Model calculation of two-ion magnetostriction in the itinerant uniaxial ferromagnet Y_2Fe_{17}

K. Kulakowski* and A. del Moral

Unidad de Magnetismo de Sólidos, Departamento de Física de Materia Condensada and Instituto de Ciencia de Materiales de Aragón, Universidad de Zaragoza and Consejo Superior de Investigaciones Científicas, 50009 Zaragoza, Spain

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Two-ion contribution to the magnetoelastic (MEL) coupling in the itinerant hexagonal iron-rich ferromagnet Y_2Fe_{17} is investigated within a Stoner-like model with an orbitally degenerate rigid $3d$ band. The *spontaneous* irreducible magnetostrictive strains $\epsilon^{\alpha,1}$ (volume distortion) and $\epsilon^{\alpha,2}$ (c-axis pure shape distortion) are calculated as well as their temperature dependences. The agreement with the experiment is reasonably good. The model includes contributions to the strains from the electron hopping within the dumbbell of $4f$ site Fe atoms and from isotropic exchange between the $4f$ Fe and $12j$ site nearest-neighbor Fe atoms, treated within the mean-field approximation. The strain derivative of the exchange integral between $4f$ and $12j$ iron atoms is obtained by the fitting of the experimental data. The one-electron hopping has been dealt with using a two-site Hubbard Hamiltonian with orbital degeneration, and within the Hartree-Fock approximation for the repulsive U term. We have also obtained the temperature dependence of the four macroscopic two-ion MEL parameters $\overline{D}^{\alpha}_{ij}$ (in Callen and Callen notation), appropriate for uniaxial symmetry.

I. INTRODUCTION

Although much is known, both experimentally and theoretically, about magnetostriction and magnetoelastic (MEL) coupling in insulators[1,2] and in $4f$-shell rare earth metals and their intermetallic compounds,[3,4] the nature of magnetostriction in $3d$ transition metals remains still unclear. It is generally accepted[2] that band involved mechanisms are active there. When the material is polycrystalline, the irreducible spontaneous strains within the grains are not easily separated out from the measured macroscopic strains.[5,6] But even for single crystals, the actual state of theory is far from enabling us to obtain the microscopic magnetoelastic coupling constants from *ab initio* calculations, and various interactions[7,8] have been invoked to explain, at least qualitatively, experimental results. Among them, the magnetostriction originated from the single-ion crystal electric field (CEF) interaction is believed to be of major importance.[9] In this case, the Brooks-Katayama-Fletcher[10] or BKF model remains as a landmark in the field. This model, when supplemented by the paramount simplifications of Kondorskii and Straube[11] and Mori, Fukuda, and Ukai,[12] has allowed the calculation of MEL constants in simple $3d$ metals, such as in cubic nickel and iron.[13]

Recently a slightly simplified model compared with the BKF, although, in our opinion, quite efficient, was introduced to evaluate some macroscopic or phenomenological constants in those cubic metals and in $3d$-amorphous alloys, and in particular to calculate their temperature dependence.[14] This model was successfully extended[15] to deal with $3d$ intermetallic compounds of uniaxial symmetry, in order to calculate the anisotropic CEF contribution to the magnetostriction α-symmetry modes[16] and their temperature dependences. These modes are the volume striction, $\epsilon^{\alpha,1}=\epsilon_{xx}+\epsilon_{yy}+\epsilon_{zz}$ and the c-axis shape distortion, $\epsilon^{\alpha,2}=(\sqrt{3}/2)[\epsilon_{zz}-(1/3)\epsilon^{\alpha,1}]$, where ϵ_{ij} are Cartesian strains. In concrete such a calculation was done for the ferromagnetic Y_2Fe_{17} hexagonal compound[15] (Ref. 15 will be termed as paper I herein). However, other MEL interactions, in particular the two-ion ones (both isotropic and anisotropic), can rarely be excluded, and for systems with lower symmetry than the cubic one, both strains $\epsilon^{\alpha,1}$ and $\epsilon^{\alpha,2}$ are coupled by symmetry.[16] Then, both isotropic and anisotropic interactions of all kinds are relevant for both kinds of observed strains.[1,3] In paper I a successful method, as we shall also see in the present one, was developed to decouple the single-ion CEF MEL interaction from the other MEL interactions. Such is the situation when $\epsilon^{\alpha,1}$ and $\epsilon^{\alpha,2}$ are obtained from the magnetostriction developed at the end of the macroscopic rotational magnetization process,[3,15,17] i.e., when the magnetization lies along the *hard* magnetization direction ($\vec{c}$ axis for Y_2Fe_{17}),[18] under the application of a magnetic field equal to the magnetocrystalline anisotropy one, H_k, and along the $\vec{c}$ axis. Such a field is usually small (at most 4 T for Y_2Fe_{17})[3,16–18] compared with the exchange one, and therefore two-ion origin magnetostriction should be negligible below H_k.[16,19] However, the above method must fail when the strains are *spontaneous*, i.e., developed along the *easy* magnetization direction ($\vec{a}$ axis for Y_2Fe_{17}). This spontaneous magnetization is formed at the crossing of the Curie temperature T_c, in zero applied field. In this case both magnetostrictive strains should come essentially from isotropic exchange and other possible *two-ion* anisotropic MEL coupling mechanisms, in anisotropic uniaxial systems. This is so because at zero applied field there is not rotation of the magnetization against single-ion CEF interaction torques. But much more important in order to search for a new mechanism to explain the spontaneous strains $\epsilon^{\alpha,1}(\vec{a})$ and $\epsilon^{\alpha,2}(\vec{a})$ is that they are about 7×10^3 and 2×10^2 bigger than the CEF rotational ones $\epsilon^{\alpha,1}(\vec{c})$ and $\epsilon^{\alpha,2}(\vec{c})$, respectively, therefore claiming for a different origin.

Little is known about anisotropic interactions, in particular in metallic systems. Theoretically, these interactions are usually obtained within perturbation calculations up to at least third order in the expansion,[7] where spin-orbit coupling energy is considered to be small when compared with mag-

netic or with CEF energies. This approach is well established for narrow band systems,[1,16,20] such as $4f$ metals, where the indirect exchange interaction is believed to be a driving force for magnetic ordering. For $3d$ metallic systems, two-ion anisotropy can be due to anisotropic direct electron hopping[21] as well, if the interatomic distances are small enough. Nevertheless both anisotropic interactions are difficult to separate experimentally from those of single-ion CEF origin. Therefore, much remains to be done to clarify the observed effects (anisotropy and magnetostriction) as coming from a well defined kind of microscopic interaction, the field remaining still open.

As mentioned above, in paper I we were able to calculate the thermal dependences of the measured $\epsilon^{\alpha,1}(\vec{c})$ and $\epsilon^{\alpha,2}(\vec{c})$ strains for Y_2Fe_{17} at H_k, i.e., when the average magnetization starts to be along the hard $\vec{c}$ direction. Besides from the data fittings we obtained the macroscopic MEL coupling parameters $\overline{M}^{\alpha}_{12}$ and $\overline{M}^{\alpha}_{22}$, of CEF origin only. Obviously we are interested in the role of other possible mechanisms for the reasons above mentioned. Therefore the aim of this paper is an attempt to explain the spontaneous magnetostrictive strains $\epsilon^{\alpha,1}(\vec{a})$ and $\epsilon^{\alpha,2}(\vec{a})$ for Y_2Fe_{17} within the model of two-ion anisotropic hopping interaction, and where the isotropic exchange interaction is treated within the simple mean field (MF) approximation.

The paper is organized in the following way: in Sec. II we describe the proposed model, together with the assumptions which have been made; in Sec. III we present the magnetostriction calculations, the numerical results, and their comparison with the experimental strictions; finally, in Sec. IV we discuss our work and extract its main conclusions.

II. MODEL OF TWO-ION MAGNETOSTRICTION

A. The model Hamiltonian

As mentioned before, our aim is to explain the thermal dependences of the $\epsilon^{\alpha,1}(\vec{a})$ and $\epsilon^{\alpha,2}(\vec{a})$ spontaneous strictions in Y_2Fe_{17}, i.e., when the average magnetization is developed below T_c, along the easy magnetization direction. Those magnetic strains can be extracted from the thermal expansion (TE) measured along the $\vec{a}$ and $\vec{c}$ directions in a single crystal, once the lattice contribution to the TE is subtracted. They are $\epsilon^{\alpha,1}(\vec{a})=(\Delta c/c_0+2\Delta a/a_0)_m$, $\epsilon^{\alpha,2}(\vec{a})=(\sqrt{3}/2)[\Delta c/c_0-(1/3)\epsilon^{\alpha,1}(\vec{a})]_m$, where m means the magnetic TE and a_0 and c_0, the lattice constant values at the paramagnetic regime ($T\gg 2T_c$). Several workers have measured such strains, e.g., Givord,[22] Andreev *et al.*,[23] and García-Landa.[24] Measurable magnetic strains are still observed up to about $2T_c$,[22] due to strong short range ferromagnetic order, although our model is, in principle, only able to deal with them up to $T_c=324$ K.[25]

The Y_2Fe_{17} crystalline structure is of Th_2Ni_{17} type, where the Fe atoms occupy four kinds of sites: $12k$, $12j$, $6g$, and $4f$.[22,26] Only the $4f$ Fe atoms have high enough symmetry (trigonal $3m$) to give a contribution to the orbital magnetic moment, supporting a representation with the following $3d$ real atomic orbitals $|\rho\rangle$ basis: $\{|xz\rangle\equiv|1\rangle,|yz\rangle\equiv|2\rangle\}$, $\{|xy\rangle\equiv|3\rangle,|x^2-y^2\rangle\equiv|4\rangle\}$, $|2z^2-(x^2+y^2)\rangle\equiv|5\rangle$, i.e., two doublets plus a singlet.[16] At the remainder sites the states are all singlets and the orbital moment is quenched by the CEF. $4f$ Fe atoms form a dumbbell, perpendicular to a hexagon of

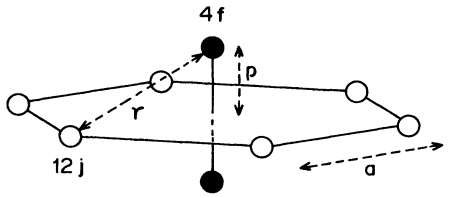

FIG. 1. The unit formed by the dumbbell of $4f$-site (trigonal $3m$ point symmetry) and the hexagon of $12j$-site Fe atoms, in the hexagonal ferromagnet Y_2Fe_{17}. The distances in the picture are $a=2.46$ Å and $p=1.195$ Å (from Ref. 33).

nearest neighbors (NN) Fe atoms in $12j$ sites (see Fig. 1). We will make the assumption that this part of the crystal cell, the dumbbell plus the hexagon, gives the major contribution to the two-ion magnetostriction. The role of the hexagon is assumed to contribute with a magnetic MF at the dumbbell atoms positions. Within this approximation we will look for the energy levels of the dumbbell atoms.

Current accuracy of band-structure calculations does not allow us to obtain the values for the MEL coupling parameters, even within the one-electron theory. Therefore we will work within a much simplified, although quite efficient scheme, where the calculations are, in principle, limited to a few high symmetry points of the Brillouin zone (BZ), which for the dumbbell plus hexagon complex, or even for the hexagonal unit cell, can be approximated by a cylinder. Such a simplification is justified by the mentioned result of Kondorskii and Straube[11] and Mori, Fukuda, and Ukai,[12] and, in our situation, is justified to consider just a single $\vec{k}$ point within the cylinder axis and close to the Fermi wave vector, $\vec{k}_F$. If, for instance, we perform our calculations within the tight binding approximation, using Bloch functions of the usual kind, only in the region close to $\vec{k}_F$ is the orbital angular momentum unquenched, being fully quenched elsewhere (see paper I for more details). Besides, the itinerant ferromagnet Hamiltonian is translationally invariant, and then it becomes $\vec{k}$ independent. This simplification reduces the problem to the analysis of an one-electron atomic model Hamiltonian of the form

$$H=H_{\mathrm{CEF}}+H_{\mathrm{SO}}+H_z+H_h\,. \tag{1}$$

The CEF Hamiltonian, H_{CEF}, was extensively discussed in paper I and it will have only a second order axial term, due to the reasons there exposed, of the form

$$H_{\mathrm{CEF}}=B_{20}\tilde{O}_{20}\,, \tag{2}$$

where $\tilde{O}_{20}=L_z^2-(1/3)L(L+1)$ is the second order or quadrupolar Stevens-Buckmaster operator and $\vec{L}$, the Fe orbital angular momentum.[27] This term produces a CEF energy level splitting of the form $-\Delta$, $+2\Delta$, -2Δ, corresponding to the singlet $|5\rangle$ and to the two doublets $\{|1\rangle, |2\rangle\}$ and $\{|3\rangle, |4\rangle\}$, respectively. Now, $\Delta=\alpha_L B_{20}\langle r^2\rangle_{3d}$, where α_L is the Stevens reduced matrix element, $\langle r^2\rangle_{3d}$, the Fe $3d$-shell second radial moment and B_{20}, the CEF strength parameter.[27] Δ is the only CEF parameter in the model.

H_{SO} is the spin-orbit (SO) interaction Hamiltonian, of the form

TABLE I. Values for the magnetostriction model parameters used for Y_2Fe_{17} intermetallic compound. The meaning of the parameters is the following: R is the ratio between the filling capacities of the wide conduction and the five $3d$-electron narrow bands; Δ is the axial crystal field energy shift for the $\{|xz\rangle,|yz\rangle\}$ doublet; W_0 is the half-bandwidth of the wide conduction electron band; W_1, the half-bandwidth for the $3d$ narrow bands; n is the total number of $3d$ electrons per Fe atom;[35] δ is the 0 K Stoner gap;[35] α, the orbital quenching and polarization parameter;[28] A, the spin-orbit coupling parameter;[9] C_{ij}^{α}, the α-symmetry stiffness elastic constants for hexagonal $PrNi_5$ (in eV/atom).[36]

R	Δ (eV)	W_0 (eV)	W_1 (eV)	n	δ (eV)	α	A (eV)	C_{11}^{α}	C_{12}^{α}	C_{22}^{α}
1	1.28	60	1.5	7.2	1.2	0.05	0.0468	55.4	5.4	166.3

$$H_{SO}=AL_z\sigma_z, \tag{3}$$

where A is the SO one-electron coupling constant. Notice that in order to simplify the calculations we have neglected all matrix elements of H_{SO} between the two doublets and between them and the singlet, an approximation which is justified because the CEF energy is much greater than the SO one. In such a situation the L_x and L_y angular momentum components are fully quenched by the CEF within the above $|\rho\rangle$ basis, i.e., $\langle\rho|L_x|\rho'\rangle=\langle\rho|L_y|\rho'\rangle=0$.

H_z is the Zeeman Hamiltonian, of the form

$$H_z=-(\vec{\sigma}+\alpha L_z)\cdot\vec{H}_{\rm eff}, \tag{4}$$

where $\vec{\sigma}$ are the Pauli matrices and $\vec{H}_{\rm eff}$ an effective magnetic field of the form

$$\vec{H}_{\rm eff}=g\mu_B\vec{H}_{\rm appl}+6J(r)\langle\vec{s}\rangle+\vec{H}_{\rm int}, \tag{5}$$

where g is the orbital Landé factor; $\vec{H}_{\rm appl}$, the external applied field (null in our situation); $J(r)$, an isotropic exchange integral of the $4f$ atom with its hexagon of NN's (Fig. 1); $\vec{H}_{\rm int}$ represents an intra-atomic mean magnetic field, whose origin will be discussed later on; and $\langle\vec{s}\rangle$, the spin thermal average of the NN atoms. Both $\langle\vec{s}\rangle$ and $\vec{H}_{\rm int}$ are assumed, within the MF approximation, to be proportional to the average magnetization. α is a constant introduced to take into account the partial quenching of L_z by the CEF, and the effect of the orbital polarization.[28] Notice that in paper I we choose $\alpha=0.40$, because there we were dealing with a part of the Brillouin zone (BZ) where the quenching of the orbital momentum was not complete, whereas here the contribution to the orbital momentum should be even smaller, inasmuch as the dumbbell units are only a small part of the unit cell. This is the reason to choose here $\alpha=0.05$ (see Table I).

We will now deal with the anisotropic one-electron hopping mechanism within the dumbbell of Fe atoms (Fig. 1), and represented in Eq. (1) by the Hubbard Hamiltonian,[29]

$$H_h=\sum_{i=1,2}\sum_{\rho,\rho',\sigma}t_{12}(\rho,\rho')a^{+}_{i\rho\sigma}a_{3-i\rho'\sigma}+U_{\rm int}, \tag{6}$$

where $t_{12}(\rho,\rho')$ are the hopping matrix elements or Slater-Koster (SK) integrals[30] (site-independent), between the $|\rho\rangle$ and $|\rho'\rangle$ orbitals, i counts the sites in the dumbbell, $\sigma(=\pm1/2)$ is the spin projection, and $U_{\rm int}$ represents the intraatomic Coulomb repulsive potential, both intraband and interbands. Its concrete expression[29] is not needed here. When treated within the MF or Hartree-Fock approximation, that potential can be added as an effective magnetic field, $\vec{H}_{\rm int}$, in Eq. (5).[29] The Slater-Koster integrals depend on the direction cosines, (l,m,n), of the dumbbell axis with respect to the OZ quantization axis (chosen such that $l=m=0$, $n=1$), therefore providing for an anisotropic hopping. Now, all matrix elements $t_{12}(\rho,\rho')=0$ for $\rho\neq\rho'$, i.e., there is not interorbital hopping,[30] the only non-null matrix elements being the intraorbital ones: $t_{12}(1,1)=t_{12}(2,2)=dd\pi$, $t_{12}(3,3)=t_{12}(4,4)=dd\delta$, $t_{12}(5,5)=dd\sigma$, where the dds symbols are the SK integrals.[30] We should mention that hopping is only active near the Fermi level, μ, where there exist unoccupied states, i.e., only states within the $\{|xz\rangle,|yz\rangle\}$ subband should be involved in the hopping. Our calculation treats hopping in the same way for all the subbands states, although this is not any drawback for our magnetostriction results, because contributions to hopping from fully occupied states vanish (see paper I). Finally, notice that only the intraorbital hopping does not quench the orbital momentum, the interorbital one fully quenching it.

So far, any kind of many-body electron effects have not been explicitly included within our Eq. (1) model Hamiltonian. Although such an effects should not be important below the paraprocess regime (i.e., for $H_{\rm appl}\gg H_k$), as it is our actual situation, nevertheless they have been implicitly accounted for within our calculations as we shall see in Sec. II B below.

B. The system magnetic energy

Our basis of system states is formed, considering the spin projections $\sigma=\pm1/2$, by ten one-electron $3d$ states $|\rho\sigma\rangle$ for each dumbbell Fe atom, i.e., 20 states overall. An exact fully analytical diagonalization of Hamiltonian (1) gives the splitting of energy levels shown underneath. We should distinguish two situations: $\vec{H}_{\rm eff}\|\vec{c}$ axis (z axis), i.e., $H_{\rm eff}=H_{\rm eff}^{z}$, and $\vec{H}_{\rm eff}$ perpendicular to $\vec{c}$ (in the basal plane), i.e., $H_{\rm eff}=H_{\rm eff}^{bp}$. In both cases we obtain for the energy eigenvalues, E_λ, the following:

$$E_{1-8}=\pm dd\pi\pm\left(\frac{A}{2}-2\alpha\sigma H_{\rm eff}^{z}\right)-\sigma H_{\rm eff}^{z}+\Delta, \tag{7a}$$

$$E_{9-16}=\pm dd\delta\pm2\left(\frac{A}{2}-2\alpha\sigma H_{\rm eff}^{z}\right)-\sigma H_{\rm eff}^{z}-2\Delta, \tag{7b}$$

$$E_{17-20}=\pm dd\sigma-\sigma H_{\rm eff}^{z}+2\Delta, \tag{7c}$$

where for $\vec{H}_{\rm eff}$ within the basal plane, the orbital momentum is quenched ($\alpha=0$), and $H_{\rm eff}^{z}$ should be substituted by $H_{\rm eff}^{bp}$ in Eqs. (7). Energy levels $\lambda=1$ to 8 result from the states $\{|1;\pm1/2\rangle,|2;\pm1/2\rangle\}$; similarly, levels $\lambda=9$–16 come from states $\{|3;\pm1/2\rangle,|4;\pm1/2\rangle\}$, and $\lambda=17$–20 ones, from $|5;\pm1/2\rangle$. For the calculation of the spontaneous magneto-

TABLE II. Slater-Koster integrals derivatives $dds' \equiv \partial dds/\partial \ln r$ (see Fig. 1) for bcc iron ($s \equiv \pi,\sigma,\delta$) (in eV);[32] $J'(r) \equiv \partial J(r)/\partial \ln r$ is the *obtained* strain derivative of the exchange integral between an Fe dumbbell atom ($4f$) and an Fe atom within the hexagon of NN (in eV) (see Fig. 1); here C_{ij}^{α} are the *fitted* elastic constants (in eV/atom) used to obtain the best theoretical fit for the $\epsilon^{\alpha,i}$ ($i=1,2$) irreducible strains temperature dependences (see Fig. 3).

$dd\pi'$	$dd\sigma'$	$dd\delta'$	$J'(r)$	C_{11}^{α}	C_{12}^{α}	C_{22}^{α}
−4.35	2.31	0.95	−0.83	15.4	5.4	166.3

strictive strains, $H_{\text{appl}}=0$ and the spontaneous magnetization is within the basal plane; therefore we are in the above second situation. We assume that the dds ($s=\pi,\delta,\sigma$) integrals and the effective field, H_{eff}, are magnetization and strain dependent. In fact this magnetization dependence is how we have effectively incorporated many-body electron effects in the calculation of the spontaneous strictions $\epsilon^{\alpha,1}(\vec{a})$ and $\epsilon^{\alpha,2}(\vec{a})$. The magnetization we are referring to is the measured spontaneous one along the $\vec{a}$-easy direction.[18] Further, within our MF approximation such a dependence has been introduced through the Stoner gap, given by $\delta=(M_+-M_-)H_{\text{eff}}$, where $M_{\pm}$ are the up and down spin plus orbital magnetizations in the direction of $\vec{H}_{\text{eff}}$ and $M_s=(M_+-M_-)$ is the average spontaneous magnetization.[29,31] Finally, as we are interested only in two-ion magnetostriction calculation, we neglect any dependence of Δ on the strains.

Within our model, the Eqs. (7) energy levels constitute the centers of 20 subbands, where we assume that the density of states has Lorentzian shape, and it is normalized to unity, i.e.,

$$\rho_{\lambda}(E)=\frac{W_1}{g_0\pi}\frac{1}{(E-E_{\lambda})^2+W_1^2}, \tag{8}$$

where $g_0=20$ is the orbital plus spin degeneracy and W_1, the half-bandwidth, the same for all of them. To those $3d$ subbands we have added two purely spin dependent subbands, much wider, with different electron filling capacity, C_0, and representing no magnetostrictive electron states, i.e., conduction electrons states. Therefore the number of $3d$ electrons filling each subband will be given by

$$n_{\lambda}=\int_{-\infty}^{\mu}\rho_{\lambda}(E)dE, \tag{9}$$

where μ is the chemical potential. μ is calculated from the condition of a constant number of electrons $n=\Sigma_{\lambda}n_{\lambda}$ ($C_{\lambda}\equiv W_1/g_0\pi$ is the electron filling capacity of the $|\lambda\sigma\rangle$ subband, with $\sigma=\pm 1/2$). In order to evaluate the system magnetic energy, U_m, we have adopted a rigid band Stoner-like approximation,[14,31] where particular subbands can mutually shift, when magnetization or strain are modified. Therefore we will write

$$U_m=\sum_{\lambda=1}^{20}\int_{-\infty}^{\mu}E\rho_{\lambda}(E)dE. \tag{10}$$

The temperature dependence of the calculated quantities is, as discussed before, introduced via the dependence of them on the spontaneous magnetization experimental thermal dependence, $M_s(T)$.[18]

III. MAGNETOSTRICTION CALCULATION AND RESULTS

A. Magnetostrictive strains

The detailed calculation of the magnetoelastic (MEL) energy for our itinerant system, within the rigid-band Stoner-like approximation, was presented in paper I, and we will recall here only the final result. Under the external solicitations (effective field and/or strains) each subband λ will shift in an energy $\Delta E_{\lambda}(H_{\text{eff}},\epsilon^{\alpha,i})$, the MEL energy becoming

$$\Delta U_{\text{me}}(\vec{H}_{\text{eff}},\epsilon^{\alpha,i})=-\sum_{\lambda}n_{\lambda}\Delta E_{\lambda}. \tag{11}$$

We add to the MEL energy, the elastic one, U_{el}, given for hexagonal symmetry by the expression,[16]

$$U_{\text{el}}=\frac{1}{2}C_{11}^{\alpha}(\epsilon^{\alpha,1})^2+C_{12}^{\alpha}\epsilon^{\alpha,1}\epsilon^{\alpha,2}+\frac{1}{2}C_{22}^{\alpha}(\epsilon^{\alpha,2})^2, \tag{12}$$

assuming only α-symmetry strains and where C_{ij}^{α} are the elastic stiffness constants. From the minimization of the overall energy, we obtain for the spontaneous equilibrium strains, when the spontaneous magnetization is in the basal plane, the following:

$$\epsilon^{\alpha,1}=\frac{1}{\Delta^{\alpha}}\left[C_{12}^{\alpha}\frac{\partial U_{\text{me}}}{\partial\epsilon^{\alpha,2}}-C_{22}^{\alpha}\frac{\partial U_{\text{me}}}{\partial\epsilon^{\alpha,1}}\right]_{\vec{M}\|\text{b.p.}}, \tag{13a}$$

$$\epsilon^{\alpha,2}=\frac{1}{\Delta^{\alpha}}\left[C_{12}^{\alpha}\frac{\partial U_{\text{me}}}{\partial\epsilon^{\alpha,1}}-C_{11}^{\alpha}\frac{\partial U_{\text{me}}}{\partial\epsilon^{\alpha,2}}\right]_{\vec{M}\|\text{b.p.}}, \tag{13b}$$

with $\Delta^{\alpha}\equiv C_{11}^{\alpha}C_{22}^{\alpha}-(C_{12}^{\alpha})^2$. It is easy to show that

$$\frac{\partial E_{\lambda}}{\partial\epsilon^{\alpha,1}}=2\left.\frac{\partial E_{\lambda}}{\partial\ln p}\right|_{\epsilon^{\alpha,2}=0},\quad \frac{\partial E_{\lambda}}{\partial\epsilon^{\alpha,2}}=\frac{9}{\sqrt{3}}\left.\frac{\partial E_{\lambda}}{\partial\ln p}\right|_{\epsilon^{\alpha,1}=0}, \tag{14}$$

where $2p$ is the Fe-Fe dumbbell distance (see Fig. 1), and therefore from Eqs. (7) and (14) we can immediately express $\partial U_{\text{me}}/\partial\epsilon^{\alpha,i}$ ($i=1,2$) in terms of the derivatives $dds'=\partial(dds)/\partial\ln p$ ($s=\pi,\delta,\sigma$). Because the values of the SK integrals and their logarithmic derivatives are not known for the dumbbell atoms in Y_2Fe_{17}, we have adopted for the latter those for bcc iron[32] (see values in Table II). This approximation is reasonable because $2p$ (Ref. 33) is similar as in bcc iron for NN.[34] The other derivative which appears in $\partial U_{\text{me}}/\partial\epsilon^{\alpha,i}$ is, according to Eq. (5), $\partial J(r)/\partial\epsilon^{\alpha,i}$, amounting $(\partial J/\partial\epsilon^{\alpha,1})_{\epsilon^{\alpha,2}=0}=(1/2)(\partial J/\partial\ln r)$ and $(\partial J/\partial\epsilon^{\alpha,2})_{\epsilon^{\alpha,1}=0}=-(3/\sqrt{3})[(r^2-2p^2)/r^2](\partial J/\partial\ln r)$, where r is the $4f-12j$ Fe atoms distance (see Fig. 1).

Three parameters were used to fit the thermal variation of the strains $\epsilon^{\alpha,1}$ and $\epsilon^{\alpha,2}$: $\partial H_{\text{eff}}^{\text{b.p.}}/\partial\epsilon^{\alpha,i}=6\langle\vec{s}\rangle J'(r)$, i.e., the in

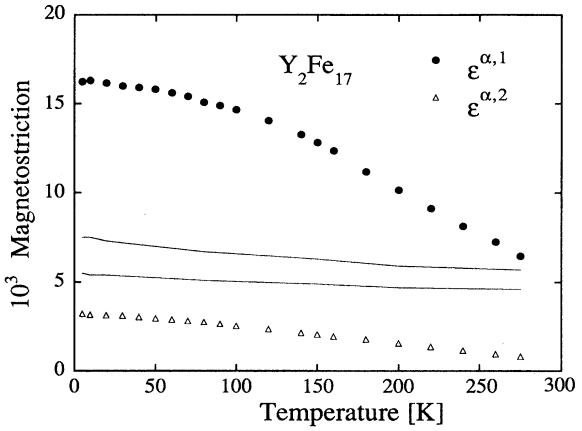

FIG. 2. Temperature dependence of the *spontaneous* irreducible magnetostrictive α strains for Y_2Fe_{17}: observed volume distortion $\epsilon^{\alpha,1}$ (●) and shape distortion $\epsilon^{\alpha,2}$ (△) (from Ref. 22). The continuous lines (—) are the result of the model calculation for $\epsilon^{\alpha,1}(\vec{a})$ (upper line) and $\epsilon^{\alpha,2}(\vec{a})$ (lower line), using the parameters collected in Tables I and II [for this calculation the elastic symmetry constants (see Table I) for hexagonal $PrNi_5$ (Ref. 36) intermetallic compound were employed].

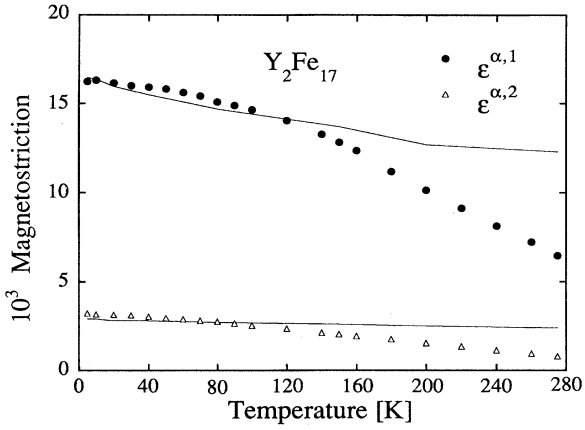

FIG. 3. The same as Fig. 2, but choosing elastic constant C_{ij}^{α} giving the "best" fit (see Table II), and keeping the same parameter values as in Fig. 2.

plane effective field strain derivatives, where $J'(r) \equiv \partial J/\partial \ln r$; the half bandwidths of the densities of states, W_1 for the $3d$ subbands, and W_0 for the two wide nonmagnetostrictive subbands, whose values are quoted in Table I. We would like to point out that the large value of W_0 is artificial, meaning that the spin subband is very flat. Such an artificial width comes from its Lorentzian shape, but has no consequences at all within our calculation, because it is only near the Fermi level that the density of states is important. Most of the remainder parameters in the model were the same as in paper I for calculating the single-ion CEF magnetostriction, and they are also quoted in Table I. In particular, the finite temperature $3d$-band Stoner gap, which at 0 K amounts to $\delta(0)=1.266$ eV,[35] has the form quoted in Sec. II B, i.e., proportional to $M_s(T)$. Also, the CEF splitting parameter was taken as in paper I, i.e., $\Delta=1.28$ eV, which is an acceptable value for $3d$ metals. Nothing is known about the elastic stiffness constants, C_{ij}^{α}, of Y_2Fe_{17} and therefore we have to take them from another intermetallic, e.g., the *hexagonal* $PrNi_5$ (Ref. 36) (see Table I), inasmuch as Th_2Ni_{17} structure is deduced from $CaCu_5$ by ordered substitutions of one rare-earth (RE) ion by the dumbell.[22] Therefore we will have for the symmetry elastic constants[1]

$$C_{11}^{\alpha}=(1/9)(2C_{11}+2C_{12}+4C_{13}+C_{33}), \quad (15a)$$

$$C_{12}^{\alpha}=(2/3\sqrt{3})(-C_{11}-C_{12}+C_{13}+C_{33}), \quad (15b)$$

$$C_{22}^{\alpha}=(1/3)(2C_{11}+2C_{12}-8C_{13}+4C_{33}). \quad (15c)$$

In Fig. 2 we present the experimental temperature variations for both modes,[22] together with the "best" fits from Eqs. (13), using all the above quoted parameters and the C_{ij}^{α} values for $PrNi_5$ (see Table I). Since the accordance attained between experiment and theory is only *qualitative*, we suspected the lack of obtaining a good enough agreement with experiment was due to the inadequacy of the elastic constants chosen. Therefore we modified one of the elastic constants, i.e., C_{11}^{α}, in an attempt to improve the fits, keeping all the other parameters unchanged. As we can see in Fig. 3, the agreement now obtained is much better, at least up to $T=150$ K. For higher temperatures the disagreement persists, but the Stoner-like theory is known to fail at high temperatures. We consider to modify the remainder elastic constants too artificial. The value of the fitted C_{11}^{α} constant is quoted in Table II, and if compared with the value for $PrNi_5$ (see Table I), we can see that the order of magnitude is preserved. In fact, this second fit was done in order to show that with a slightly different set of elastic constants, the agreement between experiment and theory is much better, in agreement with our guess. But, indeed, it was not done to state that the elastic constants for Y_2Fe_{17} can be determined in such a way. The half-bandwidths (W_0 and W_1) and $J'(r)$ values obtained from the first fit are quoted in Tables I and II, respectively. This value of $J'(r)$ could be compared with the value estimated from the slope of the Slater-Néel curve[37] at the $4f-12j$ sites distance of 2.7 Å. Such an estimation does not give a clear number; it seems only that the accepted value of $J'(r)$ (about -0.83 eV/atom) is of proper order of magnitude. However, even such an estimate does not take into account that the value quoted in Table I actually represents an effective one, which includes all kinds of Fe NN's in the Y_2Fe_{17} unit cell.[22,26] Let us add that the fitted value of the half-bandwidth W_1, 1.5 eV, is of reasonable order of magnitude for $3d$ systems.

B. Macroscopic two-ion magnetoelastic coupling parameters

Based only on symmetry arguments it is possible to show that for uniaxial symmetry the two-ion magnetoelastic energy can be written in the following phenomenological form:[16]

$$U_{\rm me}=-\overline{D}^{\alpha}_{11}\epsilon^{\alpha,1}-\overline{D}^{\alpha}_{21}\epsilon^{\alpha,2}-\frac{\sqrt{3}}{3}\overline{D}^{\alpha}_{12}\epsilon^{\alpha,1}[\alpha_3^2-\tfrac{1}{2}(\alpha_1^2+\alpha_2^2)]$$
$$-\frac{\sqrt{3}}{3}\overline{D}^{\alpha}_{22}\epsilon^{\alpha,2}[\alpha_3^2-\tfrac{1}{2}(\alpha_1^2+\alpha_2^2)], \quad (16)$$

where $(\alpha_1,\alpha_2,\alpha_3)$ are the direction cosines of the average magnetization, $\vec{M}$, with respect to the orthogonal crystal hexagonal cell axes and $\overline{D}^{\alpha}_{ij}$, the so-called two-ion phenomenological or macroscopic MEL coupling parameters, temperature and applied field dependent, i.e., $\overline{D}^{\alpha}_{ij}(H_{\rm appl},T)$. From Eq. (16) it is clearly recognized that $\overline{D}^{\alpha}_{11}$ and $\overline{D}^{\alpha}_{21}$ have their origin in isotropic two-ion interactions (i.e., the isotropic exchange), whereas $\overline{D}^{\alpha}_{12}$ and $\overline{D}^{\alpha}_{22}$ come from anisotropic interactions (i.e., anisotropic exchange and hopping). Following the discussion included in Sec. I, in Eq. (16) we have not included the single-ion CEF magnetoelastic energy [see Eq. (23) of paper I], inasmuch as this energy is irrelevant in order to calculate the *spontaneous* $\epsilon^{\alpha,1}(\vec{a})$ and $\epsilon^{\alpha,2}(\vec{a})$ strictions, as there is not magnetization rotation against magnetocrystalline anisotropy torques. As we did in paper I for the CEF origin magnetostriction, our model allows us to determine the above two-ion MEL parameters. In fact, taking the strain derivatives of Eqs. (11) and (16) and equating them, both for the spontaneous magnetization $\vec{M}_s$ along the $\vec{c}$ axis and within the basal plane (e.g., along the hexagonal unit cell $\vec{a}$ axis), it is possible to show that

$$\overline{D}^{\alpha}_{11}=-\frac{1}{3}\left[2\left.\frac{\partial U_{\rm me}}{\partial\epsilon^{\alpha,1}}\right|_{\vec{M}\|\vec{a}}+\left.\frac{\partial U_{\rm me}}{\partial\epsilon^{\alpha,1}}\right|_{\vec{M}\|\vec{c}}\right], \quad (17a)$$

$$\overline{D}^{\alpha}_{12}=\frac{2}{\sqrt{3}}\left[\left.\frac{\partial U_{\rm me}}{\partial\epsilon^{\alpha,1}}\right|_{\vec{M}\|\vec{a}}-\left.\frac{\partial U_{\rm me}}{\partial\epsilon^{\alpha,1}}\right|_{\vec{M}\|\vec{c}}\right], \quad (17b)$$

$$\overline{D}^{\alpha}_{21}=-\frac{1}{3}\left[2\left.\frac{\partial U_{\rm me}}{\partial\epsilon^{\alpha,2}}\right|_{\vec{M}\|\vec{a}}+\left.\frac{\partial U_{\rm me}}{\partial\epsilon^{\alpha,2}}\right|_{\vec{M}\|\vec{c}}\right], \quad (17c)$$

$$\overline{D}^{\alpha}_{22}=\frac{2}{\sqrt{3}}\left[\left.\frac{\partial U_{\rm me}}{\partial\epsilon^{\alpha,2}}\right|_{\vec{M}\|\vec{a}}-\left.\frac{\partial U_{\rm me}}{\partial\epsilon^{\alpha,2}}\right|_{\vec{M}\|\vec{c}}\right]. \quad (17d)$$

The derivatives of U_{me} in Eqs. (17) for $\vec{M}\|\vec{a}$ were obtained from the Y_2Fe_{17} *experimental* $\epsilon^{\alpha,i}$ strains using Eqs. (13). However, the derivatives for $\vec{M}\|\vec{c}$ were theoretically calculated from Eq. (11), because they are not experimentally accessible from the spontaneous thermal expansion strains. Notice that although the $\overline{D}^{\alpha}_{\rm ij}$ parameters do not explicitly depend on the elastic constants, the way of obtention of $\partial U_{\rm me}/\partial\epsilon^{\alpha,i}|_{\vec{M}\|\vec{a}}$ make them elastic constants dependent. We should point out again that for zero external applied magnetic field, $H_{\rm appl}$, the spontaneous two-ion magnetostriction in Y_2Fe_{17} should not include any substantial forced or paraprocess contribution,[3,16,17,19] where many-body electron effects can appear. However, if such an effect were present, our model is able to deal with the $\overline{D}^{\alpha}_{\rm ij}$ parameters calculation, in the way already discussed in Sec. II B. In Figs. 4(a) and 4(b) we present the temperature dependence of the zero applied magnetic field MEL parameters $\overline{D}^{\alpha}_{11}$,$\overline{D}^{\alpha}_{21}$ and $\overline{D}^{\alpha}_{12}$,$\overline{D}^{\alpha}_{22}$, respectively. In fact, this temperature variation is a consequence of the spontaneous magnetization temperature dependence. As we can see the values of the isotropic MEL parameters $\overline{D}^{\alpha}_{11}$ and $\overline{D}^{\alpha}_{21}$ are about *two orders* of magnitude larger than those for the anisotropic parameters $\overline{D}^{\alpha}_{12}$ and $\overline{D}^{\alpha}_{22}$. We stress that this rule was kept for a wide range of variations of the other parameters involved in the model.

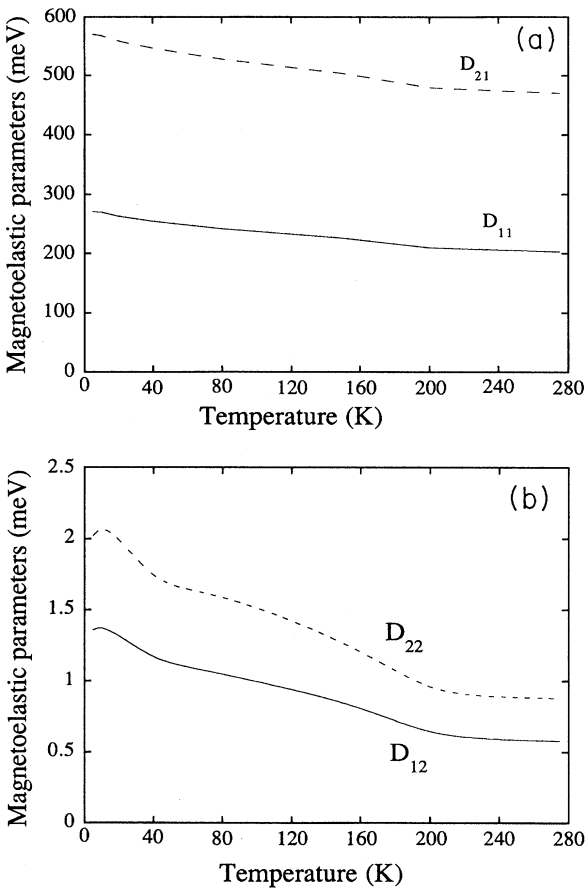

FIG. 4. (a) Model calculation of the temperature dependencies of the *macroscopic* or phenomenological two-ion isotropic magnetoelastic coupling parameters for Y_2Fe_{17} itinerant ferromagnet: $\overline{D}^{\alpha}_{11}$ (continuous line, —) and $\overline{D}^{\alpha}_{21}$ (dashed line, - - -) (see text for details and their meaning). (b) The same as (a), for the anisotropic magnetoelastic parameters: $\overline{D}^{\alpha}_{12}$ (continuous line, —) and $\overline{D}^{\alpha}_{22}$ (dashed line, - - -).

IV. DISCUSSION AND CONCLUSIONS

In this work we have performed calculations on the magnetoelastic coupling of the uniaxial itinerant ferromagnet Y_2Fe_{17} intermetallic compound, using a Stoner-like model for a degenerate rigid $3d$ band. We have assumed that yttrium has no magnetic moment, the $3d$-band magnetism coming from the Fe sublattice. Full details of the derivation of the magnetoelastic energy expression [Eq. (11)] can be found elsewhere.[15] We have made two strong, although rea-

sonable, assumptions. Because the $4f$-site Fe atoms, which form a dumbbell, are the only ones where the orbital angular momentum is not quenched by the crystal electric field, we have assumed that the unit formed by the dumbbell plus the hexagon of NN Fe atoms (see Fig. 1) gives the main contribution to the magnetostriction. In particular, the dumbbell has been treated using a two-site Hubbard Hamiltonian, and within the Hartree-Fock approximation for the Coulomb electron repulsion U term, which is strain independent. However, the exchange interaction of the dumbbell Fe atoms with the hexagon atoms have been only treated within the mean field approximation. Loosely speaking, the Y_2Fe_{17} unit cell (Th_2Ni_{17} structure) is formed by the stacking of atomic planes (perpendicular to the $\vec{c}$ axis), where the above units are inserted, surrounded by three Y^{3+} NN ions, and besides containing another Fe atoms hexagon. This layer is sandwiched by two planes containing two Fe atoms hexagons (sites $12k$ and $6g$).[26] Although for all the Fe atoms except for the $4f$ ones $\alpha=0$ in the Hamiltonian H_z [Eq. (4)], within the MF approximation they will contribute to H_z via the spin, and therefore their effect will be reflected in the energy eigenvalues of Eqs. (7). However, they will only modify the Eqs. (14) derivatives with extra terms of the same nature as $\partial H_{\rm eff}^{\rm b.p.}/\partial \epsilon^{\alpha,i}$. But we have found that such extra contributions are irrelevant compared with that provided by the dumbbell plus NN hexagon unit. More important is that for homogeneous strains, such contributions are not going to distort the $\epsilon^{\alpha,1}$ and $\epsilon^{\alpha,2}$ modes of deformation, calculated considering only the above units. In any case their little effect is also cast within our results if we consider $\partial H_{\rm eff}^{\rm b.p.}/\partial \epsilon^{\alpha,i}$ $(i=1,2)$ as effective values for the whole unit cell, and in turn the effect becomes reflected in the effective value of $J'(r)$ (by effective we understand a value which represents the whole iron sublattice). To go beyond the present approximation would make the problem practically intractable, because of the complexity of the unit cell and of the large number of exchange interactions involved.[22]

We should point out that the two-ion interaction MEL coupling parameters $\overline{D}_{ij}^{\alpha}$ for anisotropic itinerant systems are evaluated here. In paper I we evaluated the single-ion CEF anisotropic MEL parameters $\overline{M}_{12}^{\alpha}$ and $\overline{M}_{22}^{\alpha}$. There we made the assumption that two-ion interactions gave no significant contribution to the $\epsilon^{\alpha,i}$ $(\vec{c})$ strains, i.e., measured at $H_{\rm appl}=H_k$ for $\vec{M}\|\vec{c}$. Therefore two-ion contribution to the $\overline{M}_{i2}^{\alpha}$ parameters was neglected. Now we see that such an assumption was justified: the anisotropic MEL parameters $\overline{D}_{12}^{\alpha}$ and $\overline{D}_{22}^{\alpha}$, calculated on the basis of two-ion anisotropic hopping and isotropic exchange are about *one order* of magnitude smaller than the corresponding single-ion ones.

It is noticeable that the isotropic MEL parameters $\overline{D}_{i1}^{\alpha}$ are about two orders of magnitude bigger than the anisotropic $\overline{D}_{i2}^{\alpha}$ parameters [see Figs. 4(a) and 4(b), respectively]. The matter arises whether the calculation is reliable for parameters differing so much. We think that such an objection is not justified, because we have checked that the variation of the parameters of fitting does not influence the mutual relations between the values of the magnetoelastic parameters $\overline{D}_{ij}^{\alpha}$.

Some final remarks are pertinent here. For ferromagnetic insulators, it is quite usual to ascertain the origin of the observed magnetic anisotropy and magnetostriction in terms of the so-called Akulov laws, through the well known m^{α} powers of the reduced magnetization.[38] However, the theoretical interpretation of the magnetostriction results presented here and in paper I (Ref. 15), seem to indicate that the MEL phenomenological or macroscopic parameters in the uniaxial itinerant Y_2Fe_{17} iron-rich intermetallic compound can be classified into two classes of well differentiated *microscopic* mechanisms: of single-ion crystal field origin ($\overline{M}_{ij}^{\alpha}$ parameters), and of two-ion hopping and exchange origins ($\overline{D}_{ij}^{\alpha}$ parameters). We believe that this kind of classification could be very useful in order to improve our understanding of magnetostriction in $3d$ ferromagnetic metallic systems, and in general represents a valuable step forward in our understanding of the microscopic magnetoelastic coupling mechanisms.

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*On leave from the Faculty of Physics and Nuclear Techniques, University of Mining and Metallurgy, 30059 Cracow, Poland.

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