

Modeling of Mn²⁺ doped MgV₂O₆ Crystal

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ABSTRACT : The crystal field parameters (CFPs) of Mn²⁺ in magnesium meta-vanadate, MgV₂O₆ (MMV) crystal are determined using the superposition model. The zero field splitting parameters (ZFSPs) D and E are obtained using perturbation and microscopic spin Hamiltonian (SH) theory. The theoretical ZFSPs are compared with the experimental ones. The ZFSPs D and E obtained theoretically are in good agreement with the experimental values found by electron paramagnetic resonance. The results indicate that the Mn²⁺ ion occupies Mg²⁺ substitutional site in MMV.

KEYWORDS - C. Crystal structure and symmetry; D. Crystal and ligand fields; D. Optical properties; E. Electron paramagnetic resonance.

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I. INTRODUCTION

The superposition model was developed in order to find physical and geometrical information contained in crystal field parameters [1, 2]. The positions of different ligands are needed in applying this model. Therefore, the relation between the model and the theories of local distortion in crystals is of particular interest. A one-parameter model was used [3] to describe the position of the Fe³⁺ ion relative to the surrounding oxygen octahedron, assumed to be undisturbed by the substitution. Mn²⁺ spin Hamiltonian parameters were analyzed [4] using this model together with local distortion and quite reasonable results were obtained.

Theoretical studies on the spin Hamiltonian parameters of d³ ions have become the matter of interest of many researchers [5-14]. Various mechanisms have been suggested to contribute to the ground state splitting of the magnetic ions introduced in the lattices [15]. The effect of spin Hamiltonian mechanism is normally considered by perturbation procedures. In most of the used perturbation procedure, cubic field and the diagonal part of free-ion Hamiltonian are considered as unperturbed terms while the spin-orbit coupling, the low-symmetry field, and the off-diagonal part of free-ion Hamiltonian are taken as the perturbation terms [16].

Electron paramagnetic resonance (EPR) studies of Mn²⁺ doped magnesium meta-vanadate, MgV₂O₆ (MMV) single crystals have been reported [17]. Two possibilities exist for Mn²⁺ site in the MMV crystal, namely substitutional and interstitial. It is interesting to investigate the site of the impurity. It was suggested [17] that Mn²⁺ ion enters the lattice substitutionally at Mg²⁺ site. In the present study, the axial and rhombic zero-field splitting parameters (ZFSPs) are computed for the Mn²⁺ ion existing at substitutional Mg²⁺ site in MMV; using crystal field parameters (CFPs) obtained from superposition model and perturbation expressions [18]. The result derived from this model is in reasonable agreement with the experimental finding.

II. CRYSTAL STRUCTURE

The MMV single crystals are monoclinic, space group C2/m with Z = 2 [17, 19]. The unit cell dimensions are a = 0.9279 (7) nm, b = 0.3502 (2) nm, c = 0.6731 (6) nm and $\beta = 111.77(6)^\circ$ [17]. The structure consists of Mg²⁺ lying at a site of 2/m symmetry octahedrally coordinated to oxygen atoms with an average separation of 0.2140 nm. The remaining atoms lie in crystallographic mirror planes with V ion coordinated to six oxygen atoms having bond distances ranging from 0.1666 to 0.2671 nm. (Fig.1).

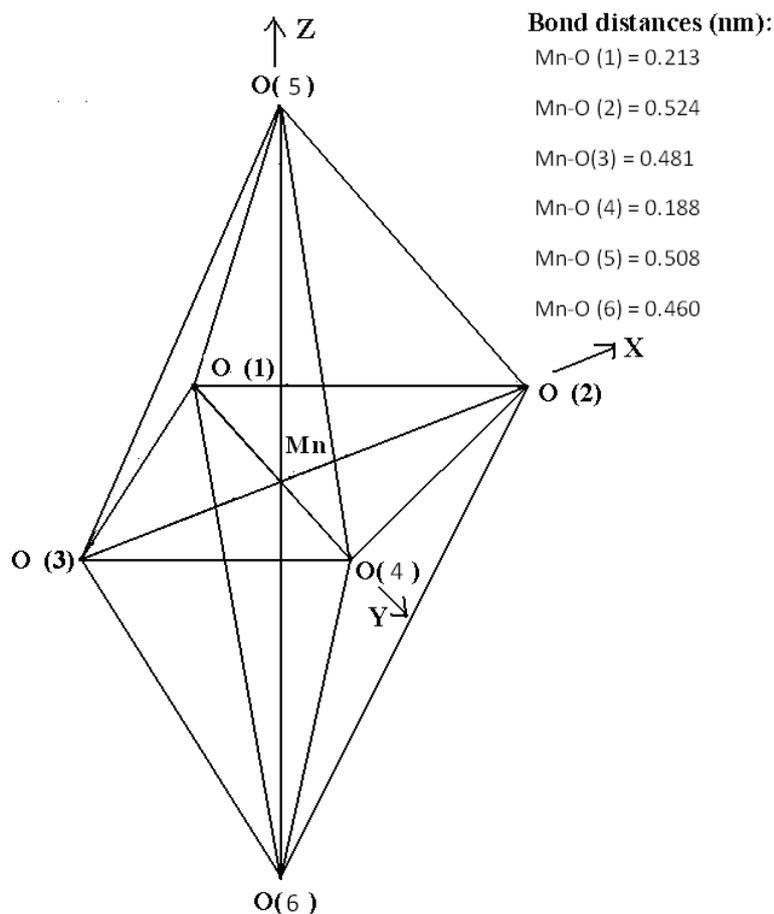


Fig. 1: Coordination around Mn^{2+} in MMV single crystal.

III. THEORETICAL INVESTIGATION

The experimental resonance fields can be obtained using the spin Hamiltonian [20, 21]

$$\begin{aligned}
 \mathcal{H} = & g\mu_B \mathbf{B} \cdot \mathbf{S} + D \left\{ S_z^2 - \frac{1}{3} S(S+1) \right\} + E(S_x^2 - S_y^2) + \left(\frac{a}{6} \right) [S_x^4 + S_y^4 + S_z^4 - \frac{1}{5} S(S+1)(3S^2 + 3S - 1)] \\
 & + \frac{F}{180} \{ 35 S_z^4 - 30 S(S+1) S_z^2 + 25 S_z^2 - 6S(S+1) + 3S^2(S+1)^2 \} + \frac{K}{4} [\{ 7S_z^2 - S(S+1) - 5 \} \\
 & (S_x^2 + S_y^2) + (S_x^2 + S_y^2) \{ 7S_z^2 - S(S+1) - 5 \}] + \mathcal{A} S_z I_z + \mathcal{B} (S_x I_x + S_y I_y)
 \end{aligned} \quad (1)$$

where g is the isotropic spectroscopic splitting factor, μ_B is the Bohr magneton, \mathbf{B} is the external magnetic field. D and E are the second-rank axial and rhombic ZFSPs, whereas a , F , and K are the fourth-rank cubic, axial and rhombic ones, respectively. The last two terms in Eq. (1) represent the hyperfine ($I = 5/2$) interaction. The F and K terms are deleted here as their effect is small [20, 22, 23]. The isotropic approximation used for the electronic Zeeman interaction is generally valid for $3d^5$ ions [20, 24]. The two approximations in question may slightly affect the fitted value of a [25]. The direction of the maximum overall splitting of EPR spectrum is taken as the z axis and that of the minimum as the x axis [26]. The laboratory axes (x , y , z) determined from EPR spectra are found to coincide with the crystallographic axes (CA). The z -axis of the local site symmetry axes, i.e. the symmetry adapted axes (SAA) is along the metal oxygen bond and the other two axes (x , y) are perpendicular to the z -axis.

In MMV, magnesium ion is located within a distorted octahedron of oxygen ions [17, 19] and the local symmetry is approximately orthorhombic of first kind (OR-I) [27]. In an OR-I symmetry, the SO contributions to the ZFSPs D and E of $3d^5$ ions were obtained [18, 28] as:

$$D^{(4)}(SO) = (3\xi^2/70P^2D) (-B_{20}^2 - 21 \xi B_{20} + 2B_{22}^2) + (\xi^2/63P^2G) (-5B_{40}^2 - 4B_{42}^2 + 14B_{44}^2) \quad (2)$$

$$E^{(4)}(SO) = (\sqrt{6} \xi^2 / 70P^2D) (2B_{20} - 21 \xi) B_{22} + (\xi^2 / 63P^2G) (3\sqrt{10} B_{40} + 2\sqrt{7} B_{44}) B_{42} \quad (3)$$

where $P = 7B+7C$, $G = 10B+5C$, and $D = 17B+5C$; B and C are the Racah parameters. Only fourth order term is taken up here as the first-, second-, third-, fifth- and sixth-order perturbations of D and E are zero [18]. Eqs. (2) and (3) are appropriate for weak-field cases, and are also correct even when the low-symmetry components are comparable with the cubic part [18].

By considering the covalency effect via the average covalency parameter N, the B, C and ξ are expressed in terms of N as [29-30]

$$B = N^4B_0, C = N^4C_0; \xi_d = N^2 \xi_d^0 \quad (4)$$

where B_0 and C_0 , and ξ_d^0 are the free ion Racah and the spin-orbit coupling parameters, respectively [29-30].

The following values of B_0 and C_0 , and ξ_d^0 for free Mn^{2+} ion are used: $B_0 = 960 \text{ cm}^{-1}$, $C_0 = 3325 \text{ cm}^{-1}$, $\xi_d^0 = 336 \text{ cm}^{-1}$ [20].

From optical absorption study of Mn^{2+} doped crystal with oxygen ligands [31]: $B = 917 \text{ cm}^{-1}$ and $C = 2254 \text{ cm}^{-1}$ were obtained. The average value [30] of $N = (\sqrt{B/B_0} + \sqrt{C/C_0}) / 2 = 0.91$ is used to calculate the ZFSPs D and E from Eqs. (2) and (3).

The superposition model is used to calculate the CFPs, B_{kq} for Mn^{2+} ion in MMV single crystal and ZFSPs are then calculated using these B_{kq} parameters.

The superposition model has been quite successful in explaining the crystal-field splitting of the $4f^n$ ions [32] and recently of some $3d^n$ ions [33, 34-35]. The superposition model expresses the CFPs as [18, 32]

$$B_{kq} = \sum \bar{A}_k(R_j) K_{kq}(\theta_j, \phi_j) \quad (5)$$

where R_j are the distances between the paramagnetic ion Mn^{2+} and the ligand ion j, R_0 is the reference distance, normally chosen near a value of the R_j 's. θ_j are the bond angles in a chosen axis system (preferably symmetry adapted axes system (SAAS)) [36, 37]. Summation is taken over all the nearest neighbour ligands. The coordination factor $K_{kq}(\theta_j, \phi_j)$ are the explicit functions of angular position of ligand [18, 36, 38-39]. The intrinsic parameter $\bar{A}_k(R_j)$ is given by the power law [16, 27]:

$$\bar{A}_k(R_j) = \bar{A}_k(R_0) (R_0 / R_j)^{t_k} \quad (6)$$

where $\bar{A}_k(R_0)$ is intrinsic parameter for a given ion host system. The symbol t_k is power law exponent. The crystal-field parameters B_{kq} may be determined using the superposition model given by Eq. (5) and are presented in Appendix A [40].

For 3d⁵ ions, $\overline{A_2(R_0)} / \overline{A_4(R_0)}$ is 8-12 [5, 34]. In the present study, we have taken $\overline{A_2(R_0)} / \overline{A_4(R_0)} = 10$. For 3d^N ions in the 6-fold cubic coordination $\overline{A_4(R_0)}$ can be found from the relation: $\overline{A_4(R_0)} = (3/4) Dq$ [18]. As $\overline{A_4(R_0)}$ is independent of the coordination [41], we have used above relation to determine $\overline{A_4(R_0)}$ in our calculation using $Dq = 756 \text{ cm}^{-1}$ [31]. The values of $R_1, R_1', R_2, R_2', R_3, R_3'; \theta_1, \theta_1', \theta_2, \theta_2', \theta_3, \theta_3'; \phi_1, \phi_1', \phi_2, \phi_2', \phi_3$ and ϕ_3' used in the calculation are: 0.213 nm, 0.524 nm, 0.481 nm, 0.188 nm, 0.508 nm, 0.460 nm; 87.4°, 87.0°, 83.4°, 93.7°, 93.1°, 97.1°; 86.5°, 85.1°, 87.7°, 94.9°, 95.2° and 92.4°, respectively.

IV. RESULT AND DISCUSSION

At first to check the substitution at Mg²⁺ site, the origin of Mn²⁺ was shifted at the Mg²⁺ ion. Since the ionic radius of the impurity Mn²⁺ ion (0.080 nm) is slightly larger than that of the host Mg²⁺ (0.072 nm), a distortion can be expected [42]. Taking the coordinates x, y, z; the bond distances of different ligands, R_j as well as the angles θ_j and ϕ_j were calculated and are given in Table 1.

Table 1: Coordinates of oxygen ligands, Mn-oxygen bond distances R_j and coordination angles θ_j and ϕ_j for Mn²⁺ ion doped MMV single crystals (without distortion).

MetMetal and Oxygen	x	y	z	Mn-oxygen bond distance R _j (nm)	Angle θ_j (Degree)	Angle ϕ_j (Degree)	Ligands
Mg	0	0	0				
O(1)	0.1517	0.5	0.1133	0.248	87.4	86.5	
O(2)	0.4607	0.5	0.2764	0.536	87.0	85.1	
O(3)	0.1930	0.5	0.5652	0.491	83.4	87.7	
O(4)	-0.1517	0	-0.1133	0.176	93.7	94.9	
O(5)	-0.4607	0	-0.2764	0.507	93.1	95.2	
O(6)	-0.1930	0	-0.5652	0.459	97.1	92.4	

In adjusting the Mn-O distances to match the experimental result, the site symmetry is preserved as well as the energy is minimised and thus the structural stability is taken into consideration. Taking R₀ as slightly larger than the minimum of R_j [43], i.e. R₀ = 0.214 nm, $\overline{A_2(R_0)} / \overline{A_4(R_0)} = 10$, t₂ = 3, t₄ = 7 [5]; consideration no distortion, we obtain B₂₀ = 16313.54, B₂₂ = -264.45, B₄₀ = -1038.5, B₄₂ = 453.77, B₄₄ = -100.91 cm⁻¹ and then |D| and |E| to be 423 × 10⁻⁴ cm⁻¹ and 14.9 × 10⁻⁴ cm⁻¹, respectively, which are inconsistent with the experimental values. Therefore, we have considered the distortion. The bond distances of different ligands R_j and the angles θ_j and ϕ_j calculated for this case are given in Table 2.

Table 2: Metal-oxygen bond distances R_j and coordination angles θ_j and ϕ_j for Mn^{2+} ion doped MMV single crystals (with distortion).

Metal-oxygen	Metal-oxygen bond distance R_j (nm)	Angle θ_j (Degree)	Angle ϕ_j (Degree)
Mn-O(1)	0.213	87.4	86.5
Mn-O(2)	0.524	87.0	85.1
Mn-O(3)	0.481	83.4	87.7
Mn-O(4)	0.188	93.7	94.9
Mn-O(5)	0.508	93.1	95.2
Mn-O(6)	0.460	97.1	92.4

The calculated B_{kq} parameters are: $B_{20} = 16444.05$, $B_{22} = -1070.07$, $B_{40} = -1053.92$, $B_{42} = -1380.02$, $B_{44} = 34.68 \text{ cm}^{-1}$. After that $|D|$ and $|E|$ are calculated taking other parameters as above, which come out to be $429 \times 10^{-4} \text{ cm}^{-1}$ and $60 \times 10^{-4} \text{ cm}^{-1}$, respectively. This provides $|D|$ and $|E|$ data (Table 3) which are in good agreement with the experimental values.

Table 3: Comparison of the ZFSPs calculated by the superposition model for the Mn^{2+} ion doped MMV single crystal with experimental values.

	Values of ZFSPs ($\times 10^{-4} \text{ cm}^{-1}$)		
	$ D $	$ E $	$ E / D $
Calculated	429	60	0.14
Experimental	428.9	60.7	0.14

Such model calculations have been done earlier in case of Mn^{2+} and Fe^{3+} doped anatase TiO_2 crystal [44]. Therefore, we can say that Mn^{2+} ion substitutes the Mg^{2+} ion. In this way, the conclusion drawn on the basis of superposition model supports the experimental result that Mn^{2+} ions take up substitutional Mg^{2+} site in the crystal [17]. For comparison we have also investigated the interstitial sites for Mn^{2+} ions. The predicted values of ZFSPs come out to be inconsistent with the experimental ones and hence we are not giving this result here.

V. CONCLUSIONS

The zero field splitting parameters (ZFSPs) have been determined using the superposition model and perturbation formulae. The experimental ZFSPs obtained for Mn^{2+} ion in MMV single crystal are in good agreement with the calculated ZFSPs at the substitutional Mg^{2+} site. We suggest that the Mn^{2+} ion occupies substitutional Mg^{2+} site in MMV. The results support the conclusion drawn from experimental study.

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