Zero field splitting parameter of Mn^{2+} in $SrCl_2$ single crystals

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Abstract— A theoretical study has been done to find crystal field parameters and zero-field splitting parameter of Mn^{2+} doped $SrCl_2$ single crystals using superposition model and the perturbation theory. The theoretical zero-field splitting parameter D agrees well with the experimental value evaluated from EPR study. The present study supports the experimental result that Mn^{2+} ions substitute at Sr^{2+} site in $SrCl_2$ single crystal.

Keywords— A. Inorganic compounds; A. Single crystal; D. Crystal fields; D. Optical properties; D. Electron paramagnetic resonance.

I. INTRODUCTION

Electron paramagnetic resonance (EPR) yields information about distortions in the lattice and local site symmetry of transition ions incorporated in different crystals [1-3]. The spin Hamiltonian (SH) parameters obtained from EPR can be correlated with optical and structural parameters using microscopic spin-Hamiltonian (MSH) theory,. The outcome of above studies is that the spin Hamiltonian parameters of transition ions (d5) in crystals are much sensitive to local distortions. Hence, the SH theory is widely used in the study of crystals.

The crystal-field (CF) parameters of d^5 ion can be obtained with the help of superposition model (SPM) [4, 5]. The zero field splitting (ZFS) parameters are then estimated using CF parameters [6]. Mn^{2+} ion of iron group is interesting due to its $^6S_{5/2}$ ground state [7-9]. The electron spins are oriented freely in applied magnetic field with high order interaction of crystalline electric field [10, 11].

The physical properties of crystals with fluorite structure have been described in [12].Transition metal ions in sixfold and fourfold cubic coordination as well as rare-earth ions in eightfold cubic coordination have been studied for a long time, while d^n ions in eightfold cubic coordination were the subject of study in the last decade. In the group of fluorite structure crystals only the compounds CaF_2, SrF_2, BaF_2, CdF_2, PbF_2, and $SrCl_2$ have been used as host lattices for the study of transition ion impurities till now.

EPR measurements on the Mn^{2+} centers in $SrCl_2$ at room temperature (RT) have been carried out [13]. In the present study, the CF parameters are determined using SPM and these parameters with MSH theory then give ZFS parameter for Mn^{2+} ions at the axial symmetry site in $SrCl_2$ single crystal at RT [14]. The ZFS parameter D obtained

with the help of SPM provides good agreement with the experimental value [13].

This section was dedicated to the brief introduction of the subject and objective of the study conducted. The rest of the paper is organized as follows. Section II gives the related work associated with the SPM analysis. Section III describes the methods considered for calculation of CF and ZFS parameters. Section IV presents the results and its discussion based on the analysis. In section V, conclusion of the study and future scope for improvement are given.

II. RELATED WORK

The SPM analysis has been done for different ion-host systems [15-31]. The crystal structure of $SrCl_2$ is cubic as shown in Fig. 1. The lattice parameter is given to be a = 6.9767 Å [14]. The crystal structure belongs to the space group O_h^5 (Fm3m). The chlorine coordination around Sr^{2+} is illustrated in Fig. 1. The site symmetry around Mn^{2+}ions may be considered to be axial, as indicated by EPR study of Mn^{2+}: $SrCl_2$ [13].
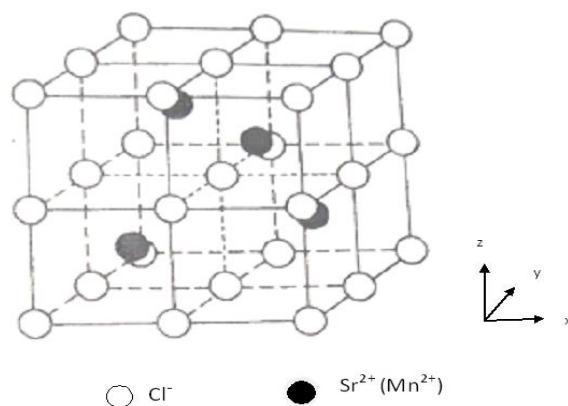

Fig. 1: Crystal structure of $SrCl_2$ together with axes (SAAS-symmetry adopted axes system).

III. MATERIALS AND METHODS

The SH of Mn^{2+} ($3d^5$) ion in crystal field of axial symmetry is written as [15-17]

$$\mathcal{H} = g\,\mu_B B.S + D\{S_Z^2 - S(S+1)\}$$
$$+ \left(\frac{a}{6}\right)[S_X^4 + S_Y^4 + S_Z^4 - \frac{1}{5}S(S+1)(3S^2+3S-1)]$$
$$+ \frac{F}{180}\{35S_Z^4 - 30S(S+1)S_Z^2 + 25S_Z^2 - 6S(S+1) + 3S^2(S+1)^2\}$$
$$+ A(I.S) \tag{1}$$

where the first term provides electronic Zeeman interaction, B is the applied magnetic field, g is the spectroscopic splitting factor and μ_B is Bohr magneton. The second, third, and fourth terms are the second order axial, fourth-rank cubic and fourth-rank axial ZFS terms [8]. The fifth term represents the hyperfine interaction term. S, D, a, F give the effective spin vector, second order axial, fourth-rank cubic and fourth-rank axial ZFS parameters, respectively. The electronic Zeeman interaction is taken to be isotropic for Mn^{2+} ions [8, 18, 19].

The Hamiltonian for a d^5 ion is written as

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{cf} + \mathcal{H}_{so}$$
$$\text{where } \mathcal{H}_{cf} = \sum_{kq} B_{kq} C_q^k \tag{2}$$

is the crystal field Hamiltonian whereas $\mathcal{H}_0$ and $\mathcal{H}_{so}$ represent free ion Hamiltonian and spin-orbit (SO) coupling, respectively. As the spin-spin coupling is very small, its contribution is neglected in Eq. (2) [20-22]. The crystal field of SO interaction is considered as perturbation term [23-25]. The strong-field scheme calculation for F-state ions has been given by Macfarlane [26]. The SO contribution to the ZFS parameter D for $3d^5$ ions in axial symmetry is given as [24]

$$D^{(4)}(SO) = \left(\frac{\xi^2}{63P^2G}\right)[14B_{44}^2 - 5B_{40}^2] - \left(\frac{3\xi^2}{70P^2D}\right)B_{20}[B_{20} - 14\xi] \tag{3}$$

where P = 7(B+C), G = 10B+5C and D = 17B+5C. P, G, and D give the energy separations between the excited quartets and the ground sextet. Racah parameters B and C provide the electron-electron repulsion. Only fourth order term is taken in Eq. (3) since other perturbation terms are negligible [24, 26]. The parameters B, C and ξ, in terms of the average covalency parameter N, are written as, B = $N^4 B_0$, C = $N^4 C_0$ and $\xi = N^2 \xi_0$, where B_0, C_0 and ξ_0 are the Racah parameters and the spin-orbit coupling parameter for free ion, respectively [27, 28]. $B_0 = 960$ cm^{-1}, $C_0 = 3325$ cm^{-1}, $\xi_0 = 336$ cm^{-1} for Mn^{2+} ion are taken in this calculation [8]. Using equation

$$N = \left(\sqrt{B/B_0} + \sqrt{C/C_0}\right)/2, \tag{4}$$

N can be evaluated taking the values of Racah parameters (B = 843 cm^{-1}, C = 3100 cm^{-1}) obtained from optical study [13].

The CF parameters for Mn^{2+} in $SrCl_2$ single crystal are evaluated using SPM and then from Eq. (3) ZFS parameter D is obtained. Similar method has been used for finding ZFS parameters by several other workers [29].

The SPM is effectively considered to interpret the crystal-field splitting. This model has also been used for $3d^n$ ions [26, 30]. The crystal field parameters B_{kq}, employing this model, are determined from the equations

$$B_{20} = -2\bar{A}_2\left(\frac{R_0}{R_{10}+\Delta R_1}\right)^{t_2} - 4\bar{A}_2\left(\frac{R_0}{R_{20}+\Delta R_2}\right)^{t_2} \tag{5}$$

$$B_{40} = 16\bar{A}_4\left(\frac{R_0}{R_{10}+\Delta R_1}\right)^{t_4} + 12\bar{A}_4\left(\frac{R_0}{R_{20}+\Delta R_2}\right)^{t_4} \tag{6}$$

$$B_{44} = 2\sqrt{70}\,\bar{A}_4\left(\frac{R_0}{R_{20}+\Delta R_2}\right)^{t_4} \tag{7}$$

where R_0 is the reference distance [31]. It is normally taken as the average value of all four bond lengths (for axial symmetry). $\bar{A}_2$, $\bar{A}_4$ and t_k are the intrinsic parameter and power law exponent, respectively.

IV. RESULTS AND DISCUSSION

The position of Mn^{2+} ion and spherical coordinates of ligands are presented in Table 1. The average of two out of four Mn^{2+}-Cl^- bond lengths are obtained as $R_{10} = 0.6042$ nm and the average value of the rest two bond lengths are found as $R_{20} = 0.6042$ nm. ΔR_1 and ΔR_2 are the distortion parameters. In octahedral coordination, $\overline{A_4}(R_0) = (3/4)Dq$ [6]. For $3d^5$ ions $\dfrac{\overline{A_2}}{\overline{A_4}}$ lies in the range 8-12 [26, 30]. The power law exponent for Mn^{2+} ion is taken as $t_2 = 3$, $t_4 = 7$. Semi-ab initio calculations are done for other transition ions to find the intrinsic parameter values in SPM; the same method is used here.

Table 1 Atomic coordinates in $SrCl_2$ crystal and spherical coordinates of ligands R θ, φ.

Position of Mn^{2+} (Fractional)				Ligands	Spherical co-ordinates of ligands		
					R(nm)	θ^0	ϕ^0
	x	y ($\mathring{A}$)	z			(degree)	
Site : Substitutional	0.2500	0.2500	0.2500	Cl (1)	0.3021	54.73	45.00
Sr (0, 0, 0)	0.7500	0.7500	0.7500	Cl (2)	0.9063	54.73	45.00
	-0.2500	-0.2500	-0.2500	Cl (3)	0.3021	125.26	45.00
	-0.7500	-0.7500	-0.7500	Cl (4)	0.9063	125.26	45.00

The values of B, C and Dq are obtained from optical absorption study as 843, 3100 and 550 cm^{-1}, respectively [13]. First no local distortion is accounted and the value of D is evaluated. For this, taking $\frac{\overline{A_2}}{A_4} = 10$ and $R_0 = 0.211$ nm, which is slightly smaller than the sum of ionic radii of $Mn^{2+} = 0.083$ nm and $Cl^- = 0.181$ nm, the B_{kq} parameters are found as: $B_{20} = -1054.1$ cm^{-1}, $B_{40} = 7.316353$ cm^{-1}, $B_{44} = 4.372357$ cm^{-1} and the value of D as: $|D| = 11.28 \times 10^{-4}$ cm^{-1}. EPR study gives the experimental value of D as: $|D| = 426.0 \times 10^{-4}$ cm^{-1}, $|D| = 572.0 \times 10^{-4}$ cm^{-1} and $|D| = 701.0 \times 10^{-4}$ cm^{-1} for centers I, II and III, respectively[13]. From above it is observed that the theoretical value is quite smaller than the experimental one.

Now, taking local distortions as $\Delta R_1 = -0.3400$ nm and $\Delta R_2 = -0.3420$ nm, $R_0 = 0.211$ nm and ratio $\frac{\overline{A_2}}{A_4} = 10$, the B_{kq} parameters are obtained as given in Table 2 and the value of D as: $|D| = 426.19 \times 10^{-4}$ cm^{-1}, in good agreement with the experimental one: $|D| = 426.0 \times 10^{-4}$ cm^{-1} for center I. Similarly taking distortions as $\Delta R_1 = -0.3590$ nm, $\Delta R_2 = -0.3520$ nm and other parameters as above, the B_{kq} parameters are found as given in Table 2 and the value of D as: $|D| = 572.74 \times 10^{-4}$ cm^{-1}, also in good agreement with the experimental value: $|D| = 572.0 \times 10^{-4}$ cm^{-1} for center II. Further taking distortions as $\Delta R_1 = -0.3646$ nm, $\Delta R_2 = -0.3650$ nm and other parameters as above, the B_{kq} parameters are evaluated as given in Table 2 and the value of D as: $|D| = 701.85 \times 10^{-4}$ cm^{-1}, also in good agreement with the experimental value: $|D| = 701.0 \times 10^{-4}$ cm^{-1} for center III. Employing B_{kq} parameters and CFA program, the optical spectra of Mn^{2+} doped $SrCl_2$ crystals are calculated [32-33]. The energy levels of Mn^{2+} ion are evaluated by diagonalizing the complete Hamiltonian within the $3d^N$ basis of states in the intermediate crystal field coupling scheme.

Table 2. Crystal field parameters and zero field splitting parameters of Mn^{2+} doped $SrCl_2$ single crystal.

	ΔR_1 (nm)	ΔR_2 (nm)	R_o(nm)	B_{20}	B_{40}	B_{44}	$|D|$
I	-0.3400	-0.3420	0.211	-12801.2	2449.525	1508.525	426.19
	0.0000	0.0000	0.211	-1054.1	7.316353	4.372357	11.28
						Exptl.	426.0
II	-0.3590	-0.3520	0.211	-14919.7	3726.366	1980.459	572.74
	0.0000	0.0000	0.211	-1054.1	7.316353	4.372357	11.28
						Exptl.	572.0
III	-0.3646	-0.3650	0.211	-16959.6	4768.008	2868.489	701.85
	0.0000	0.0000	0.211	-1054.1	7.316353	4.372357	11.28
						Exptl.	701.0

I, II, III represent three centers.

The Hamiltonian contains the Coulomb interaction (in terms of B and C parameters), Trees correction, the spin-orbit interaction, the crystal field Hamiltonian, the spin-spin interaction and the spin-other orbit interaction. The computed energy values are given in Table 3 (input parameters are given below the Table) together with the experimental values for compariso[13]. It is observed from Table 3 that there is a reasonable agreement between the computed and experimental energy values. The energy values obtained without considering distortion were not consistent from the experimental ones and so are not being given here. Thus the theoretical study supports the results of the experimental one.

Table 3. Experimental and calculated (CFA package) energy band positions of Mn^{2+} doped $SrCl_2$ single crystal.

Transition from $^6A_{1g}(S)$	Observed energy bands (cm^{-1})	Calculated energy bands (cm^{-1}) With distortion		
		I	II	III
$^4T_1g(G)$	22215	23029, 23054, 23056, 23124, 23652, 23691	21975, 22032, 22066, 22142, 23017, 23054	22183, 22218, 22657, 22710, 22771, 22881
$^4T_2g(G)$	24675	23994, 24044, 24197, 24290, 24346, 24999	23270, 23335, 23458, 23939, 23955, 24745	23640, 23652, 24200, 24214, 25442, 25448
$^4A_1g(G)$ $^4Eg(G)$	25100 25675	25016, 25442 25449, 25453, 25458, 25970	24760, 25442 25449, 25450, 25457, 26111	25449, 25457 26189, 26211, 26246, 26303
$^4T_2g(D)$	29200	28138, 28169, 28720, 28724, 29008, 29017	28377, 28410, 28499, 28508, 28825, 28836	28295, 28307, 28694, 28706, 28880, 28921
$^4Eg(D)$	30275	30263, 30303, 31678, 31800	30261, 30305, 31816, 31923	30260, 30313, 31928, 32023
$^4T_1g(P)$	31200	31901, 31996, 35011, 35458, 35515, 35802	32010, 32094, 33723, 34572, 34655, 34944	32105, 32181, 32348, 33530, 33618, 34211

Input parameters: Numbers of free ion parameters = 5, number of d shell electrons = 5, number of fold for rotational site symmetry = 1; Racah parameters in A, B and C, spin-orbit coupling constant and Trees correction are 0, 843, 3100, 280 and 76 cm^{-1}, respectively; number of crystal field parameters = 3; B_{20}, B_{40}, B_{44} are taken from Table 2, spin-spin interaction parameter, M0 = 0.2917; spin-spin interaction parameter, M2 = 0.0229; spin-other-orbit interaction parameter, M00 = 0.2917; spin-other-orbit interaction parameter, M22 = 0.0229; magnetic field, B = 0.0 Gauss; angle between magnetic field B and z-axis =0.00 degree.

V. CONCLUSION AND FUTURE SCOPE

Zero-field splitting parameter D for Mn^{2+} in $SrCl_2$ single crystal has been determined employing superposition model and perturbation theory. The theoretical D agrees well with the experimental one when distortion is taken into consideration. The theoretical study shows that Mn^{2+} ion occupies Sr^{2+} site which supports the results of the experimental EPR investigation. The CF energy values for Mn^{2+} ions at Sr^{2+} sites obtained using CFA package and CF parameters are in reasonable agreement with the experimental ones. Thus the theoretical results support the experimental finding. Modeling approach used here may be applicable in future to correlate EPR and optical data for different ion-host systems.

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