Band Theory of Anisotropy

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Until now the cubic ferromagnetic anisotropy at 0° Kelvin has been calculated by integrating the fourth order spin-orbit energy correction over the volume enclosed by the unperturbed Fermi surface S. We show that the change in occupation of states caused by the spin-orbit perturbation of the Fermi surface introduces an additional term into the cubic anisotropy which is proportional to the integral over S of the second order energy squared. The tendency for cancellation of these two terms is so strong in the case of degenerate bands such as those of iron-group metals that the effect of including the new term is to reduce the calculated anisotropy greatly. An analytic calculation based on a simple band structure resembling Fletcher's computed nickel bands suggests that the correct value may be 200 times smaller than that calculated by Fletcher.

Introduction

The band theory of cubic anisotropy was formulated by Brooks[1] and applied to nickel by Brooks[1], Fletcher[2], and Merkle[3]. Brooks assumed that the anisotropy energy is given by integrating the spin-orbit energy over the occupied states in the Brillouin zone, neglecting the changes in occupation of states caused by the spin-orbit perturbation. We show here that this neglect is invalid because consideration of the changes in occupation reduces greatly the calculated anisotropy.

General Theory

The one-electron energy E_n may be written

$$E_n(\mathbf{k}, \alpha_1, \alpha_2, \alpha_3) = \sum_{p=0}^{\infty} w_{np}(\mathbf{k}, \alpha_1, \alpha_2, \alpha_3). \quad (1)$$

Here $\mathbf{k}$ is the wave vector, n is a band index (including spin quantum number), and $\alpha_1, \alpha_2, \alpha_3$ are direction cosines of the spontaneous magnetization with respect to the cubic axes. The function w_{np} is homogeneous in $\alpha_1, \alpha_2, \alpha_3$ to degree $2p$. The term w_{no} is an eigenvalue of kinetic energy plus periodic potential plus exchange energy. For $p > 1$, w_{np} are perturbation corrections for spin-orbit energy.

By expanding the energy integral over the states occupied at 0°K, one finds that the leading terms in the cubic anisotropy are

$$W = (16\pi^3)^{-1} \sum_n \left[2\iiint dk^3 w_{n2} - \iint dS \, w_{n1}^2 \right.$$

$$\left. \times (\partial w_{no}/\partial k_\perp)^{-1} \right] \quad (2)$$

The first integral in Eq. (2), considered by Brooks, is taken over the unperturbed occupied Fermi *volume*. The second integral, which we have introduced, is taken over the unperturbed Fermi *surface* S. It takes into account the displacement of S by the perturbation. Here $k_\perp$ is the component of $\mathbf{k}$ normal to S. Both integrals are of fourth degree in $\alpha_1, \alpha_2, \alpha_3$ and both are of order λ^4/Δ^3 where λ is the spin-orbit parameter and Δ is characteristic of $w_{no} - w_{n'o}$.

The practical effect of the surface term is greater than order-of-magnitude considerations would suggest because d-bands are highly degenerate. For such bands we have shown that each of the integrals in Eq. (2) is generally dominated by contributions from regions close to points at which a degenerate axis intersects S. However, the tendency toward cancellation of the two integrals in such regions is so strong that W is *not* dominated by these regions. Therefore, the anisotropy is much smaller than evaluation of the volume term alone would suggest and knowledge of the band structure in the large is required in order to calculate it.

Band Model

To illustrate these remarks we have calculated analytically the cubic anisotropy coefficient K_1 for a simple degenerate band model which resembles to some degree the tight-binding structure of nickel[4] used by Fletcher to evaluate K_1. We assume that multiple band minima for the electron-holes

lie at the centers of the (100) faces of the Brillouin zone for a face-centered cubic lattice. The bands are assumed to be doubly degenerate along the cubic axes of k-space. Near the center of the [001] face the effective Hamiltonian H has the approximate form

$$H = \begin{bmatrix} a_1(\varphi)r^2 + bz^2 & i\lambda\, a_3 \\ -i\lambda\, a_3 & a_2(\varphi)r^2 + bz^2 \end{bmatrix} \quad (3)$$

where k is specified by the cylindrical coordinates z, r, φ centered at the center of the [001] face of the Brillouin zone. The functions $a_1(\varphi)$ and $a_2(\varphi)$ have fourfold symmetry and b is a constant. H reduces to analogous forms at the other (100) faces.

The diagonal elements are the unperturbed levels for spin state $m_s = -1/2$ and the off-diagonal elements are due to spin-orbit coupling. Exchange energy is assumed to be greater than the occupied band width so that states with $m_s = 1/2$ are neglected. The unperturbed Fermi surface for this model consists of 6 pairs of warped hemi-spheroids lying inside the zone with the equators of each pair centered on a (100)-face and the poles of each pair touching.

To obtain K_1 we have evaluated the integrals of Eq. (2), using the eigenvalues of H, taking into special account the degeneracy at $r = 0$. The result is

$$K_1 = \frac{-\lambda^4}{64\,\pi^3\zeta^{3/2}b^{1/2}} \int_0^{2\pi} d\varphi \left\{ \frac{a_1 + a_2}{(a_1 - a_2)^2} \right.$$
$$\left. - \frac{2a_1 a_2}{(a_1 - a_2)^3}\ln\!\left(\frac{a_1}{a_2}\right) \right\} \quad (4)$$

for $a_1 > a_2 \geq 0$, where ζ is the Fermi energy.

Comparison with Experiment

In applying our result to the case of nickel we assume that our band model represents the states occupied by the 0.54 holes per atom believed to occupy d-bands in nickel. We assume parameter values suggested by the tight-binding bands[4]. In this way we find that $a_2 \ll a_1$ and that a_1 is almost constant.

In this limit, and assuming a_2 is constant we find from the standard theory of the gyromagnetic ratio that the orbital moment in Bohr magnetons per atom is given accurately by

$$\mu_1 = -\lambda\zeta^{1/2}\ln(a_1/a_2)/(2\pi^2 b^{1/2} a_1 N) \quad (5)$$

where N is the atomic density. The numerical values we used to calculate μ_1 and K_1 are $\lambda = -295\ \mathrm{cm}^{-1}$ (free atom), $\zeta = 0.4$ e.v., $b = 1.1$ e.v.$\cdot\text{Å}^2$, $a_1 = 2.1$ e.v.$\cdot\text{Å}^2$, and $a_1/a_2 = 33$. (a_2 was entirely neglected in calculating K_1.) The results are given in column 1 of the following table.

The fact that our value of μ_1 agrees with Fletcher's (column 2) tends to confirm that our band model is roughly equivalent to his. Our estimate of K_1, however, is 200 times smaller. Yet the experimental value of K_1[5] (column 3) is closer to Fletcher's than to ours. If we scale the band parameters downward by a factor of 2.6 (column 4) in order to agree with the experimental value of μ_1[6], we find that our value of K_1 is 1/3 of the measured value whereas Fletcher's would probably exceed it by far. Therefore, if we regard the band structure as adjustable our results would appear to agree better than Fletcher's considering μ_1 and K_1 together.

Conclusions

We find that consideration of the displacement of the Fermi surface by spin-orbit coupling has the general effect of revising downward drastically estimates of the cubic anisotropy at 0°K. An analytic calculation based on a degenerate-band model resembling Fletcher's tight-binding bands for nickel leads to a value of K_1, 200 times smaller than his. To the questionable extent that our model represents the band structure of nickel the results suggest that Fletcher's *a priori* values of the band parameters should be scaled down by a factor of 3 or so in order to account for the orbital moment as well as the anisotropy.

	1. Present Theory	2. Fletcher's Theory	3. Experiment	4. Scaled Theory (See text.)
μ_1	0.020	0.025	0.052	0.052
$K_1 \times 10^{-5}$ erg/c.c.	−0.16	−28.	−7.5	−2.8

References

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DISCUSSION

E. P. WOHLFARTH: I would like to give a summary of an old qualitative idea of Fletcher and myself to explain the temperature variation of K_1. If two levels in the + and − spin band are "accidentally" degenerate due to exchange, there is a large contribution to K_1. Raising the temperature would dampen this contribution and thus reduce K_1. Precise calculations of this effect are of course impossible at present.

J. C. SLONCZEWSKI: We find that symmetry degeneracy alone does not lead to anomalously large anisotropy at 0°K. However it is easy to construct an accidentally degenerate structure (for example $a_1 = a_2$) which leads to anomaly.

Direct Exchange

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The direct exchange integral, defined as the exchange which enters into a Heitler-London description of a system, is discussed for the case of many electrons. The general expression, which should give equivalent results for all "good" sets of wave functions, simplifies for special choices and may be described in terms of its deviation from the hydrogen molecule form. The cases considered are where a) the one-electron functions are solutions of Hartree equations for the system, and b) solutions of the Hartree and Hartree-Fock equations for the atoms. In the latter, the principal difference between the result and hydrogen molecule exchange integral is that the electron-other nucleus potential, $-\dfrac{e^2}{|r_1 - R_2|}$, is replaced by $-\dfrac{e^2 Z(r)}{|r_1 - R_2|}$ where $Z(r)$ is the effective charge experienced by the electron. This alteration changes the sign of the exchange integral in iron from that calculated by Stuart and Marshall and makes the integral negative, or antiferromagnetic. Nickel and cobalt are presumed to be similar.

Introduction

The direct exchange of interest in this discussion is that which occurs between electrons on different atoms in a Heitler-London description of the wave function. It generally is recognized that in ferromagnetic materials direct exchange is not the dominant interaction; nevertheless, it is an important coupling which must be considered, for example, in studies of the transition between