+3/2}|S_{-1}^{(1)}|\psi_{+1/2}\rangle \\ &- \langle\psi_{+3/2}|S_{+1}^{(1)}|\psi_{+1/2}\rangle)], \end{aligned} \quad (5b)$$

where $L_q^{(k)}$ and $S_q^{(k)}$ are the irreducible tensor operators, and k is the orbital reduction factor. The eigenvectors $|\psi_{+1/2}\rangle$, $|\psi_{-1/2}\rangle$, and $|\psi_{+3/2}\rangle$ for the ground state of the $3d^3$ ions at the tetragonal site can be obtained by the diagonalization of the below actual Hamiltonian. Takeuchi and Arakawa[6] reported $D = -0.4321$ cm$^{-1} < 0$ for the tetragonal centre ion Cr^{3+} in the $KZnF_3$ crystal. Thus, we adopt Eq. (5) in our following investigation.

We note that the ZFS is a result of the actual Hamiltonian acting on the Cr^{3+} ions. This can be written as

$$\begin{aligned} H =& H_{\rm ee}(B,C) + H_{\rm CF}(B_{kq}) + H_{\rm SO}(\zeta_d) \\ &+ H_{\rm SOO}(M_0, M_2) + H_{\rm SS}(M_0, M_2) \\ &+ H_{\rm OO}(M_0, M_2), \end{aligned} \quad (6)$$

where the terms on the right-hand side are due to the electrostatic field, the crystal field (CF), the spin–orbit (SO) interaction, the spin–spin (SS) interaction, the spin–other-orbit (SOO) interaction, and the orbit–orbit (OO) interaction, respectively. B and C are the Racah parameters, B_{kq} is the crystal filed parameter, ζ_d is the SO constant, and M_0 and M_2 are the parameters for the SS, SOO, and OO. The CF Hamiltonian for the $3d^3$ ions at the tetragonal symmetry site can be explicitly expressed as

$$H_{\rm CF} = B_{20}C_0^{(2)} + B_{40}C_0^{(4)} + B_{44}(C_4^{(4)} + C_{-4}^{(4)}), \quad (7)$$

where $C_q^{(k)}$ is the irreducible tensor operator. For the tetragonal symmetry ($z \parallel C_4$), it is convenient to define[8,13]

$$B_{20} = \delta - \mu, \quad (8a)$$

$$B_{40} = 21Dq - \frac{3}{5}(3\mu + 4\delta), \quad (8b)$$

$$B_{44} = 21\sqrt{\frac{5}{14}}Dq, \quad (8c)$$

where Dq is the cubic CF parameter; the parameters μ and δ measure the net tetragonal CF components and vanish identically in the cubic site. Thus the parameters μ and δ both represent the charge compensation for the CF contribution.

For the Cr^{3+} ions in the $KZnF_3$ crystal, the parameters $B = 820$ cm^{-1}, $C = 2900$ cm^{-1}, $Dq = 1500$ cm^{-1}, and the spin–orbit coupling constant $\zeta_d = 217$ cm^{-1} have been obtained from optical spectra,[14,15] the SS and the SOO parameters $M_0 = 0.2021$ cm^{-1} and $M_2 = 0.0159$ cm^{-1} are available from atomic data.[16] In order to evaluate the orbital reduction factor k, we use the relation $k \approx (\sqrt{B/B_0} + \sqrt{C/C_0})/2$,[17,18] where $B_0 = 920.48$ cm^{-1} and $C_0 = 3330.71$ cm^{-1} are the Racah parameters of the free Cr^{3+} ion.[17] With the values of the input parameters B, C, ζ_d, k, M_0, and M_2 fixed, the microscopic SH parameters D, $g_\parallel$ and $g_\perp$, as well as the CF energy levels, each become a function of only the CF parameters B_{20}, B_{40}, and B_{44}. This enables us to theoretically study the local structure and the disorder around the Cr^{3+} centres in the $KZnF_3$ crystal.

According to the superposition model (SPM),[19,20] we establish relationships between the CF parameters and the crystal structure parameters. The expressions for the CF parameters with C_{4v} symmetry are derived as

$$B_{20} = 2\bar{A}_2 \left[\left(\frac{R_0}{R_0 - \Delta_2} \right)^{t_2} - \left(\frac{R_0}{R_0 - \Delta_1} \right)^{t_2} \right], \quad (9a)$$

$$B_{40} = 4\bar{A}_4 \left[5 \left(\frac{R_0}{R_0 - \Delta_2} \right)^{t_4} + 2 \left(\frac{R_0}{R_0 - \Delta_1} \right)^{t_4} \right], \quad (9b)$$

$$B_{44} = 2\sqrt{70}\bar{A}_4 \left(\frac{R_0}{R_0 - \Delta_1} \right)^{t_4}, \quad (9c)$$

where $R_0 = 0.202$ nm is the Cr–F distance at the perfect cubic site for the Cr^{3+}:$KZnF_3$ crystal[6] and is taken as a reference distance. The t_k are the power-law exponents, and $\bar{A}_k$ are the intrinsic parameters. For an ionic crystal, we take the power-law exponents $t_2 = 4$ and $t_4 = 6$.[19,20] The $\bar{A}_4$ can be found from the relation for the cubic CF parameter Dq, $\bar{A}_4 \approx 3Dq/4$.[21,22] It then follows that $\bar{A}_4 = 1125$ cm^{-1} from the experimental value of $Dq = 1500$ cm^{-1}.[14] We take $\bar{A}_2 = 10.8\bar{A}_4 = 12150$ cm^{-1} by considering that ratio $\bar{A}_2/\bar{A}_4$ tends to be a constant for the iron-group ions.[20,21,23] We introduce the parameters Δ_1 and Δ_2 to describe the tetragonal lattice distortion in Cr^{3+}:$KZnF_3$ (see Fig. 1). By using the relationship between the ZFS and the CF contributions, we can obtain a reliable relation between the charge-compensation ZFS effect and the lattice distortion parameters Δ_1 and Δ_2.

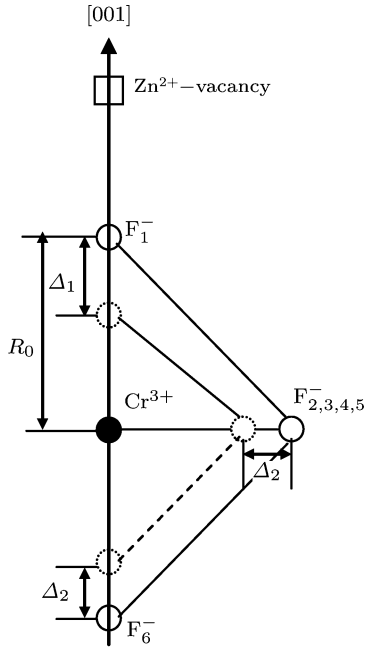


Fig. 1. Local lattice structure of Cr^{3+}–V_{Zn} tetragonal defect centre in Cr^{3+}:$KZnF_3$ crystal.

3. Results and discussion

The zero-field splitting parameter D and the anisotropic Zeeman g factor Δg ($= g_\parallel - g_\perp$) for paramagnetic transition-metal (TM) impurity ions in a crystal reflect very sensitively even a small variation in the coordination of the paramagnetic centres,[24–28] so we can study the local environments of the paramagnetic ions from these data.

The trivalent Cr^{3+} ions replace the divalent Zn^{2+} ions after they have been doped into the $KZnF_3$ crystals. When the paramagnetic impurity Cr^{3+} ions substitute the Zn^{2+} ions in the $KZnF_3$ crystals, a Zn^{2+} ion site on the [001] axis can be vacant to form a tetragonal defect centre (see Fig. 1) owing to the charge compensation. Expression (9) enables us to investigate the variation of the CF parameter B_{kq}, and via Eqs. (3) and (5) also the variations of the SH parameters (D, Δg), each as a function of the lattice distortion parameters Δ_1 and Δ_2. To obtain the SH parameters, a prior diagonalization of Hamiltonian (6) for a given set of values of the lattice distortion parameters Δ_1 and Δ_2 is required. In order to investigate the variations of D and Δg with Δ_1 and Δ_2, we must select a reasonable range of values for Δ_1 and Δ_2. Takeuchi *et al.*[29] have analysed the ZFS parameters by using the superposition

mode. They obtained that an F^- ion on the [001] axis of the crystal moves towards the central Fe^{3+} ion by $\Delta_1 = 0.0104$ nm $= 0.0517R_0$ (note: Takeuchi *et al.* ignored the movement of the other five F^- ions around the central Fe^{3+} ion) for the Fe^{3+}–V_{Cd} tetragonal defect centre in the $RbCdF_3$ crystal. Since the tetragonal local structural distortion in Fe^{3+}:$RbCdF_3$ is similar to that induced by Zn^{2+} vacancy on the [001] axis in Cr^{3+}:$KZnF_3$, we select Δ_1 to be in a range from $0.0R_0$ to $0.1R_0$, and Δ_2 varies from $0.0R_0$ to $0.04R_0$.

The variations of ZFS parameter D and anisotropic Zeeman g factor Δg for Cr^{3+} at the tetragonal site in $KZnF_3$ with Δ_1/R_0 are plotted in Fig. 2 with parameters $\Delta_2/R_0 = 0.0$, 0.013, 0.03, 0.04. The experimental values[6] $D = -542.1 \times 10^{-4}$ cm^{-1} and $\Delta g = -2.2 \times 10^{-3}$ are plotted as horizontal lines in Fig. 2 for direct comparison among the various options considered in the present calculations. The best match $\Delta_1 = 0.06R_0 \approx 0.0121$ nm and $\Delta_2 = 0.013R_0 \approx 0.0026$ nm are obtained, which yields a good agreement between the theoretical results and the experimental findings for the ZFS parameter D and g factors $g_\parallel$, Δg (see Table 1 and Fig. 2). The theoretical results of D, $g_\parallel$, and Δg for the three cases considered are listed in Table 1 together with the experimental data for Cr^{3+}:$KZnF_3$. These results indicate that the parameters D and Δg depend strongly on the lattice distortion parameters Δ_1 and Δ_2. Under the assumption of an undistorted host lattice, i.e., $\Delta_1 = \Delta_2 = 0$, we obtain $D = 0$ and $\Delta g = 0$. This shows that a lattice distortion must occur and plays a significant role in making contributions to the zero-field splitting D and g factor Δg. In fact, owing to the differences in mass, charge and ionic radius between Cr^{3+} and Zn^{2+}, the mutual interaction between the Cr^{3+} and the surrounding F^- ions in the doped crystal must differ from that between the Zn^{2+} and the F^- ions in the host crystal. Moreover, because the radius of the Cr^{3+} (0.063 nm) ion is much smaller than that of the host Zn^{2+} (0.083 nm) ion and the charge of the Cr^{3+} ion is more than that of the Zn^{2+} ion, the Coulomb interaction between the Cr^{3+} and the F^- ions is greater than that between the Zn^{2+} and the F^- ions. Thus it is reasonable to assume that the six F^- ions move towards the central magnetic Cr^{3+} ion in an ionic crystal in which the Coulomb interaction acts as a main crystallization source. The fitted value of the distortion parameter Δ_1 is larger than that of Δ_2, which confirms that the Zn^{2+} vacancy is located above the Cr^{3+} centres. In fact, because the effective charge of the Zn^{2+} vacancy on the [001] axis is negative and the interaction force between the V_{Zn} and the nearest F^- ions is repulsive, Δ_1 must be much larger than Δ_2 of the other five F^- ions. The SH parameters D and Δg are very sensitive to changes in the structural parameters,[24–28,30,31] hence the values of the lattice distortion parameters Δ_1 and Δ_2 obtained from the fitting are unlikely to be random.

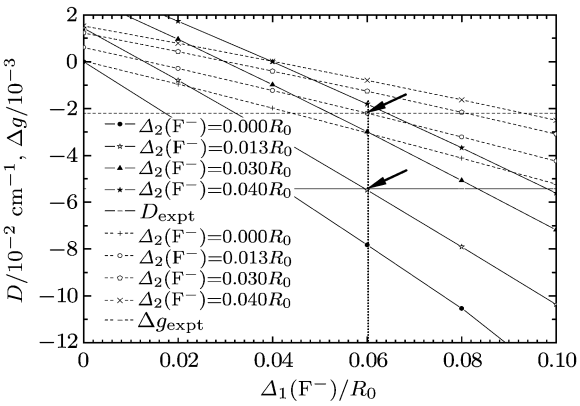


Fig. 2. Variations of ZSF parameter D and Zeeman g factor $\Delta g = g_\parallel - g_\perp$ with Δ_1 $(F^{-1})/R_0$. The horizontal lines denote the experimental values of $D = -5.421 \times 10^{-2}$ cm^{-1}[6] and $\Delta g = -2.2 \times 10^{-3}$[6] respectively.

Table 1. ZFS parameter D and g factors from various sources for Cr^{3+} ions in $KZnF_3$ crystal.

	Crystal field parameters					SH parameters		
	μ	δ	B_{20}	B_{40}	B_{44}	$D/10^{-2}$ cm^{-1}	$\Delta g/10^{-3}$	$g_\parallel$
Case *a*	0	0	0	31500.0	18824.9	0	0	1.9695
Case *b*	–3064.7	919.0	3983.6	37383.6	20362.4	–7.27	–2.5	1.9683
Case *c*	–3064.7	919.0	3983.6	37383.6	20362.4	–5.48	–2.2	1.9720
Expt.[6]	–	–	–	–	–	–5.421(5)	–2.2	1.9720(3)

Case *a*: perfect lattice.
Case *b*: $\Delta_1 = 0.06R_0$, $\Delta_2 = 0.013R_0$, only with SO magnetic interaction.
Case *c*: $\Delta_1 = 0.06R_0$, $\Delta_2 = 0.013R_0$, with SO, SS, SOO, and OO magnetic interactions.

In order to illustrate the relative importance of the other three magnetic interactions (i.e., SS, SOO, and OO)[32–34] contributing to the SH parameters with respect to that due to the SO interaction, it is convenient to define a percentage ratio as

$$\eta_X = \frac{|X_{\mathrm{SO+SS+SOO+OO}} - X_{\mathrm{SO}}|}{|X_{\mathrm{SO+SS+SOO+OO}}|} \times 100\%, \quad (4)$$

where X is D or Δg. It is found from Table 1 that the contribution from the other three interactions including SS, SOO, and OO for Cr^{3+} in the $KZnF_3$ crystals are 32.7% for D and 13.6% for Δg. This result shows that reliable information about the local structure distortion, the pressure behaviour and the observed magnetic and spectroscopic properties could not be acquired if the contributions to the SH parameters from the other three interactions including SS, SOO, and OO were omitted.

4. Summary

The SH parameters and the tetragonal charge-compensation defect of the Cr^{3+} centre in the $KZnF_3$ crystal are theoretically studied by using the complete diagonalization method. In the doped Cr^{3+}:$KZnF_3$ crystal, the Cr^{3+} impurities substitute the Zn^{2+} after they have been doped into the $KZnF_3$ crystal. Owing to the charge compensation, some Zn^{2+} sites on the [001] axis will be vacant. Moreover, the Zn^{2+} vacancy and the differences in mass and radius between the Cr^{3+} and the Zn^{2+} ions induce the lattice distortion. The local lattice distortions are shown to give rise to the tetragonal crystal field, which in turn results in the tetragonal zero-field splitting D and the anisotropic g factor Δg. The ZFS parameter D and the Zeeman g factors $g_{\|}$ and Δg calculated in the Cr^{3+}:$KZnF_3$ crystal are in good agreement with the experimental data if we assume the ligand F^- ion is along the [001] direction and the other five F^- ions move towards the central Cr^{3+} by distances of $\Delta_1 = 0.0121$ nm and $\Delta_2 = 0.0026$ nm (see Fig. 1), respectively. Hence, the local structure distortion effect plays an important role in explaining the spectroscopic properties of the Cr^{3+} ions in the Cr^{3+}:$KZnF_3$ crystal. Our approach takes into account the spin–orbit interaction as well as the spin–spin, spin–other-orbit, and orbit–orbit interactions omitted in the previous studies. It is found for the Cr^{3+} ions in the Cr^{3+}:$KZnF_3$ crystal that although the SO mechanism is the most important one, the contribution to the SH parameters from the other three magnetic interactions including SS, SOO, and OO is appreciable and should not be omitted, especially for the ZFS parameter D.

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