

**First-principles calculation of magnetocrystalline anisotropy for rare-earth–iron ternary compounds**

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(Received 1 June 1993; revised manuscript received 27 October 1993)

Crystalline electric field (CEF) parameters and magnetic anisotropic energies for rare-earth atoms  $R$  in  $R_2\text{Fe}_{17}L_8$  compounds are calculated based on first-principles electronic-structure calculations. The parameter  $A_{20}$  of CEF is obtained by using the real charge distribution from the corresponding cluster-model calculation and by directly calculating the crystal CEF parameters from the expansion coefficients of the local potential in the embedded-cluster model. The magnetic anisotropic energy is studied by taking the spin-orbit coupling as a perturbation into account in the semirelativistic embedded-cluster approach. The obtained results are in agreement with the experiments.

**I. INTRODUCTION**

Since the discovery of  $\text{Nd}_2\text{Fe}_{14}\text{B}$  in 1983, an intensive search has been made for new high-performance magnetic materials. The nitride  $R_2\text{Fe}_{17}\text{N}_\delta$  ( $R$  is the rare-earth atom,  $\delta$  is the concentration of the light element N) discovered in 1990 (Ref. 1) is the most promising of the hard-magnetic compounds. Two intrinsic properties are necessary for applications, a high Curie temperature, and easy-axis magnetic crystalline anisotropy (MCA). In  $R_2\text{Fe}_{17}$  compounds, the uptake of nitrogen leads to an increase in the Curie temperature by a factor varying between 1 and 5 for different  $R$  elements, and to transition to easy-axis MCA from easy-plane MCA for  $R = \text{Sm}$  only, at room temperature.<sup>2</sup>

Some theoretical research based on the electronic structure<sup>3–7</sup> has been done to study the enhancement of the Curie temperature after uptake of nitrogen in these compounds. In some of these calculations, substitution of Y for the rare-earth element gives the necessary exchange enhancement. However, a more difficult task is the calculation of the MCA, which must involve unusual  $4f$ -electron properties. Gu and Lai<sup>4</sup> treated the  $4f$  electron in two limiting cases, a highly localized and a band electron. This calculation introduced an error as high as 15% in the magnetic moments, and did not examine the MCA.

There have been other efforts to study the MCA of rare-earth–iron–light-element ( $R$ -Fe- $L$ ) compounds based on their fundamental electronic structure. Early studies based on empirical parameters have been replaced by evaluation of the effect of the crystalline electric field (CEF) in first-principles electronic-structure calculations. Zhong and Ching<sup>8</sup> calculated the crystal field parameters for  $\text{Nd}_2\text{Fe}_{14}\text{B}$  based on a tight-binding energy-band method. A similar method was also applied to calculate the MCA of  $R_2\text{Fe}_{17}\text{N}_x$  ( $R = \text{Sm}, \text{Nd}$ ;  $x = 0, 3$ ) by Huang *et al.*,<sup>9</sup> and the result is in qualitative agreement with experiment. However, the problem of self-consistent first-

principles calculation of the electronic structure and proper uniform treatment of the  $4f$  electrons is still open.

Generally speaking, the MCA in  $R$ -Fe- $L$  compounds arises from the  $4f$  electrons of the rare-earth atom in the crystal field. Although the  $f$  electron displays strong localized features, the mixing between  $4f$  and other states is not small. The  $f$  electron has to be considered as a valence orbital in the self-consistent procedure in the calculation rather than as a frozen-core state. In this paper, the MCA of  $R$ -Fe- $L$  compounds has been studied by two different approaches:

(1) Evaluation of the CEF based on the results of a self-consistent first-principles electronic-structure calculation for the corresponding crystal.

(2) Direct determination of the anisotropy constant from a total-energy calculation by taking the spin-orbit coupling as a perturbation in the semirelativistic approximation.

In the evaluation of the CEF parameters, we adopt two methods. First, the parameters of the local CEF are calculated using the charge distribution around the rare-earth atom  $R$  from the corresponding embedded-cluster model, which is similar to Ref. 8. Second, the CEF parameters are obtained directly from a harmonic expansion of the local crystal potential of the rare-earth atom considered in the embedded-cluster model. When local CEF parameters are known, the MCA can be obtained by the usual CEF theory. The results of applying these methods to  $R_2\text{Fe}_{17}L_8$  compounds are discussed.

**II. THEORETICAL METHOD**

Due to the complexity of the crystal structure of  $R_2\text{Fe}_{17}L_8$  compounds, it is difficult to consider the energy band of the crystal with sufficient accuracy. According to electronic-structure studies on the  $R_2\text{Fe}_{17}L_8$  compounds, there is charge transfer between atoms.<sup>5,6</sup> The magnitude of this effect is dependent on the specific rare-earth and light-element atoms, and may be the source of the variant magnetic behaviors of the compounds

$R_2\text{Fe}_{17}\text{L}_8$ . In this work, we will discuss the MCA on the basis of an electronic-structure calculation using the discrete variational method (DVM) cluster approach.<sup>10</sup> As the MCA mainly comes from the rare-earth atom in  $R_2\text{Fe}_{17}\text{L}_8$  compounds, we take the cluster centered at the rare-earth element  $R$ , consisting of  $R(6c)\text{-Fe}(6c)\text{-6Fe}(18f)\text{-9Fe}(18h)\text{-3Fe}(9d)\text{-3L}(9e)$  ( $R\text{Fe}_{19}\text{L}_3$ ), embedded in a crystal containing 1500 atoms of the  $R_2\text{Fe}_{17}\text{L}_8$  compound in this calculation. The embedded cluster of  $R(6c)\text{-Fe}(6c)\text{-6Fe}(18f)\text{-9Fe}(18h)\text{-3Fe}(9d)$  ( $R\text{Fe}_{19}$ ) is considered for the  $R_2\text{Fe}_{17}$  compound. Here the notations  $6c$ ,  $9d$ ,  $9e$ ,  $18f$ , and  $18h$  are representative of nonequivalence atomic sites in a unit cell, respectively. The electronic structure and charge density distribution are solved by DVM self-consistently.

In our calculation, the  $4f$  state is considered as a valence orbital. The basis sets we used are the valence orbitals  $4f6s5d$  for rare-earth element,  $3d4s$  for iron, and  $2s2p$  for the light element. The other electrons are considered to be in their atomic status, in the frozen-core procedure.

The Hamiltonian for the system can be written in the molecular field  $H_m$  approximation as

$$H = \mathbf{H}_0 + \xi \mathbf{L} \cdot \mathbf{S} + \mathbf{V}_{\text{CEF}} + 2\mathbf{S} \cdot \mathbf{H}_m + (\mathbf{L} + 2\mathbf{S}) \cdot \mathbf{H}_e, \quad (1)$$

where  $\mathbf{H}_0$  is the Hamiltonian of the single atom,  $\mathbf{H}_e$  is the external magnetic field,  $\mathbf{V}_{\text{CEF}}$  is the crystalline field potential, and  $\xi$  is the spin-orbital coupling constant.

The first approach is to evaluate the CEF as the starting point for study of the MCA. In traditional crystal field theory, when the crystal field  $\mathbf{V}_{\text{CEF}}$  is known, the eigenvalue and eigenfunction of the Hamiltonian (Eq. 1) can be solved by standard methods, and the MCA can be obtained from calculation of the total energy of the system. The problem we are confronted with is how to get the CEF with enough accuracy. As an improvement on the point-charge approximation, the CEF due to the environmental charge  $\rho(\mathbf{R})$  can be written as

$$V(r, \theta, \varphi) = - \int \frac{e\rho(\mathbf{R})}{|\mathbf{r} - \mathbf{R}|} d\mathbf{R}, \quad (2)$$

where  $(r, \theta, \varphi)$  represent the coordinates of the local electron, the integral extending over the whole crystal. As usually, the crystal field potential  $V_{\text{CEF}} = V(r, \theta, \varphi)$  can be expressed in terms of Stevens operators  $O_{nm}$  as

$$V(r, \theta, \varphi) = B_{20}O_{20} + \cdots + B_{66}O_{66} + \cdots. \quad (3)$$

$B_{nm}$  are the crystal field parameters which are related to the MCA.<sup>2</sup> In this work, the parameters  $B_{nm}$  are calculated by two approximate methods.

(1) In one first method, the integral in Eq. (2) can be performed simply by an average orbital radius approximation as done by Zhong and Ching.<sup>8</sup> In this approximation, the  $r$  is replaced by the average orbital radius  $r_0 = \langle r \rangle$  of the electrons considered ( $4f$  electrons for rare-earth atoms). Then from Eq. (6)–(9) in Ref. 8, the CEF parameter is obtained as the sum of two parts

$$B_{nm}^{\text{out}} = \theta_j \langle r^n \rangle A_{nm}^{\text{out}}, \quad R > r_0, \quad (4)$$

$$B_{nm}^{\text{in}} = \theta_j \langle r^{-n-1} \rangle A_{nm}^{\text{in}}, \quad R < r_0, \quad (5)$$

where  $\theta_j$  are the Stevens factors, and  $\langle r^n \rangle$  is the radial average of  $r^n$ .  $A_{nm}^{\text{in}}$  and  $A_{nm}^{\text{out}}$  are given by

$$A_{nm}^{\text{out}} = - \frac{4\pi e}{2n+1} \int \frac{\rho(\mathbf{R})}{R^{n+1}} Z_{nm}(\Theta, \Phi) d\mathbf{R}, \quad (6)$$

$$A_{nm}^{\text{in}} = - \frac{4\pi e}{2n+1} \int R^n \rho(\mathbf{R}) Z_{nm}(\Theta, \Phi) d\mathbf{R}, \quad (7)$$

and  $Z_{nm}$  is the tesseral harmonics including the numerical factor as defined in Ref. 3.

The  $\rho(r)$  in Eqs. (6,7) includes the nucleus, core, and valence electrons. In order to reduce the error in the numerical calculation, we subtract the spherical charge density of the corresponding atom; this does not influence the MCA which comes from the aspherical distribution of the charge density around the rare-earth atom.<sup>1</sup> The CEF parameter  $B_{nm}$  defined in (3) is simply the sum of  $B_{nm}^{\text{out}}$  and  $B_{nm}^{\text{in}}$ .

(2) We propose here a different method of calculating parameters  $B_{nm}$ . We can also calculate the CEF parameter directly from the Coulomb potential surrounding the atom concerned (the rare-earth atom in this work), after the self-consistent cluster electronic-structure calculation.

The crystal field potential acting on the local electrons of the concerned atom  $R$  can be expanded in terms of spherical harmonic functions according to the local crystal symmetry of  $R_2\text{Fe}_{17}\text{L}_8$  compounds:

$$V(r, \theta, \phi) = V_{00}(r)Y_{00} + V_{20}(r)Y_{20} + \cdots + V_{66}(r)Y_{66} + \cdots, \quad (8)$$

where  $V(r, \theta, \varphi)$  is the crystal field potential  $V_{\text{CEF}}$ , and  $Y_{LM} = Y_{LM}(\theta, \varphi)$  are spherical harmonic functions.

In the case of rare-earth atoms, the wave function of  $4f$  electrons in the CEF is a linear combination of  $Y_{lm}(\theta, \varphi)$  ( $l=3$ ) as

$$\psi_{4f} = \sum_m C_m R_{43}(r) Y_{3m}(\theta, \varphi). \quad (9)$$

In the usual crystal field theory, we are interested in the matrix  $H_{ij}$ . The CEF part of matrix  $H_{ij}$  is  $\langle \psi_i | V_{\text{CEF}} | \psi_j \rangle$ . We define

$$\bar{V}_{LM} = \int V_{LM}(r) |R(r)|^2 r^2 dr, \quad (10)$$

where  $R(r)$  is the  $4f$  radial function of the concerned atom. One can express the  $V(r, \theta, \varphi)$  in terms of the irreducible tensor operators  $Y_{LM}$  with the radial average  $\bar{V}_{LM}$  instead of  $V_{LM}$  itself as follows:

$$\begin{aligned} \bar{V}(\theta, \varphi) &= \int V(r, \theta, \varphi) |R(r)|^2 r^2 dr \\ &= \bar{V}_{00} Y_{00} + \bar{V}_{20} Y_{20} + \cdots + \bar{V}_{66} Y_{66}. \end{aligned} \quad (11)$$

The  $\bar{V}_{LM}$  can be obtained by multiplying  $Y_{LM}^*(\theta, \varphi)$  on both sides of Eq. (11) when using the well-known normalization of spherical harmonics, and integrating over  $\theta$  and  $\varphi$ ,

$$\begin{aligned} \bar{V}_{LM} &= \int \bar{V}(\theta, \varphi) Y_{LM}^*(\theta, \varphi) \sin\theta d\theta d\varphi \\ &= \int V(r, \theta, \varphi) |R(r)|^2 Y_{LM}^*(\theta, \varphi) d\mathbf{v}. \end{aligned} \quad (12)$$

These integrations over total volume can be performed conveniently in the discrete variation manner.

In practice, we calculate the crystal field potential  $V(r, \theta, \varphi)$  self-consistently using the embedded-cluster model. The relation between the coefficients  $\bar{V}_{LM}$  in Eq. (11) and the  $B_{nm}$  in Eq. (3) is as follows:

$$B_{nm} = \bar{V}_{nm} . \quad (13)$$

The main crux of this method is to get enough precision for the integration of  $V(r, \theta, \varphi)$ . In the DVM calculation, we take about 73 integration points per electron for each rare-earth atom and 23 points per electron for other kinds of atoms in the cluster. After calculating the coefficients, one can obtain the MCA following Yamada and co-workers.<sup>12-14</sup>

Another direct approach to investigate MCA is given by us. One can obtain the MCA by comparing the total energies with the direction of the magnetic moment along the different crystalline axes. Since the relativistic effect is important for the rare-earth atoms, a semirelativistic local-spin-density approximation (LSDA) cluster code has been used to obtain the zero-order approximate result  $|lsjm_j\rangle$  in the self-consistent calculation for the embedded cluster with rare-earth atom. The spin-orbit correction, small compared to the zero-order energy, is treated as a perturbation in the total-energy calculation. The spin-orbit interaction has the form

$$H_{so} = \frac{e}{2m^2c^2} \frac{1}{r} \frac{dV(r)}{dr} l \cdot s \\ = \xi(r) l \cdot s . \quad (14)$$

Although the coupling constant  $\xi(r)$ , which depends on the gradient of the potential, can be obtained in the self-consistent calculation, it is difficult to get a value accurate enough. In this preliminary work, the experimental value  $\bar{\xi}$  of the spin-orbit splitting constants from optical spectra of the trivalent rare-earth ions are used in our calculation.

The anisotropic total energy can be expressed as

$$E_t(\theta) = K_0 + K_1 \sin^2\theta + \dots , \quad (15)$$

where  $\theta$  is the angle between the moment and the  $c$  axis and  $K_1$  determines the direction of magnetization. The total energy of the cluster is calculated using the usual method described by Delley *et al.*<sup>15</sup>

In order to determine the  $K_1$ , and then the direction of magnetization, we calculate the total energy where the moment is set in the direction specified, [001] or [100], respectively. Then the anisotropy constant  $K_1$  is

$$K_1 = E_t([100]) - E_t([001]) \quad (16)$$

The constant of higher-order expansion can be obtained if a more specific direction such as [111] is taken into consideration.

### III. RESULT AND DISCUSSION

These approximate methods sketched above are used to evaluate the magnetic anisotropy of  $R_2Fe_{17}N_x$  ( $R = \text{Sm, Nd, Gd}$ ;  $x = 0, 3$ ) ( $x = 0$  means the binary com-

TABLE I. The calculated effective ionic charges in  $R_2Fe_{17}L_x$  ( $R = \text{Sm, Nd}$ ;  $x = 0, 3$ ).

Site	R (6c)	Fe(6c)	Fe(9d)	Fe(18f)	Fe(18h)	N(9e)
Sm <sub>2</sub> Fe <sub>17</sub>	0.24	0.11	0.06	0.11	-0.05	
Sm <sub>2</sub> Fe <sub>17</sub> N <sub>3</sub>	0.65	0.20	0.19	0.17	0.02	-0.45
Nd <sub>2</sub> Fe <sub>17</sub>	0.42	0.24	0.24	0.13	-0.03	
Nd <sub>2</sub> Fe <sub>17</sub> N <sub>3</sub>	0.66	0.20	0.08	0.23	0.05	-0.54

pounds  $R_2Fe_{17}$ ). The calculated effective ionic charges on all the different sites in  $R_2Fe_{17}N_x$  ( $R = \text{Sm, Nd}$ ;  $x = 0, 3$ ) are listed in Table I, as obtained from self-consistent calculations for the corresponding embedded clusters  $R_2Fe_{20}N_x$ . These effective ionic charges are obviously different from the assumed values used in the approximate point-charge model calculation.<sup>16</sup>

The calculated radial averages  $\langle r^n \rangle$  for  $4f$  atomic wave functions of Sm and Nd are listed in Table II. These values are used to calculate  $B_{nm}$  in Eqs. (4) and (5) in the first approximate method of calculating the CEF. From these equations, we can get the values of the second-order crystal field parameter  $B_{20}$  as 1.38, 0.95, 2.24, and -3.17 for Nd<sub>2</sub>Fe<sub>17</sub>, Nd<sub>2</sub>Fe<sub>17</sub>N<sub>3</sub>, Sm<sub>2</sub>Fe<sub>17</sub>, and Sm<sub>2</sub>Fe<sub>17</sub>N<sub>3</sub>, respectively. The positive parameter  $B_{20}$  indicates easy-plane anisotropy for Nd<sub>2</sub>Fe<sub>17</sub>, Nd<sub>2</sub>Fe<sub>17</sub>N<sub>3</sub>, and Sm<sub>2</sub>Fe<sub>17</sub>, and the negative parameter  $B_{20}$  for the nitride compound Sm<sub>2</sub>Fe<sub>17</sub>N<sub>3</sub> corresponds to easy-axis anisotropy; this is in good agreement with the experimental value of  $B_{20} = -4.8$  K in Sm<sub>2</sub>Fe<sub>17</sub>N<sub>2.3</sub> obtained by Coey and Otani.<sup>17</sup>

In Ref. 8, the environmental charge density is determined as the difference between the electronic charge density in the crystal from the non-self-consistent tight-binding band calculation and the charge density of the free rare-earth atom. In this work, the effect of the aspherical charge density is considered not only on the surrounding atoms but also on the rare-earth atom itself, obtained from the results of a self-consistent electronic-structure calculation for the corresponding cluster model.

The charge density distribution (in Fig. 1) of the cluster model concerned can provide an intuitive feature about the MCA. Figure 1(a) is the contour plot of charge density on the (101) plane. The distribution along the  $c$  axis for Sm<sub>2</sub>Fe<sub>17</sub>N<sub>3</sub>, which comes from charge transfer between R and N atoms, implies  $c$ -axis easy magnetization. On the other hand, the charge distribution of Sm<sub>2</sub>Fe<sub>17</sub> shown in Fig. 1(b) leads to a basal-plane anisotropy. The same idea is also described by Coehoorn.<sup>18</sup>

The second method to calculate the CEF parameter from the crystal field potential is carried out for Gd<sub>2</sub>Fe<sub>17</sub>N<sub>x</sub> ( $x = 0, 3$ ). The coefficients defined by Eqs.

TABLE II. Calculated radial averages  $\langle r^n \rangle$  for  $4f$  atomic wave functions of Sm and Nd in binary and ternary compounds.

	$r^2$	$r^4$	$r^6$	$r^{-1}$	$r^{-3}$
Sm <sub>2</sub> Fe <sub>17</sub>	0.87717	2.50692	18.26746	1.65836	12.48399
Sm <sub>2</sub> Fe <sub>17</sub> N <sub>3</sub>	0.87488	2.49290	18.14465	1.65841	10.57422
Nd <sub>2</sub> Fe <sub>17</sub>	0.88033	2.10305	11.64345	1.57753	10.03925
Nd <sub>2</sub> Fe <sub>17</sub> N <sub>3</sub>	0.88046	2.11370	11.80610	1.57794	10.37639

(11) and (16) are  $-38.14$  K for  $\text{Gd}_2\text{Fe}_{17}$  and  $-55.3$  K for  $\text{Gd}_2\text{Fe}_{17}\text{N}_3$ . The strength of the CEF in the nitride  $\text{Gd}_2\text{Fe}_{17}\text{N}_3$  is larger than that in the alloy  $\text{Gd}_2\text{Fe}_{17}$ . The experimental results for  $A_{20}=(-60\pm 40)$  K for the binary compounds  $R_2\text{Fe}_{17}$  with  $R=\text{Dy}, \text{Ho}, \text{or Er}$  are comparable with these calculated values. Since the spin-orbit coupling perturbation is inversely proportional to the interval between the energy levels constrained by selection rules, the distribution of energy levels will effect the strength of the MCA. The energy distribution below the Fermi level of the  $\text{GdFe}_{19}\text{N}_3$  cluster is closely concentrated, and the corresponding energy intervals of the  $\text{GdFe}_{19}\text{N}_3$  cluster model are smaller than those of the  $\text{GdFe}_{19}$  cluster model. This leads to stronger spin-orbit interaction, i.e., stronger MCA affected by the CEF, in  $\text{Gd}_2\text{Fe}_{17}$  after  $\text{N}_2$  uptake.

As an example, the magnetic anisotropy energy was evaluated from direct total-energy calculation for  $R_2\text{Fe}_{17}\text{N}_x$  ( $R=\text{Sm}, \text{Nd}; x=0, 3$ ) and  $\text{Nd}_2\text{Fe}_{17}\text{C}_3$ . When there is no spin-orbital coupling term in the Hamiltonian, the nonrelativistic total energies for different directions of magnetic moment are almost the same. This result indicates that the precision of our energy calculation is acceptable. The spin-orbit splitting constants  $\xi$  of  $R^{3+}$  ions

TABLE III. The magnetic anisotropy constant  $K_1$  for  $R_2\text{Fe}_{17}\text{L}_x$  ( $R=\text{Sm}, \text{Nd}; L=\text{N}, \text{C}; x=0.3$ ).

	$\xi$ (eV)	$K_1$ (eV)
$\text{Sm}_2\text{Fe}_{17}$	0.146290	-0.0888
$\text{Sm}_2\text{Fe}_{17}\text{N}_3$	0.146290	0.0506
$\text{Nd}_2\text{Fe}_{17}$	0.109107	-0.0111
$\text{Nd}_2\text{Fe}_{17}\text{N}_3$	0.109107	-0.0176
$\text{Nd}_2\text{Fe}_{17}\text{C}_3$	0.109107	-0.0199

in  $\text{RF}_3$  crystals are used in this work. The coefficients  $K_1$  obtained are listed in Table III.

The energy levels split and rearrange when the perturbation of the spin-orbit interaction is introduced into the Hamiltonian, and the MCA depends on the ordering of the energy levels. The occupied  $f$  state below the Fermi level is  $f_{y(y^2-3x^2)}$  in the  $\text{SmFe}_{19}$  cluster model used to simulate  $\text{Sm}_2\text{Fe}_{17}$ . This  $xy$ -plane behavior will result in planar MCA when the spin-orbit coupling operator is turned on with the spin moment sites in the  $ab$  plane. Due to the mixing between samarium and nitrogen in the  $\text{SmFe}_{19}\text{N}_3$  cluster model (related to  $\text{Sm}_2\text{Fe}_{17}\text{N}_3$ ), the occupied  $f$  state below the Fermi level changes to  $f_{x(5z^2-r^2)}$ . This state including  $z$ -axis behavior will exhibit  $c$ -axis MCA with the spin-orbit interaction considered. In the  $\text{NdFe}_{19}\text{N}_3$  cluster model, which is related to the  $\text{Nd}_2\text{Fe}_{17}\text{N}_3$  compound, because of the fewer electrons of Nd compared to Sm, the occupied energy levels below the Fermi level are similar to those in  $\text{Sm}_2\text{Fe}_{17}$ , i.e., the state  $f_{x(x^2-3y^2)}$ ; this compound shows planar MCA also. The results of this analysis are shown in Table III; only  $\text{Sm}_2\text{Fe}_{17}\text{N}_{2.6}$  shows  $c$ -axis MCA and all the other compounds in Table III exhibit basal-plane easy magnetization. This agrees with the experimental results. The error of this calculation (larger MCA values than experiment) may result from the selection of the approximate spin-orbit coupling constant  $\xi$  and the correspondence between the one-electron states and the multiplet of the many-body system for rare-earth atoms.

In summary, the results for MCA from first-principles electron-structure calculations using the two approaches described above may explain the magnetocrystalline anisotropy of  $R_2\text{Fe}_{17}\text{L}_8$  compounds reasonably well. The strong MCA of  $\text{Sm}_2\text{Fe}_{17}\text{N}_{2.6}$  mainly comes from the anisotropic behavior of the  $4f$  electrons in the CEF, enhancement of magnetocrystalline anisotropy with uptake of  $\text{N}_2$  takes place, and the  $c$ -axis easy magnetization is an effect related to the charge transfer between samarium and nitrogen as well as to the change of CEF. The results obtained by us show that the two approximate methods of calculating the CEF are reliable and efficient in the investigation of MCA in rare-earth-iron compounds.

#### ACKNOWLEDGMENTS

This work is partly supported by the National Natural Science Foundation of China under Grant No. 19174057, by LWZ-1298 of the Chinese Academy of Science, and by the Chinese National Laboratory of Magnetism, Beijing.

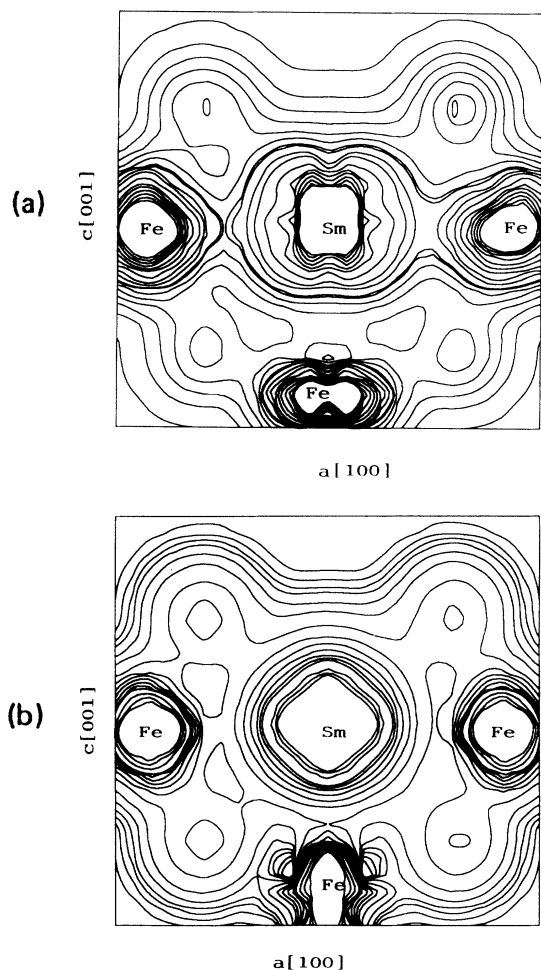


FIG. 1. Charge density contour plot on the (101) plane. (a)  $\text{Sm}_2\text{Fe}_{17}\text{N}_{2.6}$ ; (b)  $\text{Sm}_2\text{Fe}_{17}$ .

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