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The effects of magnetic annealing of transition metal alloys deduced from *ab initio* electronic structure calculations

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Abstract
A theory is presented for describing the effects of annealing magnetic alloys in magnetic fields. It has an *ab initio* spin-polarized relativistic Korringa–Kohn–Rostoker coherent potential approximation (KKR-CPA) electronic structure basis and uses the framework of concentration waves. Alloys which would otherwise be soft magnets are found experimentally to develop directional chemical order and significant uniaxial anisotropy when annealed in magnetic fields. Our approach is able to provide a quantitative description of these effects together with the underlying electronic mechanisms. We describe applications to the soft magnetic alloys permalloy and FeCo.

1. Introduction

In finding applications for magnetic materials it is very useful to be able to control the shapes of their magnetization curves by means of specific treatments. It is found that most ferromagnetic and ferrimagnetic materials develop an extra magnetic anisotropy with a 'knock-on' effect on the shape of their magnetic curves when they undergo a treatment with directional properties. For example most ferromagnetic alloys exhibit a uniaxial magnetic anisotropy associated with the roll direction when they are cold-rolled. Also induced magnetic anisotropies grow in magnetic materials heat treated under an applied stress or, pertinent to this paper, in a magnetic field as they are cooled through a phase transition [1, 2]. In this paper we give a theory for the microscopic basis for this magnetic annealing effect.

From 'first principles', magnetic anisotropy arises from relativistic interactions. The most important is spin–orbit coupling which links the spin of an electron to the crystal structure. These relativistic interactions, which arise from the high speeds of the electrons close to the atomic nuclei and are pronounced in materials with constituents with large atomic number, are small in comparison with the exchange interactions but are nonetheless important in

determining the equilibrium direction of the magnetization, coercivity, linear magnetostriction, domain wall structure, and magnetic properties in general. Consequently our theory is based on relativistic spin-polarized density functional theory [3–5] and its solution by the SPR-KKR-CPA method [6, 7] (SPR standing for spin-polarized relativistic). A detailed description of how the method can be used to describe magnetocrystalline anisotropy in homogeneously disordered ferromagnetic alloys has been provided in reference [8]. Here we describe a way to investigate the effects of compositional order, both short and long ranged, on the magnetocrystalline anisotropy (for a brief summary see reference [9] and for more details see reference [10]) and how this can be used to describe directional chemical order induced in a soft magnetic alloy when it is cooled in a magnetic field.

2. Compositional order

We consider a binary alloy A_cB_{1-c} where the atoms are arranged on a regular array of lattice sites. At high temperatures the homogeneously disordered alloy has each site occupied by an A- or B-type atom with probabilities c and $1-c$ respectively. Below some transition temperature, T_o, the system orders or phase separates. A compositionally modulated alloy can be described by 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-type (B-type) atom. The thermodynamic average, $\langle\xi_i\rangle$, of the site-occupation variable is the concentration c_i at that site. At high temperatures, $c_i = c$ for all sites. When inhomogeneity sets in below T_o, the temperature-dependent concentration fluctuations $\{\delta c_i\} = \{c_i - c\}$ can be written as superpositions of static concentration waves [11], i.e.,

$$c_i = c + \frac{1}{2}\sum_{\boldsymbol{q}}\left[c_{\boldsymbol{q}}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_i} + c^*_{\boldsymbol{q}}\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_i}\right]$$

where the $c_{\boldsymbol{q}}$ are the amplitudes of the concentration waves with wave-vectors $\boldsymbol{q}$, and the $\boldsymbol{R}_i$ are the lattice positions. Usually only a few concentration waves are needed to describe a particular ordered structure. For example (figure 1), the Cu_3Au-like $L1_2$ ordered structure is set up by three concentration waves of identical amplitude $c_{\boldsymbol{q}} = \frac{1}{4}$ and wave-vectors $\boldsymbol{q}_1 = (100)$, $\boldsymbol{q}_2 = (010)$, and $\boldsymbol{q}_3 = (001)$ ($\boldsymbol{q}$ is in units of $2\pi/a$, a being the lattice parameter).

The grand potential of a soft magnetic alloy with composition $\{c_i\}$ at temperature T and in the presence of an applied magnetic field such that it is magnetized along the direction $\boldsymbol{e}$ is given by [11–13]

$$\Omega(\{c_i\};\boldsymbol{e}) = \nu Z - \int_{-\infty}^{\infty}\mathrm{d}\varepsilon\; f(\varepsilon,\nu)N(\{c_i\},\varepsilon;\boldsymbol{e}) + \Omega_{DC}(\{c_i\};\boldsymbol{e}) \tag{2.1}$$

where ν is the chemical potential, Z is the total valence charge, $f(\varepsilon,\nu)$ is the Fermi factor, $N(\{c_i\},\varepsilon;\boldsymbol{e})$ is the integrated electronic density of states, and $\Omega_{DC}(\{c_i\};\boldsymbol{e})$ is the 'double-counting' correction to the grand potential [12]. The derivatives of the grand potential with respect to the concentration variables give rise to a hierarchy of direct correlation functions. In particular, the second derivative evaluated at the equilibrium concentration:

$$S^{(2)}_{jk}(\boldsymbol{e}) = -\left.\frac{\partial^2\Omega(\{c_i\};\boldsymbol{e})}{\partial c_j\,\partial c_k}\right|_{\{c_i=c\}}$$

is the Ornstein–Zernike direct correlation function for our lattice model [11–15] (so called in view of the close analogy with similar quantities defined for classical fluids [16]). These are related to the linear response functions, $\alpha_{ij}(\boldsymbol{e})$, through [13]

$$\left[1 + \sum_k S^{(2)}_{ik}(\boldsymbol{e})\alpha_{ki}(\boldsymbol{e})\right]\alpha_{ij}(\boldsymbol{e}) = \beta c(1-c)\left[\delta_{ij} + \sum_k S^{(2)}_{ik}(\boldsymbol{e})\alpha_{kj}(\boldsymbol{e})\right] \tag{2.2}$$

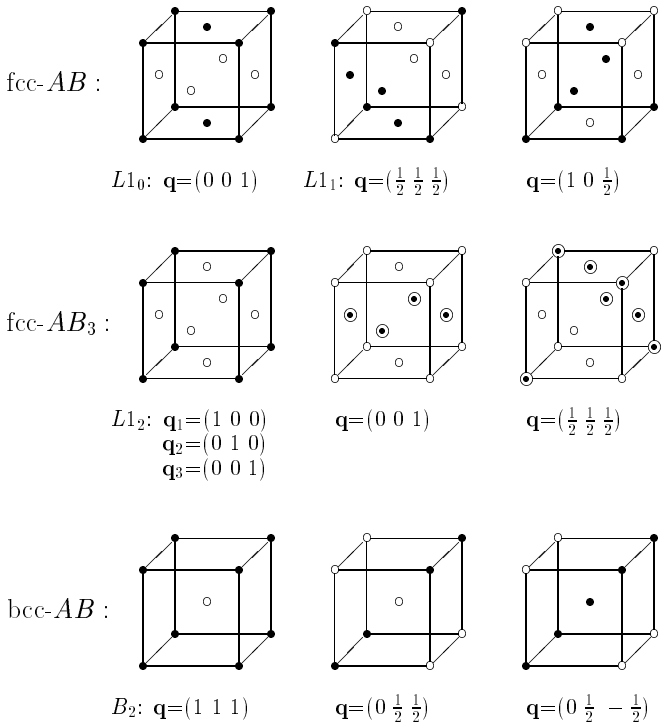

Figure 1. Some ordered structures and their representative concentration wave-vectors. For the AB-type stoichiometry, $\boldsymbol{q} = (001)$ and $\boldsymbol{q} = (\frac{1}{2}\frac{1}{2}\frac{1}{2})$ generate respectively the CuAu-type $L1_0$ layered ordered structure with layers perpendicular to the [001] direction and the CuPt-type $L1_1$ layered ordered structure with layers perpendicular to the [111] direction, and $\boldsymbol{q} = (10\frac{1}{2})$ generates a layered structure with planes of an ordered structure of A and B atoms stacked along the [001] direction. For the AB_3-type composition, a combination of $\boldsymbol{q}_1 = (100)$, $\boldsymbol{q}_2 = (010)$, and $\boldsymbol{q}_3 = (001)$ generates the Cu_3Au-type $L1_2$ ordered structure. For this composition, a single wave-vector $\boldsymbol{q} = (001)$ generates a superstructure of alternating monolayers of pure B atoms and disordered $A_{0.5}B_{0.5}$ perpendicular to the [001] direction. Similarly, $\boldsymbol{q} = (\frac{1}{2}\frac{1}{2}\frac{1}{2})$ generates a superstructure of monolayers of pure B atoms and disordered $A_{0.5}B_{0.5}$ perpendicular to the [111] direction. The full circles denote A atoms, open circles denote B atoms, and a full circle circumscribed by an open circle denotes a CPA effective atom $A_{0.5}B_{0.5}$.

where $\beta = (k_B T)^{-1}$, k_B being the Boltzmann constant. The linear response functions, $\alpha_{ij}(\boldsymbol{e})$, describe the resulting concentration fluctuations, $\{\delta c_i\}$, which are produced when a small inhomogeneous set of external chemical potentials, $\{\delta\nu_i\}$, is applied at all sites. Via the fluctuation dissipation theorem these are proportional to atomic pair-correlation functions, i.e. $\alpha_{ij} = \beta[\langle\xi_i\xi_j\rangle - \langle\xi_i\rangle\langle\xi_j\rangle]$. Upon taking the lattice Fourier transform of equation (2.2) we obtain a closed form of equations [11–15]:

$$\alpha(\boldsymbol{q}, T; \boldsymbol{e}) = \frac{\beta c(1-c)}{1 - \beta c(1-c)[S^{(2)}(\boldsymbol{q}; \boldsymbol{e}) - \lambda_c]} \tag{2.3}$$

where the Onsager cavity correction λ_c is given by [13]

$$\lambda_c = \frac{1}{\beta c(1-c)} \frac{1}{V_{BZ}} \int \mathrm{d}\boldsymbol{q}'\, S^{(2)}(\boldsymbol{q}'; \boldsymbol{e})\, \alpha(\boldsymbol{q}', T; \boldsymbol{e}).$$

Here, the $\alpha(\boldsymbol{q}, T)$, the lattice Fourier transform of α_{ij}, are the Warren–Cowley atomic short-range order (ASRO) parameters in the disordered phase and are proportional to the intensities

measured in diffuse electron, x-ray, or neutron scattering experiments. The Onsager cavity correction in equation (2.3) ensures that the spectral weight over the Brillouin zone is conserved [13, 15], so, in other words, the diagonal part of the fluctuation dissipation theorem is honoured, i.e. $\alpha_{ii} = \beta c(1-c)$.

The spinodal transition temperature T_s below which the alloy orders into a structure characterized by the concentration wave-vector $\boldsymbol{q}_{max}$ is determined by $S^{(2)}(\boldsymbol{q}_{max}; \boldsymbol{e})$, where $\boldsymbol{q}_{max}$ is the value at which $S^{(2)}(\boldsymbol{q}; \boldsymbol{e})$ is maximal. We can write [11, 12, 14]

$$T_s = \frac{c(1-c)(S^{(2)}(\boldsymbol{q}_{max}; \boldsymbol{e}) - \lambda_c(T_s))}{k_B}.$$

Full details of the expression for $S^{(2)}(\boldsymbol{q}; \boldsymbol{e})$ in terms of the electronic structure of the disordered phase are given elsewhere [9–15]. The effect of magnetic annealing is contained in the dependence of $S^{(2)}(\boldsymbol{q}; \boldsymbol{e})$ upon $\boldsymbol{e}$ and to achieve this we must include the effects of relativistic, spin-polarized electronic structure. As an example in the next section we show that for permalloy $Ni_{75}Fe_{25}$ annealed in a magnetic field along [001], $S^{(2)}(\boldsymbol{q} = (001)) > S^{(2)}(\boldsymbol{q} = (010))$, $S^{(2)}(\boldsymbol{q} = (100))$. Directional chemical order can thus be induced into the alloy.

3. Magnetic annealing of $Ni_{0.75}Fe_{0.25}$ alloy

Permalloy $Ni_{0.75}Fe_{0.25}$ is a soft magnet and is a disordered alloy on an fcc lattice above 820 K. Below this temperature it orders into an $L1_2$ structure [17]. However, when it is annealed in a magnetic field, a uniaxial magnetic anisotropy is induced depending on the direction of the applied field with respect to the crystallographic axes [1, 2]. A recent study based on magneto-optic Kerr effect measurements [18] also reveals that magnetic annealing can induce uniaxial anisotropy. In reference [9], we produced the first quantitative description of magnetic annealing from *ab initio* electronic structure calculations in $Ni_{0.75}Fe_{0.25}$. We found that ordering is favoured along the direction of the applied field. For example, when the field is applied along the [001] direction, it produces a layered structure along the [001] direction comprising alternate pure Ni layers and disordered $Ni_{0.5}Fe_{0.5}$ layers. Noting that the measured intensity in a scattering experiment is proportional to the ASRO parameter $\alpha(\boldsymbol{q})$, we present here the ASRO parameters calculated at 1 K above the ordering temperature for different $\boldsymbol{q}$-vectors in table 1. We note that when the applied magnetic field is along the [001] direction, $\alpha(\boldsymbol{q})$ for $\boldsymbol{q} = (001)$ is 40–50% larger than that at other $\boldsymbol{q}$-vectors. Therefore, when the alloy is annealed in the magnetic field, the superlattice spot in the measured intensity at $\boldsymbol{q} = (001)$ will be 40–50% more intense than that at $\boldsymbol{q} = (100)$ at a temperature 1 K above the transition temperature.

Table 1. Atomic short-range order (ASRO) parameters $\alpha(\boldsymbol{q}; \boldsymbol{e})$ calculated at a temperature 1 K above the ordering temperature 721 K at a few high-symmetry $\boldsymbol{q}$-vectors for $Ni_{0.75}Fe_{0.25}$ alloy (the respective ordered structures are shown in figure 1).

$\boldsymbol{q}$	$\boldsymbol{e} = [001]$	$\boldsymbol{e} = [100]$	$\boldsymbol{e} = [111]$
(100)	1509.7	2601.4	1756.2
(010)	1509.7	1509.7	1756.2
(001)	2601.4	1509.7	1756.2
$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	2.3	2.3	2.3
$(10\frac{1}{2})$	4.3	4.3	4.3
$(\frac{1}{2}01)$	4.3	4.3	4.3

4. Magnetocrystalline anisotropy

We now move on to show how the magnetic anisotropy that is induced by magnetic annealing can be estimated. The magnetocrystalline anisotropy energy (MAE) of the inhomogeneous alloy can be characterized by the change in the electronic grand potential arising from the change in the magnetization direction. Thus,

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

where $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ are two magnetization directions. We assume that the double-counting correction $\Omega_{DC}(\{c_i\}; \boldsymbol{e})$ is generally unaffected by the change in the magnetization direction, and, therefore, only the first two terms of equation (2.1) contribute to the MAE:

$$K(\{c_i\}) = (\nu_1 - \nu_2)Z - \int_{-\infty}^{\infty} \mathrm{d}\varepsilon\ f(\varepsilon, \nu_1) N(\{c_i\}, \varepsilon; \boldsymbol{e}_1) + \int_{-\infty}^{\infty} \mathrm{d}\varepsilon\ f(\varepsilon, \nu_2) N(\{c_i\}, \varepsilon; \boldsymbol{e}_2)$$

where ν_1 and ν_2 are the chemical potentials of the system when the magnetization is along the $\boldsymbol{e}_1$- and $\boldsymbol{e}_2$-directions respectively. The change in the chemical potential originates from a redistribution of the occupied energy bands in the Brillouin zone in the event of a change of magnetization direction. A Taylor expansion of $f(\varepsilon, \nu_2)$ about ν_1 and some algebra leads to

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

Note that the effect of the small change in the chemical potential on $K(\{c_i\})$ is of second order in $\nu_1 - \nu_2$, and can be shown to be very small compared to the first term [8]. We now expand $K(\{c_i\})$ around $K_{CPA}(c)$, the MAE of the homogeneously disordered alloy $\mathrm{A}_c\mathrm{B}_{1-c}$:

$$K(\{c_i\}) = K_{CPA}(c) + \sum_j \left.\frac{\partial K(\{c_i\})}{\partial c_j}\right|_{\{c_i=c\}} \delta c_j + \frac{1}{2}\sum_{j,k} \left.\frac{\partial^2 K(\{c_i\})}{\partial c_j\,\partial c_k}\right|_{\{c_i=c\}} \delta c_j\,\delta c_k + \mathrm{O}(\delta c)^3. \tag{4.1}$$

Within the SPR-KKR-CPA scheme, a formula for $K_{CPA}(c)$ is obtained by using the Lloyd formula [19] for the integrated density of states. The second term in equation (4.1) is independent of the site index and so vanishes if the number of A and B atoms in the alloy is to be conserved. We find

$$\left.\frac{\partial^2 K(\{c_i\})}{\partial c_j\,\partial c_k}\right|_{\{c_i=c\}} = -(S^{(2)}_{jk}(\boldsymbol{e}_1) - S^{(2)}_{jk}(\boldsymbol{e}_2))$$

i.e. in terms of the Ornstein–Zernike direct correlation functions [11]. Now taking the Fourier transform of equation (4.1), we get the MAE of the compositionally modulated alloy with wave-vector $\boldsymbol{q}$:

$$K(\boldsymbol{q}) = K_{CPA}(c) + \frac{1}{2}|c_{\boldsymbol{q}}|^2 K^{(2)}(\boldsymbol{q}) \tag{4.2}$$

where

$$K^{(2)}(\boldsymbol{q}) = -(S^{(2)}(\boldsymbol{q}; \boldsymbol{e}_1) - S^{(2)}(\boldsymbol{q}; \boldsymbol{e}_2)). \tag{4.3}$$

The technical and computational details for evaluating $K^{(2)}(\boldsymbol{q})$ and $S^{(2)}(\boldsymbol{q}; \boldsymbol{e})$ are discussed in references [8–10].

Having established how $\mathrm{Ni}_{0.75}\mathrm{Fe}_{0.25}$ can develop directional chemical order when annealed in a magnetic field along the [001] crystallographic direction we can now calculate the induced uniaxial MAE using (4.2). We find this to be of the order of 5 μeV, an increase of more than two orders of magnitude over that of the disordered phase which is very small (less than 0.1 μeV). However, in the case of perfect ordering, which is $L1_2$, the MAE becomes very small, as in the disordered phase. This is consistent with experimental observations of Chikazumi [1] and Ferguson [2].

5. $Fe_{0.5}Co_{0.5}$ alloy

FeCo alloys exhibit high saturation magnetizations, low magnetocrystalline anisotropies, and high Curie temperatures, and therefore are potential candidates as high-temperature magnets in such applications as in rotors in electric aircraft engines. The bcc disordered $Fe_{0.5}Co_{0.5}$ alloy undergoes a phase transition to an ordered $B2$ structure [20] below 1000 K, which is below the alloy's Curie temperature T_c, and both the ordered and the disordered phases have very low magnetocrystalline anisotropy but somewhat large magnetostriction [20]. The experimental value of the MAE ($E(001) - E(111)$) for both the disordered and $B2$ ordered phase is less than 1.0 μeV per atom and the easy axis is along the [111] direction of the crystal for both phases. Our estimate of the order–disorder transition temperature (1286 K) is in reasonable agreement with the experimental value of 1000 K.

Also there is good agreement between our theoretical value of the MAE and the experimental value. (It is difficult to compare the absolute values of the theoretical and experimental values of the MAE, because they are of the order of 0.1 μeV, which is the accuracy of our calculations). Moreover, on the basis of our calculations shown in table 2 we can again emphasize the role of symmetry for magnetic anisotropy. Note that $\boldsymbol{q} = (100)$, $\boldsymbol{q} = (010)$, $\boldsymbol{q} = (001)$, as well as $\boldsymbol{q} = (111)$, each generate the same $B2$ structure, unlike the case for a fcc lattice. Our calculation shows the results to be identical. This is an indicator of the accuracy and robustness of our computational procedure. Interestingly it can be seen from table 2 that the $B2$ ordering instils a tendency for the magnetic easy axis to twist from (111) to (100). Thus with a modest degree of order the MAE constant could become vanishingly small. We have also calculated the MAE for some hypothetical structures shown in figure 1. The reduced symmetry of these structures causes the MAE to be some two orders of magnitude larger than those of the equilibrium ordered structure and the disordered phase.

Table 2. Magnetocrystalline anisotropy energy $K(\boldsymbol{q})$ for several compositionally modulated $Fe_{0.5}Co_{0.5}$ alloys characterized by different $\boldsymbol{q}$-vectors (the respective ordered structures are shown in figure 1). Here the $K(\boldsymbol{q})$ are calculated with respect to the reference system which has the magnetization along the [001] direction (i.e. $\boldsymbol{e}_1 = [001]$) of the crystal. Thus, when $K(\boldsymbol{q}) < 0$ the easy axis is along [001] and when $K(\boldsymbol{q}) > 0$ the easy axis is along $\boldsymbol{e}_2$.

		$K(\boldsymbol{q})$ (μeV)			
$\boldsymbol{q}$	Structure	$\boldsymbol{e}_2 = [111]$	$\boldsymbol{e}_2 = [100]$	$\boldsymbol{e}_2 = [110]$	Easy axis
(100)	$B2$	−0.8	0.0	−0.7	[001]
(001)	$B2$	−0.8	0.0	−0.7	[001]
(111)	$B2$	−0.8	0.0	−0.7	[001]
$(\frac{1}{2}\frac{1}{2}0)$		11.1			[111]
$(-\frac{1}{2}\frac{1}{2}0)$		−95.2			[001]
$(\frac{1}{2}0\frac{1}{2})$		74.2			[111]
$(-\frac{1}{2}0\frac{1}{2})$		−32.5			[001]

6. Electronic structure

In elemental solids and the disordered alloys the MAE originates from a redistribution of electronic states around the Fermi level caused by the change in the magnetization direction [8]. The electronic structure of the disordered phase around the Fermi level is also partly responsible

for the tendency towards compositional order in some alloys [11, 13]. We believe therefore that the directional chemical ordering resulting from magnetic annealing together with the enhancement of the MAE in soft magnetic alloys is also related to this aspect of the disordered phase's electronic structure, and we demonstrate this in this section.

First we consider the electronic mechanism underlying the compositional ordering tendency. Our calculations of $S^{(2)}(\boldsymbol{q};\boldsymbol{e})$ and $\alpha(\boldsymbol{q},\boldsymbol{e},T)$ predict $L1_2$- and $B2$-type order in $Ni_{75}Fe_{25}$ and $Fe_{50}Co_{50}$ respectively in excellent agreement with experiment. $S^{(2)}(\boldsymbol{q};\boldsymbol{e})$ can be written as a sum over occupied electronic states of an electronic structure-based quantity $F(\boldsymbol{q},\varepsilon;\boldsymbol{e})$ [10, 11, 13]:

$$S^{(2)}(\boldsymbol{q};\boldsymbol{e}) = -\frac{\mathrm{Im}}{\pi}\int_{-\infty}^{\infty} \mathrm{d}\varepsilon\ f(\varepsilon,\nu)F(\boldsymbol{q},\varepsilon;\boldsymbol{e}).$$

$S^{(2)}(\boldsymbol{q})$ can also be written in terms of a sum over Matsubara frequencies, $\omega_n = (2n+1)\pi k_B T$:

$$S^{(2)}(\boldsymbol{q};\boldsymbol{e}) = 2k_B T\sum_n \mathrm{Re}\left[F(\boldsymbol{q},\nu+\mathrm{i}\omega_n;\boldsymbol{e})\right]. \tag{6.1}$$

For the interplay between the MAE and compositional order, the quantity $K^{(2)}(\boldsymbol{q})$ given by equation (4.3) can also be written as a sum of contributions evaluated at the Matsubara frequencies:

$$K^{(2)}(\boldsymbol{q}) = -\frac{\mathrm{Im}}{\pi}\int_{-\infty}^{\infty} \mathrm{d}\varepsilon\ f(\varepsilon,\nu)\,\Delta F(\boldsymbol{q},\varepsilon) = 2k_B T\sum_n \mathrm{Re}[\Delta F(\boldsymbol{q},\nu+\mathrm{i}\omega_n)] \tag{6.2}$$

where

$$\Delta F(\boldsymbol{q},\varepsilon) = F(\boldsymbol{q},\varepsilon;\boldsymbol{e}_1) - F(\boldsymbol{q},\varepsilon;\boldsymbol{e}_2). \tag{6.3}$$

As shown in figure 2, the principal contributions to $\Delta F(\boldsymbol{q},\varepsilon)$ come from near the real axis indicating that the Fermi surface plays the dominant role in directional chemical ordering by magnetic annealing and the corresponding enhancement of the MAE.

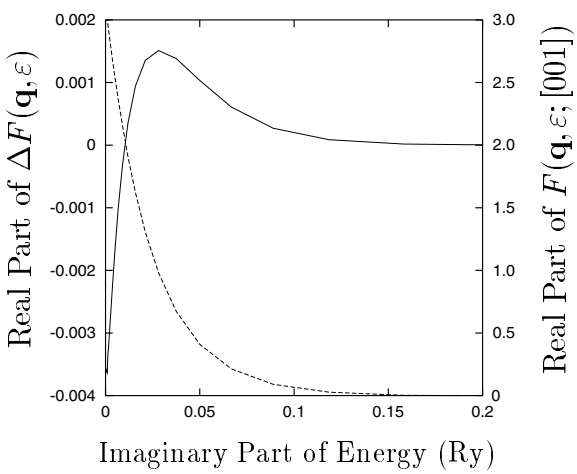

Figure 2. The real part of $\Delta F(\boldsymbol{q},\varepsilon)$ as defined in equation (6.3) with $\boldsymbol{e}_1 = [001]$ and $\boldsymbol{e}_2 = [100]$ (full line, left scale) and the real part of $F(\boldsymbol{q},\varepsilon;[001])$ as defined in equation (6.1) for $\boldsymbol{q} = (001)$ (dashed line, right scale) at complex energies along the imaginary axis perpendicular to the Fermi level for $Ni_{0.75}Fe_{0.25}$ alloy.

7. Conclusions

We have outlined our *ab initio* theory of the connection between magnetocrystalline anisotropy of ferromagnetic alloys and compositional order within the SPR-KKR-CPA scheme. We have focused upon the effect of annealing a soft magnetic alloy in an applied magnetic field and have shown how the induced uniaxial magnetic anisotropy, known to develop under these circumstances, is caused by directional compositional order related to the direction of the magnetic field. Changes to the alloy's electronic structure close to the Fermi surface are important for the details of this effect.

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References

[1] Chikazumi S 1956 *J. Phys. Soc. Japan* **11** 551
[2] Ferguson E T 1958 *J. Appl. Phys.* **29** 252
[3] MacDonald A H and Vosko S 1979 *J. Phys. C: Solid State Phys.* **12** 2977
[4] Rajagopal A K 1978 *J. Phys. C: Solid State Phys.* **11** L943
[5] Ramana M V and Rajagopal A K 1983 *Adv. Chem. Phys.* **54** 231
[6] Ebert H, Drittler B and Akai H 1992 *J. Magn. Magn. Mater.* **104–107** 733
[7] Strange P, Ebert H, Staunton J B and Gyorffy B L 1989 *J. Phys.: Condens. Matter* **1** 2959
[8] Razee S S A, Staunton J B and Pinski F J 1997 *Phys. Rev.* B **56** 8082
[9] Razee S S A, Staunton J B, Ginatempo B, Pinski F J and Bruno E 1999 *Phys. Rev. Lett.* **82** 5369
[10] Razee S S A, Staunton J B, Ginatempo B, Bruno E and Pinski F J 2001 *Phys. Rev.* B **64** at press
[11] Gyorffy B L and Stocks G M 1983 *Phys. Rev. Lett.* **50** 374
[12] Gyorffy B L, Johnson D D, Pinski F J, Nicholson D M and Stocks G M 1987 *Alloy Phase Stability (NATO ASI Series, vol 163)* ed G M Stocks and A Gonis (Dordrecht: Kluwer Academic) p 421
[13] Staunton J B, Johnson D D and Pinski F J 1994 *Phys. Rev.* B **50** 1450
[14] Staunton J B, Razee S S A, Ling M F, Johnson D D and Pinski F J 1998 *J. Phys. D: Appl. Phys.* **31** 2355
[15] Johnson D D, Staunton J B and Pinski F J 1994 *Phys. Rev.* B **50** 1473
[16] Evans R 1979 *Adv. Phys.* **28** 143
[17] Orehotsky J, Sousa J B and Pinheiro M F 1982 *J. Appl. Phys.* **53** 7939
[18] Schedin F, Hewitt L, Morrall P, Petrov V N and Thornton G 1999 *J. Magn. Magn. Mater.* **198+199** 555
[19] Lloyd P 1967 *Proc. Phys. Soc.* **90** 207
[20] Hall R C 1960 *J. Appl. Phys.* **31** 157S