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## A theoretical study of the magnetic and magneto-optical properties of Nd-substituted yttrium iron garnets

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**Abstract.** The neodymium substitution in yttrium iron garnet induces a large enhancement of the Faraday rotation although the magnetic moment of the  $\text{Nd}^{3+}$  ion in yttrium iron garnet is very small. A detailed theoretical analysis of both magnetic and magneto-optical (MO) properties in  $\text{Nd}_x\text{Y}_{3-x}\text{Fe}_5\text{O}_{12}$  using the quantum theory is developed. The intra-ionic electric dipole transitions between the  $4f^3$  and  $4f^25d$  configuration split states are studied taking into account the spin-orbit, crystal field and super-exchange interaction perturbations. For the excited configuration, the coupling scheme of Yanase is extended to the  $\text{Nd}^{3+}$  ion. A good agreement between experimental and calculated values is obtained for the temperature dependence of both the magnetic moment and Faraday rotation, and the MO resonance frequencies. Attention is paid to the mixing of the ground state multiplets. It is concluded that the Faraday rotation is well described by the intra-ionic electric dipole transition model and is unambiguously of the paramagnetic type.

### 1. Introduction

In Nd-substituted yttrium iron garnet ( $\text{Nd}_x\text{Y}_{3-x}\text{Fe}_5\text{O}_{12}$ ), the substitution of  $\text{Nd}^{3+}$  ions for the  $\text{Y}^{3+}$  ions leads to a large increase of the Faraday rotation (FR) which becomes one order of magnitude larger than the values observed in heavy rare-earth iron garnets [1]. This giant enhancement of the magneto-optical (MO) properties was observed in the near infra-red range first by Wemple *et al* [2] and later by other authors [3, 4]. The experimental data on Nd:YIG were analysed in the frame of the approach using the following widely accepted hypothesis [3, 5, 6]: the Faraday rotation and magnetization ( $M$ ) of Nd-substituted YIG (Nd:YIG) are simply the sum of the contributions of all the sublattices and the contributions of the  $\text{Fe}^{3+}$  sublattices are not affected by the substitution of  $\text{Nd}^{3+}$  because the superexchange interaction between the  $\text{Fe}^{3+}$  and  $\text{Nd}^{3+}$  ions is much weaker than that between different  $\text{Fe}^{3+}$  ions. Therefore the Faraday rotation induced by the  $\text{Fe}^{3+}$  sublattices in Nd:YIG is nearly identical to that of pure YIG (FR(YIG)) under the same experimental conditions, and the  $\text{Nd}^{3+}$ -sublattice-induced Faraday rotation (FR(Nd)) is equal to the difference of FR(Nd:YIG) (the resultant Faraday

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rotation of Nd:YIG) and FR(YIG). The Nd<sup>3+</sup>-sublattice-induced magnetization ( $M(\text{Nd})$ ) can be determined by the same method.

The analysis of the data obtained in the 77–300 K temperature range for the Faraday rotation (4.2–300 K for the magnetization) on single crystals corresponding to  $x = 1.06 \pm 0.02$ ,  $0.9 \pm 0.02$ ,  $0.63 \pm 0.02$ , and  $0.47 \pm 0.02$ , respectively allows us to establish that both FR(Nd) and  $M(\text{Nd})$  are proportional to the Nd content [4]. In other words, the superexchange interaction between different Nd<sup>3+</sup> ions is negligible. To investigate the origin of the MO enhancement, the wavelength dependence of  $\theta_F$  (the FR induced by Nd<sup>3+</sup> ions) was measured between 1050 and 1500 nm on the same single crystals but at 300 K only [4]. From the linear variations of  $|\theta_F|^{-1}$  and  $\lambda|\theta_F|^{-1/2}$  versus  $\lambda^2$  ( $\lambda$  is wavelength), two origins were proposed by Leycuras *et al* [4]. However these conclusions remain more or less at a macroscopic scale without precise analysis developed at the microscopic state. The aim of this article is to calculate simultaneously the spontaneous magnetization and Faraday rotation based on the quantum theory and to clarify the origin of the MO enhancement. On the one hand the magnetic behaviour originates from the split states of the ground configuration; on the other hand the MO phenomena depend not only on the splitting of the ground configuration but also on the splitting of the excited one, so the comparison with different experimental data is helpful for studying the origin of the MO effect and magnetization and for determining the correctness of the used model and parameters.

## 2. Theory and calculation

The magnetization of the Nd<sup>3+</sup> ion is simply determined by the splitting of the 4f<sup>3</sup> configuration taking into account the successive perturbations: spin–orbit (SO) coupling, crystal field (CF) and Nd<sup>3+</sup>–Fe<sup>3+</sup> superexchange interaction. According to Martin *et al* [7], the energy values of the four multiplets of the ground term <sup>4</sup>I of the 4f<sup>3</sup> configuration are 0, 1880, 3860 and 5910 cm<sup>-1</sup>, respectively. The gaps between them are not large enough compared with the crystal field splitting, so all of them have to be included in the calculation. However, the energy of the lowest multiplet of the second term <sup>4</sup>F is 11 290 cm<sup>-1</sup>, so the effect of this term is neglected. Then the spin-orbit interaction can be expressed as

$$H_{SO} = \lambda_{SO} L \cdot S \quad (1)$$

where  $L$  and  $S$  are the total orbital and spin angular momentum operators of the <sup>4</sup>I term;  $\lambda_{SO}$  is a spin-orbit coupling constant. The crystal field Hamiltonian is

$$H_C = \sum_{k,q} \sum_{i=1}^3 A_{kq} r_i^k Y_{kq}(\theta_i, \varphi_i) \quad (2)$$

where  $A_{kq}$  is the crystal field parameter. Neel [8] theory reduces to the assumption that the superexchange interaction acting on the rare-earth ions in the rare-earth iron garnets can be expressed as

$$H_{ex} = 2\mu_B H_{exch} \cdot S \quad (3)$$

where  $H_{exch}$  is an exchange field and is proportional to the resultant spontaneous magnetization of the two iron sublattices:

$$H_{exch} = n_0(1 + \gamma T)M(\text{YIG}) \quad (4)$$

where  $n_0(1 + \gamma T)$  is the exchange-field coefficient and  $\gamma$  is a coefficient which describes its thermal evolution. It should be noted that the exchange-field coefficient is different from the classical molecular-field coefficient. Because the lowest multiplet of the ground term plays a

more important role than other ground multiplets in the magnetic and MO behaviour, the two coefficients are of opposite sign for the light rare-earth ions. The temperature dependence of the exchange-field coefficient is first attributed to the thermal lattice expansion. When we refer to the variation of the exchange integral  $A$  versus  $(\delta - 2r)$  for many 3d, 4d, and 4f metals or alloys ( $\delta$  is the distance between two nearest atoms and  $r$  is the orbital radius of the 3d, 4d, or 4f electronic shell) proposed by Neel [9], it is well known that  $\gamma$  may be negative or positive.  $M(\text{YIG})$  is temperature dependent and, in this work, the values of  $M(\text{YIG})$  deduced from the nuclear magnetic resonance experiments by Gonano *et al* [6] will be used.

As the superexchange interaction is much weaker than the spin-orbit coupling and crystal field, at first, the splitting of the  $^4\text{I}$  term induced by  $H_{SO}$  and  $H_C$  is calculated by using the following secular equation:

$$\| \langle i | H_{SO} + H_C | j \rangle - E \delta_{ij} \| = 0 \quad (5)$$

where the bra and ket include all the states of the four multiplets. Because the crystal field acting on the  $\text{Nd}^{3+}$  ions in  $\text{Nd}:\text{YIG}$  has  $D_2$  symmetry, every SO and CF-split level is double degenerate for the Kramers'  $\text{Nd}^{3+}$  ion. They will be split by the superexchange interaction. However, the energy gaps between different SO- and CF-split levels are not always very large and the higher-order correction of the Zeeman effect has usually to be considered, therefore the Zeeman effect is calculated by solving the following secular equation:

$$\| \langle \psi_i | H_{SO} + H_C + H_{ex} | \psi_j \rangle - E \delta_{ij} \| = 0 \quad (6)$$

where  $|\psi_i\rangle$  and  $\langle \psi_i | H_{SO} + H_C | \psi_j \rangle$  are the eigen wave function and eigen-energy obtained by solving equation (5), respectively. Some high-lying SO- and CF-split levels can be neglected in solving equation (6) because their occupation probabilities are small.

The ionic magnetic moment, at a temperature  $T$ , is given by

$$m = -\mu_B \sum_g \langle g | (L_z + 2S_z) | g \rangle \rho_g \quad (7)$$

where  $|g\rangle$  is the SO-CF- and superexchange-interaction-split (mixed) state whose energy and occupation probability are  $E_g$  and  $\rho_g$ , respectively.  $\rho_g$  is given by:

$$\rho_g = \exp(-E_g/kT) / \sum_g \exp(-E_g/kT). \quad (8)$$

In some of our previous articles [10, 11], it has been proved that the MO effects induced by the rare-earth ions in some rare-earth compounds are mainly caused by intra-ionic electric dipole transitions between the ground and the parity-allowed excited configurations. In this work, this model is used as well. According to [12] and [13], when the optical absorption is weak, the specific Faraday rotation is given by the following formula:

$$\theta_F = \frac{N\pi(\bar{n}^2 + 2)^2}{9\hbar c \bar{n}} \sum_{ng} \frac{\omega^2}{\omega_{ng}^2 - \omega^2} [|\langle n | V_- | g \rangle|^2 - |\langle n | V_+ | g \rangle|^2] \rho_g \quad (9)$$

where it is assumed that the frequency of the observed light is far from magneto-optical resonance frequencies. In this equation,  $N$  is the number of  $\text{Nd}^{3+}$  ions per unit volume,  $c$  the velocity of the light in vacuum,  $\omega$  the angular frequency of the observed light,  $g$  runs over the split states  $|g\rangle$  of the  $4f^3$  configuration and  $n$  runs over split states  $|n\rangle$  of the  $4f^25d$  configuration.  $\omega_{ng} = (E_n - E_g)/\hbar$ , where  $E_n$  is the energy of the state  $|n\rangle$ .  $V_{\pm}$  are the electric dipole moment operators for right- and left-handed circularly light, respectively.

It is seen from equation (9) that to calculate the  $\text{Nd}^{3+}$ -induced Faraday rotation it is also necessary to calculate the splitting of the  $4f^25d$  configuration. However, there is no experimental value of the energies of the  $4f^25d$  terms of a free  $\text{Nd}^{3+}$  ion. Therefore the

splitting of these terms cannot easily be obtained in the  $LSJ$  representation as in the case of Ce and Pr compounds [10, 11]. It has been shown [14, 15] that for the  $4f^{n-1}5d$  configuration of  $\text{Eu}^{2+}$  and  $\text{Sm}^{2+}$  ions, the total spin angular momentum  $S(S = s_d + S_f)$  and a composite angular momentum  $J(J = S + L_f)$  can be good quantum numbers approximately, where  $s_d$  is the spin angular momentum of a 5d electron and  $S_f$  and  $L_f$  are the total spin and orbit angular momenta of the  $4f^{n-1}$  electrons, respectively. This coupling scheme is able to explain the optical absorption and MO effects induced by the  $4f^n \rightarrow 4f^{n-1}5d$  transitions within the  $\text{Eu}^{2+}$  or  $\text{Sm}^{2+}$  ions. In this article this approach will be extended to the  $\text{Nd}^{3+}$  ion. The electric part of the Hamiltonian for the  $4f^{n-1}5d$  configuration can be written as follows:

$$H = H_{Cd} + H_{Cf} + \xi_d \mathbf{l}_d \cdot \mathbf{s}_d + \xi_f \sum_i \mathbf{l}_{fi} \cdot \mathbf{s}_{fi} + H_{ff} + H_{fd} \quad (10)$$

where  $H_{Cd}$  and  $H_{Cf}$  are the crystal field Hamiltonians upon the 5d and 4f electrons, respectively;  $\xi_d$  and  $\xi_f$  are the spin-orbit coupling constants for the 5d and 4f electrons, respectively;  $H_{ff}$  denotes the Coulomb and exchange interactions between the 4f electrons, and  $H_{fd}$  denotes those between the 4f and 5d electrons. The electric interactions between the core of the ion and the 4f and 5d electrons are not included. The fourth and fifth terms in equation (10) give the energy levels of the  $4f^{n-1}$  electrons when  $H_{Cf}$  is negligible. Because  $\xi_f$  and  $H_{ff}$  change very little with the existence of the 5d electron, we can discuss effective values for these two terms from the energy levels of  $\text{RE}^{3+}$  ions in the  $4f^{n-1}$  configuration (see [15] and the references therein). Consequently, the energy levels of the 4f<sup>2</sup> electrons in the  $4f^2 5d$  configuration of free  $\text{Nd}^{3+}$  ions could be derived from the energy levels of the 4f<sup>2</sup> configuration of free  $\text{Pr}^{3+}$  ions. Furthermore, for the excited  $4f^2 5d$  configuration, the total spin and orbit angular momenta  $S_f$  and  $L_f$  of the 4f<sup>2</sup> electrons are assumed to be good quantum numbers approximately, and the total spin momentum  $S(S = s_d + S_f)$  and a composite angular momentum  $J(J = S + L_f)$  are approximately good quantum numbers as well.

Because the crystal field upon the  $4f^{n-1}$  electrons is much less than the crystal field upon the 5d electron and the energy difference between the excited and ground configurations, the effect of  $H_{Cf}$  can be neglected in calculating the splitting of the  $4f^{n-1}5d$  configuration. Then the wave functions of the CF-split  $4f^2 5d$  levels can be expressed as [15]:

$$|\Gamma\beta; (SL_f)J\rangle = \sum_{d_z} A_{\Gamma\beta}(d_z) |l_d, d_z\rangle |(s_d S_f)S, L_f; J, J_z\rangle \quad (11)$$

where  $|l_d, d_z\rangle$  are the wave functions of the 5d electron,  $A$ 's are symmetrized coefficients and  $\beta$  runs over the states within an irreducible representation  $\Gamma$ . The corresponding energy value is given by the following formula [15]:

$$\begin{aligned} E(\Gamma, S, L_f, J) = E_d(\Gamma) - J_0 S_f + \frac{(L_f + S - J)(L_f - S + J + 1)}{2S(2J + 1)} E_f(S_f L_f; J_f = J + \frac{1}{2}) \\ + \frac{(S - L_f + J)(L_f + S + J + 1)}{2S(2J + 1)} E_f(S_f L_f; J_f = J - \frac{1}{2}) \\ \text{(when } S = S_f + \frac{1}{2}\text{)} \end{aligned} \quad (12)$$

where  $E_d(\Gamma)$  is the energy of the CF-split state of the 5d electron,  $E_f$  the energy of the state of the  $4f^{n-1}$  electrons with quantum numbers  $(S_f L_f J_f)$ ,  $J_0$  is a constant determined by  $H_{df}$  and is given as a combination of Slater integrals  $G_k$  [15] and for the  $\text{Nd}^{3+}$  ion its value is  $1670 \text{ cm}^{-1}$  [16]. The matrix elements of the electric dipole transition can be calculated by using the following formula [15]:

$$\begin{aligned} \langle 4f^n (S_g L_g) J_g, J_{gz} | \chi_\eta | l_d, d_z \rangle |(s_d S_f)S, L_f; J, J_z\rangle \\ = \langle 4f | r | 5d \rangle \delta(S_g, S) \sqrt{2L_g + 1} \sqrt{2J + 1} \sqrt{2J_g + 1} \sqrt{3} \langle f^{n-1} S_f L_f | \rangle f^n S_g L_g \end{aligned}$$

$$\begin{aligned}
& \times (-1)^{2J+S_g-J_{gz}+L_f} \begin{Bmatrix} 3 & J & J_g \\ S_g & L_g & L_f \end{Bmatrix} (-1)^{f_z} \\
& \times \begin{pmatrix} 3 & 1 & 2 \\ -f_z & \eta & d_z \end{pmatrix} \begin{pmatrix} J_g & 3 & J \\ -J_{gz} & f_z & J_z \end{pmatrix} \quad (13)
\end{aligned}$$

where  $\eta$  can be  $\pm 1$ ,  $\chi_{\pm 1} = \mp(1/\sqrt{2})V_{\pm}$ . It should be noted that in equation (13), the  $LSJ$  representation is used for the  $4f^m$  states while the new coupling scheme is used for the  $4f^{m-1}5d$  states.

### 3. Results and discussion

In the calculation, the choice of the proper set of the parameters of the crystal field upon the  $\text{Nd}^{3+}$  ion is a crucial step. Following our previous works [10, 11], we determined these parameters according to the values of the crystal field parameters for the  $\text{Sm}^{3+}$  in  $\text{SmIG}$  deduced from the magnetic phase transition experiments by Nekvasil *et al* [17] and the ratios of the values of  $\langle r^2 \rangle$ ,  $\langle r^4 \rangle$  and  $\langle r^6 \rangle$  of different rare-earth ions. The non-zero parameters are reported in table 1. The values of  $n_0$  and  $\gamma$  in equation (4) were determined from the fitting of the experimental values of the  $\text{Nd}^{3+}$  magnetic moment. The optimum values of  $\gamma$  and  $n_0$  are  $5.0 \times 10^{-4} \text{ K}^{-1}$  and  $-5.2 \times 10^4 \text{ Oe}$  ( $\mu_B/\text{two formulae of YIG}$ ) $^{-1}$ , respectively. Our  $\gamma$  value is close to the one ( $3.84 \times 10^{-4} \text{ K}^{-1}$ ) determined by Krinchik *et al* [3].

**Table 1.** The non-zero parameters of the CF upon the  $\text{Nd}^{3+}$  ions in  $\text{Nd:YIG}$  (in  $\text{cm}^{-1}$ ).

	$A_{20}\langle r^2 \rangle$	$A_{2\pm 2}\langle r^2 \rangle$	$A_{40}\langle r^4 \rangle$	$A_{4\pm 2}\langle r^4 \rangle$	$A_{4\pm 4}\langle r^4 \rangle$	$A_{60}\langle r^6 \rangle$	$A_{6\pm 2}\langle r^6 \rangle$	$A_{6\pm 4}\langle r^6 \rangle$	$A_{6\pm 6}\langle r^6 \rangle$
4f	-615	325	-6730	362	2390	966	-237	1801	107
5d	-3998	2113	-182 921	7240	23 900				

**Table 2.** The calculated and measured magnetization ( $m$ , in  $\mu_B/\text{ion}$ ) of the  $\text{Nd}^{3+}$  ions in  $\text{Nd:YIG}$ .

	4.2 K	50 K	100 K	150 K	200 K	250 K	300 K
$m(\text{calc.})$	1.61	1.29	0.85	0.60	0.44	0.33	0.26
$m(\text{meas.})$ [4]	1.68	1.30	0.95	0.67	0.45	0.37	0.40

**Table 3.** Contributions of the  $\text{Nd}^{3+}$  ions in  $\text{NdY}_2\text{IG}$  to Faraday rotation (in degrees/ $\text{cm}^{-1}$ ):  $\theta_F^A$  and  $\theta_F^B$  correspond to 1150 and 633 nm wavelengths, respectively.

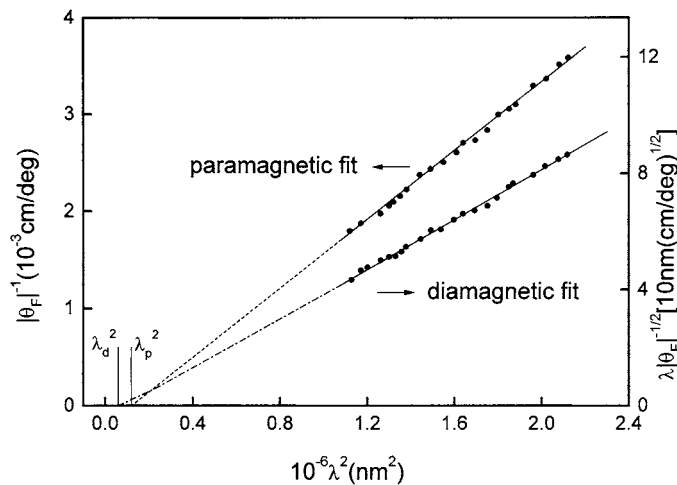
	77 K	100 K	150 K	200 K	250 K	300 K
$\theta_F^A(\text{calc.})$	-1341	-1133	-847	-668	-533	-439
$\theta_F^A(\text{meas.})$ [4]	-900	-850	-700	-590	-510	-450
$\theta_F^B(\text{calc.})$	-3331	-3016	-2600	-2273	-1948	-1687

Some theoretical values of the magnetization of a  $\text{Nd}^{3+}$  ion are listed in table 2. They are in good agreement with the measured results [4] although the measured  $M(\text{Nd})$  was derived from the difference of two large values:  $M(\text{Nd:YIG})$  and  $M(\text{YIG})$ . In table 3, we list the temperature dependence of the Faraday rotation at 1150 and 633 nm wavelengths and the measured values at 1150 nm [4]. Above 100 K the agreement between the calculated and measured results appears reasonable. However, at low temperatures the absolute value of the

calculated Faraday rotation increases too rapidly as temperature decreases. Table 4 shows that the agreement between the measured wavelength dependence of the Faraday rotation [3] and the calculated one is reasonable as well.

**Table 4.** The wavelength dependence of Faraday rotation (in  $^{\circ} \text{cm}^{-1}$ ) induced by the  $\text{Nd}^{3+}$  ions in  $\text{NdY}_2\text{IG}$  at temperature 300 K.

	8696 $\text{cm}^{-1}$	10 000 $\text{cm}^{-1}$	12 000 $\text{cm}^{-1}$	14 000 $\text{cm}^{-1}$
$\theta_F$ (calc.)	-439	-591	-878	-1249
$\theta_F$ (meas.) [3]	-344	-530	-670	-1000



**Figure 1.** The plots of  $|\theta_F|^{-1}$  versus  $\lambda^2$  and of  $\lambda|\theta_F|^{-1/2}$  versus  $\lambda^2$  for the Faraday rotation in  $\text{NdY}_2\text{Fe}_5\text{O}_{12}$  at 300 K (after Leycuras *et al* [4]).

As noted in section 1, Leycuras *et al* [4] showed that both the plots of  $|\theta_F|^{-1}$  versus  $\lambda^2$  and of  $\lambda|\theta_F|^{-1/2}$  versus  $\lambda^2$  were straight lines (figure 1). The extension of the plot of  $|\theta_F|^{-1}$  versus  $\lambda^2$  gives its intersection with the abscissa. From the location of the intersection point, they obtained a resonance frequency at  $27\,700 \pm 250 \text{ cm}^{-1}$ . The transitions related to this resonance frequency lead to a paramagnetic Faraday rotation. From the intersection point of the second plot, they obtained another resonance frequency at  $39\,400 \pm 500 \text{ cm}^{-1}$ . The transitions associated with this resonance lead to a diamagnetic Faraday rotation. They suggested that the MO resonance at  $27\,700 \text{ cm}^{-1}$  might be due to the  $\text{Nd}^{3+}\text{-Fe}^{3+}$  pair excitations; but they did not give any explanation for the transition at  $39\,400 \text{ cm}^{-1}$ . Our calculation shows that the MO resonance frequencies are mainly determined by the splitting of the 5d state of the  $4f^25d$  configuration induced by the crystal field and, besides a minor resonance at  $21\,600 \text{ cm}^{-1}$ , there are two resonances below 7 eV photon energy. They are located at  $25\,400$  and  $50\,600 \text{ cm}^{-1}$ , respectively. The former is close to the value of the paramagnetic MO resonance frequency ( $27\,700 \text{ cm}^{-1}$ ) proposed by Leycuras *et al* [4]. Furthermore, in our calculation, only the Zeeman effect of the ground configuration is included (the superexchange interaction on the excited configuration is neglected) and consequently our calculated Faraday rotation corresponds effectively to the paramagnetic type rotation [11]. So, our study confirms that the observed Faraday rotation is mainly of the paramagnetic type and the theoretical resonance frequency is in good agreement with experiment. However, the assignment for the

MO transition at  $27\,700\text{ cm}^{-1}$  suggested by Leycuras *et al* [4] is denied by our theoretical study. Our calculation allows to conclude that this resonance frequency corresponds simply to the intra-ionic electric dipole transitions from the lowest CF–SO- and superexchange-interaction-split  $4f^3$  states to the split  $4f^25d$  ones located at about  $24\,900\text{ cm}^{-1}$ , taking the energy of the lowest multiplet of the ground term of a free  $\text{Nd}^{3+}$  ion as zero.

The Zeeman splitting of the excited configuration is very small compared with the crystal field splitting and the energy difference between the ground and excited configurations. As a result, the theoretical resonance frequencies of the diamagnetic Faraday rotation are almost the same as those of the paramagnetic Faraday rotation. So, contrarily to [4], we cannot justify a transition which corresponds to the MO resonance frequency near  $39\,400\text{ cm}^{-1}$ . Furthermore, the diamagnetic Faraday rotation is important only in the vicinity of the resonance frequencies. So, we concluded that the observed Faraday rotation could not be of diamagnetic type.

At last, we would like to discuss briefly why we could not rule out the possibility, that the observed Faraday rotation is of diamagnetic type, by the analysis used in [4]. Both the linear relations between  $|\theta_F|^{-1}$  and  $\lambda^2$  and between  $\lambda|\theta_F|^{-1/2}$  and  $\lambda^2$  are tenable under the following two conditions. First, the frequency of the observed light has to be far from the resonance frequencies. Second, the observed Faraday rotation has to be produced only by the transitions related to one magneto-optical resonance frequency. Furthermore, the measured wavelength range of the Faraday rotation should be as wide as possible to guarantee the accuracy of the thus-obtained resonance frequency. It is mentioned above that there are several MO resonance frequencies for the studied MO effect. Although the contributions of the transitions related to the resonance at  $25\,400\text{ cm}^{-1}$  are of first importance, the contributions of other transitions are non-negligible. In addition, the measured wavelength range of [4] is rather small (see figure 1). From these facts, we can conclude that an unambiguous judgment on the type of the observed Faraday rotation cannot be obtained by this method. The discrepancy between our calculated resonance frequency ( $25\,400\text{ cm}^{-1}$ ) and the paramagnetic MO resonance frequency deduced by Leycuras *et al* [4] is explained by the above discussion as well.

#### 4. Conclusion

In this work, the theoretical calculations of both magnetic and MO properties leads to a good interpretation of the observed results. They show that the large MO enhancement of the  $\text{Nd}^{3+}$  ions in Nd:YIG originates mainly from the intra-ionic electric dipole transition. Our study confirms also that there exists a MO resonance frequency at about  $27\,700\text{ cm}^{-1}$  and that the observed Faraday rotation is of the paramagnetic type. The assignment of the involved transitions is totally different from that previously proposed [4].

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