

***Ab Initio* Theoretical Description of the Interrelation between Magnetocrystalline Anisotropy and Atomic Short-Range Order**

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The cubic lattice symmetry of ferromagnetic homogeneously disordered alloys is broken when a compositional modulation is imposed. This can have a profound influence on the magnetocrystalline anisotropy energy (MAE). We describe our *ab initio* theory of this effect and use the framework of concentration waves with the electronic structure described within the spin-polarized relativistic Korringa-Kohn-Rostoker coherent-potential approximation. We find that ordering produces a 2 order of magnitude increase in the MAE as well as altering the equilibrium direction of magnetization. Using the same theoretical framework we also examine directional compositional order produced by magnetic annealing with an explicit study of permalloy. [S0031-9007(99)09484-3]

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Magnetocrystalline anisotropy (MCA) of ferromagnetic materials containing transition metals has become the subject of intensive theoretical and experimental research because of the technological implications for high-density magneto-optical storage media [1,2]. Potential materials for these applications need to exhibit a substantial perpendicular magnetic anisotropy (PMA), which is evidently due to an intrinsic magnetic anisotropy in the crystal lattice strong enough to overcome the extrinsic macroscopic shape anisotropy favoring an in-plane magnetization. Whereas in ultrathin films and multilayers the PMA is due to surface [3] and interface [4,5] effects, respectively, in thick films of transition metal alloys it is an intrinsically bulk magnetic property which leads to PMA. Such systems are particularly interesting for magneto-optic recording because in addition to PMA they exhibit large Kerr effect signals as well as being chemically stable and easy to manufacture. There has been much effort directed towards an understanding of the mechanism of MCA from a first-principles electronic structure point of view to aid future magnetic material design but since MCA arises from spin-orbit coupling, which is essentially a relativistic effect [6], this means that a fully relativistic electronic structure framework is desirable.

Empirically compositional structure is found to have a profound influence on both the magnitude of the magnetocrystalline anisotropy energy (MAE) as well as the equilibrium or *easy* magnetization direction. Compositional order lowers the lattice symmetry of the homogeneously disordered alloy and this enhances its MAE. For example, the measured MAE ($\sim 130 \mu\text{eV}$) of ordered CoPt alloy (CuAu or $L1_0$ type) [7] is some 2 orders of magnitude larger than that of its disordered counterpart ($\sim 3 \mu\text{eV}$), and with a different easy axis. In this Letter we provide the first quantitative calculations of the effect of compositional order on MAE via a study of CoPt.

We also note that thick fcc- $\text{Co}_c\text{Pt}_{1-c}$ [8–10] and fcc- $\text{Co}_c\text{Pd}_{1-c}$ [8] films exhibit PMA of a size comparable with that of multilayers. Such a large PMA is quite unexpected for systems which should have effectively bulk cubic structure. Now whereas tensile strain and large negative magnetostriction coefficients may account for some of this in the $\text{Co}_c\text{Pd}_{1-c}$ films, it cannot for the thick $\text{Co}_c\text{Pt}_{1-c}$ ones [11]. Rather recent experiments have confirmed that although $\text{Co}_c\text{Pt}_{1-c}$ films seem to be nearly homogeneously disordered there are actually more Co-Co nearest neighbors in plane and very few out of plane [9,12,13]; i.e., there is presence of some atomic short-range order (ASRO). The existence of this compositional order produces *internal interfaces* analogous to Co/Pt multilayers and this has been suggested as a likely cause of the strong PMA in fcc- $\text{Co}_c\text{Pt}_{1-c}$ films [10,12]. This suggestion is strengthened by the fact that films grown at higher temperatures, in which enhanced bulk diffusion tends to destroy the in-plane compositional order, show no PMA. Very recently Kamp *et al.* [14] have shown from magnetic circular x-ray dichroism measurements that chemical ordering is also responsible for the enhanced MAE in thick $\text{Fe}_{0.5}\text{Pd}_{0.5}$ films. These observations clearly underline a correlation between MCA and ASRO. In this Letter we provide, for the first time, a detailed theoretical analysis based on first-principles calculations which shows how chemical order significantly influences MCA and compare the MAE of ordered and disordered CoPt alloys. Moreover, we use the same approach to model other hitherto unfabricated structures. This is pertinent now that it is possible to *tailor* compositionally modulated films to obtain better magneto-optic recording characteristics [15].

Upon ordering CoPt undergoes a modest tetragonal lattice distortion ($c/a = 0.98$) which also lowers the symmetry. From magnetostriction data, however, we

can estimate this to contribute only 15% of the MAE. The measured magnetostriction coefficient, λ , of pure fcc Co (5×10^{-5}) is of the same size as that of CoPt (-4×10^{-5}) although with a different sign. From “first-principles” electronic structure calculations Wu *et al.* [16] have shown that the rate of change of the MAE with lattice strain is proportional to λ and thus in fcc-Co and CoPt should be roughly of the same magnitude. Thus from Wu *et al.*'s [16] calculation of the MAE of Co for a range of c/a ratios we estimate that a 2% tetragonalization will change the MAE only by about $20 \mu\text{eV}$. Consequently we conclude that it is the compositional order that is primarily responsible for the large MAE of CoPt.

In previous work, we presented a theory of MCA of disordered bulk cubic alloys [17,18] within the framework of spin-polarized relativistic Korringa-Kohn-Rostoker coherent-potential approximation (SPR-KKR-CPA) [19]. In this Letter we set up a new framework to investigate the effects of compositional order, both short and long ranged. Any compositionally modulated alloy can be specified by site-dependent concentrations $\{c_i\}$ which themselves can be written as a superposition of static concentration waves (CWs) [20], i.e.,

$$c_i = c + \frac{1}{2} \sum_{\mathbf{q}} [c_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{R}_i} + c_{\mathbf{q}}^* e^{-i\mathbf{q}\cdot\mathbf{R}_i}],$$

with wave vectors \mathbf{q} and amplitudes $c_{\mathbf{q}}$. Usually only a few CWs are needed to describe a particular ordered structure. For example, the CuAu-like $L1_0$ structure (Fig. 1) is set up by a single CW with $c_{\mathbf{q}} = \frac{1}{2}$ and $\mathbf{q} = (001)$, and the [111]-layered CuPt-like $L1_1$ structure is set up by a CW with $c_{\mathbf{q}} = \frac{1}{2}$ and $\mathbf{q} = (\frac{1}{2}\frac{1}{2}\frac{1}{2})$ (\mathbf{q} is in units of $\frac{2\pi}{a}$, a being the lattice parameter).

The grand potential for the interacting electrons in an alloy with composition $\{c_i\}$ and magnetized along the direction \mathbf{e}_1 at a finite temperature T is given by [21,22],

$$\Omega(\{c_i\}; \mathbf{e}_1) = \nu Z - \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon, \nu) N(\{c_i\}; \varepsilon; \mathbf{e}_1) + \Omega_{DC}(\{c_i\}; \mathbf{e}_1),$$

where ν is the chemical potential, Z is the total valence charge, $f(\varepsilon, \nu)$ is the Fermi factor, $N(\{c_i\}; \varepsilon; \mathbf{e}_1)$ is the in-

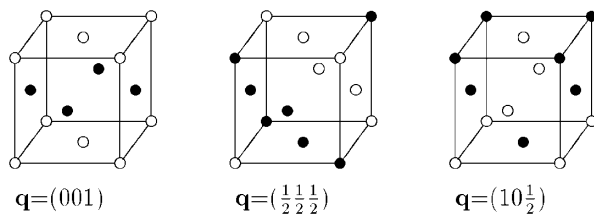


FIG. 1. Some ordered structures and their representative wave vectors. $\mathbf{q} = (001)$ generates the CuAu-type structure with ordering along the [001] direction. $\mathbf{q} = (\frac{1}{2}\frac{1}{2}\frac{1}{2})$ generates the CuPt-type structure. $\mathbf{q} = (10\frac{1}{2})$ generates a layered structure with planes of an ordered structure of A and B atoms stacked along the [001] direction.

tegrated electronic density of states, and $\Omega_{DC}(\{c_i\}; \mathbf{e}_1)$ is the “double-counting” correction. The MAE of the inhomogeneous alloy can be characterized by the difference

$$K(\{c_i\}) = \Omega(\{c_i\}; \mathbf{e}_1) - \Omega(\{c_i\}; \mathbf{e}_2).$$

Assuming that $\Omega_{DC}(\{c_i\}; \mathbf{e})$ is generally unaffected by the change in the magnetization direction, we get

$$K(\{c_i\}) = \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon, \nu_1) [N(\{c_i\}; \varepsilon; \mathbf{e}_1) - N(\{c_i\}; \varepsilon; \mathbf{e}_2)] + O(\nu_1 - \nu_2)^2.$$

Note that the correction due to the change in the chemical potential (from ν_1 to ν_2) with the magnetization direction is of second order in $(\nu_1 - \nu_2)$ and can be shown to be very small compared to the first term [17]. We now expand $K(\{c_i\})$ around $K_{CPA}(c)$, the MAE of the homogeneously disordered alloy $A_c B_{1-c}$,

$$K(\{c_i\}) = K_{CPA}(c) + \sum_j \left. \frac{\partial K(\{c_i\})}{\partial c_j} \right|_{\{c_i=c\}} \delta c_j + \frac{1}{2} \sum_{j,k} \left. \frac{\partial^2 K(\{c_i\})}{\partial c_j \partial c_k} \right|_{\{c_i=c\}} \delta c_j \delta c_k + O(\delta c)^3. \quad (1)$$

The second term in Eq. (1) vanishes if the number of A and B atoms in the alloy is to be conserved. Now taking the Fourier transform, we get the MAE of the compositionally modulated alloy with wave vector \mathbf{q} ,

$$K(\mathbf{q}) = K_{CPA}(c) + \frac{1}{2} |c_{\mathbf{q}}|^2 [S^{(2)}(\mathbf{q}; \mathbf{e}_1) - S^{(2)}(\mathbf{q}; \mathbf{e}_2)], \quad (2)$$

and so, for example, the MAE of the CuAu-type $L1_0$ ordered alloy is obtained by choosing $\mathbf{q} = (001)$ and $c_{\mathbf{q}} = \frac{1}{2}$. Here $S^{(2)}(\mathbf{q}; \mathbf{e})$ are the Fourier transforms of the so-called direct correlation functions [21] which determine the ASRO parameter $\alpha(\mathbf{q})$ in the disordered phase, $\alpha(\mathbf{q}) = \beta c(1-c)/[1 - \beta c(1-c)S^{(2)}(\mathbf{q})]$, ($\beta = 1/k_B T$, k_B being the Boltzmann constant). These have been calculated for many alloys, both nonmagnetic and ferromagnetic, in which up to now relativistic effects were largely ignored and were compared with diffuse x-ray and neutron scattering data [21,22]. $S^{(2)}(\mathbf{q})$ is given by

$$S^{(2)}(\mathbf{q}) = -\frac{\text{Im}}{\pi} \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon, \nu) \sum_{L_1 L_2 L_3 L_4} (X^A - X^B)_{L_1 L_2} \times I_{L_2 L_3; L_4 L_1}(\mathbf{q}) \Lambda_{L_3 L_4}(\mathbf{q}),$$

where

$$\Lambda_{L_1 L_2}(\mathbf{q}) = (X^A - X^B)_{L_1 L_2} - \sum_{L_3 L_4 L_5 L_6} X_{L_1 L_5}^A I_{L_5 L_3; L_4 L_6}(\mathbf{q}) X_{L_6 L_2}^B \Lambda_{L_3 L_4}(\mathbf{q}),$$

$$I_{L_5 L_3; L_4 L_6}(\mathbf{q}) = \frac{1}{V_{BZ}} \int d\mathbf{k} \tau_{L_5 L_3}(\mathbf{k} + \mathbf{q}) \tau_{L_4 L_6}(\mathbf{k}) - \tau_{L_5 L_3}^{00} \tau_{L_4 L_6}^{00}, \quad (3)$$

and $X^{A(B)} = [(t_{A(B)}^{-1} - t_c^{-1})^{-1} + \tau^{00}]^{-1}$. Here, τ^{00} is the site-diagonal path-operator matrix, $t_{A(B)}$ and t_c are the t matrices for electronic scattering from sites occupied by $A(B)$ atoms and the CPA effective potentials, respectively, $\tau(\mathbf{k}) = [t_c^{-1} - g(\mathbf{k})]^{-1}$, and $g(\mathbf{k})$ is the KKR structure constants matrix [23]. The spinodal ordering temperature below which the alloy orders into a structure characterized by concentration wave vector \mathbf{q}_{\max} is given by [21,22] $T_c = c(1 - c)S^{(2)}(\mathbf{q}_{\max}; \mathbf{e})/k_B$, where \mathbf{q}_{\max} is the value at which $S^{(2)}(\mathbf{q}; \mathbf{e})$ is maximal.

As with all MAE calculations, given the sizes of the energies involved, numerical computation of $K(\mathbf{q})$ needs to be done very carefully. The energy integration is done using a complex contour described elsewhere [17]. The Brillouin zone (BZ) integration is done using the adaptive grid method [24] which has been found to be very efficient and accurate. In this method one can preset the level of accuracy of the integration by supplying an error parameter ϵ . The integration in Eq. (3) is done with $\epsilon = 10^{-6}$ which means that $S^{(2)}(\mathbf{q}; \mathbf{e})$ which are of the order of 0.1 eV are accurate up to 0.1 μeV . To achieve such a level of accuracy, we had to sample a large number of \mathbf{k} points in the BZ. Also, owing to the form of the integrand in Eq. (3) the integration has to be done using the full BZ. Typically, in our calculations, we needed around 35 000 \mathbf{k} points for points on the energy contour 0.5 Ry above the real axis. When the energy was 0.0001 Ry above the real axis (and that is the closest point to the real axis that we need) we required as many as 3×10^6 \mathbf{k} points for the same level of accuracy. Furthermore, we have calculated $S^{(2)}(\mathbf{q}; \mathbf{e}_1)$ and $S^{(2)}(\mathbf{q}; \mathbf{e}_2)$ simultaneously ensuring that they are calculated on the same grid and thus canceling out the systematic errors if there are any. Therefore, we claim that the values of $K(\mathbf{q})$ are accurate to within 0.1 μeV .

We summarize the results for the fcc- $\text{Co}_{0.5}\text{Pt}_{0.5}$ alloy in Tables I and II. We note that $S^{(2)}(\mathbf{q})$ is maximum for the $L1_0$ structure, implying that the alloy would order into this structure at 1360 K as it is cooled from high temperature in good agreement with experiment (ordering temperature of 1000 K [7]). From Table II we note that for $\mathbf{q} = (001)$ and $\mathbf{q} = (100)$ which correspond to CuAu-like $L1_0$ ordered structure, with Co and Pt layers stacked along the [001] and [100] directions, respectively, the direction of spontaneous magnetization is along the [001] and [100] directions, respectively, in excellent agreement with experiment. Also, the MAE (58.6 μeV) is comparable to the experimental value (~ 130 μeV [7]).

In order to probe the relationship between the compositional structure and MAE further, we also performed calculations for some hypothetical structures. These are also summarized in Table II. The case of $\mathbf{q} = (\frac{1}{2}\frac{1}{2}\frac{1}{2})$ corresponding to the CuPt-type $L1_1$ ordered structure with Co and Pt layers perpendicular to the [111] direction of the crystal produces a spontaneous magnetization along the [111] direction of the crystal. This may be close to the structure of the thick [111] oriented disordered CoPt alloy films exhibiting PMA [8–10] which is attributed to the

TABLE I. Direct correlation function $S^{(2)}(\mathbf{q}; [001])$ for different \mathbf{q} vectors for the $\text{Co}_{0.5}\text{Pt}_{0.5}$ alloy.

\mathbf{q}	Structure	$S^{(2)}(\mathbf{q}; [001])$ (eV)	T_c (K)
(000)	Clustering	-1.51	...
(001)	$L1_0$	0.47	1360
(100)	$L1_0$	0.47	1360
$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$L1_1$	0.29	
$(10\frac{1}{2})$		0.19	

existence of internal interfaces [12], analogous to Co and Pt layers along the [111] direction. Our result is clearly consistent with these observations. The point is that the magnetic anisotropy (152 μeV) intrinsic to this structure is nearly 3 times larger than that of the $L1_0$ structure. Indeed, we predict that a [111]-oriented film will exhibit a markedly stronger PMA than that of a [100]-oriented film.

The structure set up by CWs with $\mathbf{q} = (10\frac{1}{2})$ and $(01\frac{1}{2})$ is also a [001]-oriented layered structure, but the layers are not alternately pure Co and Pt planes; rather they are layers of ordered Co and Pt (Fig. 1). Even in this case, we note that the magnetization is perpendicular to the layered structure, and the magnitude of MAE is large. Similarly, for $\mathbf{q} = (\frac{1}{2}01)$ and $(\frac{1}{2}10)$ where the planes are stacked along the [100] direction the magnetization is also along the [100] direction.

Evidently, the spontaneous magnetization always tends to align itself perpendicular to any layering in the structure. In addition, the magnitude of MAE depends strongly on the symmetry of the system, i.e., it increases when the symmetry is lowered. The cubic symmetry of the homogeneously disordered alloy quenches the orbital magnetic moment. In the $L1_0$ ordered alloy the symmetry is lower and in the $L1_1$ layered structure it is lower still, thus increasing the MAE in each case. On detailed examination of the electronic structure of the disordered alloy around the Fermi energy we find that the large values of $K(\mathbf{q})$ near the BZ boundary arise from Van Hove singularities of the Bloch spectral function [23]. The number, location, and occupation of these depend on the magnetization direction and produce a large contribution to the difference in the convolution integrals [Eqs. (2) and (3)].

TABLE II. Magnetocrystalline anisotropy energy $K(\mathbf{q})$ for several compositionally modulated CoPt alloys characterized by different \mathbf{q} vectors (the respective ordered structures are shown in Fig. 1). The reference system has the magnetization along the [001] direction (i.e., $\mathbf{e}_1 = [001]$).

\mathbf{q}	$\mathbf{e}_2 = [111]$	$\mathbf{e}_2 = [100]$	Easy axis
	$K(\mathbf{q})$ (μeV)	$K(\mathbf{q})$ (μeV)	
(001)	-58.6	-105.6	[001]
(100)	39.6	105.9	[100]
$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	152.0	0.0	[111]
$(10\frac{1}{2})$	-158.7	-236.5	[001]
$(\frac{1}{2}01)$	85.0	236.3	[100]

TABLE III. Direct correlation function $S^{(2)}(\mathbf{q}; \mathbf{e})$ for different \mathbf{q} vectors for $\text{Ni}_{0.75}\text{Fe}_{0.25}$ alloy.

\mathbf{q}	$\mathbf{e} = [001]$		$\mathbf{e} = [100]$		$\mathbf{e} = [111]$	
	$S^{(2)}(\mathbf{q})$ (meV)	T_c (K)	$S^{(2)}(\mathbf{q})$ (meV)	T_c (K)	$S^{(2)}(\mathbf{q})$ (meV)	T_c (K)
(100)	330.880		331.158	720.9	330.973	720.5
(010)	330.880		330.880		330.973	720.5
(001)	331.158	720.9	330.880		330.973	720.5
$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	-99.291		-99.291		-99.475	
$(10\frac{1}{2})$	99.284		99.096		99.222	
$(\frac{1}{2}01)$	99.096		99.285		99.222	

Our theory can also be used to produce the first quantitative description of the phenomenon of magnetic annealing. Here a soft magnetic material develops directional chemical order when annealed in a magnetic field [25]. We demonstrate this effect for $\text{Ni}_{0.75}\text{Fe}_{0.25}$ (permalloy) and Table III is a summary of the results. We calculate $S^{(2)}(\mathbf{q}, \mathbf{e})$ for permalloy in an applied magnetic field of strength 600 Oe (same as used in the experiment [25]) orientated along $\mathbf{e} = [001]$, $[111]$, and $[100]$ directions of the crystal. We find that when the magnetic field is along $[001]$ (column 2) $S^{(2)}(\mathbf{q})$ is maximum for $\mathbf{q} = (001)$ confirming that ordering is favored along the direction of applied field. Similar is the case when the magnetic field is along $[100]$. However, when the applied field is along $[111]$ (column 6) all three orderings, namely, (100), (010), and (001) are favored equally. Thus, in this case, we will get a CuAu_3 -type $L1_2$ ordering. The calculated transition temperature 721 K is in good agreement with the experimental value of 820 K [26]. Noting that the measured intensity in a scattering experiment is proportional to the ASRO parameter $\alpha(\mathbf{q})$, we estimate that for an alloy cooled in a magnetic field along the $[001]$ direction the superlattice spot at $\mathbf{q} = (001)$ will be 20% more intense than that at $\mathbf{q} = (100)$ at a temperature 1 K above the transition temperature.

In conclusion, we have presented a fully relativistic electronic structure scheme to study the MCA of alloys and its dependence upon compositional structure. We applied this theory to fcc- $\text{Co}_{0.5}\text{Pt}_{0.5}$ and found that when the system is cooled it tends to order into $L1_0$ layered-ordered structure and that the spontaneous magnetization tends to align itself perpendicular to the layer stacking. These observations are in complete accord with experiment. We also found that if the layers are stacked along the $[111]$ direction then the MCA becomes larger which may be the case in $[111]$ -textured films. Within the same framework we have also been able to explain the appearance of directional order in $\text{Ni}_{0.75}\text{Fe}_{0.25}$ when it is annealed in a magnetic field.

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