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Magnetism of rare-earth-transition-metal nanoscale multilayers. II. Theoretical analysis of magnetization and perpendicular magnetic anisotropy

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Systematic studies of rare-earth-transition-metal amorphous compositionally modulated films (CMF) permit the development of a detailed model for understanding the magnetization and perpendicular magnetic anisotropy and their distributions along the film normal. It is shown that the single-ion anisotropy of rare-earth ions with orbital angular momentum is the major contributor to the perpendicular anisotropy for this class of CMF. The calculated results agree well with the experimental data for Dy/Co and Tb/Fe CMF when the individual layer thicknesses are small enough ($< 10 \text{ \AA}$); these films have structures which can be characterized as compositionally modulated amorphous alloys.

I. INTRODUCTION

The magnetism and especially the perpendicular magnetic anisotropy (PMA) in compositionally modulated films (CMF) are of great interest because of both interface magnetic and low-dimensional effects, and also their promising properties with possible applications to perpendicular magnetic and magneto-optical recording. In recent years, a number of CMF have been studied. Some examples are $A^{\text{RE}}/B^{\text{TM}}$ ($A^{\text{RE}} = \text{Tb, Dy, Nd, and } B^{\text{TM}} = \text{Co, Fe}$),¹⁻¹⁴ Pd/Co,¹⁵⁻²² Au/Co,²³ Fe/Ag,²⁴ and the results suggest that the CMF constitute a fertile area of pure and applied science, particularly in view of their controllable properties.

The existence of the compositional modulation of the constituent atoms offers an extra degree of freedom to control the local atomic environments in CMF structure, which permits the tailoring of magnetic properties, such as the perpendicular anisotropy, in artificially structured CMF. However, this also introduces complications in understanding the magnetic properties analytically because of the inhomogeneous distribution of constituents. Thus far, there has not been a thorough study of the micromagnetic structure of CMF: Sato^{1,2} suggested that the anisotropic distribution of Tb-Fe pairs aligned perpendicular to the film plane was the most probable origin of the perpendicular anisotropy in amorphous Tb/Fe multilayers, but his suggestion is only qualitative. Further, he does not indicate which mechanism is responsible for perpendicular anisotropy, e.g., the dipolar-interaction or single-ion anisotropy. Draaisma²¹ gave a phenomenological expression for the anisotropy energy based on the dipolar interaction for Pd/Co multilayers, where the interfaces were assumed to be polycrystalline, however, Carcia¹⁵ and de Broeder¹⁸ proposed that the stress-induced anisotropy contributes to PMA for this system. Suzuki²⁵ and Yoshihara *et al.*²⁶⁻²⁹ claimed that single-ion anisotropy is the main source of anisotropy, but their discussion was confined to homogeneous alloys.

Suzuki *et al.*⁷ suggested that for Nd/Co CMF the perpendicular anisotropy is induced from Nd atoms which are adjacent to Co atoms in the vicinity of the interface. It seems that two points are oversimplified in their discussion. (1) The modulated composition was replaced by a fixed composition of Nd-Co alloy during the mean-field fitting, i.e., the compositionally modulated structure has not been considered there. (2) The mechanism responsible for anisotropy has not been pointed out clearly. To our knowledge there have been no attempts to describe the micromagnetic structure of an $A^{\text{RE}}/B^{\text{TM}}$ amorphous CMF in detail, namely, the distribution of magnetization and anisotropy, the origin of the anisotropy, and the relationship between anisotropy and the distributions of magnetization and constituent atoms.

We have performed systematic studies of $A^{\text{RE}}/B^{\text{TM}}$ CMF including the case of $A^{\text{RE}} = \text{Tb, Dy, Gd, Er, Nd, and } B^{\text{TM}} = \text{Fe, Co, Ni}$.^{8-14,30} These experiments have permitted us to develop a model¹³ in terms of which the detailed properties, including PMA, can be understood. A modified mean-field model is used to analyze magnetization, and a single-ion model is used for analyzing the anisotropy. The calculated data based on these models agree with the experimental results reasonably well, and the origin of the anisotropy will be clarified.

II. MAGNETIZATION

The mean-field model has been used extensively to calculate the magnetization of $A^{\text{RE}}/B^{\text{TM}}$ homogeneous alloys.³¹⁻³⁵ This method is adopted to the CMF structure in the present paper. The main physical ideas are as follows. (1) The compositional dependence of magnetization for $A^{\text{RE}}/B^{\text{TM}}$ homogeneous alloys is calculated by mean-field theory and fitted to the experimental data. (2) The $A^{\text{RE}}/B^{\text{TM}}$ CMF is divided into thin slices each of which can be regarded as a two-dimensional amorphous film as shown in Fig. 1(a). (3) A trial distribution of TM concentration, e.g., a sinusoidal function, is assumed for

FIG. 1. The schematic diagram of A^{RE}/B^{TM} CMF regarded as the synthesis of homogeneous $A_{1-c}^{RE}B_c^{TM}$ slices (a), and the concentration distributions of Dy and Co along the film normal.

the thin layer-thickness CMF as shown in Fig. 1(b) because of the interdiffusion between RE and TM atoms, and also that the results of small angle x-ray diffraction pattern shows only the first-order peak for Dy/Co, Dy/Fe, Tb/Fe CMF with thin individual layer thicknesses (see Fig. 2 in paper I and Refs. 36 and 30). The magnetization σ_j of the j th slice is determined and then the resultant magnetization is obtained by taking the average of σ_j over the whole volume of the CMF. (4) The trial distribution is adjusted by repeatedly comparing the calculated results with the experimental data to achieve a good fit. This fitting gives the possible distributions of the constituent atomic fraction, the total magnetization, and its constituent magnetization along the film normal. In the following sections the calculation procedures and discussions to obtain a deeper physical understanding of the properties are described.

A. Magnetization for homogeneous $A^{RE}-B^{TM}$ alloys

For homogeneous $A_{1-c}^{RE}B_c^{TM}$ alloys, the spontaneous magnetization σ_s is governed by the following set of equations based on the mean-field model.³¹

1. Basic equations for magnetization of $A_{1-c}^{RE}B_c^{TM}$ alloys

In the mean-field model we have

$$\sigma_s = N\mu_B(C_1g_1\bar{S}_1 \pm C_2g_2\bar{S}_2), \quad (1)$$

$$\bar{S}_1 = S_1B_{S_1} \left[\frac{g_1\mu_B S_1 H_1}{k_B T} \right], \quad (2)$$

$$\bar{S}_2 = S_2B_{S_2} \left[\frac{g_2\mu_B S_2 H_2}{k_B T} \right], \quad (3)$$

$$H_1 = 2 \left[\frac{J_{11}Z_{11}\bar{S}_1}{g_1\mu_B} + \frac{J_{12}Z_{12}\bar{S}_2}{g_1\mu_B} \right], \quad (4)$$

$$H_2 = 2 \left[\frac{J_{21}Z_{21}\bar{S}_1}{g_2\mu_B} + \frac{J_{22}Z_{22}\bar{S}_2}{g_2\mu_B} \right], \quad (5)$$

where the subscript i ($i=1,2$) refers to TM and RE subnetworks and $+$ ($-$) sign refers to light RE (heavy RE), and C_i is the atomic fraction of the i th constituent, so that $C_2=1-C_1$ (we will use C simply to denote C_1 below), g_i is the gyromagnetic factor of the i th atom and H_i is the effective field of the i th subnetwork. $\bar{S}_i$ and S_i are the effective subnetwork spin at room and zero temperatures, respectively. J_{ij} are the exchange constants and Z_{ij} is the number of nearest neighbors. N is the total number of atoms per unit volume, k_B is the Boltzmann constant, and μ_B is the Bohr magneton. B_{S_i} denotes the Brillouin function.

We take Dy/Co CMF as an example, but this method is also suitable for the other similar A^{RE}/B^{TM} systems.

In the fitting procedure we first calculate the Co compositional dependence of magnetization for amorphous $Dy_{1-c}Co_c$ in terms of Eqs. (1)–(5). The calculated σ_s can be fitted optimally to the experimental σ_s over a wide range of composition C with the following parameters: $J_{11} = (2.35C - 0.95) \times 10^{-14}$ erg, $J_{22} = 8.00 \times 10^{-17}$ erg, $J_{12} = -(1.3 - 0.6C) \times 10^{-15}$ erg, $g_1 = 2$, $S_1 = 0.735$, $g_2 = \frac{4}{3}$, $S_2 = 5.47$. These values are subject to a certain degree of nonuniqueness. For example, the value of $g_2S_2 = 7.3$ which is smaller than the value appropriate for free Dy^{3+} ion ($g_2S_2 = 10$). This is interpreted as decreasing from a fanning of the Dy moments into a cone of half angle 63 degrees. The origin of this is the well-known random anisotropy effect. In addition, one could imagine allowing the Co spin, the J_{ij} values, and the coordination numbers to be functions of composition. However, our assumptions, which correspond to those used by other workers who have treated homogeneous $A^{RE}-B^{TM}$ alloys, are the simplest ones which lead to

FIG. 2. The Co concentration dependence of magnetization for Dy-Co alloys: the total magnetization σ_s , Dy-subnetwork magnetization σ_{Dy} , and Co-subnetwork magnetization σ_{Co} .

physically reasonable results.

Using these data, the magnetization curves $\sigma_s(C)$, $\sigma_1(C)$, and $\sigma_2(C)$, i.e., the total spontaneous magnetization, the magnetization of Co and Dy constituents, are shown in Fig. 2. Here

$$\sigma_1(C) = NC\mu_B g_1 \bar{S}_1, \quad \sigma_2(C) = N(1-C)\mu_B g_2 \bar{S}_2. \quad (6)$$

These curves are the basis of describing the magnetic structure of Dy/Co CMF.

2. Discussion

a. Physical origin of the magnetic ordering for Dy-Co binary alloys. Physically the Dy subnetwork is disordered magnetically at room temperature if the Co subnetwork does not exist. It is the exchange interaction between Co and Dy which causes magnetic ordering for Dy subnetwork. If there is no such exchange interaction, i.e., $J_{12} = J_{21} = 0$, obviously Eqs. (2) and (3) become linearly independent and $\bar{S}_2$ becomes zero because the Dy moment is disordered at room temperature.

Further analysis shows that the effective subnetwork spin $\bar{S}_i$ depends on the argument $y_i = g_i \mu_B S_i H_i / k_B T$ [see Eqs. (2) and (3)]. If y_i is less than the critical value corresponding to the Curie temperature, the i th subnetwork will be disordered magnetically. For the binary Dy-Co alloys, two parameters affect the argument y at least: they are temperature T , and effective field H_i [see Eqs. (4) and (5)] which in turn depend on $\bar{S}_i$, J_{ij} , and the composition C through the expression of Z_{ij} as³¹

$$Z_{11} = Z_{21} = 12C, \quad Z_{22} = Z_{12} = 12(1-C),$$

where C is the atomic fraction of Co atoms. In the above equations the approximation of 12-fold coordination has been adopted.

Using these relations, Eqs. (4) and (5) may be written as

$$H_1 = \frac{24}{g_1 \mu_B} [J_{11} C \bar{S}_1 - |J_{12}| (1-C) \bar{S}_2], \quad (7)$$

$$H_2 = \frac{24}{g_2 \mu_B} [|J_{12}| C \bar{S}_1 + J_{22} (1-C) \bar{S}_2], \quad (8)$$

and we notice that $J_{11} > 0$, $J_{22} > 0$, and $J_{12} = J_{21} < 0$ for heavy $A^{\text{RE}}/B^{\text{TM}}$.

The compositional dependences of H_i and $\bar{S}_i$, and consequently the argument y are of great importance in the interpretation of the origin and main features of magnetization curves in Fig. 2.

b. The compositional dependence of the subnetwork internal field. the compositional dependence of the calculated internal field of Dy and Co subnetworks, i.e., the $H_{\text{Dy}}(C)$ and $H_{\text{Co}}(C)$, is illustrated in Fig. 3. It is seen that (1) the internal field $H_{\text{Co}}(C)$ increases linearly with composition C over a wide range and its maximum value is about 1.3×10^7 Oe. (2) The internal field $H_{\text{Dy}}(C)$ is much smaller than that of $H_{\text{Co}}(C)$ and its value is about 10^6 Oe over a wide range of C . (3) To make a numerical estimation it is reasonable to ignore the external applied field H_a for large values of C , e.g., $C > 65$ at. %. In the case of small C , either the external field H_a has to be in-

FIG. 3. The Co concentration dependence of subnetwork internal field H_{Co} and H_{Dy} at 300 K.

involved or the spontaneous magnetization σ_s should be adopted.

c. The compositional dependence of the effective subnetwork spins. The compositional dependence of the calculated subnetwork spins $\bar{S}_{\text{Dy}}(C)$ and $\bar{S}_{\text{Co}}(C)$ is illustrated in Fig. 4. Both of them change their values smoothly for $C > 75$ at. %, and decrease rapidly as C becomes less than ~ 65 at. %. Finally they are disordered at $C \sim 53$ at. %. We notice that both $\bar{S}_{\text{Dy}}$ and $\bar{S}_{\text{Co}}$ change smoothly through the compensation point at $C \approx 74$ at. %. This feature implies that both Dy and Co subnetworks are ordered magnetically at the compensation point, but their magnetic moments cancel each other because of antiferromagnetic coupling.

Figures 2–4 illustrate the pictorial behavior of the compositional dependence of magnetization, internal field, and spin, and this is valuable to understand the micromagnetic characteristics of the Dy-Co alloys.

The general behavior of σ_{Co} and σ_{Dy} can be interpreted in terms of Eqs. (7) and (8) and Figs. 3 and 4. The internal field H_1 increases monotonically as C increases (see Fig. 3) and consequently σ_{Co} increases correspondingly. This character also can be seen in Eq. (7) because

FIG. 4. The Co concentration dependence of the subnetwork spins $\bar{S}_{\text{Dy}}$ and $\bar{S}_{\text{Co}}$ at 300 K.

the term $J_{11}C\bar{S}_1$ dominates in comparison with the term $|J_{12}|(1-C)\bar{S}_2$ and becomes larger as C increases. At small C , which is about 53 at. % in Fig. 2, the Co subnetwork is disordered because $J_{12}(1-C)\bar{S}_2$ term gives an appreciable negative contribution so that H_1 becomes less than the critical value corresponding to the Curie temperature. The behavior of the compositional dependence σ_{Dy} (see Fig. 2) follows because H_2 is small at small C and at large C the factor $(1-C)$ in Eq. (6) reduces the σ_{Dy} value. Consequently σ_{Dy} has larger values at intermediate C and vanishes at both small and large values, as shown in Fig. 2. This may also be seen in Eq. (8) wherein H_2 is small at small C because the term $|J_{12}|C\bar{S}_1$ gives a small contribution. At large C , each Dy atom has large spin $\bar{S}_2$ (see Fig. 4). The decrease of σ_{Dy} value is because of the small Dy atomic fraction $(1-C)$ [see Eq. (6)].

B. Magnetization and its distribution for $A^{\text{RE}}/B^{\text{TM}}$ CMF

To determine the magnetization of the $A^{\text{RE}}/B^{\text{TM}}$ CMF we evaluate the magnetizations σ_{sj} , σ_{1j} , and σ_{2j} of the j th slice from Fig. 2 (assume that $A^{\text{RE}}=\text{Dy}$, $B^{\text{TM}}=\text{Co}$) if the trial distributions of Co and Dy concentrations (at. number/cm³) along the film normal direction [see Fig. 1(b)] are assumed. Then the C value of each slice can be calculated and the magnetization of the CMF is equal to

$$\sigma_s = \frac{1}{\lambda} \sum_j \sigma_{sj} \Delta Z_j = \frac{1}{\lambda} \sum_j (\sigma_{1j} - \sigma_{2j}) \Delta Z_j, \quad (9)$$

where λ is the bilayer thickness and ΔZ_j the thickness of the j th slice. The parameters of the distribution function were adjusted until the σ_s values calculated from Eq. (9) fitted the experimental data within the given error (1 emu/cm³ in this work).

For Dy/Co, Dy/Fe, and Tb/Fe CMF of the thin individual layer thickness, the distribution of the constituent atoms has the sinusoidal form

$$\eta_j(Z) = A_{j0} \pm A_j \sin \left[\frac{2\pi Z}{\lambda} \right], \quad (10)$$

where $j=1$ and “+” sign refer to TM, and $j=2$, and “−” sign refer to RE and the Z axis is along the film normal. A_{j0} is a constant and A_j the modulation amplitude of the j th constitute concentration.

When the parameters A_{j0} and A_j are determined by the optimum fitting, the distributions of the constituent atomic fraction, the total magnetization $\sigma_s(Z)$, and the constituent magnetization $\sigma_1(Z)$ and $\sigma_2(Z)$ along the film normal are obtained.

To ensure that the fitting is reasonable, some constraints should be considered. (1) The conservation of the total number of TM and RE atoms is necessary during the process of assuming the trial distributions of TM and RE concentrations. (2) The summation of TM and RE atomic fractions is equal to unity. (3) The trial distribution curves of TM and RE have to be transferred smoothly through the nominal boundary. These constraints have to be obeyed to choose the trial distribution of TM and RE concentration. Further details of the constraints

imposed are described in Appendix A.

Detailed examples of the magnetization distributions for Dy/Co and Tb/Fe CMF are discussed in Sec. IV.

III. ANISOTROPY

A. The origin of the anisotropy in amorphous $A^{\text{RE}}/B^{\text{TM}}$ CMF

Many efforts have been made to investigate magnetic anisotropy and its origin in thin films. In principle, the necessary conditions to create PMA include the following.

(1) The anisotropic distributions of the constituent atoms which are determined by (a) the crystal structure for the crystalline RE (or TM) layers or the artificial multilayered structure which follows from the fabrication procedure, (b) the strain induced by the mismatch between the substrate and the $A^{\text{RE}}/B^{\text{TM}}$ CMF, and the tension (or compression) exerted on one layer (say RE layer) by its neighboring layers (say TM layers), and (c) the CSRO (compositional short-range order) and bond-orientational order.^{37,38}

(2) The interactions among the constituent atoms which include mainly the following two interactions: (a) magnetic dipolar interactions and (b) spin-orbit interactions which lead to single-ion anisotropy.

As outlined above, it is clear that once the anisotropic atomic structure is determined, this will then affect the magnitudes of both of the possible origins of PMA. Often, three sources of anisotropy are mentioned as candidates for PMA of thin films. These include dipolar-interaction,^{39,40} single-ion anisotropy,^{25–29,41,42} and stress-induced or “magnetostrictive” anisotropy.^{15,18} In fact, the third of these involves PMA induced by the distortion of the structure resulting from strains of the magnetic layers by the nonmagnetic layers or by the substrate.

The following three facts suggest that the main magnetic origin of PMA is due to single-ion anisotropy, as opposed to dipolar interactions, for amorphous $A^{\text{RE}}/B^{\text{TM}}$ ($A^{\text{RE}}=\text{Dy}$, Tb, and $B^{\text{TM}}=\text{Fe}$, Co) CMF.

(1) Figure 5 illustrates our experimental results for the behavior of K_u for $A^{\text{RE}}/B^{\text{TM}}$ CMF ($A^{\text{RE}}=\text{Tb}$, Dy, Gd, and $B^{\text{TM}}=\text{Fe}$, Co). This figure demonstrates that the anisotropy K_u for Dy/Fe, Dy/Co, and Tb/Fe CMF is roughly an order of magnitude larger than that of Gd/Fe CMF. The K_u of Gd/Co CMF is even smaller than that of Gd/Fe CMF. Since, to first order, the Gd atom has no single-ion anisotropy, it is reasonable to attribute the main origin of the perpendicular anisotropy of the Dy and Tb CMF to single-ion anisotropy of Dy and Tb atoms.

(2) The dipolar-interaction model has been successful in explaining the perpendicular anisotropy in terms of an anisotropy parameter “ p ” for Gd-Co amorphous alloys.^{39,40} Here p is a measure of the anisotropy in the distribution of unlike nearest-neighbor pairs, and its value is only about 0.015 for bias-sputtered Gd-Co. We used this model, which has been modified, for Dy/Co CMF, and found that the average value $\langle p \rangle$ is about 0.2, and its peak value may reach 0.4, because the K_u value of

FIG. 5. The anisotropy for (4.5 Å Tb)/(X Å Fe), (5 Å Dy)/(X Å Fe), (6 Å Dy)/(X Å Co), and Gd/Fe CMF. The anisotropy data of (2.3 Å Gd)/(3 Å Fe), (3 Å Gd)/(3 Å Fe), (3 Å Gd)/(5 Å Fe), etc., are in the shaded area.

Dy/Co CMF is an order magnitude larger than that of Gd/Co alloy. We noticed the p value seems unreasonably large, which implies that the dipolar-interaction model is inadequate for $A^{\text{RE}}/B^{\text{TM}}$ CMF ($A^{\text{RE}} = \text{Dy, Tb}$, $B^{\text{TM}} = \text{Co, Fe}$). But the dipolar-interaction model seems to be appropriate for Gd/ B^{TM} CMF ($B^{\text{TM}} = \text{Fe, Co}$).

(3) We have discovered that detailed layer-thickness dependence of the perpendicular anisotropy, as exhibited in Fig. 5, can be understood on the basis of the following expression:

$$K_u = \xi \frac{A}{\lambda} \langle \sigma_z^2 \rangle f \left(\frac{l_1}{l_2} \right), \quad (11)$$

where $\langle \sigma_z^2 \rangle$ is the average of magnetization squared of the rare-earth subnetwork, ξ a constant, " A " the peak to peak compositional modulation of the TM, λ the bilayer thickness, and $f(l_1/l_2)$ is a smooth function depending on the ratio of TM layer thickness to RE layer thickness. $f(l_1/l_2) = 1$ when the TM and RE have equal layer thickness. Equation (11) can be derived in terms of a single-ion model and this is a strong evidence that single-ion anisotropy of the rare-earth atom is the main source of the perpendicular anisotropy.

The subject of PMA and its origin via crystal-field interaction in $A^{\text{RE}}/B^{\text{TM}}$ multilayers has been considered recently by Baczewski *et al.*⁴² and Fert.⁴³ In addition, Lee *et al.*⁴⁴ and den Broeder *et al.*⁴⁵ have discussed PMA in Co/Au and Ni/Pd multilayers on the basis of magnetostrictive effects.

In the next section, Eq. (11) is derived briefly based on single-ion model assuming TM and RE have equal layer thickness. The derivation for the general case is given in Appendix B.

B. The anisotropy for $A^{\text{RE}}/B^{\text{TM}}$ CMF

Equation (11) can be obtained as follows. For the i th slice of the CMF, the local single-ion anisotropy is given by (see Appendix B)

$$K(i) \propto \alpha_J \langle r^2 \rangle O_2^0 A_2^0, \quad (12)$$

where α_J is Steven's factor, $\langle r^2 \rangle$ the average radius squared of the $4f$ orbit, O_2^0 is Steven's operator O_n^m with $n = 2$ and $m = 0$. O_2^0 is a factor proportional to J_z^2 if Z is the easy-axis direction. A_2^0 is a crystal-field term which is given by

$$A_2^0 \propto \sum_j \frac{q_j (3 \cos^2 \theta_j - 1)}{r_j^3}.$$

Then Eq. (10) becomes

$$K(i) \propto \alpha_J \langle \sigma_z^2 \rangle_i \sum_j \frac{q_j (3 \cos^2 \theta_j - 1)}{r_j^3}, \quad (13)$$

where j is the index of the j th ion in the neighborhood of the RE ion at the i th slice. The summation is over the neighboring ions with charge q_j and distance r_j from RE ion and θ_j is the angle with respect to the moment direction [see Fig. 6(a)]. The average notation $\langle \rangle_i$ means the statistical average of the RE ion over the i th slice. In the above derivation the relation " $\sigma_z \propto J_z$ " has been used.

For the amorphous CMF structure the sum over j in Eq. (13) has to be replaced by an integral weighted with an anisotropic probability function.²⁵ This function for

FIG. 6. The crystal field created by the neighbor ions (a), the local anisotropy $K(i)$ at Z_i (b). The resultant anisotropy K_u is the average of $K(i)$ over the whole volume of CMF. The concentration distribution C_j ($j = 1$ refers to Co, and $j = 2$ refers to Dy) along the film normal (c).

CMF structure may be expressed as

$$P_{ij}(\mathbf{r}) = \eta_j R_j(r) [1 + \beta_j(r) \cos \alpha_j + \dots], \quad (14)$$

where η_j is the atomic fraction of the j th surrounding ion consisting of RE and TM ions which have the sinusoidal form as shown in Eq. (10). $R_j(r)$ gives the isotropic part of the distribution, while $\beta_j(r)$ is the lowest-order anisotropic contribution. The parameter β_j , the anisotropy in the pair distribution function, is determined by the structural inhomogeneities produced by stress at the interfaces and chemical short-range order.

In the CMF structure C_j varies along the film normal, and then

$$P_{ij}(\mathbf{r}) \approx [\eta_j(Z_i) + \eta'_j(Z_i) r \cos \alpha_j] R_j(r) [1 + \beta_j(r) \cos \alpha_j], \quad (15)$$

where the relation $\Delta Z_i = r \cos \alpha_j$ is adopted, i.e., the RE ion at the i th slice is assumed to be the origin of the spherical coordinate and the polar axis is along the Z direction, i.e., the film normal direction. Then the local anisotropy $K(i)$ of a RE ion at the i th slice is found as follows:

$$K(i) \propto \alpha_j \langle r^2 \rangle \langle \sigma_z^2 \rangle_i \int \frac{(3 \cos^2 \theta - 1) \rho_j}{r_j^3} P_{ij}(r) d\Omega_j \\ \propto K_0 \langle \sigma_z^2 \rangle_i \left[\frac{A_j}{\lambda} \right] \cos \left[\frac{2\pi Z_i}{\lambda} \right], \quad (16)$$

where

$$K_0 = \alpha_j \langle r^2 \rangle \left[\frac{\rho_1 R(r_1) \beta_1}{r_1^2} - \frac{\rho_2 R(r_2) \beta_2}{r_2^2} \right]. \quad (17)$$

In the above derivation, the integral is calculated over the neighboring atoms with charge density ρ_j and distance r_j from RE ion, usually nearest-neighbor atoms only, and ρ_j , $R(r_j)$, and β_j are assumed to be different, but constant for the TM ($j=1$) and RE ($j=2$) ions.

The anisotropy K_u of the $A^{\text{RE}}/B^{\text{TM}}$ CMF can be obtained as the average of $K(i)$ over all the slices as shown in Fig. 6(b). If the magnetization σ_z changes smoothly along the film normal, which is true for the sample with thin layer thickness, K_u can be written as

$$K_u = \xi \langle \sigma_z^2 \rangle \left[\frac{A}{\lambda} \right] \quad (18)$$

as has been indicated in Eq. (11) while $f(I_1/I_2)=1$. A detailed derivation from Eq. (10) to Eq. (17) is given in Appendix B. The data for $\langle \sigma_z^2 \rangle$ and “ A ” can be obtained from Sec. II.

An important feature following from Eq. (16) is that the local anisotropy $K(i)$ is proportional to $\cos(2\pi Z_i/\lambda)$; since the cosine function has its peak value at $Z_i=0$, i.e., the nominal boundary position, the interface region will give the main contribution to the anisotropy.

IV. ANALYSES FOR Dy/Co AND Tb/Fe CMF

Physically all the experimental data are the results of statistical average over the whole sample. However, it is desirable to clarify the origin of the perpendicular anisotropy and obtain the distributions of magnetization and anisotropy since the composition of samples is modulated along the film normal. Two examples of analyses for (6 Å Dy)/(X Å Co) and (4.5 Å Tb)/(X Å Fe) are given below. It will be seen that the calculated results agree well with the experimental data and some micromagnetic information can be obtained based on this model.

A. Analysis for Dy/Co CMF

The distributions of the magnetizations (the total magnetization σ , Co- and Dy-subnetwork magnetization σ_{Co} and σ_{Dy}) for (6 Å Dy)/(3.5 Å Co) and (6 Å Dy)/(6 Å Co) are shown in Fig. 7. It is seen that σ_{Dy} dominates in Dy region and σ_{Co} dominates in Co region for (6 Å Dy)/(6 Å Co), and this is understandable from their higher atomic concentrations in their respective regions. But for (6 Å Dy)/(3.5 Å Co), σ_{Dy} dominates through the whole sample and shows maximum value at the central Co region. This feature follows because the Dy moment is disordered at room temperature and the exchange interaction between Co and Dy moments, which is proportional to the Co atomic concentration, makes the Dy moment ordered if the Co atomic concentration is high enough ($C_{\text{Co}} > 53$ at. %). In Fig. 7(a) σ_{Dy} shows maximum value at the central region of Co layer because of the higher Co atomic concentration there.

FIG. 7. The magnetization distribution along the film normal for (6 Å Dy)/(3.5 Å Co) (a), and (6 Å Dy)/(6 Å Co) (b).

FIG. 8. The Co concentration distribution along the film normal for (6 Å Dy)/(3.5 Å Co) (a), (6 Å Dy)/(6 Å Co) (b), and (6 Å)/(8 Å Co) (c).

The distributions of Co atomic fraction for (6 Å Dy)/(X Å Co) ($X=3.5, 6, 8$) are given in Fig. 8. Apparently the C_{Co} has its maximum value at the center of the Co region and the modulation amplitude increases as the Co layer thickness becomes thicker, and consequently the magnetization changes its value along the film normal as shown in Fig. 7.

Figure 9 shows the Co layer-thickness dependence of the total magnetization σ [Fig. 9(a)] and the Co-atomic-fraction modulation “ A ” [Fig. 9(b)]. The average magnetization of Co and Dy subnetworks are also drawn in this figure. It is noticed that the calculated and experimental magnetization data agree very well; the A value is only about 0.1 for the thinnest Co layer thickness of 3.5 Å and its value increases as the Co layer becomes thicker.

The intrinsic anisotropy K_u , which is expressed with Eq. (11) is fitted to the K_u data for (6 Å Dy)/(X Å Co) CMF with ξ as an adjustable parameter and the results are shown in Fig. 10. The agreement between the experimental data and calculated results is remarkable. The fitted value of $\xi=5.26 \times 10^{-6}$ cm leads to an average value of the single-ion anisotropy parameter $D=2 \times 10^{-17}$ erg, which is reasonable in terms of the typical value of the single-ion random-anisotropy parameter in amorphous alloys. The good agreement between the calculated and experimental data further confirms the suggestion that the Dy-ion anisotropy is the major source of perpendicular anisotropy is reasonable. This also can be found intuitively from the fact that $\langle \sigma_{Dy} \rangle$ curve in Fig. 9(a) is similar to the K_u curve in Fig. 8 and $\langle \sigma_{Co} \rangle$ curve

FIG. 9. The comparison of the calculated magnetization with the experimental data for (6 Å Dy)/(X Å Co) ($X=3.5, 5, 6, 8, 10$, and 11) (a), and the Co layer-thickness dependence of the Co atomic fraction modulation (b).

has a totally different shape which hints the Co subnetwork magnetization cannot be the origin of PMA.

B. Analysis for Tb/Fe CMF³⁰

Figure 11 shows the compositional dependence of the total magnetization σ , Tb subnetwork magnetization σ_{Tb} , and Fe subnetwork magnetization σ_{Fe} . The σ values are basically consistent with those in Ref. 46. σ value de-

FIG. 10. A comparison between the calculated and experimental anisotropy for (6 Å Dy)/(X Å Co) ($X=3.5, 6, 8, 10, 11$).

FIG. 11. The Fe concentration dependence of magnetization for Tb-Fe alloys: the total magnetization σ , Tb-subnetwork magnetization σ_{Tb} , and Fe-subnetwork magnetization σ_{Fe} .

creases rapidly as C approaches unity because the pure amorphous Fe is disordered magnetically.⁴⁷ The σ_{Tb} dominates for $53 \text{ at. \%} < C < 74 \text{ at. \%}$ and σ_{Fe} dominates for $C > 74 \text{ at. \%}$. We notice that both the Tb- and Fe-subnetwork moments change their value smoothly through the compensation point, i.e., both σ_{Tb} and σ_{Fe} are ordered, but the antiferromagnetic coupling causes the net magnetization to vanish.

FIG. 12. The magnetization distribution along the film normal for $(4.5 \text{ Å Tb})/(X \text{ Å Fe})$ ($X = 2.5, 3.75, 5, 6.25, 8.75$).

FIG. 13. The distributions of Fe atomic fraction (a), and magnetizations (the total, Tb-subnetwork and Fe-subnetwork magnetizations) for $(4.5 \text{ Å Tb})/(6.25 \text{ Å Fe})$ sample.

The distribution of the magnetization σ is illustrated in Fig. 12 for $(4.5 \text{ Å Tb})/(X \text{ Å Fe})$ ($X = 2.5, 3.75, 5, 6.25, 8.75$). It is seen that the Tb subnetwork moment dominates through the whole sample for the sample with the thinnest Fe layer thickness ($X = 2.5 \text{ Å}$) and then σ has the negative value. As Fe layer thickness increases, the moments of Tb and Fe subnetwork dominate in their own region, respectively. It should be pointed out for $(4.5 \text{ Å Tb})/(8.75 \text{ Å Fe})$ that there is a depression of the σ curve at the central Fe region because the Fe atomic fraction approaches 98% there and Fig. 11 has shown the rapid fall of the σ curve at this Fe concentration.

An example of the distributions of Fe atoms and magnetizations (σ , σ_{Tb} , and σ_{Fe}) along the film normal for $(4.5 \text{ Å Tb})/(6.25 \text{ Å Fe})$ is shown in Fig. 13. The Fe atom distribution $C_{Fe}(Z)$ has its maximum value of 0.94 at the center of the Fe region and minimum value of 0.57 at the center of the Tb region. At the nominal boundary σ is equal to zero approximately because σ_{Tb} and σ_{Fe} have about the same magnitude, but they are antiferromagnetically coupled.

FIG. 14. A comparison between the calculated and experimental anisotropy for $(4.5 \text{ Å Tb})/(X \text{ Å Fe})$ ($X = 2.5, 3.3, 3.75, 5, 6.25, 7.5, 8.75$).

Figure 14 shows the Fe layer-thickness dependence of intrinsic anisotropy. The calculated data agree with the experiment fairly well. Since the calculation is based on Eq. (11), this result implies that the model developed in this paper is reasonable.

V. SUMMARY AND CONCLUSION

In summary, a detailed model has been developed to understand the occurrence and control of perpendicular anisotropy in $A^{\text{RE}}/B^{\text{TM}}$ CMF. Single-ion anisotropy of the RE ion, which possesses orbital angular momentum, is the major source of PMA and the nominal interface region gives the main contribution to the anisotropy. The distribution of the constituent atoms, the total and constituent magnetization are determined in this model as well. The experimental data only show the magnetic properties resulting from a statistical average over the whole sample; however, the modeling analysis permits the determination of more information about the micro-magnetic structure. In this paper we have not investigated in detail the effects of inverse magnetostriction. This remains an important topic for future study. The understanding and control of the microstructure, and thus the magnetic properties may find important applications in various magneto-optic or other data-storage technologies.

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APPENDIX A: CONSTRAINTS FOR THE DISTRIBUTION FUNCTIONS OF TM AND RE SUBNETWORKS

The trial distribution should be a sinusoidal curve for the thin-layer CMF. We may imagine that the original distribution of TM and RE are square curves as shown in Figs. 15(b) and 15(c). It is the combination of interdiffusion and the surface roughness that makes the distribution curve sinusoidal.

A. The character of TM distribution function

(1) The distribution function of normalized TM concentration may be expressed as

$$\eta_1(Z) = \frac{N_1(Z)}{N_{10}} = \begin{cases} A_{10} + K A_1 \sin \left[\frac{\pi}{l_2} Z \right] & \text{as } -l_2 \leq Z \leq 0, \\ A_{10} + A_1 \sin \left[\frac{\pi}{l_1} Z \right] & \text{as } 0 \leq Z \leq l_1, \end{cases} \quad (\text{A1})$$

FIG. 15. The constraints between the concentration distributions of TM and RE: the block diagram of $A^{\text{RE}}/B^{\text{TM}}$ bilayer (a), the TM concentration distribution with constraints of $S_{11}=S_{12}$ and $K=l_2/l_1$ (b), and the Dy concentration distribution with constraints of $S_{21}=S_{22}$ and $K=l_2/l_1$ (c).

where N_{10} is the concentration of TM (at. number/cm³) and the meaning of parameters A_{10} , A_1 , K , l_1 , and l_2 can be found intuitively from Fig. 15.

(2) Since the TM concentration should vary smoothly from the nominal TM region to the RE region, the first derivative of $[N(Z)/N_{10}]$ has to be continuous and this leads to

$$K = \frac{l_2}{l_1}. \quad (\text{A2})$$

(3) Because of the conservation of TM atom number, there is a constraint between the areas of S_{11} and S_{12} , as shown in Fig. 15(b). S_{11} and S_{12} are proportional to the reduced number of TM atom in nominal TM region and the increased number of TM atom in nominal RE region due to the interdiffusion. The constraint requires

$$S_{11} = S_{12}, \quad (\text{A3})$$

which leads to

$$A_{10} = \begin{cases} \frac{1}{2} & \text{if } l_1 = l_2, \\ \frac{(2A_1/\pi)(Kl_2 - l_1) - l_2}{l_1 + l_2} & \text{if } l_1 \neq l_2. \end{cases} \quad (\text{A4})$$

B. The character of the RE distribution function

Analogous to the TM subnetwork the following expressions exist for RE subnetwork:

$$\eta_2 = \frac{N_2(Z)}{N_{20}} = \begin{cases} A_{20} - K A_2 \sin \left[\frac{\pi}{l_2} Z \right] & \text{if } -l_2 \leq Z \leq 0, \\ A_{20} - A_2 \sin \left[\frac{\pi}{l_1} Z \right] & \text{if } 0 \leq Z \leq l_1, \end{cases} \quad (\text{A5})$$

$$S_{22} = S_{21}, \quad (\text{A6})$$

$$A_{20} = \begin{cases} \frac{1}{2} & \text{if } l_1 = l_2, \\ \frac{l_2 - (2/\pi) A_2 (K l_2 - l_1)}{l_1 + l_2} & \text{if } l_1 \neq l_2. \end{cases} \quad (\text{A7})$$

C. The constraints between TM and RE subnetworks

If the parameters of V_1 and V_2 are defined as the volume per TM atom and the volume per RE atom, respectively, then the following constraint should hold at any position Z :

$$N_1(Z)V_1 + N_2(Z)V_2 = 1, \quad (\text{A8})$$

since N_1V_1 and N_2V_2 are the volumes of TM and RE atoms in unit volume, respectively.

To simplify Eq. (A8), Eqs. (A1) and (A5) are substituted into Eq. (A8) at $Z=0$, so that Eq. (A8) becomes

$$A_{10}N_{10}V_1 + A_{20}N_{20}V_2 = 1.$$

Since $N_{10}V_1 = N_{20}V_2 = 1$ by their definition, the above equation becomes

$$A_{10} + A_{20} = 1. \quad (\text{A9})$$

If this result is substituted into Eqs. (A4) and (A7) we will find

$$A_1 = A_2. \quad (\text{A10})$$

Equations (A9) and (A10) are the constraints between TM and RE subnetworks.

Once the parameters A_{10} , A_{20} , A_1 , and A_2 have been determined, the atomic fraction of TM atoms may be expressed as

$$C(Z) = \frac{N_1(Z)}{N_1(Z) + N_2(Z)}, \quad (\text{A11})$$

and consequently the magnetization values of $\sigma_s(Z)$, $\sigma_1(Z)$, $\sigma_2(Z)$ at Z position can be obtained from Fig. 2 (if $A^{\text{RE}} = \text{Dy}$, $B^{\text{TM}} = \text{Co}$) and Fig. 11 (if $A^{\text{RE}} = \text{Tb}$, $B^{\text{TM}} = \text{Fe}$), i.e., the distribution of magnetizations is determined. The rationality of this calculation is confirmed further by the anisotropy calculation where the data of $\sigma_2(Z)$ were adopted and the calculated result agreed with experiments fairly well.

APPENDIX B: SINGLE-ION ANISOTROPY IN $A^{\text{RE}}/B^{\text{TM}}$ CMF

Single-ion anisotropy arises from the interaction between the $4f$ electron of the RE atom and the local electric field created by the neighboring ions. If the charge distribution of the $4f$ electrons is nonspherical, i.e., $L \neq 0$, the electric field forces the distribution, the orbital angular momentum, and consequently the magnetic moment into a preferred orientation through the strong spin-orbit coupling. The expressions for the electric potential energy and anisotropy energy of a RE atom are derived on this basis, and the expression for the anisotropy in the CMF is obtained as well.

A. The expression of electric potential energy

Coulomb interaction W_{ef} between the $4f$ electrons and the local electric field can be expressed as^{25,48}

$$W_{ef} = -|e| \sum_i V(\mathbf{r}_i) = -|e| \sum_i \sum_j \frac{q_j}{|\mathbf{r}_j - \mathbf{r}_i|} = -|e| \sum_i \left[\sum_j q_j \sum_{n=1}^{\infty} \frac{r_i^n}{r_j^{n+1}} \frac{4\pi}{2n+1} \sum_{m=-n}^n (-1)^m Y_n^{-m}(\hat{\mathbf{r}}_j) Y_n^m(\hat{\mathbf{r}}_i) \right], \quad (\text{B1})$$

where $V(\mathbf{r}_i)$ is the electric potential of $4f$ electron at $\mathbf{r}_i$ surrounded by the neighboring ions with charge q_j at $\mathbf{r}_j$. The summation “ i ” is over all $4f$ electrons of a RE ion at the origin [Fig. 6(a)], and summation “ j ” is over all neighboring ions; usually only the nearest neighbor is taken into account.

The term related to the uniaxial anisotropy along the polar axis Z_M , which is parallel to the magnetic moment of the RE ion, is that with $n=2$, $m=0$. Taking this term only, W_{ef} becomes

$$W_{ef} = -|e| \sum_i \left[\sum_j q_j \frac{r_i^2}{r_j^3} \frac{4\pi}{5} Y_2^0(\hat{\mathbf{r}}_j) Y_2^0(\hat{\mathbf{r}}_i) \right] = -\frac{|e|}{4} \sum_j \frac{q_j (3 \cos^2 \theta_j - 1)}{r_j^3} \sum_i (3r_i^2 \cos^2 \theta_i - r_i^2) = -\frac{|e|}{4} \sum_j \frac{q_j (3 \cos^2 \theta_j - 1)}{r_j^3} \sum_i (3Z_i^2 - r_i^2) = -\frac{|e|}{4} \alpha_j \langle r^2 \rangle O_2^0 \sum_j \frac{q_j (3 \cos^2 \theta_j - 1)}{r_j^3}, \quad (\text{B2})$$

where θ_j and θ_i are the angles between $\mathbf{r}_j$ and Z_M axis, and $\mathbf{r}_i$ and Z_M axis, respectively.

In the last step of Eq. (B2) the following relationship has been used to simplify the summation over i :

$$\sum_i (3Z_i^2 - r_i^2) = \alpha_J \langle r^2 \rangle O_2^0, \quad (\text{B3})$$

where α_J is Steven's factor and $\langle r^2 \rangle$ is the quantum-mechanical average of the square of the radius of the $4f$ orbit. O_2^0 is Steven's operator O_n^m with $n=2$ and $m=0$. It is noticed (i) the values of α_J , $\langle r^2 \rangle$, and O_2^0 are determined by the charge distribution (or wave function) of the $4f$ electrons. For the rare-earth atom of nonzero orbital angular momentum the spin-orbit coupling H^{so} ($\sim 10^4$ K) is much larger than that of the electric field H^{ef} ($\sim 10^2$ K), so that the charge distribution of $4f$ electron is almost unchanged when the polar axis (or the direction of the magnetic moment of RE ion) changes its direction. This feature will be used to derive the anisotropy expression in the next section. (ii) The summation over j has the meaning of potential at the origin created by all the neighbors. In case of an amorphous structure, the summation over j has to be replaced by an integral weighted with a probability function $P_j(\mathbf{r}_j)$, which is the probability to find a j th neighbor ion with charge density ρ_j separated from the origin by vector $\mathbf{r}_j$ [Fig. 6(a)]. Therefore the electric potential energy W_{ef} may be rewritten as

$$W_{\text{ef}} = -\frac{|e|}{4} \alpha_J \langle r^2 \rangle O_2^0 \int \rho_j (3 \cos^2 \theta - 1) P_j(\mathbf{r}_j) / r_j^3 d\Omega_j, \quad (\text{B4})$$

for the amorphous structure. The probability function $P_j(\mathbf{r}_j)$ depends strongly on the spatial distribution of RE and TM atoms. In the next section the expressions for $P_j(\mathbf{r}_j)$ and subsequently W_{ef} will be derived.

B. The anisotropy for a RE ion in CMF

1. The probability function for CMF

Analogous to the probability function for nominally homogeneous $A^{\text{RE}}B^{\text{TM}}$ alloys,^{25,39,40} the probability function for CMF may be expressed as

$$\begin{aligned} P_j(\mathbf{r}_j) &= \eta_j(Z_i + \Delta Z_i) R(r_j) (1 + \beta_j \cos \alpha_j + \dots) \\ &= [\eta_j(Z_i) + \eta'_j(Z_i) \Delta Z_i] R(r_j) (1 + \beta_j \cos \alpha_j) \\ &= [\eta_j(Z_i) + \eta'_j(Z_i) r_j \cos \alpha_j] R(r_j) (1 + \beta_j \cos \alpha_j), \end{aligned} \quad (\text{B5})$$

here $\eta_j(Z_i)$ is the atomic fraction of RE and TM ions ($j=1$ refers to TM ion and $j=2$ refers to RE ion) at i th slice, $R(r_j)$ is the isotropic and β_j the lowest order of the anisotropic part of the probability function. α_j is the angle between $\mathbf{r}_j$ and the film normal Z (or the easy-axis Z if the CMF has perpendicular anisotropy).

FIG. 16. The direction of the moment $\mathbf{M}_i$ (or $\mathbf{M}_{\parallel}$) and its corresponding potential energy $W_{\text{ef}(i)}$ ($W_{\text{ef}(\parallel)}$) (a), the relations between the angles of θ_j and α_j as $\mathbf{M}_i$ parallel to Z (b), and $\mathbf{M}_{\parallel}$ perpendicular to Z (c).

2. The anisotropy of a RE ion in CMF

a. The general concept of the single-ion anisotropy. As was pointed out above, the electric field forces the magnetic moment into a preferred orientation, i.e., the easy magnetization direction, if the charge distribution of $4f$ electron is nonspherical. Thus W_{ef} has its minimum value in the easy direction and W_{ef} increases as the magnetic moment turns away from the easy axis. By the definition the anisotropy energy $K(Z_i)$ per RE ion at Z_i is equal to

$$K(Z_i) = W_{\text{ef}(\parallel)} - W_{\text{ef}(\perp)}, \quad (\text{B6})$$

where $W_{\text{ef}(\parallel)}$ is the electric field potential energy as the magnetic moment parallel to the film plane (or perpendicular to the easy axis Z) and $W_{\text{ef}(\perp)}$ as the magnetic moment parallel to the easy axis Z (or perpendicular to the film plane) as shown in Fig. 16(a).

Equation (B5) shows that the term $\beta_j \cos \alpha_j$ gives the anisotropic distribution. We notice that the $\cos \theta_j$ may be

FIG. 17. The concentration distribution $\eta_j(Z)$ [$\eta_1(Z)$ refers to TM and $\eta_2(Z)$ refers to RE].

expressed as

$$\cos\theta_j = \cos\alpha_j, \quad (\text{B7})$$

if the magnetic moment of RE ion along the easy-axis Z [see Fig. 16(b)] and the $W_{ef(\perp)}$ is going to be calculated. If the magnetic moment of RE ion falls along the film plane [see Fig. 16(c)], then the $\cos\theta_j$ may be expressed as

$$\cos\theta_j = \sin\alpha_j \cos\phi_j, \quad (\text{B8})$$

where ϕ_j is azimuthal angle of the spherical coordinate.

Substituting Eqs. (B7) and (B8) into Eq. (B2) we are able to calculate the $W_{ef(\perp)}$ and $W_{ef(\parallel)}$, respectively.

b. The calculations of $W_{ef(\perp)}$, $W_{ef(\parallel)}$, and $K(Z_i)$. The calculation is performed under the following assumptions. (a) The charge density ρ_j , isotropic parameter $R(r_j)$, anisotropic parameter β_j , and radius r_j ($j=1$ refers to TM ion and $j=2$ refers to RE ion) are constants, but different for TM and RE ions. (b) The RE ion at Z_i is surrounded by both of the TM and RE neighbor ions. We assume that the integral in Eq. (B4) is the sum of the integrals performed for TM ($j=1$) and RE ($j=2$), respectively.

The calculation of $W_{ef(\perp)}$ can be performed as follows.

First consider the following integral, which is the main part of Eq. (B4), in spherical coordinates (r_j, α_j, ϕ_j) :

$$\begin{aligned} \mathcal{J}(j) &= \int \rho_j (3 \cos^2\theta_j - 1) \frac{P_j(r_j)}{r_j^3} d\Omega_j \\ &= \int \rho_j (3 \cos^2\theta_j - 1) [\eta_j(Z_i) + \eta'_j(Z_i) r_j \cos\alpha_j] \frac{R(r_j)(1 + \beta_j \cos\alpha_j)}{r_j^3} d\Omega_j \\ &= \int \rho_j (3 \cos^2\alpha_j - 1) [\eta_j(Z_i) + \eta'_j(Z_i) r_j \cos\alpha_j] \frac{R(r_j)(1 + \beta_j \cos\alpha_j)}{r_j^3} d\Omega_j. \end{aligned} \quad (\text{B9})$$

In the last step of the above derivation Eq. (B7) has been used. After a tedious integration the above equation can be simplified as

$$\mathcal{J}(j) = \frac{16}{15} \pi \left[\frac{\rho_j R(r_j) \beta_j}{r_j^3} \right] \eta'_j(Z_i). \quad (\text{B10})$$

Using definitions of $W_{ef(\perp)}$ and Eq. (B4), $W_{ef(\perp)}$ can be expressed as

$$\begin{aligned} W_{ef(\perp)} &= -\frac{|e|}{4} \alpha_J \langle r^2 \rangle O_2^0 [\mathcal{J}(1) + \mathcal{J}(2)] \\ &= -\frac{|e|}{4} \alpha_J \langle r^2 \rangle O_2^0 \frac{16}{15} \pi \left[\left[\frac{\rho_1 R(r_1) \beta_1}{r_1^3} \right] \eta'_1(Z_i) + \left[\frac{\rho_2 R(r_2) \beta_2}{r_2^3} \right] \eta'_2(Z_i) \right] \\ &= -\frac{|e|}{4} \alpha_J \langle r^2 \rangle O_2^0 \frac{16}{15} \pi \left[\left[\frac{\rho_1 R(r_1) \beta_1}{r_1^3} \right] - \left[\frac{\rho_2 R(r_2) \beta_2}{r_2^3} \right] \right] \eta'_1(Z_i). \end{aligned} \quad (\text{B11})$$

In the last step of the above derivation, the relation $\eta'_2(Z_i) = -\eta'_1(Z_i)$ has been used.

The calculation of $W_{ef(\parallel)}$ can be performed similarly. We consider the following integral in spherical coordinates (r_j, α_j, ϕ_j) :

$$\mathcal{J}(j) = \int \rho_j (3 \cos^2\theta_j - 1) \frac{P_j(r_j)}{r_j^3} d\Omega_j = \int \rho_j (3 \sin^2\alpha_j \cos^2\phi_j - 1) [\eta_j(Z_i) + \eta'_j(Z_i) r_j \cos\alpha_j] \frac{R(r_j)(1 + \beta_j \cos\alpha_j)}{r_j^3} d\Omega_j. \quad (\text{B12})$$

In the last step of the above derivation Eq. (B8) has been used. After the tedious integration the above equation can be simplified to

$$\mathcal{J}(j) = -\frac{8}{15} \pi \left[\frac{\rho_j R(r_j) \beta_j}{r_j^3} \right] \eta'_j(Z_i). \quad (\text{B13})$$

Using the definition of $W_{ef(\parallel)}$ and Eq. (B4), $W_{ef(\parallel)}$ may be expressed as

$$W_{ef(\parallel)} = -\frac{|e|}{4} \alpha_J \langle r^2 \rangle O_2^0 [\mathcal{J}(1) + \mathcal{J}(2)] = +\frac{|e|}{4} \alpha_J \langle r^2 \rangle O_2^0 \frac{8}{15} \pi \left[\frac{\rho_1 R(r_1) \beta_1}{r_1^3} - \frac{\rho_1 R(r_2) R(r_2) \beta_2}{r_2^3} \right] \eta'_1(Z_i). \quad (\text{B14})$$

In the last step of the above derivation, the relation $\eta'_2(Z_i) = -\eta'_1(Z_i)$ has been used as well.

Comparing Eq. (B14) with Eq. (B11) we find

$$W_{ef(\parallel)} = -\frac{W_{ef(\perp)}}{2}. \quad (\text{B15})$$

The anisotropy energy $K(Z_i)$ per RE ion at Z_i is equal to

$$K(Z_i) = W_{ef(\parallel)} - W_{ef(\perp)} = -\frac{3}{2}W_{ef(\perp)}. \quad (\text{B16})$$

Substituting Eq. (B11) into Eq. (B16), the anisotropy of a RE ion in CMF $K(Z_i)$ can be expressed as

$$K(Z_i) = \frac{2\pi|e|}{5}\alpha_J\langle r^2 \rangle O_2^0 \left[\frac{\rho_1 R(r_1)\beta_1}{r_1^2} - \frac{\rho_2 R(r_2)\beta_2}{r_2^2} \right] \eta'_1(Z_i). \quad (\text{B17})$$

In Eq. (B17) O_2^0 can be expressed as $(2J_Z^2)$ if Z is the easy axis. Thus the local anisotropy energy $K(Z_i)$ per RE ion is

$$K(Z_i) = K_0(\sigma_Z^2)\eta'_1(Z_i), \quad (\text{B18})$$

where

$$K_0 = \frac{4\pi|e|}{5N^2\mu_B^2g_2^2} \left[\frac{\rho_1 R(r_1)\beta_1}{r_1^2} - \frac{\rho_2 R(r_2)\beta_2}{r_2^2} \right] \alpha_J\langle r^2 \rangle \quad (\text{B19})$$

is treated as a constant for given $A^{\text{RE-B}}^{\text{TM}}$ alloy, and the relation $J_Z = \sigma_Z / N\mu_B g_2$ has been used.

C. The anisotropy for $A^{\text{RE}}/B^{\text{TM}}$ CMF

The anisotropy of the $A^{\text{RE}}/B^{\text{TM}}$ CMF is the average of $K(Z_i)$ throughout the whole volume, i.e., see Fig. 17:

$$K_u = \langle K(Z_i) \rangle = \frac{2}{\lambda} \int_{-l_2/2}^{l_1/2} N_{20}\eta_2(Z_i)K(Z_i)dZ_i = \frac{2}{\lambda} \int_{-l_2/2}^{l_1/2} N_{20}\eta_2(Z)K_0(\sigma_Z^2)\eta'_1(Z)dZ. \quad (\text{B20})$$

In the last step of the above derivation, the subscript “ i ” is omitted. The expressions of $\eta_2(Z)$ and $\eta_1(Z)$ [or consequently $\eta'_1(Z)$] can be found in Fig. 17.

Because the parameters A_1 , A_{10} , A_{20} , and σ_Z can be obtained in terms of mean-field model as shown in the text and Appendix A, the anisotropy K_u may be calculated numerically if the constant K_0 is regarded as an adjustable parameter.

If the magnetization σ_Z changes smoothly, which is true for the sample with thin layer thicknesses l_1 and l_2 , the K_u expression may be rewritten as

$$\begin{aligned} K_u &= \frac{2}{\lambda} N_{20} K_0 \langle \sigma_Z^2 \rangle \int_{-l_2/2}^{l_1/2} \eta_2(Z) \eta'_1(Z) dZ \\ &= \frac{2}{\lambda} N_{20} K_0 \langle \sigma_Z^2 \rangle \left\{ \int_{-l_2/2}^0 \left[A_{20} - K A_1 \sin \left[\frac{\pi}{l_2} Z \right] \right] \frac{\pi}{l_2} K A_2 \cos \left[\frac{\pi}{l_2} Z \right] dZ \right. \\ &\quad \left. + \int_0^{l_1/2} \left[A_{20} - A_1 \sin \left[\frac{\pi}{l_1} Z \right] \right] \frac{\pi}{l_1} A_1 \cos \left[\frac{\pi}{l_1} Z \right] dZ \right\}. \end{aligned} \quad (\text{B21})$$

After lengthy operation the anisotropy K_u for CMF may be expressed as

$$K_u \simeq 2N_{20}K_0\langle\sigma_Z^2\rangle A_{20}\frac{A}{\lambda} \left[1 - \frac{A_1(1-K)}{2A_{20}} \right]. \quad (\text{B22})$$

Obviously

$$K_u \simeq 2N_{20}K_0\langle\sigma_Z^2\rangle A_{20}\frac{A}{\lambda}, \quad (\text{B23})$$

as $K=1$, i.e., TM and RE have equal layer thicknesses. This is the case of equal RE and TM layer thicknesses which has been pointed out in Eq. (18).

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