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A first-principles theory of magnetocrystalline anisotropy in metals

P Strange^{†‡}, H Ebert^{†§}, J B Staunton^{||} and B L Gyorffy[†]

[†] Physics Department, Bristol University, Tyndall Avenue, Bristol BS8 1TL, UK

^{||} Physics Department, Warwick University, Coventry, West Midlands, UK

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Abstract. A first-principles theory of the zero-temperature magnetocrystalline anisotropy in metals is discussed. It is based on a relativistic spin-polarised multiple-scattering theory. The magnetic moment can point along any direction with respect to the crystal lattice and the total energy is calculated. The difference between total energies for two different moment directions is the magnetocrystalline anisotropy energy. We show that this energy difference can be written as the difference in single-particle energies for the same charge density. The theory is illustrated with a calculation of the anisotropy in energy and spin contribution to the magnetic moment in nickel. It is found that the theory gives good qualitative agreement with experiment in this case. Numerical difficulties involved in the calculation are discussed.

1. Introduction

Compared with a non-relativistic description, relativistic quantum mechanics of electrons in condensed matter has a number of qualitatively new features. One of these is the coupling of the spin to the orbital degrees of freedom. Evidently its consequences are particularly striking in spin-polarised systems of itinerant electrons such as occurs in metallic magnets. For instance, it is this coupling that gives rise to the magnetocrystalline anisotropy energy (Landau *et al* 1984, March *et al* 1984). Also, as has been shown by Staunton *et al* (1988), a relativistic treatment of the RKKY interaction leads to anisotropic effects. Recently, this interesting subject has been attracting considerable theoretical attention. Feder (1985) (see also references therein), Strange *et al* (1984, 1989a) and Schadler *et al* (1987) have all developed theories of the electronic structure of solids in which both relativity and spin polarisation are treated on an equal footing.

Fritsche *et al* (1987) have used an apparently equivalent theory to calculate the magnetocrystalline anisotropy energy in nickel and iron. They assumed the difference in total energies for the moment pointing in two different directions in the unit cell can be written as the difference in single-electron energies. Their results were of the correct order of magnitude, but gave the wrong sign for iron.

In this paper we report a calculation of the magnetocrystalline anisotropy energy and the anisotropy in the magnitude of the magnetic moment when the moment points along

[‡] Present address: Neutron Division, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, UK.

[§] Present address: Siemens AG, ZFE TPH 11, Paul Gossen-Strasse 100, D-8520 Erlangen, Federal Republic of Germany.

the (001) and the (111) axes in nickel. This calculation is performed using a relativistic spin-polarised scattering theory (Strange *et al* 1989a). We examine the origin of the anisotropy within the formalism. The results are encouraging, having the correct sign and order of magnitude, however the numerical uncertainties in the calculation lead to large uncertainties in the final answer.

2. Formalism

It is now well established that the equilibrium properties of many-electron systems can be accurately described by density functional theory (Hohenberg and Kohn 1964, Kohn and Sham 1965). In this theory the complicated many-body problem is reduced to a set of effective single-particle Schrödinger-like equations and the many-body effects are treated by way of some local approximation (Hedin and Lundqvist 1971). More recently this theory has been generalised in order to make it applicable to systems in which relativistic effects play an important role in determining the systems' properties (Rajagopal 1978, Ramana and Rajagopal 1979, McDonald and Vosko 1979). In particular McDonald and Vosko (1979) developed the theory for a many-electron system in the presence of an external potential and a spin-only magnetic field (neglecting diamagnetic effects). Their equations can be written as (Strange *et al* 1984)

$$\{-ihc\boldsymbol{\alpha} \cdot \nabla + \boldsymbol{\beta}mc^2 + IV^{\text{eff}}[n(\mathbf{r}), m(\mathbf{r})] + \boldsymbol{\beta}\boldsymbol{\sigma} \cdot B^{\text{eff}}[n(\mathbf{r}), m(\mathbf{r})] - \varepsilon_i\}\varphi_i(\mathbf{r}) = 0 \quad (2.1)$$

$$n(\mathbf{r}) = \sum_i^{\text{occ}} \text{Tr} \varphi_i^\dagger(\mathbf{r})\varphi_i(\mathbf{r}) \quad (2.2)$$

$$m(\mathbf{r}) = \sum_i^{\text{occ}} \text{Tr} \varphi_i^\dagger(\mathbf{r})\boldsymbol{\beta}\boldsymbol{\sigma}\varphi_i(\mathbf{r}) \quad (2.3)$$

$$V^{\text{eff}}(n(\mathbf{r}), m(\mathbf{r})) = \left(V^{\text{ext}}(\mathbf{r}) + \delta E_{\text{xc}}/\delta n(\mathbf{r}) + e^2 \int (n(\mathbf{r}')/|\mathbf{r} - \mathbf{r}'|) d^3\mathbf{r}' \right) \quad (2.4)$$

$$B^{\text{eff}}(n(\mathbf{r}), m(\mathbf{r})) = (eh/2mc)(B^{\text{ext}}(\mathbf{r}) + \delta E_{\text{xc}}/\delta m(\mathbf{r})). \quad (2.5)$$

Here $V^{\text{ext}}(\mathbf{r})$ is the external potential, E_{xc} is the relativistic exchange correlation energy which is a functional of $n(\mathbf{r})$ and $m(\mathbf{r})$. φ_i is a 4-spinor, B^{ext} is a fictional magnetic field coupling to the spin of the electron only. $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are the standard Dirac matrices and $\boldsymbol{\sigma}$ are the 4×4 Pauli matrices. All other symbols have their usual meanings. McDonald and Vosko (1979) write an expression for the total energy functional in the non-magnetic case. It is a close analogy to the non-relativistic expression and is easily generalised to the spin-polarised case

$$\begin{aligned} E[n(\mathbf{r}), m(\mathbf{r})] &= \sum_i^{\text{occ}} \varepsilon_i - \frac{1}{2}e^2 \int \int (n(\mathbf{r})n(\mathbf{r}')/|\mathbf{r} - \mathbf{r}'|) d^3\mathbf{r} d^3\mathbf{r}' \\ &+ E_{\text{xc}}[n(\mathbf{r}), m(\mathbf{r})] - \int n(\mathbf{r})\delta E_{\text{xc}}[n(\mathbf{r}), m(\mathbf{r})]/\delta n(\mathbf{r}) d^3\mathbf{r} \\ &+ \int m(\mathbf{r})\delta E_{\text{xc}}[n(\mathbf{r}), m(\mathbf{r})]/\delta m(\mathbf{r}) d^3\mathbf{r}. \end{aligned} \quad (2.6)$$

It has been shown that an approximate but reliable method of finding the total energy difference between two systems with ground-state charge densities which differ by a small amount $\delta n(\mathbf{r})$ is as follows (Mackintosh *et al* 1980). One does a fully self-consistent density functional calculation in one case. The resulting charge density is used to perform a single iteration in the second case and the difference in total energy is equal to the difference in the single-particle energies to order $\delta n(\mathbf{r})^2$. This exploits the stationarity of the total energy with respect to changes in the charge density. It is trivial to generalise this argument to the spin-polarised case as follows. Consider $n^{001}(\mathbf{r})$ and $m^{001}(\mathbf{r})$ to be the self-consistent charge and magnetisation densities when the magnetic moment points along the (001) direction. Then we write

$$n^{111}(\mathbf{r}) = n^{001}(\mathbf{r}) + \delta n(\mathbf{r}) \quad (2.7)$$

and

$$m^{111}(\mathbf{r}) = m^{001}(\mathbf{r}) + \delta m(\mathbf{r}). \quad (2.8)$$

Then we write the difference in total energies for the moment pointing along (001) and the moment along (111) as

$$\begin{aligned} \Delta E &= E^{111}[n^{001}(\mathbf{r}) + \delta n(\mathbf{r}), m^{001}(\mathbf{r}) + \delta m(\mathbf{r})] - E^{001}[n^{001}(\mathbf{r}), m^{001}(\mathbf{r})] \\ &= E^{111}[n^{001}(\mathbf{r}), m^{001}(\mathbf{r})] + \delta n(\mathbf{r})\delta E^{111}[n^{111}(\mathbf{r}), m^{111}(\mathbf{r})]/\delta n(\mathbf{r}) \\ &\quad + \delta m(\mathbf{r})\delta E^{111}[n^{111}(\mathbf{r}), m^{111}(\mathbf{r})]/\delta m(\mathbf{r}) \\ &\quad + \text{HOT} - E^{001}[n^{001}(\mathbf{r}), m^{001}(\mathbf{r})]. \end{aligned} \quad (2.9)$$

HOT means terms of order $\delta m(\mathbf{r})^2$, $\delta n(\mathbf{r})^2$ and $\delta n(\mathbf{r})\delta m(\mathbf{r})$ or higher and where we have resubstituted for $n^{001}(\mathbf{r})$ and $m^{001}(\mathbf{r})$ in the second and third term on the right-hand side. Now $\delta E^{111}[n^{111}(\mathbf{r}), m^{111}(\mathbf{r})]/\delta n(\mathbf{r})$ and $\delta E^{111}[n^{111}(\mathbf{r}), m^{111}(\mathbf{r})]/\delta m(\mathbf{r})$ are both zero. Therefore we can neglect all terms on the right-hand side of (2.9) except the first and last ones. When we place the same charge and magnetisation density in both these functionals and subtract, only the single-particle energy terms of equation (2.6) remain. Finally we have

$$\Delta E = \sum_i \varepsilon_i^{111} - \sum_i \varepsilon_i^{001}. \quad (2.10)$$

We have shown that we can identify the difference in single-electron energies calculated in this way with the magnetocrystalline anisotropy energy to order $\delta n(\mathbf{r})^2$, $\delta m(\mathbf{r})^2$. Such an approach has already been used by Strange *et al* (1988b) to calculate the anisotropy energy in tetragonal iron.

3. Scattering theory

Feder *et al* (1985) and Strange *et al* (1984) showed how to solve equation (2.1). They used a single-site, scattering theory approach to calculate the scattering t -matrices. The t -matrices calculated this way are off-diagonal in spin space and this is all that is required to describe magnetic anisotropies. The properties of these t -matrices were explored in detail by Strange *et al* (1984).

Strange *et al* (1989a) have also derived a relativistic spin-polarised multiple-scattering theory for solving the approximate relativistic spin-polarised density functional equation

(2.1) for electrons on a crystal lattice. They derive an expression for the scattering Green function $G(\mathbf{r}, \mathbf{r}, E)$ and discuss how to calculate observables therefrom. The salient equations from their paper are that the density of states is given by

$$n(E) = -\pi^{-1} \text{Im} \int \text{Tr} G(\mathbf{r}, \mathbf{r}, E) d^3\mathbf{r} \quad (3.1)$$

and that the spin magnetic moment is

$$m_s(\mathbf{r}) = -\pi^{-1} \text{Im} \int_0^{E_F} \text{Tr} \boldsymbol{\beta} \boldsymbol{\sigma} G(\mathbf{r}, \mathbf{r}, E) dE \quad (3.2a)$$

and also that the orbital contribution to the magnetic moment is

$$m_o(\mathbf{r}) = -\pi^{-1} \text{Im} \int_0^{E_F} \text{Tr} \boldsymbol{\beta} l_z G(\mathbf{r}, \mathbf{r}, E) dE \quad (3.2b)$$

l_z is the z -component of the 4×4 matrix vector $l_r = \mathbf{l}_4 \otimes l$ with l the conventional angular momentum operator. The relativistic scattering Green function is given by

$$G(\mathbf{r}, \mathbf{r}', E) = \sum_{\kappa\mu\kappa'\mu'} Z_{\kappa}^{\mu}(\mathbf{r}) \tau_{\kappa\mu\kappa'\mu'}(E) Z_{\kappa'}^{\mu'}(\mathbf{r}') - \sum_{\kappa\mu} Z_{\kappa}^{\mu}(\mathbf{r}) J_{\kappa}^{\mu}(\mathbf{r}'). \quad (3.3)$$

$Z_{\kappa}^{\mu}(\mathbf{r})$ and $J_{\kappa}^{\mu}(\mathbf{r})$ are discussed in detail by Strange *et al* (1989a). They are the regular and irregular solutions of the Kohn–Sham–Dirac equation respectively. κ and μ are the usual relativistic quantum numbers (Rose 1966). If all the scatters are equivalent and placed on a periodic lattice it can be shown that each element of the τ -matrix can be written as

$$\tau_{\kappa\mu\kappa'\mu'}(E) = \int_{\text{BZ}} (t^{-1}(E) - g(\mathbf{q}, E))_{\kappa\mu\kappa'\mu'}^{-1} d^3\mathbf{q} \quad (3.4)$$

where $\tau_{\kappa\mu\kappa'\mu'}(E)$ is an element of the single-site scattering t -matrix, $g_{\kappa\mu\kappa'\mu'}(\mathbf{q}, E)$ are the usual KKR structure constants rotated into a representation in which they can be written in terms of the relativistic quantum numbers. In the non-relativistic case

$$g_{lm'l'm'}(\mathbf{q}, E) = \sum_{ij} \exp[i\mathbf{q} \cdot (\mathbf{R}_i - \mathbf{R}_j)] g_{lm'l'm'}(\mathbf{r}_{ij}, E) \quad (3.5)$$

$$g_{lm'l'm'}(\mathbf{R}_i - \mathbf{R}_j, E) = 4\pi E^{1/2} i^{l-l'+1} \sum_{L'} C_{LL'}^{L'} i^{l''} h_{l''}(E^{1/2} |\mathbf{R}_i - \mathbf{R}_j|) Y_l^m(\mathbf{R}_i - \mathbf{R}_j) \quad (3.6)$$

where h_l is a spherical Hankel function, Y_l^m is a spherical harmonic and $C_{LL'}^{L'}$ are the Clebsch–Gordon coefficients. If the calculations were all performed on the real axis the second term in the Green function would be zero.

The t -matrices are always calculated with their magnetic moments pointing along a local z axis, corresponding to the z axis of the crystal. However, they can be turned to any direction using the rotation matrices.

Substituting the rotated t -matrices into (3.4) and performing the Brillouin zone integral gives a new τ -matrix. The direction of the moment affects the point group symmetry of the crystal and the Brillouin zone integration must be done in different irreducible segments of the zone depending on the direction of the moment. For the (001) direction it is $\frac{3}{8}$ ths of the FCC zone and for the (111) direction it is $\frac{1}{4}$ ths. For an arbitrary direction it is $\frac{1}{8}$ ths.

Care must be taken to ensure that the new τ -matrix and the $Z_k^\mu(\mathbf{r})$ are in the same frame when combined to find the Green function. The density of states, magnetic moment and single-electron energies can then be calculated from the above formulae.

4. Calculation and results

We consider nickel on an FCC lattice. The nickel ions are defined by a potential found from a self-consistent non-relativistic electronic structure calculation (Moruzzi *et al* 1978). As nickel is a fairly light element, this should be a good approximation. The quantities on the right-hand side of equation (3.4) can be calculated straightforwardly. The Brillouin zone integrals were performed using a generalisation of the prism method (Stocks *et al* 1979).

The density of states and magnetic moment were calculated for the moment pointing along (001) and then the calculation was repeated for the moment along (111). The energy integrals were done on a rectangular box contour in the complex plane with maximum imaginary energy 50 mRyd.

At most stages of the calculation the numerical methods can be checked to ensure that sufficient accuracy is obtained to see the effects we are trying to describe. Numerical uncertainty was introduced into the calculation by the Brillouin zone integral. To gain some insight into this, the calculation was performed using 6, 10, 21, and 36 directions in each $\frac{1}{8}$ th of the zone. The Fermi energy can be found from

$$n = \int_0^{E_F} n(E) dE \quad (4.1)$$

and the single-electron energies are given by

$$E_s = \int_0^{E_F} E n(E) dE. \quad (4.2)$$

To find the anisotropy energy, we are taking the difference of two large numbers to find a small one. This can only be done by integrating the difference round the energy contour. When we return to the real axis there is a small difference in Fermi energy for the two directions. The region between the two Fermi energies is assumed to have a constant density of states.

Figure 1 shows the relativistic energy band structure of nickel along the Γ -X(001) direction or the moment along (001) in the unit cell. These are very similar to previous results (Wang and Callaway 1977, Moruzzi *et al* 1978). Comparison of their results with ours shows that relativity introduces some small changes in band widths and lifts degeneracies at points of high symmetry. There is also some gross movement in the bands due to the mass-velocity and Darwin effects in the Hamiltonian.

Figures 2 and 3 are magnified views of the energy bands for nickel with the moment pointing along (001) in the Γ -X(001) and the Γ -X(100) directions in the Brillouin zone, respectively. We see the major effect of rotating the moment is to prevent/allow band crossings and to alter some separations between bands. This can be understood on the basis of the $\boldsymbol{\sigma} \cdot \mathbf{B}$ term in the Hamiltonian. When the moment rotates the scalar product varies as a cosine function. Figure 4 and figure 5 are for the same directions in the Brillouin zone as figure 2 and figure 3 but with the moment pointing along (111) in the unit cell. The same effects are visible. The bands correspond very well to those shown

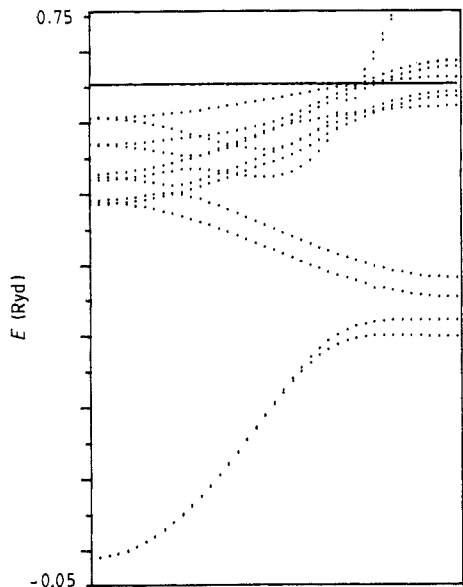


Figure 1. The relativistic spin-polarised band structure of nickel along Γ -X(001) for the magnetic moment pointing along (001).

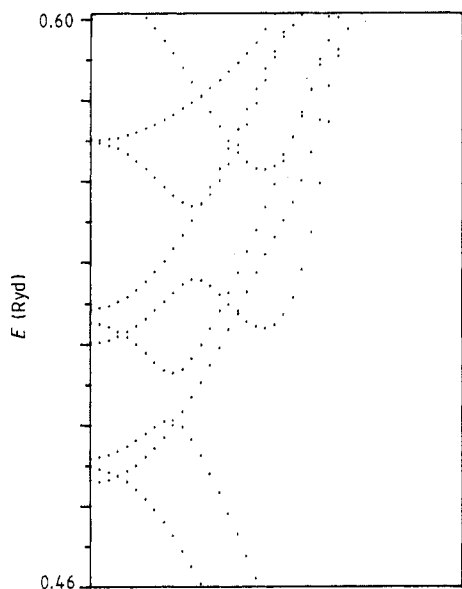


Figure 2. A magnified view just below the Fermi energy of the relativistic spin-polarised band structure of nickel along Γ -X(001) for the magnetic moment pointing along (001).

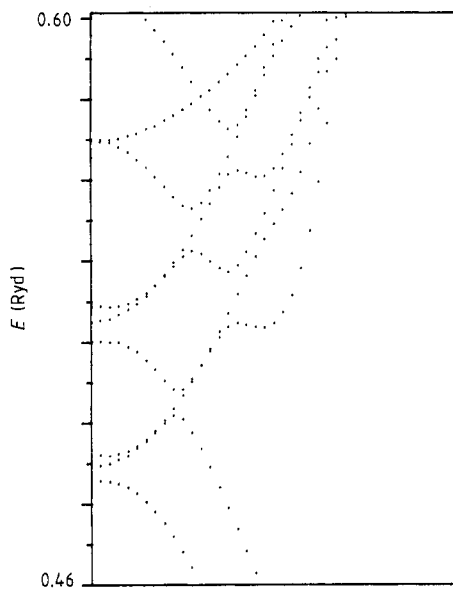


Figure 3. A magnified view just below the Fermi energy of the relativistic spin-polarised band structure of nickel along Γ -X(100) for the magnetic moment pointing along (001).

by Ebert *et al* (1988) calculated using the recently derived relativistic spin-polarised LMTO method. The density of states has been found on a complex path; it is not very meaningful in itself, and so has not been plotted.

Table 1 shows a full set of results including the orbital contribution to the magnetic moment and the value of the anisotropy in m and E . The tabulated values are those

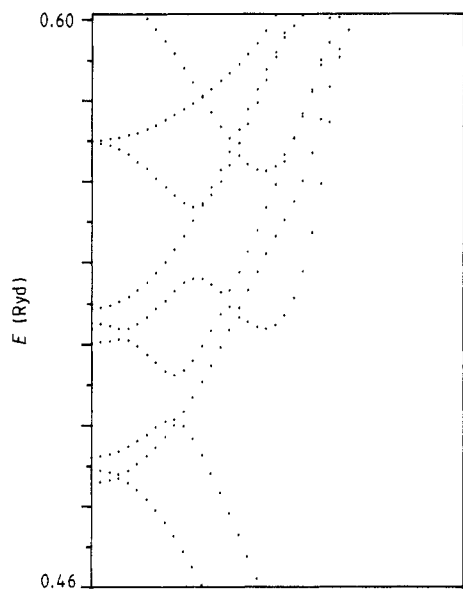


Figure 4. A magnified view just below the Fermi energy of the relativistic spin-polarised band structure of nickel along Γ -X(001) for the magnetic moment pointing along (111).

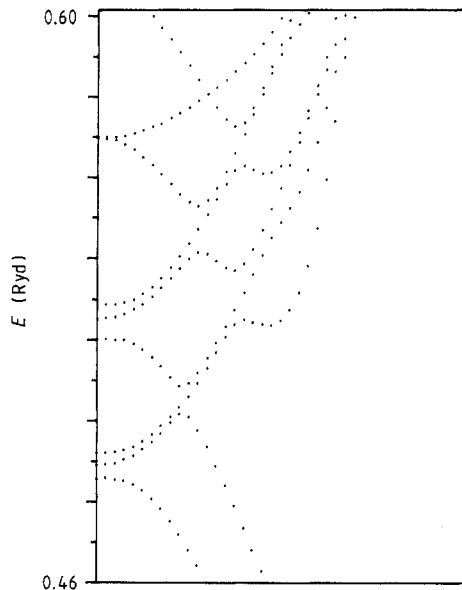


Figure 5. A magnified view just below the Fermi energy of the relativistic spin-polarised band structure of nickel along Γ -X(100) for the magnetic moment pointing along (111).

Table 1. Table showing the spin and orbital contributions to the magnetic moment of nickel, the anisotropy in the single-electron energies and the spin contribution to the magnetic moment.

	Magnetic moments			$E_s^{001} - F_s^{111}$ (10^{-6} eV)	$m^{001} - m^{111}$ (units of $10^{-4} \mu_B$)
	Spin	Orbital (units of μ_B)	Total		
Theoretical	0.598	0.046	0.644	10.5 ± 7.0	1.4 ± 0.5
Experimental	—	—	0.616	2.7	1.2

calculated when the Brillouin zone integral was performed with 36 directions per $\frac{1}{8}$ th of the zone. The errors indicated are estimated on the basis of the calculations using 10 and 21 directions in the integration. To obtain a numerically more precise value of the difference in single-electron energies would require even more precise evaluation of the Brillouin zone integral and the inclusion of higher values of the l -quantum number in the calculation. This is beyond present-day computer facilities and grants.

5. Discussion

In this section we want to examine the origin of the anisotropy in the formalism of relativistic spin-polarised scattering theory. As a consequence of this we should also

discover which electrons in nickel are predominantly responsible for the magnetic anisotropy.

If we consider equations (3.1) to (3.6), the only place where a direction with respect to the crystal lattice occurs is in the spherical harmonics in the expression for $g(\mathbf{r}, E)$. Let us take a factor of t^{-1} outside the square brackets of (3.4). We can expand what remains as a binomial series. This leads to an infinite series of terms each of which can be written $(tg)^n$ (ignoring quantum numbers), and this term includes all n -site scattering processes. We can then substitute back into (3.3) and (3.1). In the non-relativistic case, the dependence of the t -matrices and the radial part of Z on the quantum number m disappears and they can be taken outside the sum over the quantum number m in (3.3). We are then left with sums over products of Clebsch–Gordon coefficients and spherical harmonics. From simple trigonometric relations the directional dependence of $g^{ij}(\mathbf{r}, E)$ then cancels for all n .

In the relativistic case the t -matrices and the $Z_k^\mu(\mathbf{r}, E)$ cannot be taken outside the m -summation, i.e. the symmetry which allowed cancellation in the non-relativistic case has been broken. Hence magnetocrystalline anisotropy is observed. The difference in single-electron energies for the moment pointing in different directions comes from the fact that when the off-diagonal t -matrix is rotated, different elements of the t -matrix become dominant and hence the symmetry is broken in different ways for each direction of the moment. The most fundamental reason this occurs in a relativistic theory and not in a non-relativistic theory is that in the relativistic case only total angular momentum is conserved, spin and orbital angular momentum not separately being conserved. In the non-relativistic case they are conserved separately.

If we examine the origin of ΔE further by decomposing it by an quantum number l we find that the d electrons favour alignment along (111) but the s–p electrons favour the (001) direction. The d electrons dominate because they have the largest contribution to the density of states around the Fermi energy.

The conclusion to be drawn from this work is that the magnetocrystalline anisotropy energy is given with the correct sign and order of magnitude by the difference in single-electron energies. Which direction will be the axis of easy magnetisation will depend on the details of electronic structure and the symmetry of the crystal structure. The formalism we have developed may be regarded as generating t -matrices which are non-spherical in spin space. Thus one's physical intuition is supported in noting it is this non-sphericity that is responsible for the anisotropy.

The size of the anisotropy energy is an order of magnitude smaller than the single-particle energies themselves. However, we can still reproduce the experimental results to within an order of magnitude. If the lattice were not cubic the magnetocrystalline anisotropy energy would be expected to be much larger and we should be able to calculate anisotropy energies fairly straightforwardly. This leads to the hope that one could predict flips in the axis of easy magnetisation for non-cubic structures. Work is in progress on this topic (Strange *et al* 1989b).

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