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Calculation of orbital magnetism and magnetocrystalline anisotropy energy in YCo_5

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Abstract. First-principles electronic structure calculations have been performed for the intermetallic compound YCo_5 . This compound is known to have unusually large cobalt orbital magnetic moments and one of the largest magnetocrystalline anisotropies among itinerant ferromagnets. By including spin-orbit coupling and orbital polarization in the theoretical treatment the orbital magnetic moments and the magnetocrystalline anisotropy energy were calculated. It was found that in order to obtain reasonable agreement with experiments the inclusions of orbital correlation (here in the form of orbital polarization) is essential. The different contributions from the two inequivalent cobalt sites to the orbital magnetization and the anisotropy energy are discussed.

1. Introduction

Magnetocrystalline anisotropy (MA) is a most important property of permanent magnets [1, 2]. For instance, it is also an essential material parameter for the rare-earth-transition metal intermetallic compounds where, for example, SmCo_5 and $\text{Nd}_2\text{Fe}_{14}\text{B}$ are of direct technological use. The MA is very large in these two materials and provides the microscopic origin of the coercivity which for permanent magnets is so essential. The dominating contribution to MA at low temperatures in these types of compounds arises from the 4f states of the rare-earth atoms. However, at the higher temperatures, e.g. room temperature, the 4f contribution in general diminishes, but sometimes there remains a substantial contribution from the itinerant states. This is clearly seen when comparing the room temperature anisotropy constant, K_1 , for SmCo_5 , 11.2 MJ m^{-3} , with the one for the closely related non-4f compound YCo_5 , 5.5 MJ m^{-3} [1]. The MA originating from the localized 4f electrons is well understood from theoretical models where crystal-field Hamiltonians are used to describe the effect of the ligand atoms on the multiplets of the 4f shell. The contribution to MA from the itinerant ferromagnetic electrons is, however, less well understood.

It has been suggested earlier that the coupling between the spin-magnetization and the crystal lattice, which arises through the spin-orbit interaction, together with a band picture for the electrons, provide an MA of the right order of magnitude for the transition metal ferromagnets [3, 4]. Recently a thorough and accurate investigation of the magnetocrystalline anisotropy energy (MAE) for the 3d metals, Fe, Co and Ni, utilizing the

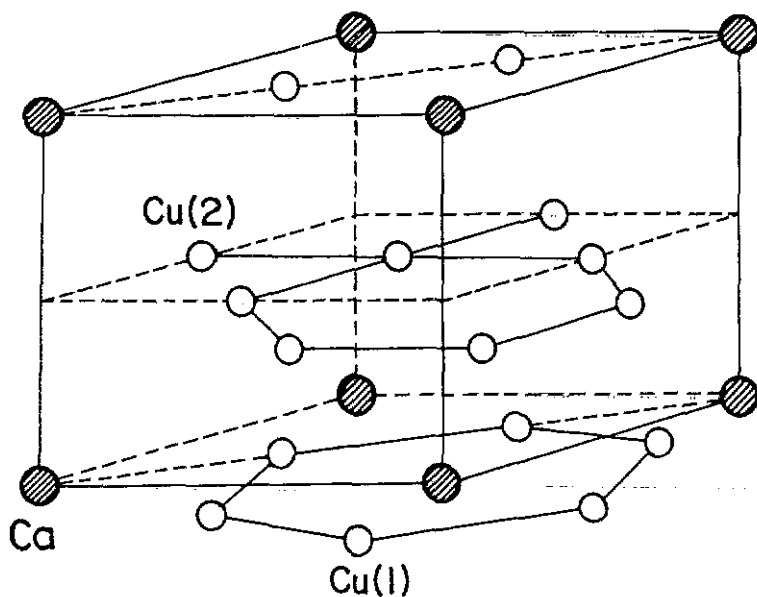


Figure 1. The CaCu_5 structure.

full machinery of modern electronic structure calculation techniques was reported [5]. In that work, the spin-orbit coupling was included in the calculations to provide the anisotropy, and the many-body problem was treated within the density functional theory in its local spin density approximation (LSDA). While the magnitude of the MAE was correctly obtained for the three metals the calculated numbers were in disagreement with experiment and for Co and Ni even the wrong easy axis was obtained. Jansen attributes this failure as being due to omitting orbital correlation in the theoretical work [6]. In the discussion of their results, however Daalderop *et al* [5], pointed out the immense numerical problem one encounters when attempting to calculate energy-differences of the order of 0.1 meV, and they stated that in order to be able to draw any conclusions about the disagreement between their calculation and experiment, one has to go beyond the approximations used, which is indeed a formidable task.

For actinide systems the spin-orbit coupling for the 5f electrons is very strong. In an early work, where the spin-orbit coupling was included, the MAE for the NaCl-compound U₅ was calculated and a very large value was predicted [7]. The order of magnitude for the anisotropy in this system was later confirmed experimentally [8].

Among ferromagnets not involving actinide or lanthanide atoms, YCo_5 has one of the largest MAEs. It is more than 50 times larger than in the elemental HCP cobalt metal and the easy axis is along the *c*-axis of the hexagonal lattice. YCo_5 is isostructural to the permanent magnet compound SmCo_5 , which makes it a suitable reference system for this technically important compound. Both YCo_5 and SmCo_5 crystallize in the hexagonal CaCu_5 structure (figure 1), which has a unit cell of six atoms and with two different types of cobalt sites, Co_I (2c) and Co_{II} (3g). Based on neutron scattering experiments, Schweizer and Tasset have reported on the existence of unusually large orbital moments on the Co_I sites in YCo_5 [9]. This suggests that it is the large Co_I orbital magnetic moments which are responsible for the large MAE. Therefore this compound is a most

interesting system for theoretical investigation—with respect to its orbital magnetism, its MAE and the interrelationship between these two properties.

Here we report on spin-polarized electronic structure calculations, including spin-orbit coupling, which were performed in order to study the orbital contribution to the magnetization and the MAE in YCo_5 . In order to investigate effects beyond the LSDA, calculations have also been performed where orbital correlations were included by means of the newly developed orbital polarization scheme [10, 11].

2. Theoretical method

Within a relativistic extension of the density functional theory an orbital contribution to the (unknown) exchange–correlation functional appears naturally [12, 13]. However, due to problems in finding an appropriate reference system as a guide for an approximate expression for this contribution (like, e.g., the local approximation LSDA for a spin-polarized system) most calculations today rely on the local spin–density approximation, where no orbital correlations enter. When a Dirac-like equation is used as the relativistic version of the Kohn–Sham equations, an orbital magnetization appears in the calculations for a spin-polarized system, due to the spin–orbit coupling present in the one particle kinetic energy. In recent years most investigations of the orbital magnetization or the magnetocrystalline anisotropy in, e.g., actinide and transition metal systems have been performed following such a strategy [5, 14–17].

In order to improve on the too small orbital moments obtained for actinide systems with this method, an orbital polarization (OP) scheme was suggested by Brooks [10]. This was later extended by Eriksson *et al* [11]. The concept of OP is taken from the theory for open shell atoms within the Russel–Saunders coupling, where it is responsible for Hund's second rule. The energy gained in the ground state by maximizing the total angular momentum, L , can be approximated by, $E_{OP} = -BL^2/2$, where B (for d states) is the Racah parameter and L is the total angular momentum. Applying this energy expression to solids one finds that it gives rise to energy shifts for the single particle states with different magnetic quantum numbers, m_l , according to

$$\delta\varepsilon_{m_l}^\sigma = \partial E_{OP}/\partial n_{m_l}^\sigma = -BL_\sigma m_l \quad (1)$$

where $n_{m_l}^\sigma$ is the occupation number for the σ , m_l state. Now L_σ may be identified as the orbital momentum (i.e. the expectation value of L_z) for states with spin σ and angular momentum l . The choice of using L_σ instead of L , as for the atom, is natural when noting that for the latter case only one spin channel is considered at a time due to Hund's first rule, i.e. already for the atom it is actually L_σ which enters the OP energy. The Racah parameter B can be expressed in terms of integrals of the single particle wave-functions and is recalculated for each iteration step.

In the present work we solve a Pauli-like Kohn–Sham equation by means of the linear muffin tin orbital method within the atomic sphere approximation (LMTO-ASA) [18], where the spin–orbit coupling only enters the variational part of the self-consistent loop. Both calculations with and without the orbital polarization corrections have been performed. The parametrization due to von Barth and Hedin [19] was used for the exchange and correlation energy. An expansion of angular momenta up to $l = 3$ was used on all sites. In the self-consistent loop a dense mesh of 225 points was sampled in the irreducible wedge (1/24) of the Brillouin zone (BZ). Integrals over the reciprocal space, e.g. when performing the sum over energy eigenvalues as described in section 4,

Table 1. The local cobalt orbital magnetic moments. SO and OP give the presently calculated values, without and with orbital polarization, respectively. S and T (S: Szpunar [22] and T: Takahashi *et al* [23]) are two earlier calculations. C (Coehoorn [25]) is an empirical estimation, and S&T and H (S&T: Schweizer and Tasset [9] and H: Heidemann *et al* [24]) are experimentally determined values. All magnetic moments are given in units of μ_B/atom .

Site	Theory				Experiment		
	SO	OP	S	T	C	S&T	H
Co _I	0.14	0.26	0.17	0.10	0.27	0.46	0.26
Co _{II}	0.10	0.17	0.04	0.13	0.20	0.28	0.24

were all carried out with the tetrahedron method, where care has been taken to weigh correctly the tetrahedra in the BZ [20]. The experimental lattice constants [21] were used in the calculations. In some of the calculations the combined correction terms to ASA were included [18].

3. Orbital moments in YCo₅

In an earlier work we reported on calculations of the orbital magnetic moments in YCo₅ [17]. In the investigation only spin-orbit coupling was included and no attempt was made to treat orbital correlations. In Table 1, the present theoretical magnetic moments are collected together with values from earlier calculations [22, 23]. In the same table, different experimental values are also listed together with estimated orbital moments [9, 24, 25]. As can be seen, the inclusion of OP increases the cobalt orbital moments significantly. However, the theoretical value for the Co_I atom is still far below the experimental value measured by spin-polarized neutron scattering [9]. In the earlier theoretical investigations in reference [22] and [23] a tight-binding approach was used, where the spin-orbit coupling constant entered as a free parameter that was either taken from experiment or used as a fitting parameter. The calculated values are smaller than the experimental ones and are close to our present calculated results, where only spin-orbit coupling was included.

On the other hand, there is a good agreement between the present calculated values, with orbital polarization included, and the local orbital moments estimated from the results of the hyperfine field measurements [24, 25]. Coehoorn [25] arrived at his estimate by subtracting from the experimentally determined values the calculated spin contributions to the hyperfine fields. The remaining orbital contribution to the hyperfine field was then assumed to be proportional to the orbital moment with the same proportionality factor as in Co metal. The values for the Co_I and Co_{II} orbital moments derived in this way agree very well with our values obtained from the OP calculations.

In our earlier investigation of the magnetization in YCo₅ a relatively large discrepancy was found for the total magnetic moment. This was then attributed as due to the fact that the calculated orbital moments were too small [17]. In the present OP calculation a total magnetic moment of $7.8 \mu_B/\text{f.u.}$ is obtained which should be compared with the experimental value of $8.3 \mu_B/\text{f.u.}$ [26]. There is still a discrepancy, although considerably smaller than before, which is actually equal to the difference between the

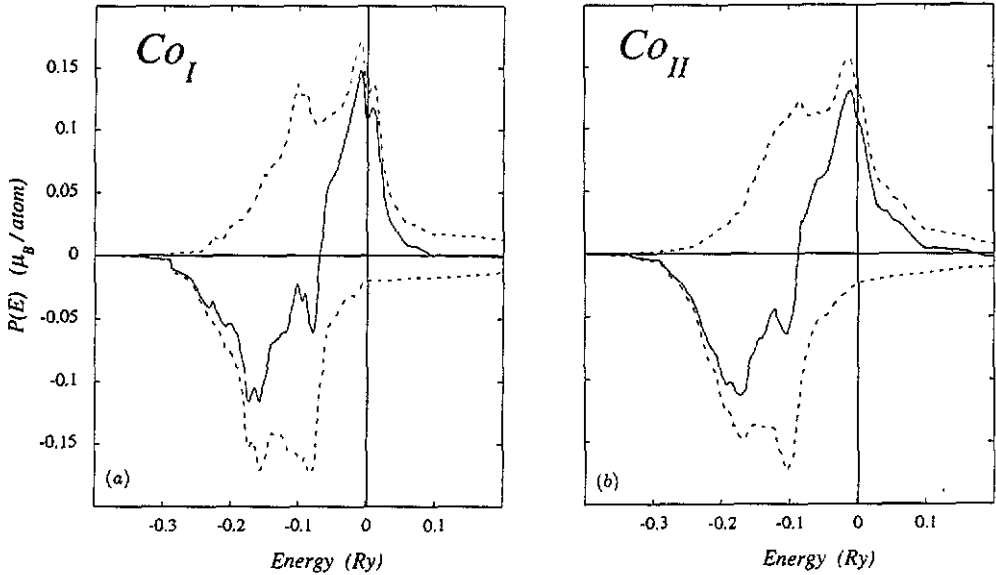


Figure 2. The energy integrated orbital moment density of states, $P(\varepsilon)$, (full curve) and its spin projected contribution, $P^\sigma(\varepsilon)$, (dashed curves) for the (a) cobalt I and (b) II atoms in YCo_5 . The negative (positive) contribution is due to the majority (minority) spin.

OP calculated orbital moments and those measured in the neutron scattering experiment [9].

In order to clarify the nature of the cobalt orbital moments and the effect due to the OP, we introduce a quantity, $P(\varepsilon)$, defined as

$$P(\varepsilon) = P^+(\varepsilon) + P^-(\varepsilon) \quad (2)$$

where

$$P^\sigma(\varepsilon) = \sum_{m_l} m_l \int_{-\infty}^{\varepsilon} N_{m_l}^\sigma(\varepsilon') d\varepsilon' \quad (3)$$

and $N_{m_l}^\sigma(\varepsilon)$ is the m_l -orbital density of states in the energy interval $(\varepsilon, \varepsilon + d\varepsilon)$. $P(\varepsilon)$ can be interpreted as the integrated orbital moment density of states and, accordingly, $P(\varepsilon_F)$ (ε_F = Fermi energy) is equal to the orbital moment. In figure 2 the local, i.e. the site projected, $P_i(\varepsilon)$ is shown for the two crystallographic inequivalent cobalt sites together with $P_i^\sigma(\varepsilon)$ for the two spin channels. (In the calculations that follows the combined correction to ASA was not included. This explains the difference between values in Table 1 and figures 2 and 3. This deviation might be taken as a measure of the numerical accuracy of the calculations.) Although the detailed structure of $P_i(\varepsilon)$ depends on the crystallographic environment of the cobalt atoms, the overall sinus-like shape is a general form for spin-polarized systems. The spin-orbit coupling within the majority spin states gives rise to a negative $P_i^+(\varepsilon)$ while $P_i^-(\varepsilon)$ is positive. Since $P_i^\sigma(\varepsilon)$ vanishes below and above the bands and the majority bands are lower in energy, the shape of total local $P_i(\varepsilon)$ follows naturally. The amplitude of $P_i(\varepsilon)$ is closely related to the strength of the spin-orbit coupling.

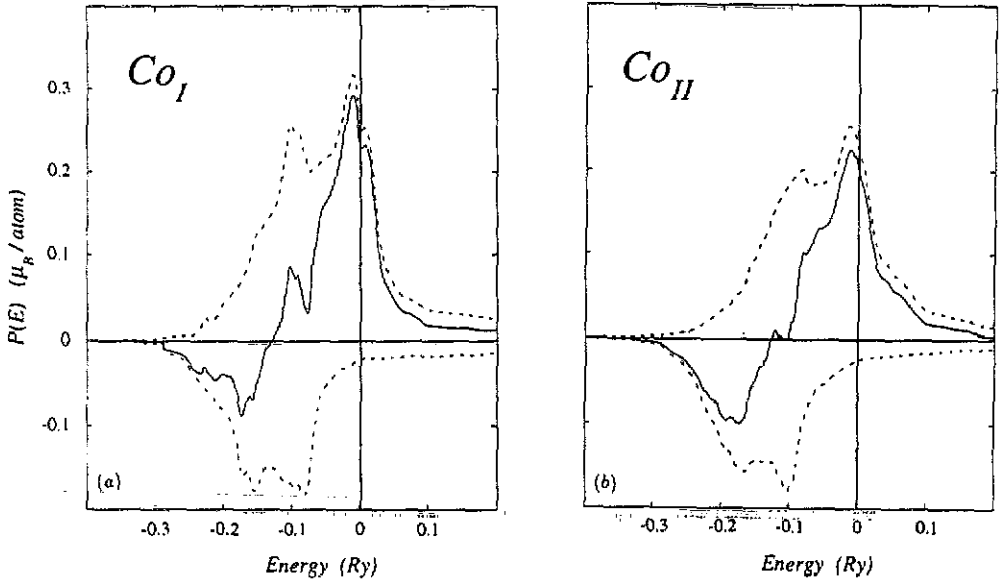


Figure 3. The same as in figure 2 but for the calculations including the orbital polarization.

As the majority spin d bands are almost filled it follows that $P^+(\varepsilon)$ contributes only very little to the orbital magnetic moment in YCo_2 . The two cobalt sites show very similarly shaped $P_i(\varepsilon)$ curves, and since the spin moments are of similar size they also have similar orbital magnetic moments.

When OP is included, it follows immediately from (1) that the major effect should occur for the minority spin for which L_o is largest. This is also what happens in the actual calculations as can be seen in figure 3, where the corresponding plots of $P_i^o(\varepsilon)$ for the OP case are shown. While the shape of $P_i^o(\varepsilon)$ is almost unchanged with the addition of OP for both spins, the height of $P_i^-(\varepsilon)$ is clearly enhanced due to OP, and hence increased cobalt orbital magnetic moments are obtained for both the Co_I and Co_{II} sites.

4. The magnetocrystalline anisotropy

Due to the anisotropy of the spin-orbit coupling there is a difference in the total energy when the magnetization is along different axes of the hexagonal lattice. This energy difference is, however, very small compared with the total energies. Therefore, a direct subtraction between total energies from two self-consistent calculations becomes numerically very cumbersome owing to the extremely high numerical convergence which is then necessary. Instead, we will here follow the same approach as in some earlier investigations [5, 7, 15] and make use of the so-called force theorem, which exploits the variational nature of the ground state energy. This theorem states that, to the second-order change in the charge and magnetization densities, the difference in total energies, ΔE_A , is given by the difference in the sum of eigenvalues between two calculations performed with the same densities. That is, we have,

$$\Delta E_A \approx \sum_{k,i}^{\text{occ}} \varepsilon_i^o(k) - \sum_{k,i}^{\text{occ}} \varepsilon_i^f(k) \quad (4)$$

where $\varepsilon_i^d(k)$ is the i th eigenvalue at the wavevector k for a calculation with magnetization

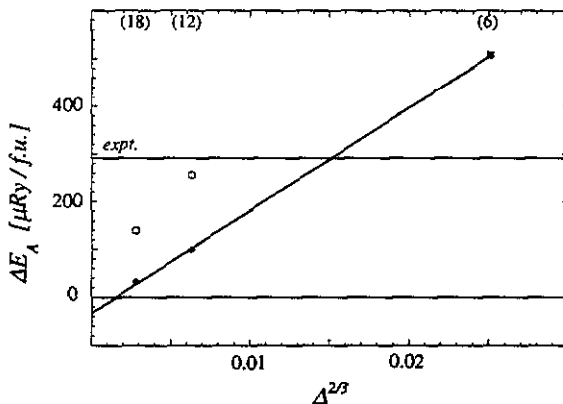


Figure 4. The MAE calculated for different meshes in the BZ for the two types of calculations. The figures in parentheses give the number of k points along the reciprocal a -axis. Δ is the volume of one tetrahedron (normalized to the volume of the full BZ). Results from the spin-orbit coupling (SO) calculations are given by full diamonds. The results of the OP calculations are denoted by squares. The straight line gives the best least square fit to a $\Delta^{2/3}$ dependence of the SO-calculation. The horizontal line marked 'expt.' is the experimental MAE (reference [26]). The fact that the two calculations give the same energy for the mesh corresponding to 6 k -points along the a -axis, is just a coincidence.

along direction d . Owing to the different magnetic space groups for the two cases the sums are performed over different irreducible parts of the BZ. These sums are calculated by means of the tetrahedron method. Numerically ΔE_A will depend on the number of k -points used in the calculations, and therefore care has to be taken to achieve convergence in the number of k -points. Also, in order to avoid numerical noise, it is essential that equivalent k -points are in the two sums in equation (4).

The calculated energy difference, ΔE_A , is plotted in figure 4 for different samplings of the BZ. The axes in reciprocal space are first divided by six in the basal plane and by seven along the uniaxial direction, where this ratio, 6:7, corresponds approximately to c/a . These numbers are then doubled (12:14) and tripled (18:21) when increasing the sampling density of the irreducible parts of the BZ. This strategy is used to facilitate the judgement of a smooth convergence of the difference between the sums in equation (4). The most dense mesh used corresponds to 6804 k -points in the full BZ.

Experimentally, it is known that YCo_5 and also SmCo_5 have an easy magnetization direction along the c -axis, i.e. in the [001] direction. Here we calculate the difference in energy between this situation and the case where the magnetization lies in the basal plane along the a -axis, i.e. the [100] direction.

While all the calculated energy differences ΔE_A are positive they decrease with refined mesh and have not reached full convergence even for the calculation with the finest mesh. However, if the errors of using a finite mesh are mainly due to the linear interpolation within the tetrahedra for the occupied states, i.e. if rearrangements occurring in the immediate neighbourhood of the Fermi level are of minor importance, ΔE_A should show a $\Delta^{2/3}$ dependence [5], where Δ is the volume of the tetrahedron. In figure 4 ΔE_A is plotted against $\Delta^{2/3}$ and, fortunately, a relatively linear dependence is found. Extrapolations to $\Delta = 0$ are then possible and are shown with straight lines in the plot. To check this linear dependence further, calculations with intermediate mesh samplings

were also performed. A result corresponding to a 10:11 division of the reciprocal lattice vectors is found to be rather close to the linear curve. This strengthens our belief that the linear behaviour found is not an artefact due to the fact that only relatively few different meshes were calculated. This linear behaviour has earlier been found for Co metal, while both Fe and Ni show a more complicated convergence [5].

Although all calculated ΔE_A values are positive for the case where only the spin-orbit coupling was included in the calculations, the extrapolation to $\Delta = 0$ gives a negative value, $-30 \mu\text{Ryd}$. Hence, when ignoring orbital correlations the wrong easy axis is predicted. For calculations with the OP correction included, the MAE remains positive and comparatively large. Unfortunately the linear relation found above, for the calculation without OP, is lost. The result at the finest mesh is $140 \mu\text{Ryd}$, which is of the same order of magnitude as the experimental value, $292 \mu\text{Ryd}$ [26] (indicated by a horizontal line in the figure). The experimental value is actually the difference between the magnetization directions [210] and [001] but, since the in-plane anisotropy is supposed to be negligible, this is an appropriate value for comparison with our calculations.

A comment about the use of OP in connection with the force theorem is in order. The splitting according to equation (1) depends on the magnitude of the orbital moment, which may vary between different magnetization axes. We have here neglected this possible dependence and used the orbital moment obtained from a self-consistent calculation with the magnetization along the [001] direction. In the calculations we also investigated the different orbital moments for the two cases. It is found that the anisotropy of the size of the orbital magnetization is small. The local orbital magnetic moments on cobalt decrease by 1% and 5% for sites I and II, respectively, when rotated from the [001] to [100] directions. These small changes in the orbital moments seem to justify our calculations *a posteriori*. This calculation of the change in the size of the orbital magnetic moments must, however, be regarded only as an estimate, since the orbital moments do not satisfy a variational principle, which was the basis for the use of the frozen densities when calculating the energy difference. There are reports on experimental observations of much larger magnetization anisotropies than those calculated here [26, 27].

In order to check how sensitive the anisotropy energy is to the exact position of the Fermi level, equation (4) is generalized to the following form

$$\Delta E(n) \approx \sum_{k,t}^{\varepsilon_F^a(n)} \varepsilon_i^a(k) - \sum_{k,t}^{\varepsilon_F^c(n)} \varepsilon_i^c(k). \quad (5)$$

Here $\varepsilon_F^d(n)$ ($d = c, a$) is the Fermi energy corresponding to n valence electrons and the direction d . The quantity $\Delta E(n)$ is plotted in figure 5 for the OP calculation with the mesh corresponding to 12 points along the a -axis. The anisotropy energy is found to vary rather strongly for occupation numbers between 46 and 48. As a matter of fact, for n around 48, which is the true value for YCo_5 , $\Delta E(n)$ is close to a local minimum. For an occupation number of 47 a much larger MAE is found. This corresponds, however, to a large displacement of the Fermi level and is far outside any deviations caused by numerical inaccuracy.

As mentioned in the introduction, there are speculation in the literature that it is the cobalt atoms of type I that are responsible for the anisotropy energy in YCo_5 . We therefore investigated the contributions to ΔE_A from the different sites. The energy

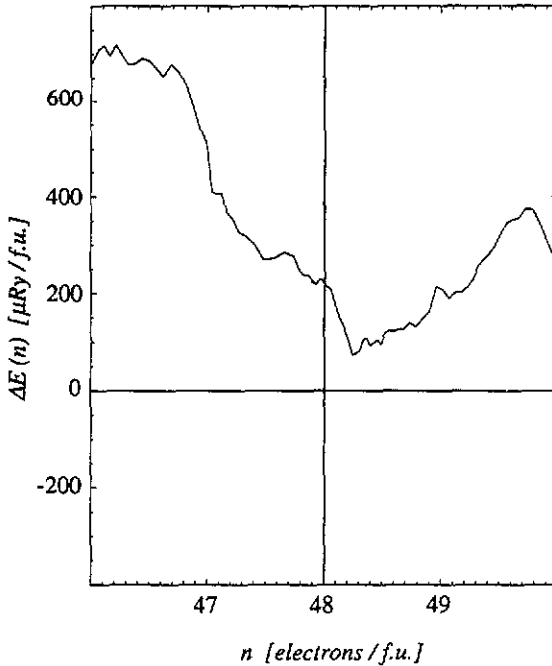


Figure 5. The MAE as a function of the number of valence electrons per formula unit. The vertical line denotes the number of valence electrons in YCo_5 .

difference in equation (4) is divided into separate contributions from the three atom types according to

$$\Delta E_A = \sum_{i=1}^3 \Delta E_A(i) = \sum_{i=1}^3 \left\{ \int_{-\infty}^{\varepsilon_F^d} \varepsilon N_i^d(\varepsilon) d\varepsilon - \int_{-\infty}^{\varepsilon_F^c} \varepsilon N_i^c(\varepsilon) d\varepsilon \right\}. \quad (6)$$

N_i^d is here the site projected density of states from a calculation with magnetization in direction d . The sum is over the three different crystallographic sites and the integrals correspond to the eigenvalue sums in equation (4). $\Delta E_A(i)$ can, in turn with a good accuracy, be approximated with

$$\Delta E_A(i) \approx F_i^c(\varepsilon_F) - F_i^d(\varepsilon_F) \equiv \Delta F_i(\varepsilon_F) \quad (7)$$

where ε_F is the average Fermi energy. Here

$$F_i^d(\varepsilon) = \int_{-\infty}^{\varepsilon} n_i^d(\varepsilon') d\varepsilon' = \int_{-\infty}^{\varepsilon} d\varepsilon' \int_{-\infty}^{\varepsilon'} N_i^d(\varepsilon'') d\varepsilon'' \quad (8)$$

where $n_i^d(\varepsilon)$ is the site projected number of states. In figure 6 the quantity $\Delta F_i(\varepsilon)$ corresponding to the 3d states (calculated with the OP included and with 12 k -points along the a -direction) is plotted for the two different types of cobalt sites. For $\varepsilon = \varepsilon_F$ these correspond to the site projected MAE. Looked upon over the whole energy range the contributions from Co_I and Co_{II} are strikingly dissimilar, but in the region of special interest around ε_F they are quite similar with a sharp minimum just above the Fermi level. It is found that the largest contribution to ΔE_A originates from the cobalt atoms at site II, which is in conflict with the suggestions mentioned in the introduction.

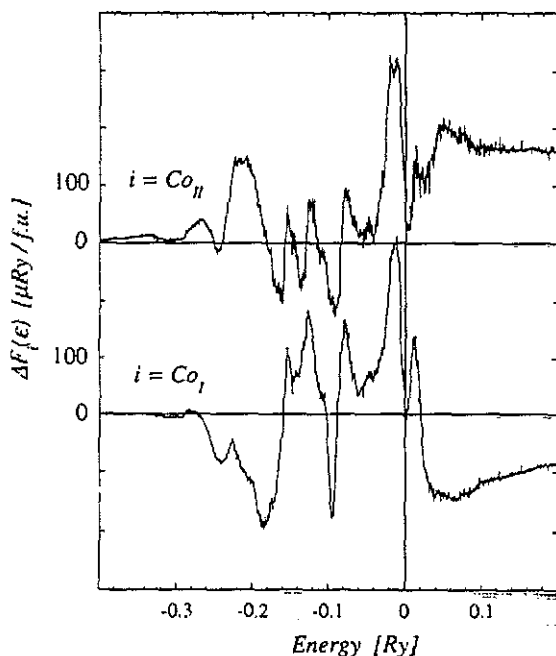


Figure 6. The energy resolved individual d state contributions from the two cobalt sites to the MAE. The Fermi level is denoted by a vertical line.

Surprisingly large contributions arise from non- d states of the cobalt atoms and from states on the yttrium atom. In numbers, the contributions to MAE from the three different sites are $27 \mu\text{Ryd/f.u.}$, $58 \mu\text{Ryd/f.u.}$ and $171 \mu\text{Ryd/f.u.}$ from Y, Co_I and Co_{II} , respectively. The observation that the largest anisotropy energy is to be attributed to the Co_{II} atoms is interesting in connection with the above observation that the largest magnetization anisotropy is also found on this atom. Thus, the MAE seems to be related to the change of the orbital moment and is less dependent on the absolute magnitude, which was actually found to be somewhat larger for the Co_I atoms than for the Co_{II} atoms (see table 1).

5. Conclusions

In this work we have applied the force theorem to calculate the MAE from first principles in YCo_5 . If orbital correlation is not included in the calculation the MAE is found to be too small and even the sign is wrong. This disagreement is in accordance with earlier theoretical studies. From a tight-binding approach a MAE of the wrong sign was obtained in [23] and in [5] a preliminary result for YCo_5 in disagreement with experiment was mentioned.

It should be noticed that, in the present investigation, effects from changes of the lattice constants have not been considered. As an input to the calculations we have used the experimentally determined lattice constants, but it is believed that if the total energy were optimized smaller lattice constants would be obtained. Such calculations are very time consuming and outside the scope of the present investigation. We are, however, of

the opinion that the present approach of using the experimentally determined crystal data is often superior when examining magnetic properties. One can, however, not overlook the possibility that these experimental data are not perfect and small changes would affect our calculated MAE. This effect was examined for the elemental metals Fe, Co and Ni in [5] where it was found to have minor importance. There are also small changes in the lattice constants connected with the rotation of the magnetization. An analysis of these magnetostriction effects, which are typically of the order 10^{-5} , suggests that they are too small to be of importance for MAE in YCo_5 .

As regards the orbital magnetization, OP calculations give moments which are considerably larger than when only the spin-orbit coupling is considered, and which are in agreement with at least some experimental data. However, the experimental total magnetic moment is not fully reproduced with the present formulation of OP.

From their calculation of MAE in Fe, Co and Ni, Daalderop *et al* [5] conclude that, today, it is not possible to calculate reliably the MAE from first principles. They relate this difficulty mainly to the use of the force theorem, and point out the necessity to go beyond it. On the other hand Jansen [6] attributes the difficulties to the neglect of orbital correlation in the theoretical treatment.

Although we have not tried to go beyond the force theorem, and although we have found that calculations of MAE are very hard to perform, the present result seems to give some support to Jansen's standpoint. It is found that when orbital polarization is included in the calculation a MAE much closer to the experimental value is calculated for YCo_5 . Hence, our results suggest that in order to determine the MAE for itinerant ferromagnets it is not enough to include just the spin-orbit coupling; instead, orbital correlation has to be introduced. In the present work this was done by means of the orbital polarization scheme.

After completion of the present work we became aware of the work by Daalderop *et al* [28] where results similar to ours were obtained for YCo_5 .

Acknowledgments

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