Magnetic anisotropy energy of disordered tetragonal Fe-Co systems from *ab initio* alloy theory

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We present results of systematic fully relativistic first-principles calculations of the uniaxial magnetic anisotropy energy (MAE) of a disordered and partially ordered tetragonal Fe-Co alloy using the coherent potential approximation (CPA). This alloy has recently become a promising system for thin ferromagnetic films with a perpendicular magnetic anisotropy. We find that existing theoretical approaches to homogeneous random bulk Fe-Co alloys, based on a simple virtual crystal approximation (VCA), overestimate the maximum MAE values obtained in the CPA by a factor of 4. This pronounced difference is ascribed to the strong disorder in the minority spin channel of real alloys, which is neglected in the VCA and which leads to a broadening of the d-like eigenstates at the Fermi energy and to the reduction of the MAE. The ordered Fe-Co alloys with a maximum $L1_0$-like atomic long-range order can exhibit high values of the MAE, which, however, get dramatically reduced by small perturbations of the perfect order.

I. INTRODUCTION

The binary ferromagnetic Fe-Co alloy has been known for a long time as a system with maximum spontaneous magnetization among the transition-metal systems.[1] Its basic magnetic properties, such as the concentration dependence of the alloy magnetization (the Slater-Pauling curve) in the ground-state body-centered-cubic (bcc) structure, have been reproduced successfully by *ab initio* electronic structure calculations in a number of studies.[2–4] This system attracted renewed interest several years ago, after a theoretical prediction of a giant uniaxial magnetic anisotropy energy (MAE) of the body-centered-tetragonal (bct) $Fe_{1-x}Co_x$ alloys.[5] The uniaxial MAE is defined quantitatively as the difference of total energies for the magnetization direction parallel to the tetragonal a and c axis $K_u = E^{(100)} - E^{(001)}$. The calculated MAE reached high values, $K_u \approx 800\ \mu eV/atom$, obtained however only in a narrow range of the Co concentration $0.55 \leqslant x \leqslant 0.65$ and of the tetragonal strain $1.2 \leqslant c/a \leqslant 1.25$. The combination of the high MAE with the high magnetization makes the bct Fe-Co system a promising material for fabrication of ferromagnetic thin films with a perpendicular magnetic anisotropy (the magnetic easy axis perpendicular to the film plane), which might be relevant as high-density magnetic recording media.

Most of the experimental realizations of this tetragonal system employed the possibility to grow epitaxially strained Fe-Co alloy films of varying composition on different non-magnetic transition-metal substrates with face-centered-cubic (fcc) structure, such as Pd(001), Rh(001), and Ir(001).[6,7] The different lattice parameters of the substrates enable one to scan a relatively wide interval of the c/a ratio of the Fe-Co films, namely $1.13 \leqslant c/a \leqslant 1.24$ (note that $c/a = 1$ and $c/a = \sqrt{2}$ refer, respectively, to the ideal bcc and fcc lattices). The measurements of the *in situ* magneto-optical Kerr effect[7] (MOKE)

confirmed the theoretical prediction of Ref. 5 on a qualitative level; in particular, a strong perpendicular magnetic anisotropy of the films was observed for compositions and tetragonal distortions in rough agreement with the calculated trends of the bulk K_u. However, systematic quantitative experimental studies of the MAE of the films have not been performed yet; available values of the K_u for a few selected systems[8–10] are appreciably smaller than the calculated ones. The missing information on the MAE has partly been compensated by measurements of x-ray magnetic circular dichroism (XMCD) spectra, which provide orbital magnetic moments of both alloy constituents.[6] The latter measurements, performed on the Rh(001) substrate corresponding to $c/a \approx 1.24$, revealed enhanced orbital moments in $Fe_{1-x}Co_x$ films around $x \approx 0.6$, in close relation to the predicted maximum of the bulk uniaxial MAE.

Nevertheless, the existing agreement between theory and experiment should be taken with caution. The original approach of Ref. 5 employed the so-called virtual crystal approximation (VCA), in which the true species of a random binary alloy are replaced by a single element with an effective atomic number given by the alloy composition. The VCA has been implemented in various *ab initio* methods and used for a number of alloys of neighboring elements in the Periodic Table.[3,11,12] Its application to the bcc Fe-Co and fcc Co-Ni systems[3,13] yields concentration trends of the spin magnetic moment in very good agreement with experiment;[1] the orbital magnetic moments seem to be described reliably in the VCA as well. However, a recent first-principles study of the random bct $Fe_{1-x}Co_x$ alloys,[14] based on a supercell technique applied to a few special Co concentrations ($x = 0.5, 0.625,$ and 0.75), has shown that a realistic treatment of the chemical disorder can reduce the MAE by a factor of 1.5–3 as compared to the simple VCA.

The main purpose of this work is to present and discuss the results of a systematic *ab initio* calculation of the MAE for the disordered bulk tetragonal Fe-Co systems obtained by using the coherent potential approximation (CPA) as a basic tool of the theory of metallic alloys.[15,16] For homogeneous bct alloys, we compare results of the VCA and the CPA, show the big difference between them, and identify the underlying physical mechanism in terms of the electronic structure. Moreover, we investigate the effect of a complete and an incomplete atomic long-range order on the MAE; this study is motivated by the existing prediction of a large uniaxial MAE in stoichiometric perfectly ordered tetragonal FeCo and $FeCo_3$ systems.[14] Similar theoretical studies have so far been done mainly for tetragonal FePt alloys[17–19] and very recently also for the FeCo alloy.[20] These works are confined to stoichiometric equiconcentration alloys; in general, their results reveal a decrease of the MAE due to imperfect chemical ordering.

II. MODELS AND COMPUTATIONAL DETAILS

All calculations of this study employed a bct lattice with the Wigner-Seitz s radius equal to that of pure bcc iron $s = 2.662\, a_0$, where $a_0 = 5.292 \times 10^{-11}$ m denotes the Bohr radius. The neglect of volume relaxations on the MAE in a broad range of lattice parameters and of alloy concentrations is justified by a more general study of Ref. 14 within the VCA. This structure model—the volume conserving tetragonal distortion (the Bain path)—coincides with that used in the original study[5] and in the recent study of the partially ordered FePt alloy.[19]

The effect of atomic long-range ordering has been studied for the case of $L1_0$ (CuAu) order relevant for compositions not far from the equiconcentration $Fe_{0.5}Co_{0.5}$ system. The bct structure is partitioned into two simple tetragonal sublattices (alternating atomic planes perpendicular to the tetragonal c axis). For the $Fe_{1-x}Co_x$ system, an additional concentration variable y is introduced, such that $0 \leqslant y \leqslant \min\{x, 1 - x\}$, which defines the chemical composition of both sublattices: $Fe_{1-x+y}Co_{x-y}$ in the Fe-enriched planes and $Fe_{1-x-y}Co_{x+y}$ in the Co-enriched planes. Note that the homogeneous solid solution corresponds to $y = 0$, while the other end of the y interval describes the maximum $L1_0$ order compatible with the given total Co concentration x. This model is a natural generalization of the model used for the stoichiometric FePt systems.[17–19]

The electronic structure calculations were done by means of the tight-binding linear muffin-tin orbital (TB-LMTO) method in the atomic sphere approximation (ASA)[21,22] with a full inclusion of relativistic effects by solving the one-electron Dirac equation[23,24] with the spd basis of the valence orbitals. The effective spin-polarized potential was constructed in the local spin-density approximation (LSDA) using the parametrization of the exchange-correlation term according to Ref. 25. The effects of alloying were treated in the CPA for all systems;[22,24] for the homogeneous random alloys ($y = 0$), the simple VCA was used as well.

The reliable evaluation of the MAE in metallic systems represents a difficult task, especially for cubic 3d transition metals owing to the weakness of the spin-orbit interaction and the high symmetry of cubic structures.[26,27] The situation is more favorable for uniaxial systems (tetragonal, trigonal, hexagonal)[28,29] and for systems with f electrons (see Ref. 30 for a review). In a number of existing studies, including the very recent ones,[5,14,19] the magnetic force theorem[31] is used and the total energy difference K_u is approximated by the change in the sum of occupied valence one-particle eigenvalues. In this study we go beyond this approximation and evaluate the MAE directly from the total energies of the fully self-consistent solutions for both magnetization directions,[14,26,32] which requires high accuracy in total-energy calculations. We have used uniform sampling meshes of about 10^5 **k** points for averages over the full Brillouin zone (BZ) of the bct lattices, while about 5×10^4 **k** points have been used for the BZ of the simple tetragonal Bravais lattices of the $L1_0$ ordered systems. The total energies were converged to 0.1 μeV/atom for all systems; this accuracy is sufficient in view of the resulting values of K_u (see below).

III. RESULTS AND DISCUSSION

A. Homogeneous random alloys

1. Magnetic anisotropy energy

The dependence of the uniaxial MAE of the random $Fe_{1-x}Co_x$ alloys on the chemical composition and the c/a ratio, calculated in the VCA and in the CPA, is shown in Fig. 1; for better transparency, only the positive values of the K_u are displayed in the plots, while the cases with negative K_u have been omitted (marked by white color). The VCA results [Fig. 1(a)] agree nicely with both previous
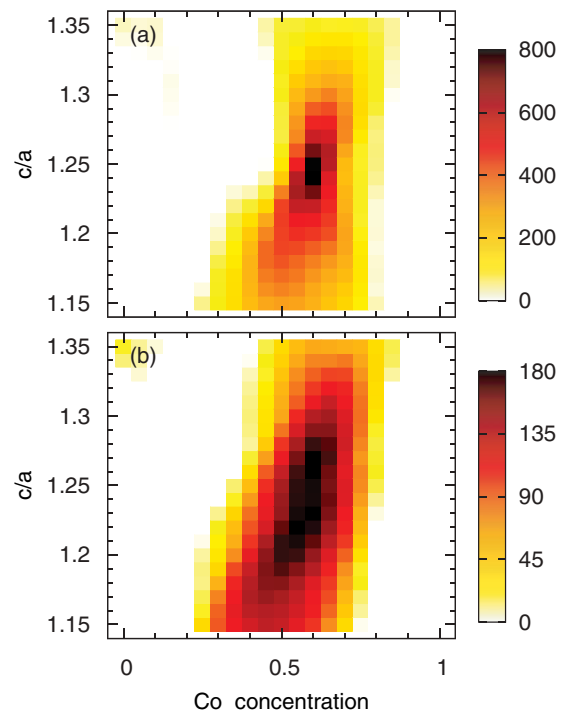

FIG. 1. (Color online) The uniaxial MAE of random bct $Fe_{1-x}Co_x$ alloys as a function of the Co concentration and of the tetragonal strain c/a: Calculated in the VCA (a) and in the CPA (b). Only positive values of the K_u are displayed in both plots; the corresponding colored scales are in μeV/atom.

studies;[5,14] in particular, a sharp maximum of the MAE, $K_u \approx 809\ \mu eV/atom$, obtained for $x = 0.6$ and $c/a = 1.24$, is clearly visible. The maximum MAE of $K_u \approx 800\ \mu eV/atom$ for $x = 0.6$ and for c/a between 1.22 and 1.24 was reported in Ref. 14 (with a slight sensitivity to the particular model of the volume relaxation employed) and practically the same values were obtained in the original VCA study.[5] Minor quantitative differences might be ascribed to different computational schemes employed. The MAE in the CPA [Fig. 1(b)] exhibits a similar trend as in the VCA; however, the CPA maximum is significantly smaller, $K_u \approx 183\ \mu eV/atom$. The latter value is obtained for $x = 0.6$ and $c/a = 1.23$, but the maximum is very flat and essentially the same K_u values can be found in a broad region of $0.5 \leqslant x \leqslant 0.65$ and $1.21 \leqslant c/a \leqslant 1.28$, see Fig. 1(b). The maximum K_u in the CPA is reduced by a factor of 4 as compared to that in the VCA, which is an even stronger reduction than that reported in Ref. 14.

The small MAE values in the CPA might be used to explain the difference between the large K_u values predicted in the VCA and the much smaller values inferred from measurements on thin Fe-Co films.[8–10] Undoubtedly, the better description of the chemical disorder in the CPA as compared to the VCA contributes to the reduction of the MAE of prepared alloy thin films. However, a thorough quantitative analysis of this point is impossible at present and it could even be misleading because of the well-known uncertainty of the LSDA to yield quantitatively correct MAEs in $3d$ transition-metal systems. For this reason, an analysis of the trends seems to be more appropriate (see, e.g., Ref. 29 and references therein).

In general, the LSDA underestimates both the MAEs and the orbital magnetism.[13,14,26,33] A counterexample to this rule is represented by the MAE of the ordered FePt alloy,[18,34] which is overestimated in the LSDA probably owing to an interplay of intra-atomic Coulomb correlations, weak exchange splitting, and strong spin-orbit interaction of Pt atoms.[34] The present results for the bct $Fe_{1-x}Co_x$ alloys seem to confirm the general rule as can be documented by two facts. First, the effective MAE of strained Fe-Co thin films, given by the difference of the bulk K_u and the magnetostatic shape anisotropy energy K_{sh}, comes out positive for alloys in the vicinity of $x \approx 0.6$ and $c/a \approx 1.25$ (near the maximum of K_u in the CPA). This situation would thus lead to an out-of-plane orientation of the thin-film magnetization, in a qualitative agreement with existing experiments.[7–10] Note that $K_{sh} = (\mu_0/2)M^2/V$, where μ_0 is the permeability of the vacuum and where M and V denote, respectively, the alloy magnetic moment per atom and the atomic volume. In the present case, $M \approx 2.14\ \mu_B$, where μ_B is the Bohr magneton, one obtains $K_{sh} \approx 132\ \mu eV/atom$, which lies below the bulk MAE $(K_u \approx 180\ \mu eV/atom)$. However, for the case of $x = 0.5$ and $c/a = 1.13$, corresponding roughly to the $Fe_{0.5}Co_{0.5}$ films grown on the Pd(001) substrate, our calculated values are $K_u = 124\ \mu eV/atom$, $M \approx 2.27\ \mu_B$, and $K_{sh} \approx 148\ \mu eV/atom$, which indicates an in-plane orientation of the magnetization, in contrast to the out-of-plane orientation observed at low temperatures.[7] Second, the calculated orbital magnetic moments in the bulk $Fe_{1-x}Co_x$ alloys, plotted in Fig. 2 for $x = 0.6$, are appreciably smaller than the values obtained from the measured XMCD spectra by employing the sum rules.[6] In particular, the measured values for films with $x = 0.6$ and $c/a = 1.24$, namely, $M_{orb}^{Fe} = 0.21 \pm 0.03\ \mu_B$

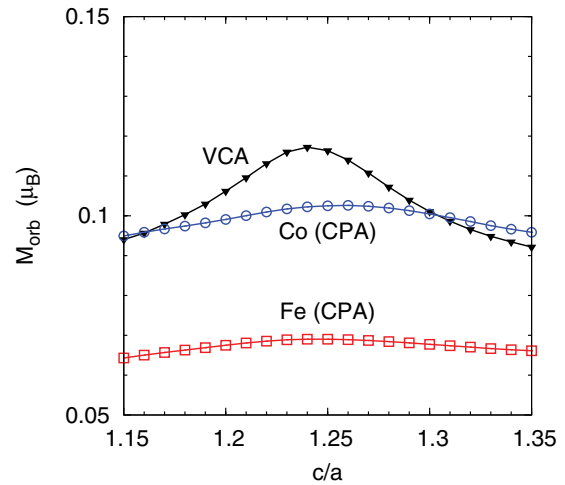FIG. 2. (Color online) The orbital magnetic moments in the random bct $Fe_{0.4}Co_{0.6}$ alloy with magnetization along z axis as functions of the c/a ratio: The alloy orbital moment in the VCA and the species-resolved orbital moments in the CPA.

and $M_{orb}^{Co} = 0.32 \pm 0.04\ \mu_B$, exceed their bulk theoretical counterparts by a factor of 3. A similar relation of the experiment and the LSDA theory (quantified roughly by a factor between 1.5 and 2) was obtained for bcc Fe-Co alloys.[3,13,33] Moreover, the data in Fig. 2 prove that the VCA and the CPA yield qualitatively different trends of the orbital magnetism versus the c/a ratio: The pronounced maximum at $c/a = 1.24$ in the VCA is replaced by very flat maxima of both local orbital moments in the CPA. This difference indicates that applicability of the VCA to all details of magnetism of the Fe-Co system is limited, being confined probably only to the cubic structures.[3,13]

In view of the above mentioned problems to evaluate reliably the MAEs and the orbital magnetic moments, we have not attempted to recalculate our results by techniques going beyond the LSDA,[26,29,30,33] but have focused on the strong difference between the VCA and the CPA and on the role of disorder on the MAE in the tetragonal Fe-Co systems.

2. Electronic structure

The giant MAE obtained in the VCA was ascribed originally to the changes in the band structure accompanying the tetragonal distortion of the effective FeCo crystal.[5] The explanation rests on a coincidence of two particular eigenvalues at the Γ point, which occurs in the minority spin (spin-down) channel. For a special alloy composition and a special c/a ratio, this coincidence takes place just at the Fermi energy corresponding to the particular filling of the spin-down band. The large contribution of this eigenvalue pair to the MAE can be understood in terms of the second-order perturbation theory, in which the effect of the weak spin-orbit interaction can be safely included.[35] In this approach the enhanced value of the K_u of the bulk Fe-Co alloys can be explained due to the coupling between $d_{x^2-y^2}$ and d_{xy} states mediated by the orbital momentum operator L_z (see Ref. 5 for details). The physical origin of the perpendicular magnetic anisotropy of the strained Fe-Co films is thus similar to that of Au covered Co monolayers on an Au(111) substrate.[36] In the latter case, however, the
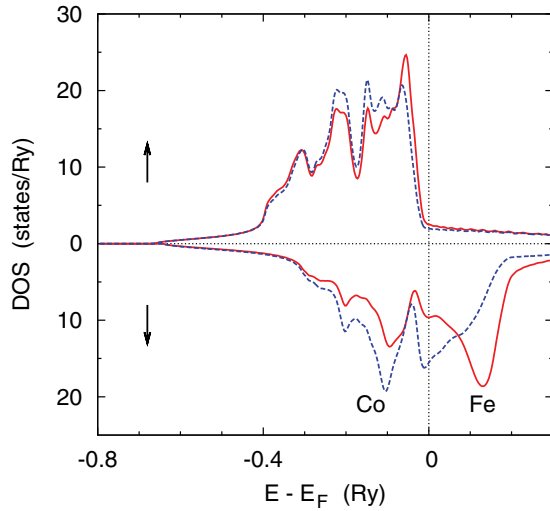
FIG. 3. (Color online) The spin-polarized local densities of states of the random bct $Fe_{0.4}Co_{0.6}$ alloy with $c/a = 1.25$ as functions of the energy. The dotted vertical line denotes the position of the Fermi level.

resulting positive MAE is caused by the L_z coupling between d_{xz} and d_{yz} states.

The usual band structures are not relevant for the electronic structure of random alloys, for which more appropriate quantities, such as the densities of states (DOS) and the Bloch spectral functions (BSF), have to be studied.[15,16,37] Motivated by the above explanation of the giant MAE, we present these quantities for the random bct $Fe_{1-x}Co_x$ alloys in the CPA, evaluated without the spin-orbit interaction, that is, in the scalar-relativistic approximation.[22,38]

The spin-polarized local DOSs are shown in Fig. 3 for the system with $x = 0.6$ and $c/a = 1.25$. The shapes of the individual DOSs prove a very weak disorder in the majority spin (spin-up) channel, whereas the spin-down band exhibits a regime of a stronger scattering. This type of spin-dependent disorder was found in the bcc Fe-Co system a long time ago;[2,4] it is responsible, for example, for the observed concentration trend of the residual resistivity.[39] Note that the strong disorder is present in the spin-down d band, which is only partially occupied and which thus contributes a lot to the alloy total energy and, consequently, to the MAE.

The spin-polarized BSFs at the Γ point for the $Fe_{0.4}Co_{0.6}$ alloy with three tetragonal distortions are plotted in Fig. 4. The BSFs were resolved according to the irreducible representations of the point group D_{4h} of the bct lattice.[40] The odd (ungerade) representations, belonging to p orbitals, have been omitted in the plots since their contribution is negligible in the displayed energy interval. The relevant even (gerade) representations are A_{1g} (orbitals s and d_{z^2}), B_{1g} ($d_{x^2-y^2}$), B_{2g} (d_{xy}), and E_g (d_{xz} and d_{yz}). One can see that all spin-up BSFs, consisting of narrow Lorentzian peaks, can be interpreted as Bloch-like eigenstates with finite lifetimes due to a weak disorder. The spin-down BSFs above the Fermi energy (mainly A_{1g}-like) reflect effects of strong disorder (nonquasiparticle behavior); the profiles at and below the Fermi energy are Lorentzian peaks again. However, their widths are clearly
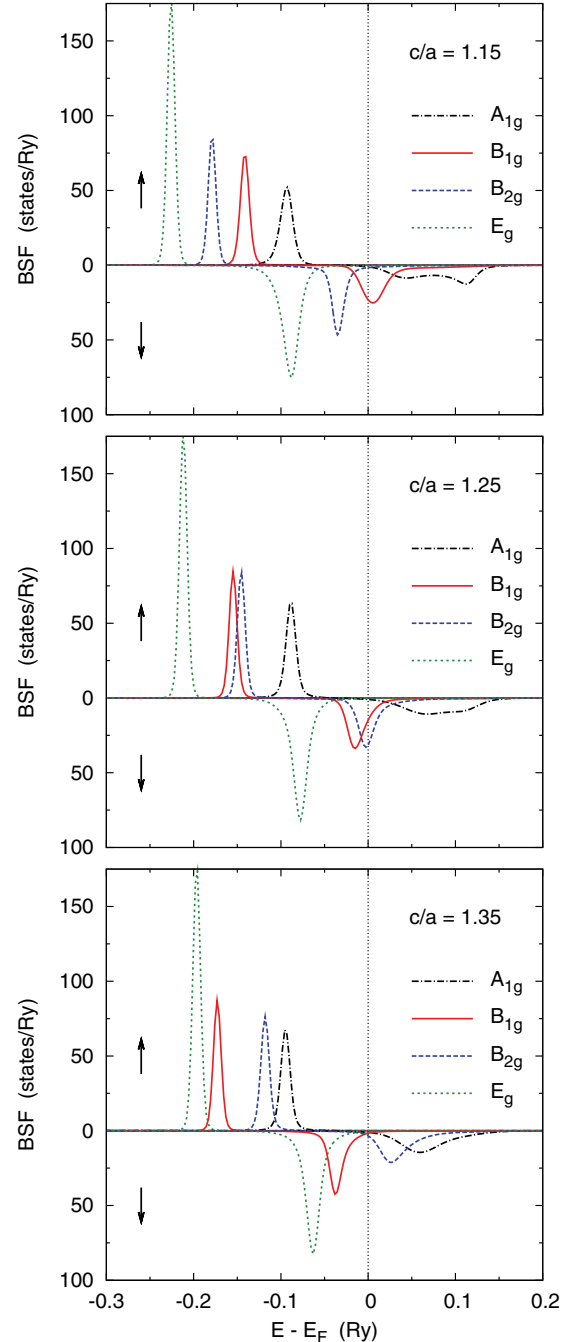

FIG. 4. (Color online) The spin-polarized symmetry-resolved Bloch spectral functions of the random bct $Fe_{0.4}Co_{0.6}$ alloy at $\mathbf{k} = \Gamma$ as functions of the energy for three values of the c/a ratio. The dotted vertical lines denote positions of the Fermi levels. For details see the text.

bigger than the spin-up widths, in agreement with the spin-dependent disorder manifested in the DOS.

The maximum of the MAE in the VCA is found for an alloy with $x = 0.6$ and with the tetragonal strain close to $c/a = 1.25$; its spin-down BSF in the CPA (Fig. 4, middle panel) shows an analogy of the coincidence of the B_{1g} ($d_{x^2-y^2}$) and B_{2g} (d_{xy}) levels at the Fermi energy. However, the disorder-induced smearing of both peaks is at least as big as their separation, which suppresses the contribution of

this eigenvalue pair to the MAE in the framework of the second-order perturbation theory. This feature proves that the minority-spin Fe-Co disorder is strong enough to reduce significantly the MAE, which explains the very big difference between the VCA and the CPA results, see Sec. III A 1.

B. Partially ordered alloys

The adopted model of the partially ordered tetragonal $Fe_{1-x}Co_x$ alloys, namely, the model of two sublattices with chemical compositions $Fe_{1-x+y}Co_{x-y}$ and $Fe_{1-x-y}Co_{x+y}$ (Sec. II) and the use of the CPA (in contrast to supercell techniques) enable one to study the MAE as a function of three continuous variables x, y, and c/a. Such a full three-dimensional scan is, however, computationally very demanding; we have thus confined our study to Co concentrations close to $x = 0.6$, for which the maximum MAE was found in the homogeneous bct alloys both in the VCA and in the CPA. The dependence of the calculated K_u on the tetragonal distortion for $x = 0.6$ is shown in Fig. 5 for three degrees of the $L1_0$ order. One can see that the very flat low maximum $K_u \approx 183\ \mu eV/atom$ for the completely disordered alloy ($y = 0$) treated in the CPA is replaced by a significantly enhanced pronounced maximum $K_u \approx 450\ \mu eV/atom$ obtained for the alloy with the maximum order ($y = 0.4$) compatible with the given Co concentration ($x = 0.6$). The latter maximum is about two times smaller than that in the VCA ($K_u \approx 809\ \mu eV/atom$), which can be ascribed to the fact that the system with $x = 0.6$ and $y = 0.4$ has one sublattice without disorder (pure Co), whereas the other one is disordered, containing the rest of Co and all Fe atoms. The MAE of the system with an intermediate degree of
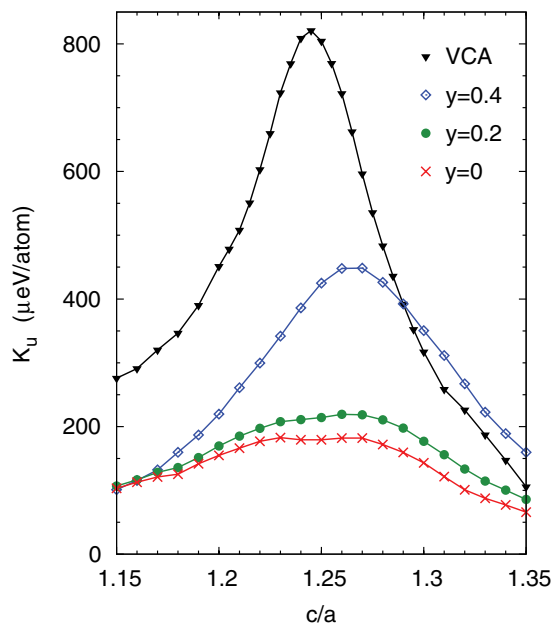

FIG. 5. (Color online) The uniaxial MAE of the bct $Fe_{0.4}Co_{0.6}$ alloy as a function of the tetragonal strain c/a for different degrees of the $L1_0$-like atomic order: The maximum order ($y = 0.4$, diamonds), an intermediate order ($y = 0.2$, full circles), and the complete randomness ($y = 0$, crosses), all treated in the CPA. For a comparison, the MAE of the completely random alloy in the VCA is displayed as well (triangles).
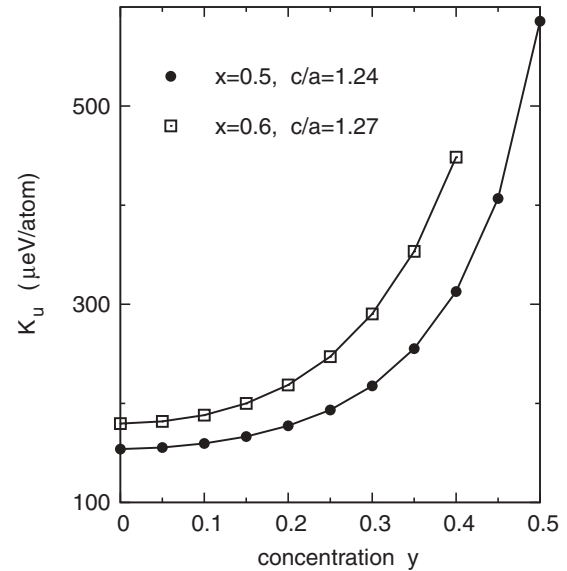

FIG. 6. The uniaxial MAE of two bct $Fe_{1-x}Co_x$ alloys as a function of the degree of the $L1_0$-like atomic order for $x = 0.5$ and $c/a = 1.24$ (full circles), and for $x = 0.6$ and $c/a = 1.27$ (open squares).

the $L1_0$ order ($y = 0.2$) exhibits the maximum and the trend very close to the fully disordered alloy.

The detailed dependence of the K_u on the concentration variable y is presented in Fig. 6 for two cases: The stoichiometric alloy ($x = 0.5$, $c/a = 1.24$) and the previous off-stoichiometric alloy ($x = 0.6$, $c/a = 1.27$). The particular values of the c/a ratio chosen in both cases correspond to the maximum K_u value obtained for alloys with the maximum order, that is, for $x = 0.6$, $y = 0.4$ (Fig. 5) and for $x = y = 0.5$. One can see that the perfectly ordered ($y = 0.5$) stoichiometric alloy leads to a very high MAE of $K_u \approx 580\ \mu eV/atom$. This value agrees well with Ref. 14, where the maximum MAE for the same $L1_0$ ordered system was obtained as $K_u \approx 520\ \mu eV/atom$. The convex shape of both dependencies in Fig. 6 proves that the very high MAEs can be obtained only for systems with the maximum order; even a small amount of additional disorder is detrimental to the MAEs and reduces them to much lower values of the completely random alloys.[20]

Strong sensitivity of the MAE to the degree of the $L1_0$ atomic order has recently been reported for the stoichiometric FePt alloy on an fcc lattice with small tetragonal distortions.[19] The results of Ref. 19 indicate that the chemical ordering is a more important factor for high MAE values than the tetragonal distortion. Our results for the Fe-Co system witness that both factors are of equal importance (see Fig. 5). We believe that validity of this type of conclusions depends also on the range of relevant variables: The tetragonal distortion was varied over a narrower interval ($0.94 \leqslant c/a \leqslant 1.06$) in Ref. 19, whereas a wider interval ($1.15 \leqslant c/a \leqslant 1.35$) has been covered in our study. Another difference between the two systems lies in the dependence of the MAE on the c/a ratio: The MAE is an ever increasing function of c/a in FePt,[19] in contrast to the maxima found for the Fe-Co systems around $c/a \approx 1.25$ (see Figs. 1 and 5). These trends reflect probably the different origins of the

high MAE in these systems. In the FePt alloys, the iron sites are responsible for strong exchange fields and the platinum sites provide strong spin-orbit interaction, both effects being only little dependent on the tetragonal distortion of the lattice. In the Fe-Co alloys, both species are featured by strong exchange splittings and weak spin-orbit couplings; the high MAEs are heavily based on collective properties (band structure) of the tetragonal systems.

IV. CONCLUSIONS

We have shown by means of first-principles LSDA calculations that chemical disorder has a strong influence on the uniaxial MAE of the bulk tetragonal Fe-Co systems. First, the complete neglect of the disorder, inherent to the simple VCA, overestimates the MAE by a large factor, whereas the more sophisticated CPA leads to a drastic reduction of the MAE. The latter low MAEs are quite close to the magnetic shape anisotropy energy and the resulting estimated stability of the perpendicular magnetic anisotropy of thin strained Fe-Co films comes out probably smaller than the measured one. Second,

the disorder-induced reduction of the MAE is due to the strong scattering regime in the minority-spin channel, which smears the Bloch-like eigenstates at the Fermi energy. Third, an analysis of the calculated orbital magnetic moments points to a non-negligible underestimation of the orbital magnetism and, most probably, of the MAEs by the LSDA. Fourth, the $L1_0$-like atomic long-range order leads to an enhancement of the MAE values. The most pronounced enhancement is obtained for the maximum degree of the order, while imperfect ordering reduces the MAE very rapidly as compared to the perfectly ordered systems. Similar correlations between the atomic order and the MAE have recently been found in the FePt alloy[17–19] and observed in artificially synthesized FeNi films.[41] We believe that this interplay should be taken into account in a future search of advanced materials for high-density magnetic recording.

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