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## The method of calculating the spin–lattice coupling coefficients $F_{ij}$ in cubic symmetry from the formulae for the $g$ -factor

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**Abstract.** Similar to the case of the spin–lattice coupling coefficients  $G_{ij}$  in cubic symmetry, in this paper the simple correlations between the coupling coefficients  $F_{ij}$  ( $F_{11}$ ,  $F_{12}$  and  $F_{44}$ ) in a cubic field and the  $g$ -factor in cubic and low symmetries have been established, and hence a simple and uniform method suitable for calculating the coefficients  $F_{ij}$  for all  $d^n$  ions is given. As an example, the analytic expressions for  $F_{ij}$  for  $d^3$  ions in a cubic field are obtained from the high-order perturbation formulae for the  $g$ -factor. From these expressions, the coefficients  $F_{ij}$  for  $\text{MgO}:\text{Cr}^{3+}$  crystals have been calculated. The results are close to the experimental values and the errors are, as in the case of  $G_{ij}$ , attributed mainly to the fact that the local elastic constants  $s_{ij}$  in the vicinity of impurity ions are different from the host values. The coefficients  $F_{ij}$  for  $\text{MgO}:\text{V}^{2+}$  crystals, in which the local values are very similar to the bulk values, are also predicted. The results should be, as shown for the coefficients  $G_{ij}$ , closer to the experimental values calculated from the bulk elastic constants. This point remains to be verified.

### 1. Introduction

The interaction of phonons with paramagnetic spin systems is best characterised by spin–lattice coupling coefficients which relate the energy shift in the spin system to the strain introduced into the lattice. The coupling tensor elements applicable to the shift of the  $g$ -factor with strain are the coefficients  $F_{ij}$  and those applicable to the change in zero-field splitting with strain are the coefficients  $G_{ij}$ . As is well known, these coupling coefficients are of importance since they intervene explicitly in the calculation of the spin–lattice relaxation time of the magnetic centre [1, 2], as well as in the elucidation of the microscopic mechanisms of zero-field splitting and anisotropic  $g$ -factor [1, 3–5]. So, in the past few decades, a great many theoretical studies have been done to explain these coefficients. Usually, these theoretical calculations are directly related to the strain tensor elements [4–6]. The method is complex and it is sometimes easy to make mistakes. In addition, it does not clearly provide the physical meaning of these coefficients. In our previous papers [7–11], for the coefficients  $G_{11}$  and  $G_{44}$  in cubic symmetry, a simple and uniform method suitable for all  $d^n$  ions has been established and the clear physical

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meaning of  $G_{11}$  and  $G_{44}$  can be found. On this basis, we calculated the coefficients  $G_{11}$  and  $G_{44}$  in cubic symmetry for  $d^3$  ions ( $V^{2+}$  and  $Cr^{3+}$  in MgO crystals [8] and  $Cr^{3+}$  in  $SrTiO_3$  crystal (9)),  $d^5$  ions ( $Mn^{2+}$  in MgO and CaO crystals [10]) and  $d^8$  ions ( $Ni^{2+}$  in MgO crystals [11]) from the distinctive complex high-order perturbation formulae of zero-field splitting in low symmetries. The calculated results show good agreement with the experimental findings. However, for the coupling coefficients  $F_{ij}$  in a cubic field, no similar method has been put forward until now. In this paper, as in the case of  $G_{ij}$ , we shall also provide a simple and uniform method for the calculations of the coefficients  $F_{ij}$ . As an example, the analytic expressions for  $F_{ij}$  for  $d^3$  ions have been derived from the high-order perturbation formulae for the  $g$ -factor and the point-charge-dipole model in accordance with the method. From the expressions, the coefficients  $F_{ij}$  for MgO:  $Cr^{3+}$  crystals have been calculated by using only two adjustable parameters which were obtained from the optical spectra and applied to the calculations of the coefficients  $G_{11}$  and  $G_{44}$  [8]. It can be seen that, similar to the coefficients  $G_{ij}$ , the results of  $F_{ij}$  are close to but somewhat greater than the observed values. Equally, this is attributed mainly to the fact that the local elastic constants  $s_{ij}$  are smaller than the host values. The coefficients  $F_{ij}$  for MgO:  $V^{2+}$  crystals are also predicted. Because the local elastic constants are very similar to the host values for MgO:  $V^{2+}$ , the coefficients  $F_{ij}$  should be, as in the case of  $G_{ij}$ , closer to the observed values. This point remains to be verified experimentally.

## 2. Formulae for $F_{ij}$ in cubic symmetry

During the application of uniaxial stress, the EPR spectra can be described by the spin Hamiltonian

$$H_S = \beta S \delta g H + S \delta D S. \quad (1)$$

The strain-induced shifts  $\delta g_{ij}$  of the  $g$ -factor and  $\delta D_{ij}$  of the zero-field splitting can be expanded in terms of the strain tensor elements  $e_{ij}$ . For  $\delta g_{ij}$  to first order,

$$\begin{bmatrix} \delta g_{11} \\ \delta g_{22} \\ \delta g_{33} \\ \delta g_{13} \\ \delta g_{23} \\ \delta g_{12} \end{bmatrix} = \begin{bmatrix} F_{11} & F_{12} & F_{12} & 0 & 0 & 0 \\ F_{12} & F_{11} & F_{12} & 0 & 0 & 0 \\ F_{12} & F_{12} & F_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & F_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & F_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & F_{44} \end{bmatrix} \begin{bmatrix} e_{11} \\ e_{22} \\ e_{33} \\ e_{13} \\ e_{23} \\ e_{12} \end{bmatrix}. \quad (2)$$

Obviously, there are only three independent coefficients  $F_{11}$ ,  $F_{12}$  and  $F_{44}$  for cubic groups because of symmetry requirement. So, these coefficients  $F_{ij}$  can be completely studied experimentally and theoretically from three pressure behaviours; usually, they are those under the hydrostatic pressure, and the uniaxial stresses along [001] and [111] directions. This is the basis of our investigations.

Under the hydrostatic pressure  $P$  ( $P > 0$ ), the crystal maintains a cubic symmetry and the stress components along the cubic axes are

$$X_{ii} = -P \quad X_{ij}(i \neq j) = 0. \quad (3)$$

Then

$$e_{ii} = -(s_{11} + 2s_{12})P \quad e_{ij}(i \neq j) = 0. \quad (4)$$

From (2), we have

$$\delta g = \delta g_{ii} = -(F_{11} + 2F_{12})(s_{11} + 2s_{12})P. \quad (5)$$

So

$$dg/dP = [\partial g/\partial (\ln R)][\partial (\ln R)/\partial P] = -(F_{11} + 2F_{12})(s_{11} + 2s_{12}) \quad (6)$$

where  $R$  denotes the bonding length. Because

$$\partial (\ln R)/\partial P = -(s_{11} + 2s_{12}) \quad (7)$$

then

$$F_{11} + 2F_{12} = \partial g/\partial (\ln R). \quad (8)$$

When the stress  $P$  is along the [001] axis, the tetragonal distortions are induced and the stress components are

$$X_{33} = -P \quad X_{11} = X_{22} = X_{ij}(i \neq j) = 0. \quad (9)$$

Then

$$e_{11} = e_{22} = -s_{12}P \quad e_{33} = -s_{11}P \quad e_{ij}(i \neq j) = 0. \quad (10)$$

Let the axis of fourfold rotation be the  $z$  axis; from (2), we obtain

$$\begin{aligned} \delta g_{\perp} = \delta g_{xx} = \delta g_{yy} &= -(s_{11}F_{12} + s_{12}F_{11} + s_{12}F_{12})P \\ \delta g_{\parallel} = \delta g_{zz} &= -(2s_{12}F_{12} + s_{11}F_{11})P. \end{aligned} \quad (11)$$

Then

$$d(g_{\perp} - g_{\parallel})/dP = (F_{11} - F_{12})(s_{11} - s_{12}). \quad (12)$$

The tetragonal distortions can be represented by the bonding angle  $\alpha$  ( $\tan \alpha = R_{\perp}/R_{\parallel}$ ; see [7]), and

$$d\alpha/dP = \frac{1}{2}(s_{11} - s_{12}). \quad (13)$$

So,

$$F_{11} - F_{12} = \frac{1}{2}[\partial(g_{\perp} - g_{\parallel})/\partial \alpha]_0 \quad (14)$$

where the subscript '0' denotes that the differentiation is done for the case of cubic symmetry.

Similarly, if the stress is along the [111] axis, the trigonal distortions are induced and  $X_{ij} = -P/3$ ; then

$$e_{ii} = -(s_{11} + 2s_{12})P/3 \quad e_{ij}(i \neq j) = -s_{44}P/3. \tag{15}$$

From (2), one can get

$$\begin{aligned} \delta g_{ii} &= -(F_{11} + 2F_{12})(s_{11} + 2s_{12})P/3 \\ \delta g_{ij}(i \neq j) &= -F_{44}s_{44}P/3. \end{aligned} \tag{16}$$

Rotating the coordinate axes to the directions of principal axes ( $z \parallel C_3$ ) for the tensor  $\delta g_{ij}$ , i.e. let the matrix  $\delta g_{ij}$  be diagonal, we have

$$\begin{aligned} \delta g_{\perp} &= [F_{44}s_{44} - (F_{11} + 2F_{12})(s_{11} + 2s_{12})]P/3 \\ \delta g_{\parallel} &= -[2F_{44}s_{44} + (F_{11} + 2F_{12})(s_{11} + 2s_{12})]P/3. \end{aligned} \tag{17}$$

Then

$$d(g_{\perp} - g_{\parallel})/dP = F_{44}s_{44}. \tag{18}$$

The trigonal distortions can be represented by the angle  $\beta$  which was defined in [7], and

$$d\beta/dP = (\sqrt{2}/6)s_{44}. \tag{19}$$

So,

$$F_{44} = (\sqrt{2}/6)[\partial(g_{\perp} - g_{\parallel})/\partial\beta]_0. \tag{20}$$

From equations (8), (14) and (20), it can be seen that the coupling coefficients  $F_{ij}$  denote the simple correlations between the isotropic and anisotropic  $g$ -factors and the distinctive distortions of binding length and bonding angles. The simple and clear physical meaning of  $F_{ij}$  enables us to calculate these coefficients from the formulae for the  $g$ -factor in cubic, tetragonal and trigonal symmetries very easily. Obviously, the method is simpler than the usual calculations directly from the strain tensor elements and would be effective for all  $d^n$  ions.

Interestingly, if we let  $F_{ij} \rightarrow G_{ij}$ ,  $\delta g_{ij} \rightarrow \delta D_{ij}$  and consider that  $G_{12} = -G_{11}/2$ , and  $D = D_{\parallel} - D_{\perp}$  for axial symmetry, we have

$$F_{11} - F_{12} = \frac{1}{2}[\partial(g_{\perp} - g_{\parallel})/\partial\alpha]_0 \rightarrow G_{11} - G_{12} = \frac{3}{2}G_{11} = -\frac{1}{2}(\partial D/\partial\alpha)_0. \tag{21}$$

Then

$$G_{11} = -\frac{1}{3}(\partial D/\partial\alpha)_0 \tag{22}$$

and

$$F_{44} = (\sqrt{2}/6)[\partial(g_{\perp} - g_{\parallel})/\partial\beta]_0 \rightarrow G_{44} = -(\sqrt{2}/6)(\partial D/\partial\beta)_0. \tag{23}$$

Obviously, the formulae for  $G_{11}$  and  $G_{44}$  are the same as those obtained in our previous papers [7–11]. Considering that, under the stresses,

$$\delta g_i = \sum_j F_{ij}e_j \quad \delta D_i = \sum_j G_{ij}e_j \tag{24}$$

the above similarity can be understood. The only difference between the coefficients  $F_{ij}$  and  $G_{ij}$  is  $G_{11} + 2G_{12} = 0$ , but  $F_{11} + 2F_{12} = \partial g/\partial(\ln R) \neq 0$ . This is because the tensor  $\delta D_{ij}$  is traceless, but  $\delta g_{ij}$  is not.

### 3. Analytic expressions for $F_{ij}$ for $d^3$ ions

As an example, we apply equations (8), (14) and (20) to  $d^3$  ions. In cubic symmetry,

$$g = g_e - 8\xi/3\Delta. \quad (25)$$

Then

$$F_{11} + 2F_{12} = \partial g/\partial(\ln R) = -\frac{8}{3}\xi/Dq. \quad (26)$$

In the case of tetragonal symmetry, the high-order perturbation formulae for the anisotropic  $g$ -factor based on the strong-field coupling scheme can be obtained from those in  $C_2$  symmetry (let  $R_1 = R_2$  and  $\varphi = 90^\circ$ ) [12]:

$$g_\perp - g_\parallel = - (2\xi/9\Delta^2)(35D_t + 7D_\eta). \quad (27)$$

So,

$$F_{11} - F_{12} = -\frac{1}{3}(\xi/\Delta^2)[\partial(35D_t + 7D_\eta)/\partial\alpha]_0 = \frac{2}{3}\xi/Dq. \quad (28)$$

The above result is obtained from the definitions of the tetragonal field parameters  $D_t$  and  $D_\eta$  [12].

From (26) and (28), one can find that

$$F_{11} = -\frac{8}{27}\xi/Dq \quad F_{12} = -\frac{14}{27}\xi/Dq. \quad (29)$$

For trigonal symmetry, from the high-order perturbation formulae for the  $g$ -factor based on the strong-field coupling scheme [13],

$$g_\perp - g_\parallel = (4\sqrt{2}\xi k/D_1 D_4)v' - (4\xi k/3D_1^2)v. \quad (30)$$

So,

$$F_{44} = \frac{4}{3}(\xi k/D_1 D_4)(\partial v'/\partial\beta)_0 - (2\sqrt{2}\xi k/9D_1^2)(\partial v/\partial\beta)_0 \quad (31)$$

where  $D_1 (= \Delta)$  and  $D_4 (= \Delta + 12B)$  are the zero-order energy separations, and

$$\begin{aligned} (\partial v/\partial\beta)_0 &= (18\sqrt{2}/7)eq(1 + 3\mu/eR_0)\langle\gamma^2\rangle/R_0^3 + (60\sqrt{2}/7)Dq \\ (\partial v'/\partial\beta)_0 &= -\frac{12}{7}eq(1 + 3\mu/eR_0)\langle r^2\rangle/R_0^3 + \frac{30}{7}Dq. \end{aligned} \quad (32)$$

They are calculated in accordance with the definitions of the trigonal-field parameters  $v$ ,  $v'$  and from the point-charge-dipole model.  $q$  is the ligand charge and  $\mu$  the dipole. In the calculations, the value of  $\mu/eR$  is kept unchanged under the pressure because the dipole  $\mu$  varies in proportion to the bonding length  $R$ . Obviously, our calculated equations (29) and (31) for  $F_{ij}$  of  $d^3$  ions are very simple and convenient.

### 4. Calculations of $F_{ij}$ for $Cr^{3+}$ and $V^{2+}$ in MgO crystals

Now let us focus attention on the  $Cr^{3+}$  and  $V^{2+}$  ions in MgO crystals. For  $Cr^{3+}$  ions, by using the empirical  $d$  orbital obtained from the optical spectra data of many crystals containing  $Cr^{3+}$  ions [14], we have

$$\begin{aligned} \langle r^2 \rangle_0 &= 2.4842 \text{ au} & \langle r^4 \rangle_0 &= 16.4276 \text{ au} \\ B_0 &= 920.48 \text{ cm}^{-1} & C_0 &= 3330.71 \text{ cm}^{-1} & \xi_{d0} &= 240 \text{ cm}^{-1}. \end{aligned} \quad (33)$$

Introducing the average covalency reduction factor  $N$  ( $k = N^2$ ), then

$$\langle r^n \rangle = N^2 \langle r^n \rangle_0 \quad B = N^4 B_0 \quad C = N^4 C_0 \quad \xi_d = N^2 \xi_{d0}. \quad (34)$$

From the optical spectra of MgO:  $Cr^{3+}$ , in [8] we obtained  $N = 0.954$ ,  $\mu = 0.086eR_0$ .

**Table 1.** The spin–lattice coupling coefficients  $F_{ij}$  and  $G_{ij}$  per unit strain for  $d^3$  ions in MgO crystals.

|                                  | MgO:Cr <sup>3+</sup> |                     | MgO:V <sup>2+</sup> |          |
|----------------------------------|----------------------|---------------------|---------------------|----------|
|                                  | Calculated           | Observed            | Calculated          | Observed |
| $F_{11}$                         | -0.041               | +0.004 ± 0.010 [15] | -0.031              |          |
| $F_{12}$                         | -0.071               | -0.060 ± 0.005 [15] | -0.054              |          |
| $F_{44}$                         | +0.041               | +0.029 ± 0.006 [15] | +0.036              |          |
| $G_{11}$ (cm <sup>-1</sup> ) [8] | 1.08                 | 0.6                 | 0.42                | 0.42     |
| $G_{44}$ (cm <sup>-1</sup> ) [8] | 4.86                 | 4.2                 | 3.04                | 3.0      |

Substituting the parameters  $N$ ,  $\mu$  and structural parameter  $R_0$  ( $= 2.1 \text{ \AA}$ ) for MgO into the above formulae, it can be found that (in units of per unit strain)

$$F_{11} = -0.041 \quad F_{12} = -0.071 \quad F_{44} = 0.041. \quad (35)$$

The results are compared with experimental values in table 1.

Similarly, for V<sup>2+</sup> ions, from the empirical d orbital, we obtain [16]

$$\begin{aligned} \langle r^2 \rangle_0 &= 2.565 \text{ au} & \langle r^4 \rangle_0 &= 13.1132 \text{ au} \\ B_0 &= 848.5 \text{ cm}^{-1} & C_0 &= 3101.9 \text{ cm}^{-1} & \xi_{d0} &= 167 \text{ cm}^{-1}. \end{aligned} \quad (36)$$

The parameters  $N$  and  $\mu$  obtained from optical spectra in [8] are

$$N = 0.911 \quad \mu = 0.126eR_0. \quad (37)$$

Applying the parameters  $N$ ,  $\mu$  and  $R_0$  to the above formulae, we obtain

$$F_{11} = -0.031 \quad F_{12} = -0.054 \quad F_{44} = 0.036. \quad (38)$$

Unfortunately, no measurement has yet been made for MgO:V<sup>2+</sup> crystals; the predicted values await experimental verification.

## 5. Discussion

In [15] the coupling coefficients  $F_{ij}$  for MgO:Cr<sup>3+</sup> crystals were measured by means of a strain-modulated EPR technique 10 years ago, but no satisfactory theoretical explanation of them has been given. In [5] this problem was first of all studied using a high-order perturbation approach and some progress was made. From the complex expressions [5] for  $F_{ij}$ , it was found that

$$F_{11} \approx -0.0005 \quad F_{12} = -0.06--0.07 \quad F_{44} = 0.036-0.042. \quad (39)$$

Clearly, for  $F_{12}$  and  $F_{44}$ , the results in [5] are close to the experimental values and our results (see table 1) but, for  $F_{11}$ , the value is too small. Considering that, for MgO:Cr<sup>3+</sup> crystals,  $G_{11} = 0.6 \text{ cm}^{-1}$  and  $G_{44} = 4.2 \text{ cm}^{-1}$ , this enables us to predict that  $F_{ij} \sim 10^{-2}$  from crystal-field theory ( $|F_{ij}| \sim G_{ij}/\lambda$  [15]). So, such a small value of  $F_{11}$  given in [5] cannot be regarded as reasonable. It is noteworthy that, in our work, all the calculated results for  $F_{ij}$  for MgO:Cr<sup>3+</sup>, as well as for MgO:V<sup>2+</sup> (where  $G_{11} = 0.42 \text{ cm}^{-1}$ ,  $G_{44} =$

$3.0 \text{ cm}^{-1}$  and hence  $|F_{ij}| \sim 10^{-2}$ ) are of the order of  $10^{-2}$ . In this sense, our result for  $F_{11}$  is more reasonable than that in [5].

On comparison with the experimental findings, it can be seen that our results are close to but somewhat greater than the experimental values. The sources of error, in our opinion, are as follows.

(i) The point-charge-dipole model and the empirical  $d$  orbital are, as is well known, only simple approximations.

(ii) The isotropic and anisotropic  $g$ -factor formulae are also approximations.

(iii) Most importantly, the observed values of  $F_{ij}$  are calculated from the assumption that the local elastic constants  $s_{ij}$  and hence local strains in the vicinity of impurities are equal to the host values [15]. However, a great number of theoretical and experimental studies show that the assumption is unreliable and unreasonable in the case of charge and/or size mismatch [17–19]. For example, in [17], it was pointed out that, in MgO crystals, for divalent impurities the local strains are close to those in the bulk crystal but, when the impurity carries extra charge, large and symmetry-dependent reductions arise. In fact, the experimental values of  $F_{ij}$  in some literature arising from this assumption are also doubted. For instance, for MgO:Cr<sup>3+</sup> crystals, in [20], where the hydrostatic pressure dependence of the  $g$ -factor was studied, it was thought that the assumption appears rather dubious in the case of Cr<sup>3+</sup> in MgO since the local binding energy is probably significantly higher in a cell containing a trivalent cation and the neglect of decreased local compressibility certainly decreases the experimental value of  $\partial[\ln(g - g_0)]/\partial(\ln V)$  (and hence of  $F_{11} + 2F_{12}$ ). In [15], where experimental values of  $F_{ij}$  for MgO:Cr<sup>3+</sup> were given, it was also considered that the local values are not the same as the bulk values. Unfortunately, no such calculations about the local values have yet been made for Cr-doped MgO; so we made the *ad hoc* assumption that  $c_{ij}(\text{local}) = c_{ij}(\text{macroscopic})$ . Obviously, the observed values of  $F_{ij}$  based on this assumption are not reliable.

In reality, because the charge of Cr<sup>3+</sup> ions is evidently greater than that of Mg<sup>2+</sup> ions, the local strains and elastic constants  $s_{ij}$  should decrease and hence the real observed values of  $F_{ij}$  increase in accordance with equations (6), (12) and (18). This case is very similar to that for the coefficients  $G_{11}$  and  $G_{44}$  in MgO:Cr<sup>3+</sup> (for clarity, the comparison of coefficients  $G_{ij}$  is also shown in table 1). This can explain why all our calculated results of  $F_{ij}$ , as well as of  $G_{ij}$  shown in a previous paper [8], are greater than the experimental values obtained from the above assumption. In addition, contrary to the value in the original literature [15], the calculated value of  $F_{11}$  is negative (this point is similar to that in [5]). The reason is, in our opinion, due to the fact that the tensor  $\delta g_{ij}$  is not traceless. So, unlike the coefficients  $G_{11}$  and  $G_{12}$ , the coefficients  $F_{11}$  and  $F_{12}$  may have the same sign. The main source giving rise to the different signs of  $F_{11}$  between theory and experiment is perhaps also due to the local elastic constants. As has been said before, the local compressibility should be smaller than the bulk value and hence the value of  $F_{11} + 2F_{12}$  has a larger negative value ( $-0.184$  in this work compared with  $-0.116$  in [15]). This leads to the fact that the coefficient  $F_{11}$  is negative.

In order to verify further the opinion that the source of error of  $F_{ij}$  in MgO:Cr<sup>3+</sup> crystals mainly arises because the local elastic constants are different from the host values, we predict the coefficients  $F_{ij}$  for MgO:V<sup>2+</sup> crystals. Considering that the local values of  $s_{ij}$  are very similar to the bulk values because the V<sup>2+</sup> and Mg<sup>2+</sup> ions have the same charge and similar sizes, the calculated values of  $F_{ij}$  for MgO:V<sup>2+</sup> should be, as in



the case of the coefficients  $G_{ij}$  [8], closer to the observed values than those for  $\text{MgO}:\text{Cr}^{3+}$  crystals. This point remains to be verified experimentally.

In conclusion, since the optical spectra and the spin–lattice coupling coefficients  $F_{ij}$  and  $G_{ij}$  can be explained in a unified way from our very simple methods by using only two adjustable parameters, our methods and expressions can be regarded as reasonable and would be effective for only similar cases.

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