Long-range chemical order effects upon the magnetic anisotropy of FePt alloys from an *ab initio* electronic structure theory

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Abstract

The magnetocrystalline anisotropy (MCA) of bulk and thick films of FePt is calculated from a 'first-principles' theory. The starting point is a description from electronic density functional theory for systems of interacting electrons moving in lattices of ions. Relativistic effects such as spin–orbit coupling are included. FePt readily transforms into a CuAu-type ($L1_0$) ordered phase and this coincides with the material's high anisotropy. Here we describe how to calculate the MCA of a partially ordered alloy and to extract its dependence on the long range chemical order parameter η. We present calculations of the MCA of FePt as a function of η and find excellent agreement with the experimental data of Okamoto *et al* (2002 *Phys. Rev.* B **66** 024413) and others with respect to the magnetic easy axis, the magnitude of the MCA and its trend with decreasing η. We also study the paramagnetic phase of the ordered alloy using the 'disordered local moment' picture of metallic magnetism at finite temperatures. We calculate a Curie temperature of 935 K in reasonable agreement with experiment (710 K) and find the easy axis for the onset of ferromagnetic order to coincide with the magnetic easy axis found at low temperatures.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

For many years alloys comprised of approximately equal amounts of iron and platinum have attracted much attention owing to their relatively high magnetocrystalline anisotropies (MCA). Films of these alloys are easy to manufacture and are found to be chemically stable so that their potential for high density [1] and magneto-optic recording [2] applications is being vigorously investigated [3]. When annealed at appropriate temperatures, the equiatomic FePt system undergoes a transformation from the high-temperature disordered fcc γ phase, observed clearly at $T > 1300\,^{\circ}C$, to the ordered face-centred tetragonal (fct) $L1_0$ phase. The phase is ferromagnetically ordered below a Curie temperature of 710 K and acquires a saturation magnetization per iron atom of roughly 3 μ_B and possesses one of the highest uniaxial anisotropy constants K_u, up to $\sim 10^8$ erg cm^{-3} (0.88 meV/FePt pair) [4]. The easy axis is perpendicular to the iron/platinum layer stacking of the $L1_0$ structure. K_u depends strongly on the extent of the tetragonal $L1_0$ ordering whereas the disordered fcc γ solid solution, when quenched to low temperatures, is magnetically soft owing to its inherent cubic structure.

Much work has focused on the growth and microstructure of FePt thin films. Whereas the as-deposited FePt films are magnetically soft due to many imperfections, after annealing the $L1_0$ structure develops with a consequent high coercivity of $\sim$3–4 kOe [5]. The annealed films consist of anisotropic FePt nanoparticles within a non-magnetic matrix [6] with grain sizes as small as 3 nm making the films promising for high-density magnetic recording applications. The extent of the all-important $L1_0$ long-range chemical order depends on the preparation of these nano-composite films. Recently Okamoto *et al* [7] carried out Hall effect measurements on a set of FePt $L1_0$ films with different long-range order parameters, η. They find a significant drop of the first order uniaxial magnetic anisotropy constant as the size of the order parameter diminishes.

The chemical stability of thick FePt alloy films makes them easy to manufacture. Thick FePt films adopt the structure and magnetic properties of the bulk system and when the magnetic surface anisotropy becomes negligible, the measured anisotropy constant K_u relates directly to the bulk MCA term, which owes its origin to the spin–orbit coupling (SOC) of the electrons in the material. This MCA can be calculated within the tenets of relativistic density functional theory [8–12]. In this paper we explore how the MCA of a partially ordered alloy can be calculated from this 'first principles' theory. We obtain the MCA as a function of the long-range order parameter of the $L1_0$ FePt phase and carry out, to our knowledge, the first such calculation of this effect. The magnetic anisotropy also varies strongly with temperature. We therefore also examine the paramagnetic phase of the ordered alloy and determine the easy axis for the onset of magnetic order in this system.

In ordered magnetic binary alloys, the MCA can reach values of the order of meV per unit cell which is several orders of magnitude larger than those of the 3d ferromagnetic transition metals and their alloy solid solutions. Using perturbative approaches for SOC, there have been some theoretical attempts to calculate the MCA of ordered FePt [13]. These calculations readily find the easy axis perpendicular to the layering as found experimentally but the values reported are typically somewhat larger than empirical values. In an earlier work [14] we used the spin-polarized fully relativistic Korringa–Kohn–Rostoker electronic structure method within the coherent-potential approximation (SPR-KKR-CPA) [15] to describe the MCA of the compositionally disordered FePt solid solution. The SPR-KKR-CPA has also been applied to give rather realistic estimates of the MCA of $(Fe_c Pt_{1-c})_n/Pt$ superstructures [16]. We also calculated [14] the enhancement of the MCA of the alloy when significant atomic short-range order (ASRO) is present [17]. Similar studies had already been made of $Fe_{0.5}Co_{0.5}$, $Co_{0.5}Pt_{0.5}$

and $Fe_{0.5}Pd_{0.5}$ alloys [18]. In this paper we follow the MCA into the long-range ordered $L1_0$ FePt phase and monitor its increase with that of the order parameter.

In the next section we describe briefly how to model the partially ordered $L1_0$ FePt alloy and in the following section detail how to calculate the MCA of such a system. We also outline how the temperature dependence of the MCA can be modelled culminating with a calculation of the easy axis for the onset of magnetic order in FePt alloys at high temperatures. We then present our results for the dependence of the MCA of FePt alloys on the long-range order parameter. We complete the paper with a short summary.

2. Compositional order

Ordering in alloys can be succinctly classified in terms of static concentration waves [19]. In a binary alloy A_cB_{1-c} the A and B atoms occupy a regular array of lattice sites. At high temperatures the solid solution has each of its sites occupied by either an A- or B-type atom with probabilities c and $(1-c)$, respectively, i.e. a uniform concentration profile. In terms of a set of site-occupation variables $\{\xi_i\}$, (with $\xi_i = 1(0)$ when the ith site in the lattice is occupied by an A(B)-type atom) the thermodynamic average, $\langle \xi_i \rangle$, of the site-occupation variable is the concentration c_i at that site and for the solid solution $c_i = c$ for all sites. Below some transition temperature, T_0, the system orders (or phase separates) so that a compositionally ordered alloy forms, and c_i varies from site to site tracing out a superposition of static concentration waves [19, 20], i.e.

$$c_i = c + \frac{1}{2} \sum_{\mathbf{q}} \left[c_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{R}_i} + c_{\mathbf{q}}^* e^{-i\mathbf{q} \cdot \mathbf{R}_i} \right], \tag{2.1}$$

where $c_{\mathbf{q}}$ are the amplitudes of the concentration waves with wavevectors $\mathbf{q}$ and $\mathbf{R}_i$ are the lattice positions. Usually only a few concentration waves are needed to describe a particular ordered structure. For example, the CuAu-like $L1_0$ tetragonal ordered structure in an alloy with $c = 0.5$ is set up by a single concentration wave with $c_{\mathbf{q}} = \frac{1}{2}$ and $\mathbf{q} = (0, 0, 1)$ ($\mathbf{q}$ is in units of $2\pi/a$, a being the lattice parameter). The $L1_0$ long-range order parameter η is equal to twice $c_{(0,0,1)}$, 0 in the disordered phase ranging up to unity for the completely ordered phase.

Elsewhere [20–22] there are detailed discussions on how to describe theoretically the atomic short range order in the compositionally disordered phase in terms of a quantity $S_{ij}^{(2)}$

$$S_{jk}^{(2)} = -\left. \frac{\partial^2 \Omega(\{c_i\})}{\partial c_j \partial c_k} \right|_{\{c_i = c\}}, \tag{2.2}$$

i.e. a second derivative with respect to concentration of the grand potential (from density functional theory) describing the interacting electron system which constitutes the alloy. $S_{ij}^{(2)}$, formally a direct pair correlation function, can loosely be pictured as an effective atom–atom interchange energy and when set by the electronic structure of the disordered phase, $c_i = c$, it leads to the atomic short-range order parameter, $\alpha_{ij} = \beta[\langle \xi_i \xi_j \rangle - \langle \xi_i \rangle \langle \xi_j \rangle]$. The lattice Fourier transform $\alpha(\mathbf{q}, T)$ can be measured by diffuse scattering experiments and is connected directly to $S_{ij}^{(2)}$ by $\alpha(\mathbf{q}, T) = \beta c(1 - c)/(1 - \beta c(1 - c) S^{(2)}(\mathbf{q}))$ where $S^{(2)}(\mathbf{q})$ is the lattice Fourier transform of $S_{ij}^{(2)}$. The spinodal transition temperature T_0, below which the alloy orders into a structure characterized by the concentration wavevector $\mathbf{q}_{max}$, is determined by $S^{(2)}(\mathbf{q}_{max})$, where $\mathbf{q}_{max}$ is the value at which $S^{(2)}(\mathbf{q})$ is maximal ($\mathbf{q}_{max} = (0, 0, 1)$ for $L1_0$ order). We can write [20, 22], $T_0 = c(1 - c) S^{(2)}(\mathbf{q}_{max})/k_B$. Calculations of $S^{(2)}(\mathbf{q})$ then can provide a quantitative description of the propensity of an alloy to order when thermally annealed.

As shown elsewhere [22–24] the electronic origins of $S^{(2)}(\mathbf{q})$ describe how the state of magnetic order present at the ageing temperature can affect this propensity. In the

ferromagnetic state the electronic bands are spin-polarized. As the temperature of a metallic magnet is raised, spin fluctuations are excited which eventually destroy the long-range magnetic order and, hence, the overall spin polarization of the system's electronic structure. In many materials a simple model of 'local moments', which produce local magnetic fields on the lattice sites, effectively describes this phenomenon. The moments are assumed to vary their orientations slowly on the timescale of the electronic motions [25] and to be self-consistently maintained by them. The average over the local moments' orientations produces zero overall magnetization in the paramagnetic state.

This 'disordered local moment' (DLM) picture has been formulated so that the magnetic fluctuations are dealt with using KKR-CPA techniques. It is one of very few fully first-principles approach to the problem of the onset of ferro- and antiferromagnetism in metals [26, 27]. At no stage does it map the many-electron problem onto an effective Heisenberg model, and yet it deals, qualitatively, with both the ground state and the demise of magnetic long-range order at the Curie temperature in a material-specific, parameter-free manner. It is based on the combination of constrained density-functional theory (DFT) with the first-principles, spin-polarized multiple scattering (KKR-CPA) description of electrons in states with random orientation of local moments. Among its many successes are the prediction of the experimentally observed local exchange splitting in bulk Fe and the onset of magnetic order in Fe and Co alloys as well as in ultra-thin Fe and Co films [28]. Using this theory for ordered FePt we find a Curie temperature of 930 K. This estimate from a mean field theory compares reasonably well with the experimental value [29] of 710 K and shows that the energy scale of the magnetic fluctuations is produced adequately by the local moment picture. The easy axis for the onset of magnetic order can also be found from this DLM picture which we now discuss.

In the DLM scenario, for times, $\tau \gg \hbar/w$, ($\hbar/w$ is electronic hopping time) but $\tau < \tau_{sf}$ (τ_{sf} is typical spin fluctuation time), the spin orientations of the electrons leaving an atomic site are sufficiently correlated with those arriving that the magnetization integrated over a unit cell and averaged over τ is non-zero. The probability of having a particular arrangements of local moments with orientations $\{\hat{e}_i\}$ is given by

$$P(\{\hat{e}_i\}) = \frac{\exp[-\beta\Omega(\{\hat{e}_i\})]}{\prod_j \int d\hat{e}_j \exp[-\beta\Omega(\{\hat{e}_i\})]}$$

where $\Omega(\{\hat{e}_i\})$ is the 'generalized' electronic grand potential from SDFT and $\beta = (k_B T)^{-1}$. $\Omega(\{\hat{e}_i\})$ plays the part of a classical 'spin' or 'local moment' Hamiltonian. A tractable theory is produced by a suitable choice of a 'reference' Hamiltonian $\Omega_0\{\hat{e}_i\}$ and use of the Feynman inequality [27] $F \leqslant F_0 + \langle\Omega - \Omega_0\rangle^0$ with

$$F_0 = -(1/\beta) \ln \prod_i \int d\hat{e}_i \exp(-\beta\Omega_0) \tag{2.3}$$

and

$$\langle X\rangle^0 = \prod_i \int d\hat{e}_i X \exp(-\beta\Omega_0) \Big/ \prod_i \int d\hat{e}_i \exp(-\beta\Omega_0) = \prod_i \int d\mathbf{e}_i P_0\{\hat{e}_i\}X\{\hat{e}_i\}$$

with Ω_0 in the form

$$\Omega_0 = \sum_i \omega_i^{(1)}(\hat{e}_i) \tag{2.4}$$

and a 'first-principles' mean field theory is set up where the averaging is performed using techniques adapted from theory of the electronic structure of disordered alloys (SCF-KKR-CPA).

By including relativistic effects on the electronic structure we can develop the DLM theory to find the temperature dependence of the MCA. For a ferromagnetic metal magnetized along a direction $\hat{n}$ at temperature T and using the 'reference local moment Hamiltonian' of the form $\Omega_0^{(\hat{n})} = \sum_i h_i^{(\hat{n})} \hat{n} \cdot \hat{e}_i$, the free energy of the system at T is given by

$$F^{(\hat{n})} = \langle \Omega^{(\hat{n})} \rangle + \frac{1}{\beta} \sum_i \int P_i^{(\hat{n})}(\hat{e}_i) \ln P_i^{(\hat{n})}(\hat{e}_i) \, d\hat{e}_i$$

where $P_i^{(\hat{n})}(\hat{e}_i) = \exp(-\beta h_i^{(\hat{n})} \hat{n} \cdot \hat{e}_i) / \int \exp(-\beta h_i^{(\hat{n})} \hat{n} \cdot \hat{e}_i) \, d\hat{e}_i$ and the Weiss field $h_i^{(\hat{n})} = \frac{3}{4\pi} \int \langle \Omega^{(\hat{n})}\{\hat{e}_l\}\rangle_{\hat{e}_i} \hat{n} \cdot \hat{e}_i \, d\hat{e}_i$. The magnetization $\mathbf{M} = M\hat{n}$ is given by $M = \int P_i^{(\hat{n})}(\hat{e}_i) \hat{n} \cdot \hat{e}_i \, d\hat{e}_i$. The magnetic anisotropy is found by taking the difference between the energies for different magnetization directions. Full details of this approach will be given elsewhere [30].

By considering the response of the paramagnetic DLM state to the addition of a small external magnetic field, a mean field estimate can be made of the temperature below which a magnetization will spontaneously form in the direction of the applied field. For a infinitesimal field in the $(0, 0, 1)$ direction we have calculated a Curie temperature of 935 K, whereas if we consider the external field to be oriented parallel to the Fe and Pt layers of the $L1_0$ structure, T_c is 922 K. This shows that the easy axis for the onset of magnetic order in this system is along the c-axis, the same direction as the easy axis found at low temperatures.

In alloys the electronic interactions, which support such thermal, local-moment, spin fluctuations at high temperatures in the paramagnetic state, are also responsible for determining the nature of compositional ordering there. In a separate paper [14] we have calculated $S^{(2)}(\mathbf{q})$ for both ferromagnetic and paramagnetic (DLM) phases of the $Fe_{0.5}Pt_{0.5}$ solid solution and our calculations provide an explanation for the experimental observation that the atomic ordering set up in $Fe_{0.5}Pt_{0.5}$ annealed at a temperature above T_c is similar to that in samples aged below in the ferromagnetically ordered state. We find FePt in both paramagnetic and ferromagnetic states to be unstable to $L1_0$-type compositional ordering modulations ($\mathbf{q}_{max} = (0, 0, 1)$) below temperatures of 1450 and 1575 K, respectively. These *ab initio* values also compare well with what is observed experimentally, namely $L1_0$-type order below temperatures of roughly 1600 K. In the next section we calculate the effect of this ordering upon the uniaxial magnetic anisotropy of ordering the alloy.

3. Magnetocrystalline anisotropy

The magnetic anisotropy of a partially ordered alloy (omitting the finite temperature spin fluctuation effects) can be found together with its dependence on the long-range order parameter η. The MAE $K(\eta)$ of such an alloy can be written as the difference in the electronic grand-potential of the system magnetized along two directions $\mathbf{n}_1$ and $\mathbf{n}_2$. Thus,

$$K(\eta) = \Omega(\eta; \mathbf{n}_1) - \Omega(\eta; \mathbf{n}_2). \tag{3.1}$$

We assume that the double-counting correction $\Omega_{DC}(\eta; \mathbf{n})$ is generally unaffected by the change in the magnetization direction [15], and therefore $K(\eta)$ is given as the difference between the sum over effective single electron energies $K(\eta) = \int d\varepsilon \, f(\varepsilon, \nu_1)\varepsilon n(\eta, \varepsilon, \mathbf{n}_1) - \int d\varepsilon \, f(\varepsilon_1\nu_2)\varepsilon n(\eta, \varepsilon, \mathbf{n}_2)$ where $f(\varepsilon, \nu)$ is the Fermi–Dirac function and $n(\eta, \varepsilon, \mathbf{n})$ the electronic density of states of the partially ordered material magnetized along $\mathbf{n}$. Integrating by parts gives [15]

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

where $N(\eta, \varepsilon; \mathbf{n})$ is the integrated density of states and ν_1 and ν_2 are the chemical potentials of the system when the magnetization is along the $\mathbf{n}_1$ and $\mathbf{n}_2$ directions, respectively. The

change in the chemical potential originates from a redistribution of the occupied energy states as the magnetization direction is changed. Note that the effect, the second term in the equation above, on $K(\eta)$ is second order in $(\nu_1 - \nu_2)$, and can be shown to be very small compared to the first term [15]. In the following we use spin-polarized, relativistic, multiple-scattering theory and the Lloyd formula [31] for $N(\eta, \varepsilon; \mathbf{n})$.

A partially ordered $L1_0$-FePt alloy is comprised of four interpenetrating simple cubic (or tetragonal) lattices and each site of a given sub-lattice n has the probability c_n of being occupied by a Fe atom. For an alloy with long-range order parameter η, the sites of two of the sublattices have the probability $(1 + \eta)/2$ of being occupied by an Fe atom whilst the other two have the probability $(1 - \eta)/2$. For $\eta = 1$, two sublattices are entirely Fe-occupied whilst the other two are wholly platinum. The coherent-potential approximation adapted for a multi-sublattice system [32–34] is used to deal with the averaging over disorder for $\eta \neq 1$. We choose $\mathbf{n}_1 = (0, 0, 1)$, and $\mathbf{n}_2 = (1, 0, 0)$ and the uniaxial magnetic anisotropy constant of $L1_0$-FePt as a function of the order parameter η is

$$K_u(\eta) \approx - \int_{-\infty}^{\infty} d\varepsilon \, f(\varepsilon, \nu_{(0,0,1)}) \left[N(\eta, \varepsilon; (0, 0, 1)) - N(\eta, \varepsilon; (1, 0, 0)) \right] \tag{3.2}$$

and $N(\eta, \varepsilon; \mathbf{n})$ is the multi-sublattice generalization of the expression for the integrated density of states of a disordered alloy [15].

$$N(\eta, \varepsilon; \mathbf{n}) = N_0(\varepsilon) - (\text{Im}/\pi) \int_{\text{BZ}} d\mathbf{k} \, \log \| \underline{t}_c^{-1} - \underline{G}(\mathbf{k}, \varepsilon) \|$$

$$- (\text{Im}/\pi) \sum_{n=1}^{4} (c_n \log |\underline{1} + (\underline{t}_{\text{Fe}}^{-1} - \underline{t}_{c,n}^{-1}) \underline{\tau}^{c,nn}|$$

$$+ (1 - c_n) \log |\underline{1} + (\underline{t}_{\text{Pt}}^{-1} - \underline{t}_{c,n}^{-1}) \underline{\tau}^{c,nn}|)$$

where $\underline{t}_c$ is the scattering t-matrix for the effective CPA medium which is a matrix with elements labelled by sublattice n and orbital (l, m) and spin (s) angular momentum quantum numbers. It is diagonal with respect to n. $\underline{G}(\mathbf{k}, \varepsilon)$ is the structure constant matrix with elements $G_{l,m;l',m'}^{n,n'} \delta_{s,s'}(\mathbf{k}, \varepsilon)$. The integral of the first term is over the Brillouin zone of the simple cubic $(c/a = 1)$ or tetragonal lattice. $\underline{t}_{\text{Fe}}$ and $\underline{t}_{\text{Pt}}$ are the single site t-matrices describing scattering from Fe and Pt sites, respectively. $\underline{\tau}^{c,nn}$ is the site diagonal scattering path operator describing scattering from and to a site on the nth sublattice. It is given by an integral over the Brillouin zone
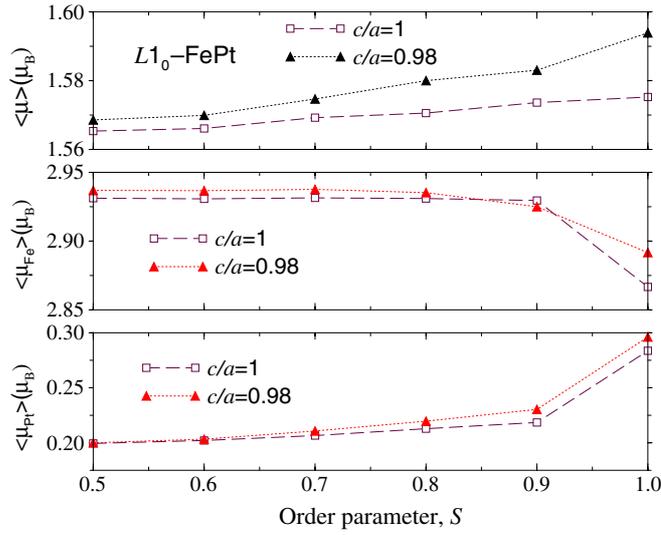
$$\underline{\tau}^{c,nn} = \int d\mathbf{k} \, (\underline{t}_c^{-1} - \underline{G}(\mathbf{k}, \varepsilon))_{n,n}^{-1} \tag{3.3}$$

and the CPA condition which sets $\underline{t}_c$ and $\underline{\tau}^{c,nn}$ is
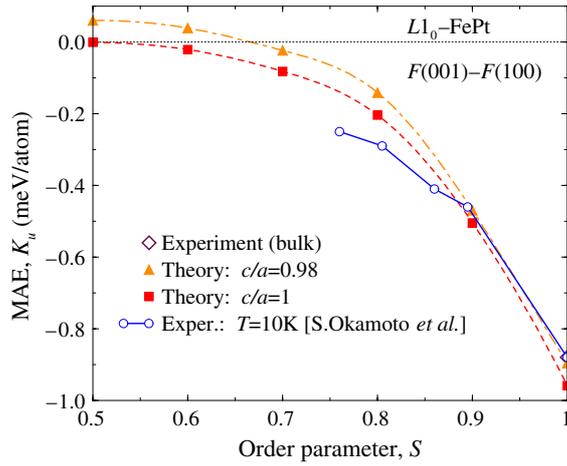
$$\underline{\tau}^{c,nn} = c_n((\underline{\tau}^{c,nn})^{-1} + (\underline{t}_{\text{Fe}}^{-1} - \underline{t}_{c,n}^{-1}))^{-1} + (1 - c_n)((\underline{\tau}^{c,nn})^{-1} + (\underline{t}_{\text{Pt}}^{-1} - \underline{t}_{c,n}^{-1}))^{-1}. \tag{3.4}$$

4. Results and discussion

The first step in calculating the MCA from equation (3.2) is to generate self-consistently the appropriate one-electron Fe and Pt potentials for partially ordered FePt alloys [33, 34]. Two sets of calculations were carried out. The first for crystal structures with the unit-cell volume fixed at the experimental volume and $c/a = 0.981$ and secondly, for the same unit cell volume but c/a set equal to one. Values of the average magnetic moments per iron and platinum sites are shown as a function of η ($\eta = 2S - 1$) in figure 1. The moments of the iron sites are rather independent of the extent of ordering of the alloy until nearly complete order ($\eta > 0.8$,

Figure 1. Total average and site-projected average spin magnetic moments of Fe and Pt in $L1_0$-FePt with $c/a = 0.98$ and 1 as calculated by the SPR-KKR-CPA for a range of long-range order parameters, $S = (1 + \eta)/2$.

Figure 2. The MCA of $L1_0$-FePt with $c/a = 0.98$ and 1, calculated as a function of order-parameter $S = (1 + \eta)/2$. Experimental data [7] are also shown for comparison.

$S > 0.9$) when μ_{Fe} drops slightly from 2.93 to 2.88 μ_B. As η increases from 0 to 0.8, the moments on the Pt sites increase very slightly from 0.20 to 0.22 μ_B. Thereafter there is a climb to 0.3 μ_B for complete order. These trends can be understood along the same lines as described by Brown *et al* [35] for their calculations of the magnetic properties of partially ordered FePt alloys. The overall average magnetic moment per site is shown in the upper panel of figure 1. Our results are in good agreement with experimental findings [7].

Figure 2 shows the main results of the paper. The value of the uniaxial magnetic anisotropy constant, $K_u(\eta)$ is shown as a function of long range order parameter η ($=2S - 1$). The measurements of Okamoto *et al* [7] are also shown for comparison. There is excellent

agreement with the experimental data with the easy axis, the magnitude of the anisotropy and its trend with the order parameter.

These results highlight the potential of this method for finding ways of designing materials based on FePt in which the magnetic properties are optimized for applications.

5. Conclusions

The high magnetocrystalline anisotropy of equiatomic FePt makes this material suitable for many magnetic applications. The $L1_0$ ordered phase of alternating Fe and Pt planes is a key factor for its significant MCA. In this paper we have shown how the MCA of a partially ordered alloy can be calculated from 'first-principles' relativistic density functional theory. The first application of this approach has been for FePt. The calculated MCA of completely ordered FePt is in excellent agreement with experimental values and its sharp drop with diminishing long-range chemical order parameter is also very well described. We have also studied the paramagnetic phase of the ordered alloy, using a model of 'disordered local moments' for the magnetic fluctuations and determined its Curie temperature and also the easy axis for the onset of ferromagnetic order. This coincides with the magnetic easy axis found at low temperatures. Future work will involve the study of the DLM picture in the ferromagnetic phase where we shall calculate the temperature dependence of the magnetic anisotropy constants [30].

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