

Giant magnetocrystalline anisotropy energy in Fe-Co alloy under uniaxial compression: A first-principles prediction

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Uniaxially strained Fe-Co disordered alloys have emerged as promising candidates for cost-effective (especially Fe-rich alloy), high Curie temperature (both Fe-rich and Co-rich), rare-earth-free permanent magnets due to their high magnetocrystalline anisotropy energy (MAE). Using first-principles, fully relativistic calculations within the coherent potential approximation and Perdew-Burke-Ernzerhof exchange-correlation potential, we explore the MAE of tetragonal Fe-Co alloys under uniaxial compression. Our results reveal a previously uncharted region of high MAE (exceeding 3 MJ m^{-3}) accessible via uniaxial compression. This phase, which lies between hexagonal-close-packed and body-centered-cubic structures, exhibits a high magnetic moment and Curie temperature, and thus offers a more stable candidate for experimental realization than the currently known high-MAE uniaxially strained Fe-Co.

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I. INTRODUCTION

The 2011 *rare-earth crisis* highlighted the vulnerability of the rare-earth elements market and spurred efforts to identify cost-effective, rare-earth-free permanent magnets [1]. This renewed interest also prompted a thorough revision of ideas proposed in the mid and late 20th century [2,3]. In particular, the disordered Fe-Co alloy with nearly 60 at.% of cobalt and an uniaxial tetragonal strain close to 22% has emerged as a promising candidate for a rare-earth-free permanent magnet already in 2004. Virtual crystal approximation (VCA) calculations predict for this alloy exceptional magnetic properties, including a giant magnetocrystalline anisotropy energy (MAE) of $\sim 800 \mu\text{eV atom}^{-1}$, a significant magnetic moment of $2.5 \mu_{\text{B}} \text{ atom}^{-1}$ [4], and a high Curie temperature (T_{C}) exceeding 1000°C [5,6].

The synthesis of epitaxial films along Bain's path [7] has been proposed as a viable fabrication route for this alloy [4], leading to several experimental realizations in 2006–2009 [8–11]. At the same time, progress towards obtaining bulk structures was made [12,13], and epitaxial FeCo growth on AuCu substrates was demonstrated [14,15]. A limitation, however, is that both ordered and disordered Fe-Co alloys have been shown to rapidly relax into the cubic bcc structure beyond a critical thickness of about 15 atomic monolayers ($\sim 2 \text{ nm}$) [16]. This structural relaxation can be partly mitigated by interstitial doping with smaller atoms such as B, C, or N—as supported by both theoretical predictions [17,18] and experimental evidence [14,19–21].

Further theoretical studies—conducted between 2011 and 2016—explain this relaxation and lower-than-expected measured MAE values. It has been shown that VCA applied to model chemical disorder in Ref. [4] tends to overestimate the MAE in Fe-Co systems. More advanced chemical disorder treatment methods yield substantially smaller MAE, approaching $200 \mu\text{eV atom}^{-1}$ ($\sim 2.5 \text{ MJ m}^{-3}$) for an optimal lattice parameter c/a ratio of 1.22 [17,18,22,23]—a value in agreement with experimental data, yet still of considerable technological importance.

The distinctive magnetic properties of Fe-Co alloy in the body-centered-tetragonal (bct) structure, with c/a ratio close

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to 1.22, are attributed to symmetry changes in hybridized orbitals of iron and cobalt [4], together with the strong Fe-Co exchange interactions [24]. Since other symmetry changes can similarly alter the chemical environment, it is also essential to investigate the magnetic properties of Fe-Co alloys along alternative lattice transformation pathways.

Thus, in this work, we complement the transformation along Bain's path with a particular bcc $\leftrightarrow$ hcp martensitic phase transition pathway, first described by Burgers [25]. This transition involves two steps: uniaxial compression along one of the main crystallographic axes, followed by the perpendicular slip of one of the two hexagonal atomic planes formed during such deformation. In general, incorporating hexagonal cell shear in addition to the plane slip allows the description of broader fcc $\leftrightarrow$ hcp $\leftrightarrow$ bcc $\leftrightarrow$ fcc transitions [26–28]. In practice, combined uniaxial deformation and shear (or slip) is often considered the most likely path [29,30]. The described deformation continues the well-known tetragonal distortion along Bain's path into the $c/a < 1$ regime [31]. The intermediate structure, for which the coordination number of the atoms changes to 10, is denoted further as bct₁₀ and has been studied for various elements [32].

II. MAGNETOCRYSTALLINE ANISOTROPY ENERGY AND MONTE CARLO CURIE TEMPERATURE

First, we examined the Fe_{1-x}Co_x system under a broad range of uniaxial tetragonal distortion. We chose the phase-space region spanning from $c/a \approx 1.42$ (fcc structure) through the bcc phase, the bct₁₀ phase in the Burgers transformation [$c/a = \sqrt{2/3} \approx 0.82$, in which the bct (110) plane is transformed into the hexagonal (0001) plane], down to $c/a \approx 0.7$. Below, we summarize the computational approach used to evaluate the MAE and to obtain an initial estimate of T_C , followed by a discussion of the results.

We employed the spin-polarized relativistic Korringa-Kohn-Rostoker method, implemented in SPR-KKR version 7.7.1 [33]. A two-atom basis and space group $P4/mmm$ were used to ensure consistency in basis and symmetry across the full distortion range. Each site was occupied evenly, with chemical disorder treated via the coherent potential approximation (CPA). We use the single-site CPA since we are considering only perfectly disordered alloys. In such cases, the nonlocal scattering path operator accounts equally for scattering from all possible atomic configurations. Furthermore, for C-doped disordered FeCo, it has been shown that probing a substantial portion of the configuration space does not significantly alter the magnetic properties, unless the mixing enthalpy is taken into account [18]. For the exchange-correlation potential, we used the generalized gradient approximation (GGA) with the Perdew, Burke, and Ernzerhof (PBE) parametrization [34], without the shape approximation (full potential approach).

We optimized the unit-cell volume for various cobalt concentrations x in Fe_{1-x}Co_x, with a 10% step. Convergence tests indicated a requirement of at least 10 000 **k**-points and an angular momentum expansion cutoff $l_{\max} = 4$ to properly capture the hybridization of Fe/Co 3d orbitals [35].

To assess the dependence of MAE on c/a and cobalt concentration x , we employed a constant-volume approach, in

which the lattice parameters were rescaled to preserve the computational cell volume optimized for each cobalt concentration. The MAE of each structure was determined by calculating the energy difference between the [001] and [100] magnetization directions as follows:

$$\text{MAE} = E_{100} - E_{001}, \quad (1)$$

with the energies calculated in the four-component relativistic formalism, including the spin-orbit coupling.

The nonmagnetic global energy minimum of fcc iron has been thoroughly investigated in numerous works, including key Fe_{1-x}Co_x studies [22,23,31,36]. Thus, we focus on the high-spin (HS) fcc phase [37], which has recently attracted attention in layered and nanoscale systems [38,39].

We began by comparing the MAE of the tetragonally strained structure, shown in Fig. 1(a), to the results of works by Burkert *et al.* [31], Turek *et al.* [22], Steiner *et al.* [23], and Neise *et al.* [36]. Our calculated MAE maximum—of about 200 $\mu\text{eV atom}^{-1}$ (2.5 MJ m^{-3}) for $c/a = 1.22$ and $x = 0.6$ —is in good agreement with results obtained previously using CPA and explicit random alloy models. As expected, this value is about four times lower than the 800 $\mu\text{eV atom}^{-1}$, initially predicted by Burkert *et al.* The overall features, such as the observed uniaxial MAE maximum and the in-plane anisotropy region for the Co-rich system, are consistent with previous findings. The noticeable difference is the complete vanishing of the MAE when considering the fcc iron HS phase, whereas prior studies reported a minor residual MAE. Importantly, we uncover a second, prominent MAE maximum for Fe_{1-x}Co_x under strong uniaxial compression, spanning a wide range of x for the Co-rich structures. The MAE value near this maximum easily exceeds 3 MJ m^{-3} and is an order of magnitude higher than that of the bulk hcp cobalt [40,41].

Qualitatively, the aspects of our results corresponding to stoichiometric FeCo are consistent with the recent findings of Wolloch and Suess [42]. However, quantitative comparisons are limited, as our approach neglects surface effects, and their study employs only a limited number of special quasirandom structure models. In Fig. 1(b), we see that the MAE increases sharply with c/a decreasing to around 0.85 and remains stable during further compression down to around $c/a = 0.78$ —a region neighboring the bct₁₀ structure. Afterward, it increases sharply even more, then drops again. This extreme compression, however, is accompanied by a rapid increase in total energy, as discussed below.

We find that for cobalt concentrations around 0.75, a high uniaxial MAE in the strained structure is accompanied by a similarly high MAE under equivalent compression. Consequently, when the average distance between certain neighbors increases (e.g., due to interstitial doping or finite-temperature vibrations), other interatomic distances decrease, which can further enhance MAE. This explains the appearance of a broader MAE maximum, shifted toward higher cobalt concentrations, as observed in studies using various configurational space sampling methods in B- and C-doped Fe-Co [17,18,36]. Related phonon-assisted magnetic effects have also been discussed for Co-doped iron garnets [43].

Based on the self-consistently converged electron density, for $x = 0.7$, we calculated exchange integrals J_{ij} up to the ninth neighboring cell using the Lichtenstein *et al.* method [44]

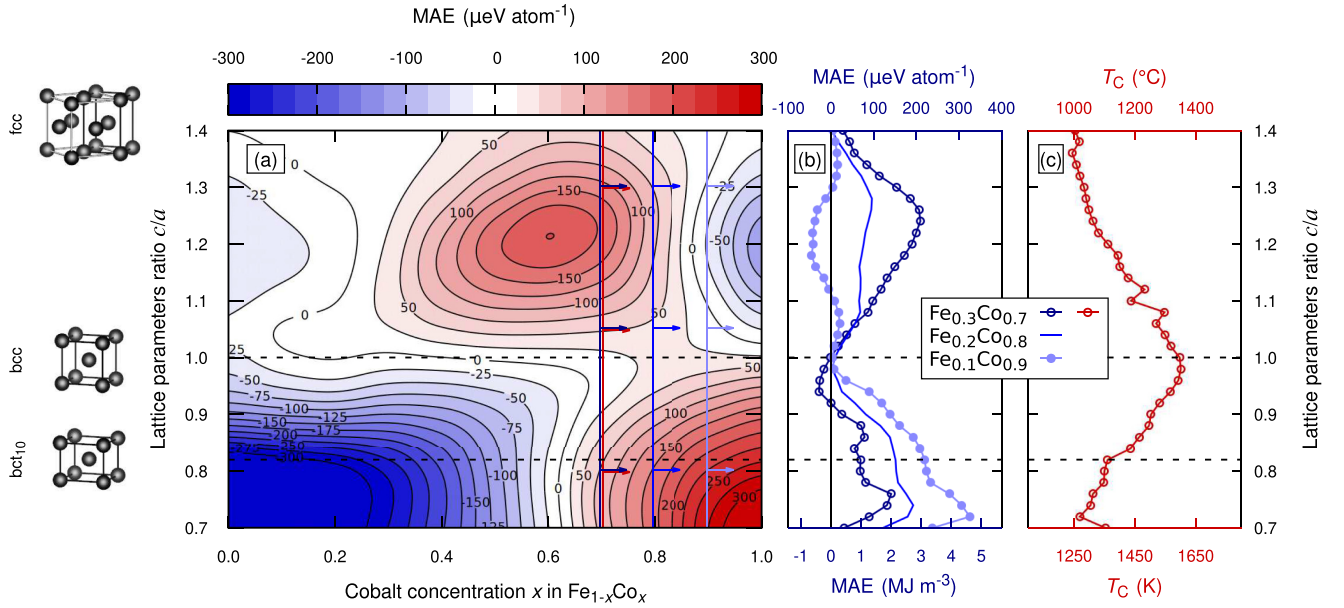


FIG. 1. Magnetic properties of $\text{Fe}_{1-x}\text{Co}_x$ alloys under tetragonal deformation. Icons on the left present the structure distortion, with light gray lines in the fcc structure depicting the conventional four-atom unit cell. Panel (a) presents a Gaussian-smoothed map of MAE calculated in the coherent potential approximation (CPA) of chemical disorder treatment. Panel (b) displays the raw, nonapproximated data for three different cobalt concentrations: $x = 0.7$ (dark blue, empty circles), $x = 0.8$ (blue, solid line), and $x = 0.9$ (light blue, filled circles). Panel (c) shows T_C as obtained from Monte Carlo simulations for $x = 0.7$.

implemented in the SPR-KKR package. Those were subsequently used for Monte Carlo simulations in the Uppsala Atomistic Spin Dynamics (UPPSAD) package [45]. The Curie temperature was determined using the Binder cumulant method, incorporating finite-size scaling [45–47].

Figure 1(c) shows the estimated T_C values derived from the intersection of the Binder cumulant versus temperature curves in two supercells—sized 25^3 and 30^3 —based on the methodology outlined in Ref. [47]. Our calculations suggest that for the bct₁₀ structure, the expected T_C ranges between 1250 and 1350 K, a highly suitable value for high-temperature permanent magnet applications. These estimates align with prior results from the group of Blügel using mean-field theory [5,48], which reported T_C values of 1550 K for bcc $\text{Fe}_{0.3}\text{Co}_{0.7}$ and 1520 K for bcc $\text{Fe}_{0.25}\text{Co}_{0.75}$, with an approximate 20% T_C reduction under uniaxial compression. It also fits well within the limits set by experimental measurements—1044 K for bulk bcc Fe [49,50], 1450 K for the high-temperature fcc Co phase (γ -Co) [51], and about 1250 K in $\text{Fe}_{1-x}\text{Co}_x$ alloys near $x \sim 0.35$ –0.45. Additionally, we observe that the T_C versus c/a dependence is slightly asymmetric, favoring uniaxial compression over uniaxial strain.

III. CURIE TEMPERATURE WITH DISORDERED LOCAL MOMENTS AND SPIN MAGNETIC MOMENT

Due to computational limitations, we were restricted in performing high-accuracy Monte Carlo T_C calculations. In this section, we complement this limited quantitative result with a broader qualitative overview of Curie temperatures and magnetic moments across the entire range of simulated distortions.

As the main computational approach, we employed the disordered local moment (DLM) method to derive a qualitative map of the critical temperature across the same c/a and x ranges as described above. In DLM, the paramagnetic state is approximated by a CPA-like configuration, in which each atomic site hosts mixed antiparallel magnetic moments (DLM state). The critical temperature of the ferromagnetic system can then be related to thermal energy and estimated approximately as follows [52,53]:

$$T_{\text{critical}}^{\text{DLM}} = \frac{2}{3} \frac{E_{\text{DLM}} - E_{\text{FM}}}{k_B \cdot c_{\text{mag}}}, \quad (2)$$

if the ferromagnetic state is energetically favorable, and

$$T_{\text{critical}}^{\text{DLM}} = 0 \quad (3)$$

otherwise, where E_{DLM} and E_{FM} are the energies of the DLM and ferromagnetic states, respectively, c_{mag} is the total concentration of magnetic atoms in the system, and k_B is the Boltzmann constant.

In Fig. 2, we present a calculated T_C^{DLM} map alongside the corresponding magnetic moments map. Since the DLM state is susceptible to a collapse of the magnetic moment, we could not obtain a stable paramagnetic HS state. Consequently, as shown in Fig. 2(a), T_C tends toward zero when approaching the iron fcc phase. In contrast, as depicted in Fig. 2(b), the ferromagnetic HS phase was successfully reproduced, with a magnetic moment value of $2.5 \mu_B \text{ atom}^{-1}$, consistent with previous studies [37,39]. This value is slightly higher than $2.22 \mu_B$ measured experimentally in bcc Fe and comes mainly from the spin contribution, similarly to experiment [49]. On the Co side, comparison to experiment also shows a good agreement. The stable hcp and fcc phases of Co exhibit a total magnetic moment of 1.67 – $1.75 \mu_B \text{ atom}^{-1}$.

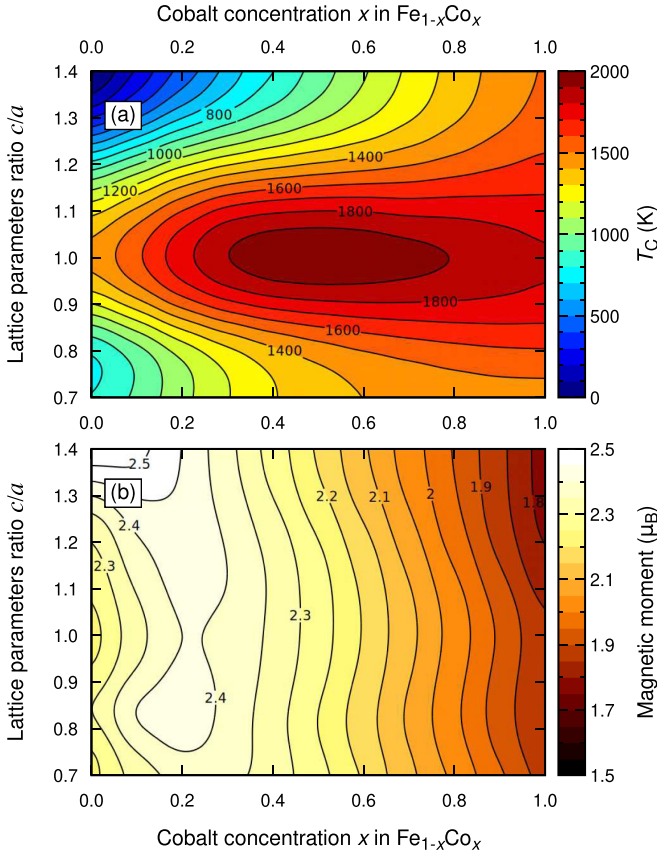


FIG. 2. (a) Curie temperature (T_C) vs c/a lattice parameters ratio and cobalt concentration x for the $\text{Fe}_{1-x}\text{Co}_x$ alloy under tetragonal deformation. (b) Corresponding total (spin + orbital) magnetic moment map of the ferromagnetic $\text{Fe}_{1-x}\text{Co}_x$. Calculations were performed using the SPR-KKR 7.7.1 package, employing CPA for chemical disorder and the PBE exchange-correlation potential. T_C was estimated using the disordered local moments (DLM) method.

[54–56], whereas metastable bcc Co phases show a broader range (1.26–1.77 μ_B atom⁻¹) due to epitaxial stress [56–59]. We fall exactly within this range, close to its upper limit ($\sim 1.75 \mu_B$ atom⁻¹) in the case of bcc Co.

Both T_C and the magnetic moment display Slater-Pauling-like [60] maxima for near-cubic structures: around $x \approx 0.5$ for T_C and $x \approx 0.2$ for the magnetic moment. This maximum is slightly shifted relative to experiments, where it occurs at $x \approx 0.35$. It results from an increase in the spin moment of the Fe atoms to a value of 2.4–3.0 μ_B , while the local spin moments of Co remain stable at 1.7–1.8 μ_B [61–63]. Both maps show promising results, with slightly asymmetric dependencies that favor the compressed structure across most cobalt concentrations. Weak minima are observed in the magnetic moment versus c/a dependency at $c/a \approx 0.82$ and cobalt concentrations above $x = 0.4$. Given that the DLM method typically overestimates the result by approximately 30% [33,64,65], we estimate that T_C for Co-rich bct₁₀ structures should lie between 1250 and 1350 K. We also expect the average magnetic moment to remain considerably high, between 1.8 and 2.2 μ_B atom⁻¹. After accounting for the expected overestimation by the DLM method, our results

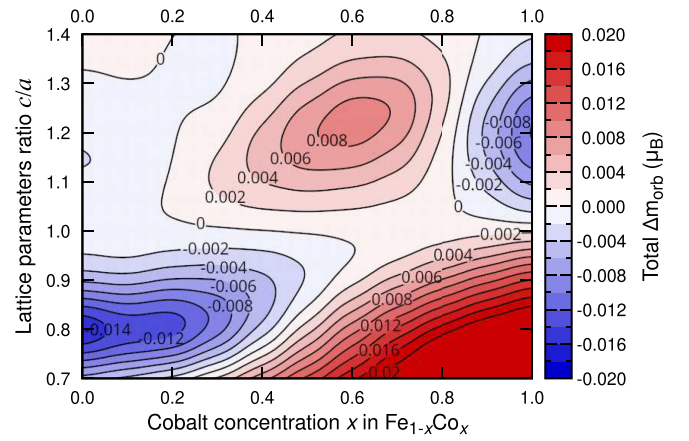


FIG. 3. Total (weighted by composition) anisotropy in orbital magnetic moment per atom vs c/a lattice parameters ratio and cobalt concentration x for the $\text{Fe}_{1-x}\text{Co}_x$ alloy under tetragonal deformation. Calculations were performed using the SPR-KKR 7.7.1 package, employing CPA for chemical disorder.

agree with both our Monte Carlo calculations [Fig. 1(c)] and previous work by the group of Blügel [5,48]. Specifically, our findings align with the high T_C values predicted for body-centered-tetragonal cobalt [5].

IV. MICROSCOPIC ORIGIN OF THE MAGNETOCRYSTALLINE ANISOTROPY ENERGY

In this section, we discuss the microscopic mechanisms that lead to the formation of local MAE maxima in deformed FeCo alloys. We focus on analyzing (i) the correlation between magnetocrystalline anisotropy and orbital magnetic moment anisotropy, and (ii) the orbital-resolved densities of states. We base our analysis on the detailed description of MAE in a tetragonal crystal provided by Miura and Okabayashi [66]. They expressed MAE based on contributions from orbital magnetic moment (Bruno [67]) and spin density quadrupole moment (van der Laan [68]). In their formulation,

$$\text{MAE} \approx \underbrace{\frac{1}{4} \sum_I \xi_I \Delta m_{\text{orb}}^I}_{\text{Bruno}} + \underbrace{\frac{21}{8} \sum_I \frac{\xi_I^2}{\Delta_{\text{exc}}} m_T^I}_{\text{van der Laan}}, \quad (4)$$

where ξ_I is the spin-orbit coupling parameter at site I , Δ_{exc} is the exchange splitting, Δm_{orb}^I is the orbital moment anisotropy, and m_T^I is the intra-atomic magnetic dipole term, which can be expressed via orbital-projected spin moments.

A. The correlation between MAE and orbital magnetic moment anisotropy

We start by looking at the anisotropy of the orbital magnetic moments Δm_{orb}^I , see Fig. 3. For the uniaxially strained alloys, the Δm_{orb} map qualitatively coincides with the MAE map shown in Fig. 1, which confirms that the Burkert MAE maximum in Fe-Co is dictated by the Bruno contribution from Eq. (4). For the structure under moderate compression of up to 10%, the situation is similar. Such a result agrees with

the findings and interpretation of voltage-controlled magnetocrystalline anisotropy measurements and calculations for thin layers performed for Co by Kawabe *et al.* [69], for Fe by Kobayashi *et al.* [70], and for FeCo by Ong *et al.* [71]. The cited works attribute the interfacial magnetism in both biased and unbiased systems to the anisotropy of the orbital magnetic moment. However, in the strongly compressed structure ($c/a \lesssim 0.9$), the similarity between Δm_{orb} and MAE maps is not conserved, indicating a possible significant contribution from another source. We observe particularly large discrepancies across a wide range of intermediate concentrations. In conclusion, for both the strained and compressed structures, near the MAE maxima, the main contributions to the MAE are clearly related to the anisotropy of the orbital magnetic moment. At the same time, the contributions to MAE in strongly compressed phases are mixed, and another component becomes significant at intermediate Co concentrations.

To further investigate the contribution stemming from orbital magnetic moment, in Fig. 4 we present the element-resolved contributions to the orbital magnetic moments in the system, along with the total per-site m_{orb} . The total m_{orb} shows trends analogous to the absolute values of the data presented in Figs. 1 and 3. It rises from $0.047 \mu_B$ for bcc Fe to $0.08 \mu_B$ for bcc Co. For intermediate concentrations, m_{orb} rises when the tetragonal distortion is introduced and drops again for the fcc structure. Due to the method used (plain GGA-PBE), those values are expected to be lower than experimental ones, but they adhere to the qualitative trends.

As determined experimentally, in the bcc Fe the orbital magnetic moment per atom is strongly quenched and equals $0.086\text{--}0.092 \mu_B$ [54,72]. For pure Co the value of m_{orb} is higher and reaches $0.13 \mu_B$ in the hcp phase [73] and $0.147 \mu_B$ in cubic systems [54,55]. For the intermediate Fe/Co concentrations, the orbital magnetic moment is quenched and equal to about $0.05\text{--}0.08 \mu_B \text{ atom}^{-1}$ [74]. By contrast, when tetragonal deformation is introduced ($c/a \neq 1$), x-ray magnetic circular dichroism (XMCD) experiments demonstrate a partial unblocking of the orbital magnetic moment, raising it to $0.15\text{--}0.20 \mu_B \text{ atom}^{-1}$ [74]. This effect is further underscored by measurements on bct films, which showed that near $c/a \approx 1.2$, the anisotropy of the orbital magnetic moment (Δm_{orb}) increases from about zero to $0.06\text{--}0.09 \mu_B$ [75]. Our results are consistent with this behavior, as m_{orb} calculated by us is roughly half of the experimentally measured systems in each of those cases.

Looking at the element-resolved contributions, one can see that the orbital magnetic moment on Fe does not show significant changes over the considered concentration range. It is the contribution from Co that mostly accounts for the qualitative agreement between orbital magnetic moments and MAE maps. Hence, we conclude that the giant MAE in $\text{Fe}_{1-x}\text{Co}_x$ follows the Bruno formula, and the main contribution to MAE for both maxima comes from the Co orbital magnetic moment. As the main contribution comes from the orbital magnetic moment, it arises in the configurational space regions associated with the symmetry transition—halfway between bcc and fcc along the Bain path in the case of the Burkert maximum [4], and for the bct₁₀ structure in the case of our newly reported maximum.

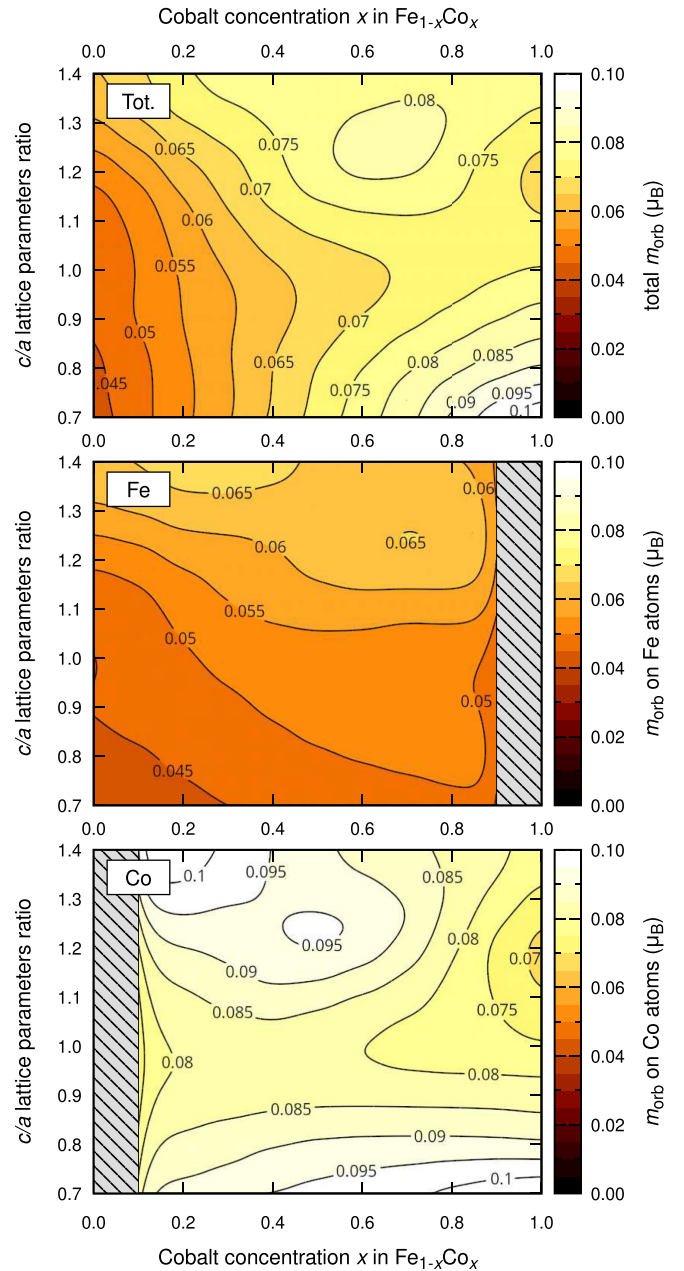


FIG. 4. Total (weighted by composition) orbital magnetic moment per atom, orbital magnetic moment per Fe atom, and orbital magnetic moment per Co atom vs c/a lattice parameters ratio and cobalt concentration x for the $\text{Fe}_{1-x}\text{Co}_x$ alloy under tetragonal deformation. Calculations were performed using the SPR-KKR 7.7.1 package, employing CPA for chemical disorder. Grayed-out regions in Fe and Co partial magnetic moment maps denote a virtual alloy with under 10% of Fe and Co, respectively.

B. Orbital-resolved densities of states

Figures 3 and 4 show that changes in the MAE values are largely due to the Co contributions, especially in the interesting range of high Co concentrations and strong compression. Therefore, we select pure Co for the analysis of the orbital-resolved densities-of-states contribution to MAE, within the framework of second-order perturbation theory. We perform our qualitative analysis in the spirit of more advanced

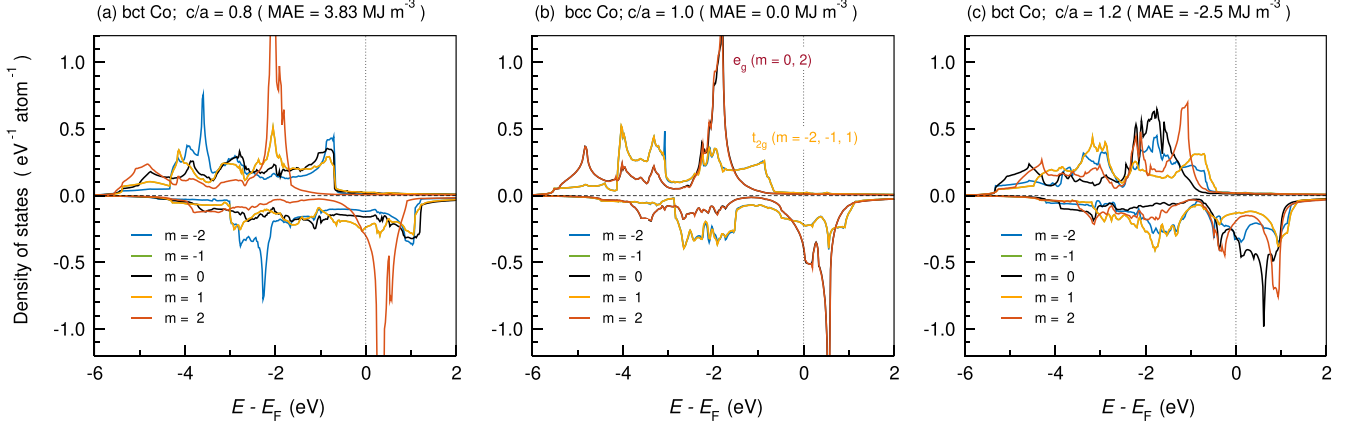


FIG. 5. Density of 3d states of body-centered-tetragonal Co, split according to magnetic quantum number (m). Panels (a), (b), and (c) for lattice parameter ratios c/a of 0.8, 1.0, and 1.2, respectively. For the cubic case [$c/a = 1.0$, panel (b)], the five 3d states split into two nearly degenerate groups in accordance with the crystal-field-splitting theory. The t_{2g} group consists of states with $m = -2, -1, 1$ (which correlate with the d_{xy} and d_{xz}/d_{yz} real orbitals). The e_g group consists of states with $m = 2, 0$ (corresponding to the $d_{x^2-y^2}$ and d_{z^2} real orbitals). For the deformed cases [(a) and (c)], only the solutions with quantum numbers $m = -1$ and 1 (d_{xz}/d_{yz}) overlap. Fully relativistic results with the [001] magnetization axis were obtained with the FPLO-PBE approach.

quantitative studies, such as those made by Masuda and Miura [76]. For this, we use fully relativistic calculations with the full-potential local-orbital FPLO18.00-52 code [77,78].

Figure 5 presents the orbital-resolved densities of states calculated for the Co 3d states for c/a ratios of 0.8, 1.0, and 1.2. For the cubic Co [panel (b)], the five states with different magnetic quantum number m split into two nearly degenerate groups—in accordance with the crystal-field splitting theory. The first group, t_{2g} , consists of states $m = -2, -1$, and 1 (corresponding to the d_{xy} and d_{xz}/d_{yz} real orbitals). The second group, e_g , consists of states $m = 2$ and 0 (corresponding to the $d_{x^2-y^2}$ and d_{z^2} real orbitals). In this cubic phase, the magnetocrystalline anisotropy vanishes (MAE = 0) due to the perfect balance of the orbital contributions.

Conversely, tetragonal deformation breaks the cubic symmetry and significantly redistributes the t_{2g} and e_g states. For the compressed bct Co phase with $c/a = 0.8$ [panel (a)], the majority spin channel is located below the Fermi level and nearly fully occupied, which severely limits the possibility of spin-flip processes (van der Laan term). According to second-order perturbation theory, the giant positive MAE of 3.83 MJ m^{-3} of this phase arises from the interaction of spin-conserving states in the minority spin channel (Bruno term). In the discussed minority spin channel, a notable feature is a nondegenerate peak of the orbital with quantum number $m = 2$ ($d_{x^2-y^2}$). Its sharp maximum is located at approximately 0.4 eV above the Fermi level. In our case, the MAE can be estimated by considering only spin-conserving transitions between occupied and unoccupied states in the minority spin channel:

$$\text{MAE} \approx \xi^2 \sum_{o,u} \frac{|\langle \psi_o | \hat{L}_z | \psi_u \rangle|^2 - |\langle \psi_o | \hat{L}_{x,y} | \psi_u \rangle|^2}{\epsilon_u - \epsilon_o}, \quad (5)$$

where ξ is the spin-orbit coupling constant, and $\hat{L}_z$ and $\hat{L}_{x,y}$ denote, respectively, the out-of-plane and in-plane components of the orbital angular momentum operator. The indices o and u denote occupied and unoccupied states, respectively,

with single-particle energies ϵ_o and ϵ_u . The presence of a nonbinding van Hove singularity with $m = 2$ in the immediate vicinity of the Fermi level minimizes the energy denominator $\epsilon_u - \epsilon_o$ in Eq. (5). This helps to understand the high positive MAE value for this compressed phase and stays in agreement with our interpretation based on the Bruno relationship and the anisotropy of orbital magnetic moments.

For the strained phase with $c/a = 1.2$ [panel (c)], the majority spin channel is also almost completely filled and shifted below the Fermi level, which results in the quenching of the spin-flip contributions to the MAE. When comparing the minority-spin channels for $c/a = 1.0$ and 1.2, the tetragonal elongation causes the $m = 2$ ($d_{x^2-y^2}$) states to split into two main peaks, one of which shifts below the Fermi level and the other toward higher energies. Just above the Fermi level, the most prominent contribution comes from the now isolated, nondegenerate $m = 0$ (d_{z^2}) orbital, which previously formed the cubic e_g pair together with the $m = 2$ state. At the Fermi level itself, the highest density of states is achieved by the contribution from the $m = -2$ orbitals. According to second-order perturbation theory, the calculated negative MAE value (-2.5 MJ m^{-3}) results from the balance of contributions between out-of-plane and in-plane coupling channels around the Fermi level. Although the high density of $m = -2$ states in the vicinity of the Fermi level promotes out-of-plane mixing via the operator $\hat{L}_z$, this positive contribution is outweighed by the matrix elements of the in-plane angular momentum operators, $\hat{L}_x$ and $\hat{L}_y$. These in-plane operators strongly couple the dominant unoccupied state $m = 0$ (d_{z^2}) with the coexisting degenerated states $m = \pm 1$ (d_{xz}/d_{yz}) ($\langle d_{z^2} | \hat{L}_{x,y} | d_{xz/yz} \rangle \neq 0$), which form a continuous profile just below the Fermi level. Importantly, the $m = 0$ orbital creates a steep slope that passes through the Fermi level and forms a sharp peak just above it. This close proximity causes a significant reduction in the energy denominator $\epsilon_u - \epsilon_o$ for an interaction $\Delta m = \pm 1$, which maximizes the negative contribution in the plane and stabilizes the easy axis in the plane.

In summary, the systematic evolution of the orbital-resolved density of states shows that the sign and magnitude of the MAE in bct Co result from strain-induced shifts and splitting of the contributions of specific 3d orbitals.

V. EFFECT OF LATTICE RELAXATION ON MAE AND STRUCTURAL STABILITY

Two important concerns arise when analyzing MAE of tetragonally distorted Fe-Co alloys. First, the constant volume approximation employed in the previous sections may introduce distortions in the description of a quantity as sensitive as the MAE. Second, from an application-oriented perspective, it is essential to assess whether the bct₁₀ structure can be stabilized—and thus realized experimentally—and whether such stabilization would be technologically feasible.

Despite the fact that the equilibrium structure of cobalt is hexagonal close-packed, bcc cobalt layers exceeding 30 nm in thickness have been experimentally obtained [57], and tetragonal cobalt structures have been shown to be energetically favorable under suitable conditions [79]. Motivated by these observations, in the last part of this work, we focus on evaluating the impact of lattice relaxation on the MAE and on examining the energetic stability of the bct₁₀ structure.

To optimize the unit-cell volume along the bcc $\leftrightarrow$ fcc $\leftrightarrow$ hcp transformation path, we used the FPLO code, version 5.00-18, which includes CPA. We applied the local density approximation (LDA) of exchange-correlation potential, based on the Perdew and Wang (PW92) parametrization [80], and we used *P1* symmetry. For computational efficiency—and in order to adhere to the initial presumption of using CPA—we did not include fully relativistic effects at this stage, as they are not essential for structural optimization. Although absolute equilibrium volumes differ between LDA- and GGA-based approaches, we assume that the relative volume changes between different distorted structures are only weakly dependent on the chosen exchange-correlation functional. Thus, we used the V/V_{bcc} profile to rescale the system volume for further calculations of the system's energy change (ΔE) and MAE along the selected transformation paths. These calculations were performed within the full-potential, fully relativistic SPR-KKR/PBE framework described earlier. The resulting volume ratios, energy profiles, and MAE values are summarized in Fig. 6.

As expected, the optimized unit cell volume decreases as it approaches the fcc and hcp (close-packed) structures. Overall, the volume variation remains within $\pm 1.25\%$ relative to the bcc reference structure [Figs. 6(a) and 6(d)]. This value is slightly lower than the approximately 2% reported in experiments, but it is consistent with results of earlier density functional theory calculations [37,81].

A comparison of the MAE obtained using the constant-volume approximation with that calculated after volume rescaling indicates that lattice relaxation has only a minor influence on the MAE [Fig. 6(c)]. The overall shape and magnitude of the MAE curves remain essentially unchanged, suggesting that the constant-volume approximation provides a reasonable description of the MAE trends in the present system.

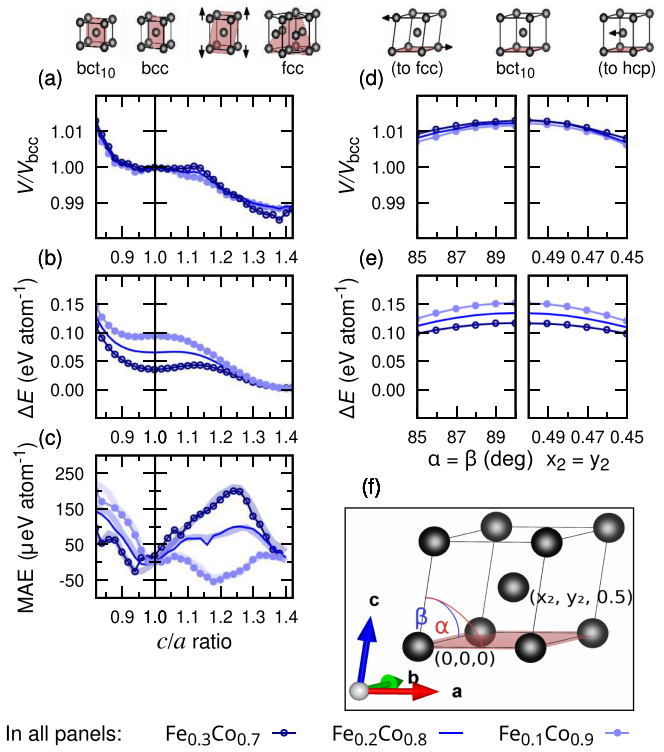


FIG. 6. Analysis of the $\text{Fe}_{1-x}\text{Co}_x$ alloy stability across Bain and Burgers pathways. Panels (a), (d) show the optimized unit-cell volume ratio V/V_{bcc} relative to the bcc reference structure. Panels (b), (e) present the transformation energy ΔE of distorted $\text{Fe}_{1-x}\text{Co}_x$ alloys along selected structural transformation paths, in comparison to the global energy minimum. Panel (c) depicts the influence of volume relaxation on MAE. Colors correspond to those used in Fig. 1; thick solid lines denote results obtained within the constant-volume approximation, while thin lines with symbols represent calculations including volume rescaling. Panels (a)–(c) correspond to tetragonal distortion along and beyond the Bain path, while panels (d), (e) show the energy variation associated with skew and slip of hexagonal planes along the Burgers transformation path. Panel (f) shows structural parameters of the *P1* unit cell varied during the Burgers transformation. The atomic plane highlighted in red in the structural miniatures indicates the hexagonal plane: (101) in the bct₁₀ structure, (111) in the fcc structure realized in the $Pm\bar{3}m$ space group, and (001) in the structures along the Burgers path described within the *P1* space group.

The energy profile along the bcc $\leftrightarrow$ bct₁₀ path [Fig. 6(b)] reveals the presence of a shallow minimum for cobalt concentrations exceeding $x > 0.8$. In contrast, along the fcc $\leftrightarrow$ bct₁₀ $\leftrightarrow$ hcp transformation path [Fig. 6(e)], the bct₁₀ structure corresponds to a local energy maximum. Taken together, these results indicate that the bct₁₀ structure is located near a saddle region of the energy landscape.

Although the minimum along the bcc $\leftrightarrow$ bct₁₀ path, near $c/a \approx 0.9$, is relatively shallow and lies close to other competing minima, the nearly flat energy profile observed along the Burgers transformation suggests that the bct₁₀ structure could be stabilized under suitable constraints. In particular, a combination of epitaxial growth on an appropriate square-lattice substrate and interstitial doping may provide viable routes toward stabilization—a solution investigated by Mehl

et al. [32]. We further note that, given the strong orbital moment contribution associated with cobalt, the MAE in Co-rich epitaxial films may be further enhanced under such conditions [41].

VI. SUMMARY AND CONCLUSIONS

In summary, we presented a comprehensive study of magnetocrystalline anisotropy energies (MAE), magnetic moments, and Curie temperatures (T_C) of Fe-Co alloys across a wide range of tetragonal deformations. We also complete the investigation of the stability of the alloy by bridging the Bain and Burgers transformation pathways. While using robust computational methods, this work covers a broader range of deformations than has been explored before. To validate the employed calculation techniques, we first reproduced key results from earlier studies, including the MAE and magnetic moment maps for body-centered-tetragonal (bct) structures with $c/a > 1$, recreating the well-known Burkert *et al.* maximum in MAE. We then extended our study to Fe-Co alloys under uniaxial stress, a region that has rarely been investigated. More in-depth investigation of the origin of high MAE in the compressed and in the strained structure shows that in both cases, the main contribution comes from the anisotropy in orbital magnetic moment, as described by Bruno.

Our findings reveal a high-MAE region in uniaxially compressed Fe-Co alloys, particularly for Co-rich alloys. This region centers near an intermediate bct₁₀ structure within the proposed Burgers bcc $\leftrightarrow$ hcp $\leftrightarrow$ fcc transition pathway. A saddle point of the energy surface is located near the aforementioned structure, at $c/a \approx 0.9$. Consequently, it could be stabilized—e.g., by epitaxial growth on suitable square-lattice substrates or/and interstitial doping. This could lead to stable structures with much thicker layers than those previously reported for uniaxially strained Fe-Co alloys. Monte Carlo simulations and DLM calculations indicate that this Co-rich structure under uniaxial tetragonal compression exhibits a higher T_C than under strain. Ultimately, our work broadens the range of stable, high-MAE structures available for various cobalt contents in tetragonal Fe-Co alloys. This now spans from ordered systems with cobalt concentrations as low as 25%, through stoichiometric FeCo, to nearly pure

cobalt—as identified in this study. Whereas Fe-Co alloys with high Co content in near-bct₁₀ geometry would be costly to manufacture, they could be an excellent candidate for high-temperature applications where their high performance outweighs the economic limitations. It is also a promising magnetic material bridging the gap between cheap Fe-based magnets and high-performance magnetic phases, such as L1₀ FePt.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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