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Citation: [Applied Physics Letters](#) **103**, 102404 (2013); doi: 10.1063/1.4819773

View online: <http://dx.doi.org/10.1063/1.4819773>

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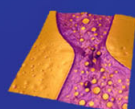
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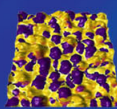
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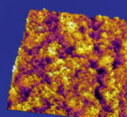


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# Tuning the Curie temperature of FeCo compounds by tetragonal distortion

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(Received 18 July 2013; accepted 16 August 2013; published online 4 September 2013)

Combining density-functional theory calculations with a classical Monte Carlo method, we show that for B2-type FeCo compounds, tetragonal distortion gives rise to a strong reduction of the Curie temperature  $T_C$ . The  $T_C$  monotonically decreases from 1575 K (for  $c/a = 1$ ) to 940 K (for  $c/a = \sqrt{2}$ ). We find that the nearest neighbor Fe-Co exchange interaction is sufficient to explain the  $c/a$  behavior of the  $T_C$ . Combination of high magnetocrystalline anisotropy energy with a moderate  $T_C$  value suggests tetragonal FeCo grown on the Rh substrate with  $c/a = 1.24$  to be a promising material for heat-assisted magnetic recording applications. © 2013 AIP Publishing LLC.

[<http://dx.doi.org/10.1063/1.4819773>]

The recording density in a commercial hard disk drive (HDD), i.e., the amount of information that can be stored per square inch, has increased by more than 7 orders of magnitude since its first introduction in 1956.<sup>1</sup> Such an increase has been achieved by a simple scaling of the dimensions of the bits recorded in storage medium. However, the recording density has an upper limit due to the superparamagnetic effect and limited write field of the writing head. This limit is around 1 Tbit/in.<sup>2</sup> for current perpendicular magnetic recording.<sup>2–5</sup> In order to further increase the recording density in future recording media, new materials with the following properties are sought: (i) they should have large uniaxial magneto-crystalline anisotropy energy (MAE)  $K_u$ , (ii) large saturation magnetization, (iii) fast magnetic response to external applied fields, and (iv) moderate Curie temperatures above the room temperature.

Retaining the magnetization of the medium over a long period of time despite thermal fluctuations is one of the major problems in designing magnetic storage media. If the ratio of the magnetic energy per grain  $K_u V$ , where  $V$  is the grain volume, to the thermal energy  $k_B T$  becomes sufficiently small, the thermal fluctuations can reverse the magnetization in a region of the medium destroying the information stored there.<sup>3,6</sup> To further increase the recording density, high- $K_u$  materials with large saturation magnetization  $M_s$  are needed. The large  $M_s$  is beneficial to reduce the write field. In addition to large  $K_u$  and  $M_s$  values, another important issue in magnetic recording applications is the magnetic switching time, which imposes physical limits on areal recording densities and data rates.<sup>5</sup> In current devices, the switching speeds have reached a point where dynamical effects are becoming important.<sup>7–13</sup> Collective magnon excitations play an important role in fast precessional magnetic switching processes because they serve as a heat bath for dissipation of the Zeeman energy and thus contribute to the relaxation of magnetization and switching time.

On the other hand, the large- $K_u$  materials require very high magnetic fields for writing the information to the

recording media. As the bit size gets smaller and smaller, at some point, the magnetic field required for switching the magnetization direction exceeds the maximal available magnetic writing fields and thus data can no longer be written to the disk. To solve this problem, the heat-assisted magnetic recording (HAMR) was proposed as a promising approach, which enables large increases in the storage density of HDD.<sup>5,14,15</sup> In HAMR, a laser is used to momentarily and locally heat the recording area of the medium to reduce its coercivity. It has been suggested that magnetic recording close to or above the Curie temperature is required to achieve the highest areal density advantage of HAMR, making the  $T_C$  an important parameter for applications and choice of materials.<sup>45,46</sup> With increasing temperature, the  $K_u$  of the medium decreases and above  $T_C$   $K_u$  vanishes, making it possible to write the information with available head fields. Thus, the  $T_C$  is an important parameter in the design of HAMR media.

Materials that combine most of necessary conditions for HAMR applications are B2-type tetragonal FeCo compounds. The large values of  $K_u$ , reaching 600  $\mu\text{eV}$ , and  $M_s$  in these compounds were first predicted by first-principles calculations<sup>16</sup> and then confirmed by experiments.<sup>17–20</sup> Experimentally, FeCo compounds have been grown on the Pd, Ir, and Rh substrates in B2-type structure, in which the in-plane lattice constant  $a$  is enforced by the substrate and the out-of-plane lattice constant  $c$  changes so as to keep the volume constant. In particular, Yildiz *et al.*<sup>19,20</sup> found in agreement with theoretical predictions that the perpendicular magnetic anisotropy is very sensitive to the tetragonal distortion and increases with increasing  $c/a$  ratio, which allows to tune the perpendicular anisotropy value by growing the alloys on different substrates. Yildiz *et al.*<sup>19,20</sup> have also shown that the structure remains stable for film thicknesses of up to 15 monolayers. Note also that microscopic atomic order in B2-type FeCo compounds is crucial to achieve high  $K_u$  values.<sup>34,41</sup>

At low temperatures, the ordered cubic FeCo takes the CsCl (B2) structure, at around 1000 K it undergoes an order-disorder transition and at around 1230 K a bcc-fcc transformation accompanied by a magnetic-nonmagnetic transition.<sup>21–23</sup>

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In a recent paper, Şaşıoğlu *et al.*<sup>25</sup> have studied the effect of the tetragonal distortion on magnon spectra of the B2-type FeCo compounds by employing the many-body perturbation theory. The authors have shown that tetragonal distortion gives rise to a significant magnon softening, which indicates a strong reduction of the Curie temperature. *Ab initio* calculations by Ležaić *et al.*<sup>24</sup> on cubic ordered and disordered FeCo alloys have shown that the calculated  $T_C$  agrees well with experiment.

The aim of this letter is to study the effect of the tetragonal distortion on the Curie temperature of the B2-type FeCo compounds from first principles. It is shown that tetragonal distortion gives rise to a strong reduction of  $T_C$  that decreases from 1575 K (for  $c/a = 1$ ) to 940 K (for  $c/a = \sqrt{2}$ ). We find that for all  $c/a$  ratios, the ferromagnetic order is stable. Combination of moderate  $T_C$  values together with large  $K_u$  suggests B2-type tetragonal FeCo grown on the Rh substrate with  $c/a = 1.24$  to be a promising material for HAMR applications.

We calculate the Curie temperature using an established approach: the adiabatic approximation for the calculation of magnon spectra.<sup>26–28</sup> *Ab initio* total-energy results, calculated within the frozen-magnon approximation, are mapped to the classical Heisenberg model

$$H = -\frac{1}{2} \sum_{i,j(i \neq j)} J_{ij} \mathbf{e}_i \cdot \mathbf{e}_j, \quad (1)$$

where  $J_{ij}$  are the exchange constants between the magnetic moments at sites  $i$  and  $j$  and  $\mathbf{e}_i$  is a unit vector along the moment of atom  $i$ . Accounting for the interactions up to the 12th nearest neighbor,  $T_C$  is calculated within this model by a Monte Carlo method by locating the crossing point of the fourth-order cumulants<sup>29</sup> for 5488 and 8192-atom supercells in the bulk limit and neglecting the anisotropy, which is a good approximation for a film thickness of 15 monolayers.<sup>32,33</sup>

The *ab initio* results are calculated within the generalized gradient approximation<sup>31</sup> to density-functional theory. We employ the full-potential linearized augmented plane-wave (FLAPW) method as implemented in the FLEUR code.<sup>30</sup> The muffin-tin radii of Fe and Co are chosen to be 1.21 Å. A dense  $16 \times 16 \times 16$   $\mathbf{k}$ -point grid is used. Keeping the volume of the B2-type unit cell constant ( $V = 23.766 \text{ Å}^3$ ), we vary the  $c/a$  ratio from 1 to  $\sqrt{2}$ . Note that if both

atoms in the unit cell were identical, we would get a bcc lattice for  $c/a = 1$  and fcc for  $c/a = \sqrt{2}$ . As FeCo with  $c/a = 1$  crystallizes in ordered B2 structure,<sup>21,22</sup> we assume the same type of structure with additional tetragonal distortion in our calculations. The mechanism behind the giant uniaxial MAE observed in tetragonal FeCo compounds has been discussed in detail in Ref. 16 and will not be analyzed here. Indeed, our calculated values of uniaxial MAE (results not shown) are very similar to those reported by Burkert *et al.*<sup>16</sup>

We begin the discussion of our results by presenting the exchange interactions. Figures 1(a) and 1(b) show the calculated sizeable intra-sublattice Co-Co and Fe-Fe exchange parameters, respectively, as a function of tetragonal distortion, i.e., from  $c/a = 1$  to  $c/a = \sqrt{2}$  (more distant coupling parameters are included in the  $T_C$  calculation but not shown here). Figure 1(c) shows the  $c/a$  dependence of the nearest neighbor inter-sublattice Fe-Co exchange parameters as well as the calculated Curie temperature of the compounds. Due to the strong ferromagnetic nature of FeCo compounds (very low majority-spin density of states (DOS), see Fig. 2) the absolute value of the exchange parameters decays quickly with increasing interatomic distance<sup>35</sup> and the main contribution to  $T_C$  comes from the interaction between atoms lying in a distance of a few first neighboring shells. The importance of each interaction ( $J_1, J_2$ , etc.) should be judged taking into account the number of neighbours in the corresponding coordination sphere, given in parentheses in Fig. 1. At  $c/a = 1$ , each Fe (Co) atom has 8 nearest neighbor Co (Fe) atoms and 6 next nearest neighbor Fe (Co) atoms, etc. With tetragonal distortion, the distances between Fe or Co atoms in the atomic plane become different compared to the adjacent planes in the direction of the  $c/a$  distortion and as a consequence the intra-sublattice Fe-Fe and Co-Co exchange parameters split into two components, which are denoted as  $J_1, J_3, J_5$  and  $J_2, J_4$  for in-plane and neighboring-plane parameters, respectively. As seen from Fig. 1, the nearest ( $J_1$ ) and next-nearest neighbor ( $J_2$ ) Fe-Fe (Co-Co) parameters stand out and are much affected by the distortion showing in part variations between ferromagnetic and antiferromagnetic values. A similar behavior is observed in the case of  $\text{Ni}_2\text{MnGa}$  and hcp Gd under distortion.<sup>36</sup>

The most decisive role for  $T_C$  is played by the nearest neighbor Fe-Co exchange as can be seen from Fig. 1(c): first, their value is significantly larger than the value of the Co-Co

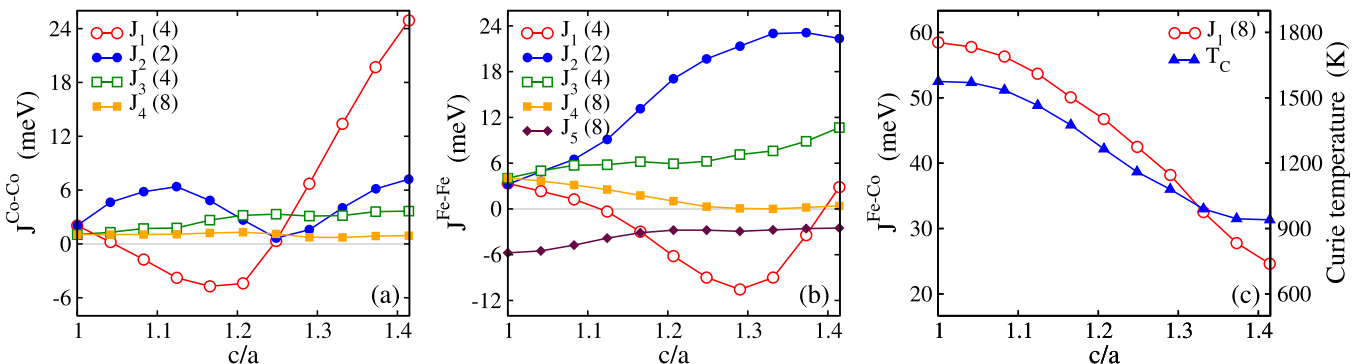


FIG. 1. (a) First four nearest neighbor intra-sublattice Co-Co exchange parameters as a function of tetragonal distortion in B2-type FeCo. (b) The same for Fe sublattice for the first five shells. (c) Nearest neighbor inter-sublattice Fe-Co exchange parameters and estimated Curie temperature of the FeCo compounds as a function of tetragonal distortion. In each panel for each exchange parameter, the number of atoms in the corresponding coordination sphere is given. Positive exchange parameters correspond to ferromagnetic coupling, negative to antiferromagnetic.

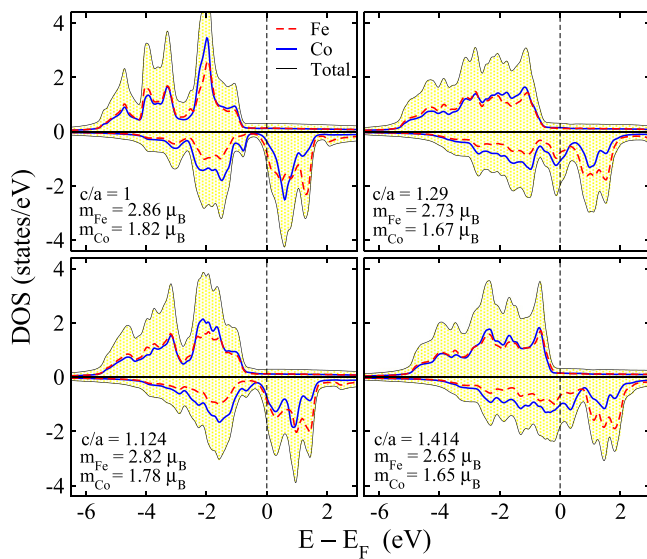


FIG. 2. Total and atom-resolved density of states of B2-type FeCo compounds for four different  $c/a$  ratios. In each panel, we include atom-resolved magnetic moments. The positive (negative) DOS axis corresponds to the majority-spin (minority-spin) channel.

or Fe-Fe parameters shown in Figs. 1(a) and 1(b) [note the different scale in Fig. 1(c) compared to Figs. 1(a) and 1(b)]; second, we witness that they closely follow the monotonical reduction of  $T_C$  with increasing distortion, except for a flattening-out of  $T_C$  close to  $c/a = \sqrt{2}$  which is not followed by the Fe-Co interaction and which we comment on later. The  $c/a$  behavior of the exchange interactions and resulting reduction of  $T_C$  can be attributed to the complex exchange coupling mechanisms and will be briefly discussed below.

Many-body model Hamiltonian approaches relevant to the problem provide useful insight into the qualitative interpretation of the density-functional results although a quantitative analysis of exchange parameters  $J$  in terms of different contributions is frequently not possible. It is meaningful to separate the interaction in two terms,  $J = J_{\text{direct}} + J_{\text{indirect}}$ .  $J_{\text{direct}}$  stems from the overlap of 3d wavefunctions of neighboring atoms and practically vanishes for distances larger than second-nearest neighbors. For FeCo, it is ferromagnetic because of the double-exchange mechanism,<sup>37–39</sup> i.e., energy gain by broadening of the half-filled minority  $d$  states due to hybridization if the moments are parallel-aligned.  $J_{\text{indirect}}$  is mediated by the Fermi sea, concerns interatomic distances from second-nearest neighbors and beyond, and is analyzed here in terms of the Anderson  $s$ - $d$  mixing model because of the localized nature of magnetic moments in these systems.

We proceed with a qualitative analysis of the calculated exchange parameters. The monotonous reduction of the nearest neighbor Fe-Co exchange interaction [see Fig. 1(c)] with tetragonal distortion can be attributed to decrease of the direct coupling  $J_{\text{direct}}$  caused by three factors. (i) The energetic distance of the majority  $d$  bands to the Fermi level decreases with increasing  $c/a$ , from 1 eV to 0.3 eV, as seen in Fig. 2, leading to a strengthening of the antiferromagnetic kinetic-exchange<sup>37</sup> contribution to  $J_{\text{direct}}$ . The latter mechanism is related to a repulsion of the occupied majority-spin with unoccupied minority-spin levels of neighboring atoms that stems from hybridization if the moments are antiparallel-

aligned and results in energy gain as the occupied levels move lower in energy. (ii) The inter-atomic Fe-Co distance increases from 2.49 Å to 2.56 Å as  $c/a$  increases from 1 to  $\sqrt{2}$  resulting in a weakening of the overlap of neighboring 3d wave functions. (iii) The magnetic moment amplitudes, that are included in the values of  $J_{ij}$  in Eq. (1), decrease from 2.86  $\mu_B$  to 2.65  $\mu_B$  for Fe and from 1.82  $\mu_B$  to 1.65  $\mu_B$  for Co.

Concerning the indirect coupling, within the Anderson  $s$ - $d$  mixing model,  $J_{\text{indirect}}$  can be separated into two contributions (see, e.g., Ref. 40):  $J_{\text{indirect}} = J_{\text{RKKY}} + J_S$ . Here, the first term is an oscillating Ruderman-Kittel-Kasuya-Yosida (RKKY)-like, which stems from a spin polarization of the conduction electron sea by the local moments. The second “superexchange” term,  $J_S$ , is antiferromagnetic, decays exponentially with spatial distance, and stems from virtual excitations in which electrons from local  $d$  states of Fe and Co are promoted above the Fermi sea.  $J_S$  depends mostly on the distance of the unoccupied Fe (Co) 3d peaks from the Fermi energy. The closer the peaks to the Fermi level, the stronger becomes  $J_S$ .

The intra-sublattice, i.e., Fe-Fe and Co-Co, exchange interactions depend strongly on  $J_{\text{indirect}}$ , showing in part stronger variations with tetragonal distortion compared to the Fe-Co interaction. However, as the nearest neighbor Fe-Fe and Co-Co pairs are relatively close (the in-plane distance decreases from 2.87 Å at  $c/a = 1$  to 2.56 Å at  $c/a = \sqrt{2}$ ), the variation of  $J_1$  also has a direct-exchange contribution. In both sublattices, we observe that  $J_1$  is sizeable and changes sign in the  $c/a$  interval. In a large section of the interval, the various intra-sublattice interactions partly compensate each other due to sizeable antiferromagnetic  $J_1$  and  $J_5$  (for Co-Co) terms. Only close to the end of the interval at  $c/a = \sqrt{2}$  do the Co-Co and Fe-Fe interactions contribute towards a stronger ferromagnetic coupling, which results in a flattening-off of the curve of  $T_C$  close to  $c/a = \sqrt{2}$  that is not witnessed in the Fe-Co coupling [see Fig. 1(c)].

Having established the possibility of tuning  $T_C$  via the  $c/a$  ratio, we should note that an additional parameter that may be used for the tuning is the film thickness. It is known that two-dimensional Heisenberg magnets without anisotropy have  $T_C = 0$ .<sup>42</sup> However, in the presence of uniaxial MAE,  $T_C > 0$  and it grows with increasing film thickness, coming close to the bulk value already at 15–20 atomic layers<sup>33,43,44</sup> (depending of course on the magnitude of  $K_u$ ). Since in HAMR applications, one could conceivably wish a lower  $T_C$  than the bulk limit shown here, this can be achieved by reducing the film thickness. Of course, the functionality will be also determined by the thickness dependence of  $K_u$  which we do not study here, however, for thin films,  $K_u$  is expected to be appreciable because of the reduced symmetry even if it differs from the value of 600  $\mu\text{eV}$  that was found for  $c/a = 1.24$ .

In conclusion, combining density-functional theory calculations with a classical Monte Carlo method, we show that for B2-type FeCo compounds a tetragonal distortion with  $1 < c/a < \sqrt{2}$  gives rise to a strong reduction of the Curie temperature  $T_C$ . In this interval, the  $T_C$  decreases monotonically from 1575 K to 940 K. We find that due to the strong ferromagnetic character of FeCo compounds the exchange interactions are strongly damped for large interatomic



distance and thus the nearest neighbor Fe-Co exchange interaction is sufficient to explain the  $c/a$  dependence of the  $T_C$ . Combination of high magnetocrystalline anisotropy energy with a moderate  $T_C$  value suggests tetragonal FeCo grown on the Rh substrate with  $c/a = 1.24$  to be a promising material for HAMR applications.

This work was partly supported by the Young Investigators Group Programme of the Helmholtz Association, Germany, Contract No. VH-NG-409. We gratefully acknowledge the support of Jülich Supercomputing Centre.

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