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Abstract

The effects of the spin–orbit (SO) interaction strength of the ground and excited configurations of rare-earth ions on the paramagnetic and diamagnetic Faraday rotation (FR) spectra in Ce-substituted yttrium iron garnets (YIG) are studied on the basis of quantum theory. It is found that the effect of the SO interaction strength of the ground configuration is stronger than the corresponding effect of the excited configuration. The reasons for this difference have been analysed in connection with the analysis of the large FR effect in Bi-substituted YIG.

1. Introduction

Over the past few decades, much attention has been paid to the magneto-optical (MO) effects, especially the MO Kerr effect (MOKE) and Faraday rotation (FR), in the visible and near-infra-red light ranges. This interest is mainly due to the technological applications of these two MO effects in optical storage devices. Numerous experimental studies of MOKE were performed first on metallic alloys of rare earths and transition metals and then on different multi-layers of suitable metals. On the other hand, most of the studies of FR were (and are) realized on magnetic ordered insulators like spinel and garnet ferrites. Besides this large domain of technological potentials, MO effects should be considered to be a very powerful tool in fundamental research that remains, up to now, incompletely explored.

A deep and unambiguous understanding of these effects requires very rigorous theoretical work using quantum theory and, to the best of our knowledge, such studies capable of supporting the tuning type of activity are rather scarce. The first investigation is that of Misemer [1], who studied the roles of both spin–orbit (SO) interaction and exchange splitting

of the electronic structure in MOKE in MnBi. Later, Oppeneer *et al* [2] studied the effect of SO coupling, exchange splitting, and lattice spacing on the MOKE in Ni, Co, and Fe. Both of them concluded that the MOKE is basically brought about by the SO coupling and scales linearly with the SO coupling strength. Besides, they found that the influence of the exchange splitting (or magnetization) on the MOKE goes far beyond simple proportionality. The same authors [2] found that in Ni, a 3–6% increase in lattice parameters would lead to a shift of about 1 eV of the main MOKE peak.

As far as the MO properties of insulators are concerned, we have to pay attention to the large enhancement of the FR induced by the bismuth substitution for yttrium in yttrium iron garnets ($Bi_xY_{3-x}Fe_5O_{12}$; Bi:YIG). Following the discovery of this amazing behaviour, the first analyses of this behaviour underline the strong SO coupling of the bismuth ion. However, as these first approaches were incomplete, an appreciable number of works have been published in the past ten years; in all of them, the key role was played by the increase in the spin–orbit (SO) coupling of Fe^{3+} ions resulting from the formation of molecular orbitals (mixing of the 3d Fe^{3+} orbitals with the 6p Bi^{3+} orbitals, which has a large SO coupling constant, through the O^{2-} ions' orbitals) [3]. Later, Dionne and Allen [4] claimed that the large splitting of the excited state induced by the large SO coupling of the Bi^{3+} ions was responsible for the FR enhancement. More recently, Helseth *et al* [5] advanced along the way of these authors and presented a good fitting of the MO spectra of Bi:YIG based on the existence of two transitions of diamagnetic character. They concluded that paramagnetic transitions seemed unable to account for the contribution from Bi. Zenkov and Moskvin [6] suggested a semi-quantitative model to explain the MO enhancement of Bi^{3+} (and of Pb^{2+})in YIG. They attributed the enhancement to $(FeO_6)^{9-}$ and $(FeO_4)^{5-}$ complexes, the main MO active centres of YIG. The covalent admixture of Bi^{3+} (or Pb^{2+}) 6p orbitals and oxygen ^{2}p states causes huge growth in the spin–orbit coupling strength of the oxygen ions. Because of this growth, the effective spin–orbit coupling of the two complexes $(FeO_6)^{9-}$ and $(FeO_4)^{5-}$ increases, then the MO effect of Bi:YIG (or Pb:YIG) is enhanced. Unfortunately, theoretical calculations for the mixing mentioned above based on quantum theory are very difficult; up to now, to our knowledge, no quantitative studies on the MO enhancement of Bi (or Pr) ions in iron garnets based on the quantum theory have been available. Furthermore, the role of temperature in the MO enhancement is generally ignored in the analyses.

Some of our previous articles [7, 8] discussed the effect of the SO coupling strength of the ground and excited configurations of rare-earth ions in garnets and trifluorides on the MO effects based on quantum theory. We concluded that the SO coupling strength of the ground configuration had a great and complex effect on FR, but the strength of the excited configuration had surprisingly only a relatively weak influence. However, we calculated FRs only at some wavelengths. So, these works could not exclude the possibility that the FR spectrum moves significantly with changing SO strength, but the change in the studied FR is small because the wavelength is far from the MO resonance frequencies. Moreover, we only paid attention to the paramagnetic FR.

In this work we extend the theoretical calculations to the influence of the SO coupling strength of both the ground and excited configurations on the spontaneous FR contributed by Ce^{3+} ions in $CeY_2Fe_5O_{12}$. Both paramagnetic and diamagnetic FR spectra are calculated. The role of temperature is considered. We choose Ce:YIG as an example to carry out all these calculations. The reasons for such a choice are as follows.

(1) The FRs in $Ce_xY_{3-x}Fe_5O_{12}$ and in $Bi_xY_{3-x}Fe_5O_{12}$ are close when x in these two compounds is almost the same. In addition, these two garnets have the largest MO enhancement among light rare-earth garnets and trifluorides.

(2) According to table 1 of the article by Zenkov *et al* [6], the order of the magnitude of the effective SO coupling constant of the main states of the two complexes, which are responsible for the large MO enhancement, is the same as that of free Ce^{3+} ions.

(3) It is well known that the MO effects in Ce:YIG are mainly produced by the intra-ionic electric dipole transitions between split levels of the ground configuration and split levels of the excited configuration. Furthermore, the electronic structure of the Ce^{3+} ion is simple. We thus can carry out quantitative calculations based on quantum theory with a very good approximation.

For $Y_{3-x}Bi_xFe_5O_{12}$, when $x < 1.5$, the substitution of Bi leads to a uniform expansion of the lattice without distortion, and this results in changes in the crystal field parameters. This work also examines the effect of the lattice expansion on the MO effect.

2. Approach

2.1. Brief outline of the calculation method for the Faraday rotation

It is supposed that the large FR in the compound discussed originates mainly from the intra-ionic electric dipole transitions between the split levels of the $4f^n$ and $4f^{n-1}5d$ configurations. The specific FR is calculated using the following formula (see [7] and the references therein):

$$\theta_F = \frac{N\pi(\bar{n}^2 + 2)^2 e^2}{9\bar{n}c\hbar} \sum_{n,g} A_{ng} \frac{\omega^2(\omega_{ng}^2 - \omega^2 - \Gamma_{ng}^2)}{(\omega_{ng}^2 - \omega^2 + \Gamma_{ng}^2)^2 + 4\omega^2\Gamma_{ng}^2} \rho_g, \tag{1}$$

where

$$A_{ng} = |\langle n|V_-|g\rangle|^2 - |\langle n|V_+|g\rangle|^2. \tag{2}$$

$|g\rangle$ and $|n\rangle$ are $4f^n$ and $4f^{n-1}5d$ levels split by the SO interaction, crystal field (CF) interaction, and superexchange interaction (SI) and/or external magnetic field. The higher-order Zeeman effect correction is included if necessary.

We use α (β) to express the ratio of a chosen SO interaction strength to the value taken from the book of Martin *et al* [9]. In other words, α (β) equal to zero means that, in the calculation, no SO coupling perturbation is taken into consideration for the ground (excited) configuration. α (β) equal to 1 means that the SO coupling strength of the ground (excited) configuration is taken from [9].

2.2. Origin of the diamagnetic Faraday rotation

In [7], the origin of the para-FR has been discussed. We now discuss the origin of the dia-FR. In the following, the FR $\theta_F(ng)$ induced by the electric dipole transition from one state $|g\rangle$ to an excited state $|n\rangle$ is written as:

$$\theta_F(ng) = K \frac{\omega^2(\omega_{ng}^2 - \omega^2 - \Gamma_{ng}^2)}{(\omega_{ng}^2 - \omega^2 + \Gamma_{ng}^2)^2 + 4\omega^2\Gamma_{ng}^2} A_{ng}\rho_g \tag{3}$$

where K is a constant which can be obtained from equation (1).

The analysis of equation (3) has to be conducted according to the nature of the levels involved in the transition and four cases have to be distinguished.

(1) There exist two nondegenerate CF–SO split levels of the excited configuration (note that the effect of SO coupling is present) and a nondegenerate CF–SO split level of the ground configuration. The matrix element associated with each of the two electric dipole

transitions is then always equal to zero. However, when the two nondegenerate CF–SO split levels of the excited configuration are mixed by a superexchange interaction (or external magnetic field), then two CF–SO split and superexchange interaction (external magnetic field) mixed levels are created (in the following, they are denoted as $|n_1\rangle$ and $|n_2\rangle$). The matrix elements associated with the two transitions may not be equal to zero. When they are not equal to zero, then the following relation is always true: $A_{n1g} = -A_{n2g}$. The total FR is the sum of the two contributions from the two transitions. Because the energy difference between $|g\rangle$ and $|n_1\rangle$ states is not the same as that between $|g\rangle$ and $|n_2\rangle$ states, the resonance frequency ω_{n1g} corresponding to the $|g\rangle \rightarrow |n_1\rangle$ transition and the resonance frequency ω_{n2g} corresponding to the $|g\rangle \rightarrow |n_2\rangle$ transition differ slightly. It should be noted that K, ρ_g and the absolute values of the two matrix elements (A_{n1g} and A_{n2g}) are the same for the two transitions. Hence the curve $|\theta_F(n_1g)|$ versus ω and the curve $|\theta_F(n_2g)|$ versus ω have the same shape, but one of the two curves shifts a small distance relative to the other curve. The total FR equals the sum of $\theta_F(n_1g)$ and $\theta_F(n_2g)$, i.e. the difference of the two curves mentioned above. The sum is almost equal to zero when the light frequency is far from the resonance frequency ($\approx \omega_{n1g}$ or ω_{n2g}), but it may have a large value near the resonance frequency and produce a narrow FR peak. Such an FR is the so-called diamagnetic FR.

(2) There exists a doubly degenerate CF–SO split level of the excited configuration and a nondegenerate CF–SO split level of the ground configuration. In this case, the matrix elements corresponding to the two transitions from the ground level to the two orthogonal states of the doubly degenerate excited level may be different from zero. But, because the two A_{ng} matrix elements are always of opposite sign with identical absolute value, the total FR is rigorously equal to zero. The above conclusion is independent of the choice for the two orthogonal states. When the degeneracy of the excited level is lifted by a superexchange interaction or external magnetic field, then two sublevels ($|n_1\rangle$ and $|n_2\rangle$) are created. The resonance frequencies ω_{n1g} and ω_{n2g} corresponding to the two transitions $|g\rangle \rightarrow |n_1\rangle$ and $|g\rangle \rightarrow |n_2\rangle$ are different. As a result, total diamagnetic FR will be produced.

(3) There exist two nondegenerate CF–SO split levels of the excited configuration and a doubly degenerate CF–SO split level of the ground configuration whose two orthogonal states are denoted as $|g_1\rangle$ and $|g_2\rangle$. For the two transitions from $|g_1\rangle$ and $|g_2\rangle$ to any nondegenerate CF–SO split level $|n\rangle$ of the excited configuration, the sum $A_{ng1} + A_{ng2}$ of the two elements is always equal to zero. If the two nondegenerate CF–SO split levels of the excited configuration are mixed by a superexchange interaction or external magnetic field, the mixed $|n_1\rangle$ and $|n_2\rangle$ levels are obtained. Now the sum $A_{n1g1} + A_{n1g2}$ may be different from zero. In this case, the two quantities $A_{n1g1} + A_{n1g2}$ and $A_{n2g1} + A_{n2g2}$ always have the same magnitude, but are of opposite sign. Now, similar to situation 1, the two transitions produce a net diamagnetic FR through the difference of ω_{n1g} and ω_{n2g} ($|g_1\rangle$ and $|g_2\rangle$ have the same energy value).

(4) There exists a doubly degenerate CF–SO split level for both the excited and ground configurations. We denote the orthogonal state of the levels as $|n_1\rangle$, $|n_2\rangle$ and $|g_1\rangle$, $|g_2\rangle$, respectively. Now it may happen that the sums $A_{n1g1} + A_{n1g2}$ and $A_{n2g1} + A_{n2g2}$ are not equal to zero. In this case, the two sums always have the same amplitude but are of opposite sign, and there is no net FR. It is only when the degeneracy of the excited level can be lifted by a superexchange interaction or external magnetic field that a net diamagnetic FR is produced through the small difference between the two resonance frequencies corresponding to the two transitions.
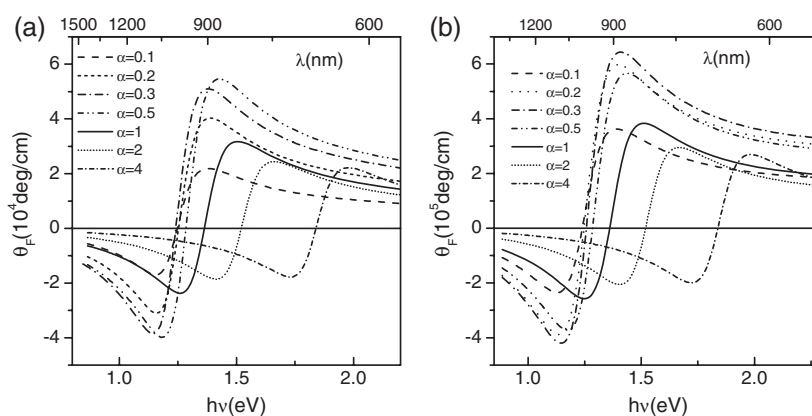
Figure 1. (a) Room-temperature spontaneous paramagnetic Faraday rotation spectrum caused by Ce^{3+} ions in $Y_2CeFe_5O_{12}$ when α varies in the range between 0.1 and 4, where β is set to 1. (b) Same as (a), but $T = 50$ K.

In summary, if the CF–SO split levels of the excited configuration are not split and not mixed by a superexchange interaction (or/and an external magnetic field), there will be no diamagnetic Faraday rotations, even though the SO split of the excited levels is present.

3. Results

3.1. Paramagnetic Faraday rotation

The room-temperature and 50 K para-FR spectra caused by the Ce^{3+} ions in $CeY_2Fe_5O_{12}$ are calculated when α varies in the range between 0.1 and 4, while β is unchanged at 1. The spectra have two resonance frequencies, at 1.36 and 3.10 eV respectively under normal conditions ($\alpha = 1$, $\beta = 1$) [10]. To make figures clearer (but without losing the main information), in figures 1(a) and (b) only the two peaks around the first resonance frequency are given. The spectra depend strongly on the α value. The dependency of the heights of the MO peaks on α value is very complex, although the resonance frequency increases monotonously with α. For room-temperature FR, the heights reach a maximum when α is about 0.5 (the corresponding value is about 0.3 for 50 K FR). It can be seen that, when α changes from 0.1 to 0.5, the height of the first peak in the room-temperature FR spectrum changes significantly (from -1.7 to -4.0×10^4 deg cm^{-1}). When α continues to increase, the peak decreases but the resonance frequency continues to increase.

Figure 2 shows the relative FR variation (defined as $[\text{FR}(\alpha)/\text{FR}(\alpha = 1) - 1] \times 100$) versus α for the dispersive part of the room-temperature FR. From the figure, it can be seen that, for light with 0.89 and 1 eV photon energies, when α takes suitable values, the FR is about 2.4 times the FR value when $\alpha = 1$. The relative FR variation for the 50 K FR is very similar to that given in figure 2 and is not shown.

Figures 3(a) and (b) show the change in the same spectrum as β changes from 0 to 4 but α is now kept unchanged at 1. Unlike in the above case, here both the resonance frequency and the peak height change only slightly. Figure 4 shows that the value of the room-temperature para-FR changes only about 10% when the value of β varies in the range of 0–4.

From the above results, we can conclude that the SO coupling strength of the ground configuration of the light rare-earth ions has a very great effect on the para-FR, however the corresponding effect of the excited-configuration SO coupling is relatively weak.
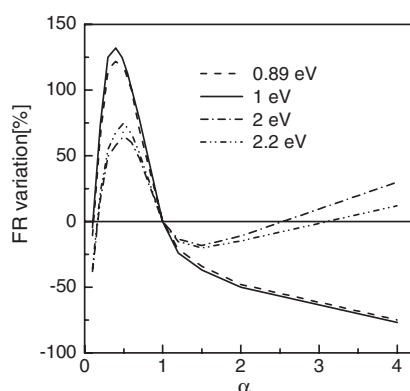
Figure 2. Relative FR variation (defined as $[\text{FR}(\alpha)/\text{FR}(\alpha = 1) - 1] \times 100$) versus α for the dispersive part of the room-temperature spontaneous para-FR spectrum caused by Ce^{3+} ions in $Y_2CeFe_5O_{12}$ (β being 1). The photon energies of the light are 0.89, 1.0, 2.0, and 2.2 eV.
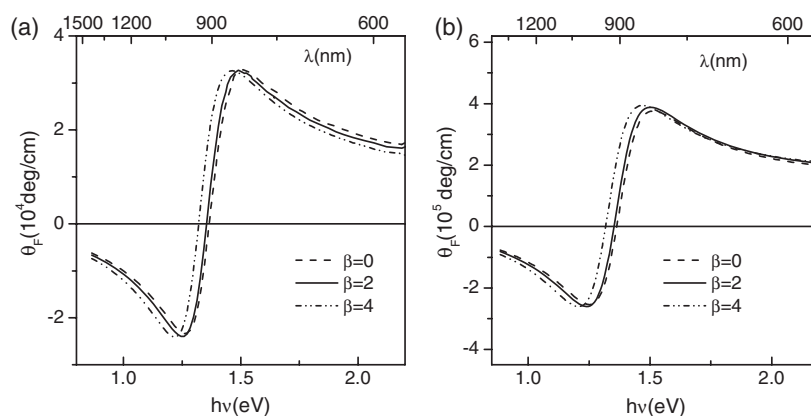

Figure 3. (a) The change in the same room-temperature spectrum as in figure 1(a) when β changes from 0 to 4, and α is kept unchanged at 1. The $\beta = 1$ curve is between the two curves with $\beta = 0$ and 2. (b) Same as (a), but $T = 50$ K.

3.2. Diamagnetic Faraday rotation

As mentioned in section 2, the dia-FR is produced when only the Zeeman effect of the excited configuration is taken into account while that of the ground configuration is neglected. So, the question is whether the excited-configuration SO coupling strength has a greater influence on the dia-FR than on the paramagnetic one. To answer this question, the variation in the dia-FR induced by the Ce^{3+} ions in $CeY_2Fe_5O_{12}$ versus β (with α kept unchanged at 1) is calculated and shown in figure 5 (the 294 and 50 K spectra being in the main diagram and inset, respectively).

When β increases from 0 to 4, the two peaks move a very small distance towards lower frequency, with their heights being basically unchanged. For comparison, the variation in the same dia-FR spectrum versus α (now with $\beta = 1$) is given in figure 6(a) (for 294 K FR) and figure 6(b) (for 50 K FR). To make the figures clearer, here only the peak at lower energy is shown. It can be seen that the peak height is seriously dependent on the value of α, especially
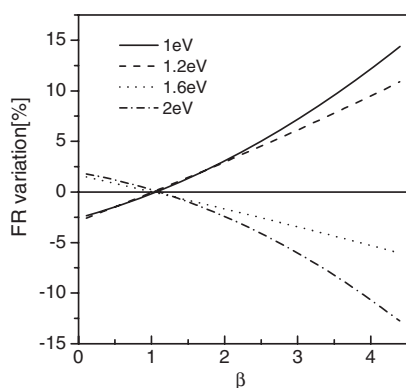
Figure 4. Relative FR variation (defined as $[FR(\beta)/FR(\beta = 1) - 1] \times 100$) versus β for the dispersive part of the room-temperature spontaneous para-FR spectrum caused by Ce^{3+} ions in $Y_2CeFe_5O_{12}$ (α being 1). The photon energies of the light are 1.0, 1.2, 1.6, and 2.0 eV.

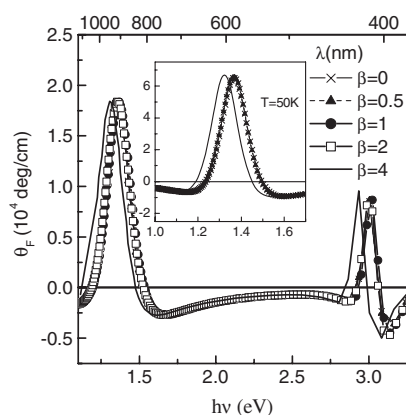**Figure 5.** Room-temperature spontaneous diamagnetic Faraday rotation spectrum caused by Ce^{3+} ions in $Y_2CeFe_5O_{12}$ when β varies in the range from 0 to 4, with α being set to 1 (the four curves corresponding to $\beta = 0$, 0.5, 1 and 2 are almost coincident with each other). Inset: 50 K dia-FR, for which only the spectrum around the first resonance frequency is given; the units are the same as the main diagram. For 50 K dia-FR, only three curves corresponding to $\beta = 0$, 0.5 and 4 are given.

when α is less than 0.5 for 294 K FR (less than 0.3 for 50 K FR) and the peak obviously moves towards lower frequency as α decreases from 4 to about 0.5.

The following important results should be noticed. For room-temperature dia-FR, as α increases from 0.1 to 0.5, the first resonance frequency almost does not change, while the height of the first peak increases obviously from about 0.45×10^4 to 1.75×10^4 deg cm^{-1}. This means that, for light with a photon energy in the range from about 1.19 to 1.4 eV, the magnitude of the dia-FR will increase by about 280% as α increases from 0.1 to 0.5. When α increases from 0.5 to 2, the location of the peak moves from 1.29 to 1.52 eV, though the change in the height of the peak is not large. For light with a photon energy between about 1.2 and 1.62 eV, the value of the dia-FR will have a very great change as α varies from 0.1 to 2. For example, for light with an energy of 1.52 eV, the value of the dia-FR will change peculiarly from a very small minus value to a large positive value (about 2.0×10^4). On the other hand, from figure 5 it can be seen that, even as β increases from 0 to 4, the changes in both the resonance frequencies and
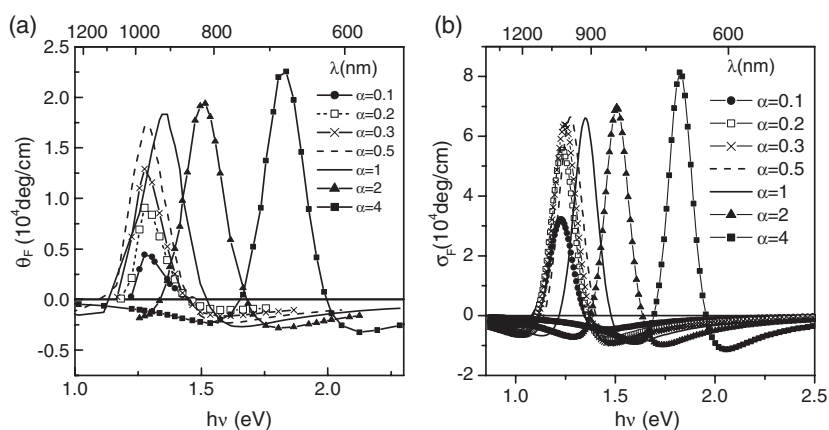
Figure 6. (a) The same spectrum as in figure 5 when α varies in the range from 0 to 4, with β being set to 1 ($T = 294$ K). (b) Same as (a), but $T = 50$ K.
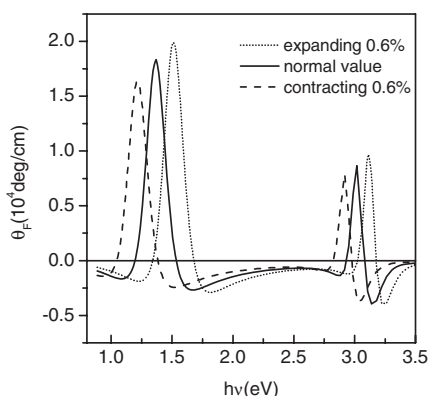

Figure 7. The change of the room-temperature spontaneous dia-FR spectrum when the lattice parameter increases or decreases by 0.6%.

the heights of the peaks are small. Therefore it can be concluded that, on the whole, the effect of the SO interaction strength of the excited configuration on the dia-FR is weaker than that of the ground configuration. However, from figure 5 it can also be seen that, on the fringes of the spectrum near the first MO resonance frequency, the change in the magnitude of the dia-FR may be large (≈ 5000 deg cm^{-1}) as β changes from 0 to 4. For light with a photon energy in a small range (≈ 0.17 eV) near 3.10 eV, the change in the magnitude of the dia-FR reaches about 8000 deg cm^{-1}.

To study the effect of the uniform lattice expansion or contraction on FR, we suppose that the lattice parameter increases by 0.6% or decreases by 0.6% and we determine the change in the parameters of the CF according to the point charge model. Then the room-temperature dia-FR spectra are calculated. The results are shown in figure 7. It can be seen that both the resonance frequency and the MO peak heights change obviously with changing the lattice parameter.

At the end of this section, we would like to point out that, in the calculation, all parameters used are the same as those in [10] except that the SO coupling strength is taken to be variable.

4. Discussion and conclusion

From the above results it can be seen that not only the para-FR but also the dia-FR in the studied compound are strongly dependent on the SO coupling strength of the ground configuration of the rare-earth ions but, surprisingly, are relatively weakly dependent on that of the excited configuration. Now the challenge is to find the reasons why the effects of the SO coupling of the two configurations are different and to draw messages for the analysis of Bi:YIG.

First, for spontaneous FR, a superexchange interaction (SI) is necessary, which acts on orbital states indirectly through SO coupling. The crystal field interaction on the excited configuration is much larger than that on the ground configuration. Taking Ce^{3+} in Ce:YIG as an example, the energy gap between the lowest and highest CF split excited-configuration levels is about $70\,000$ cm^{-1}, while the corresponding gap for the ground configuration is about 4000 cm^{-1}. So, the CF heavily decouples spin and orbit states of the excited configuration levels. Hence, although β changes over a large range, the effective SO coupling strength still varies over a relatively small range. This makes the dependence of FR on β relatively weak.

Second, all the three factors $(A_{ng}, \omega_{ng}, \rho_g)$ contained in the right-hand of equation (1) change as α changes. The height of the FR peak is determined by A_{ng} and ρ_g associated with some low-lying ground-configuration levels. Because (1) A_{ng} and ρ_g values are sensitive to the value of α (2), there are opposite effects concerning the changes in A_{ng} and ρ_g associated with the increase in α [7], the peak height in the para-FR spectrum depends strongly on the α value and is a maximum at a certain α value. As for the dia-FR, no Zeeman effect of the ground configuration is concerned. However, the occupation probabilities of the low-lying CF–SO split levels and A_{ng} related to these levels change as α changes and a large variation in the dia-FR peak height is then induced. At the same time, the MO resonance frequencies move obviously, because the energy scheme of the split ground-configuration states changes as α changes. The variation in β only leads to changes in ω_{ng} and A_{ng}. Hence, now the change in the peak height of both the para- and dia-FR is basically determined by the change in one factor A_{ng}. As a result, the change in the para-FR or dia-FR peak height due to the change in β is monotonous. Furthermore, because of the decoupling effect mentioned above, the changes in both the energy scheme and wavefunctions of the split excited-configuration states are small as β changes over a large range. This, in turn, leads to the results that both the MO resonance frequencies and the heights of the peaks of the para- and dia-FR change only relatively slightly on changing the value of β. However, for light with a photon energy in a small range near or at an MO resonance frequency, the change in the magnitude of dia-FR caused by changing the value of β may be large.

Now, we discuss the large FR in Bi:YIG. We think there are several possibilities. Some authors think that the observed FR is of the diamagnetic type. Because dia-FR peaks are always narrow, the frequency of the observed light must be close to an MO resonance frequency. So, small movements of the MO frequencies caused by the change in the SO coupling strength may lead to important changes in the observed FR magnitude. Secondly, when Fe 3d, O 2p and Bi 6p orbits form molecular orbits, both bonding and antibonding orbits contain Bi 6p components which have a great SO coupling. Then, both the initial and final levels of the MO transitions have a great SO coupling and the great FR can be attributed to the large SO coupling of the initial levels. In addition, the uniform expansion of the lattice induced by bismuth substitution has obvious effects on the FR.

All the points described above are open to further research.

Acknowledgments

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