

Calculated magneto-optical Kerr effect in Fe, Co, and Ni

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We report *ab initio* calculations of magneto-optical Kerr effect in Fe, Co, and Ni. Both real and imaginary parts of the interband optical response functions are calculated from self-consistent energy-band calculations in the presence of both a magnetic moment and spin-orbit interaction. We draw particular attention to two ways to obtain the real part of the response functions: first by direct calculation with the energy treated as a complex variable, and second by Hilbert transformation of the imaginary part of the response functions. The calculated magneto-optical Kerr effect for both the cubic metals Fe and Ni are in good agreement with measurements. Fair agreement between the theory for Co with recent measurements on Co hcp and fcc multilayers is obtained.

I. INTRODUCTION

When plane polarized light is reflected from or transmitted through a magnetic material its plane of polarization is rotated. The effect is called the Faraday effect for transmitted light and magneto-optical Kerr effect¹ for reflected light, where the angle of rotation is known as the Kerr angle. Reversing the bulk magnetism then reverses the angle of rotation. There are now several good reviews of the state of measurements of magneto-optical Kerr effect.^{2,3} The largest magneto-optical Kerr effect found to date is for CeSb, with a Kerr angle of 14°. This compares with a couple of degrees for uranium compounds and less than 0.5° for Fe, Co, and Ni.

While these effects have long been understood in terms of classical optics, a microscopic theory in terms of the application of quantum mechanics to solid-state physics is a more recent development.⁴ An attempt to estimate the absorptive part of the off-diagonal dielectric function by Argyres⁵ achieved the correct order of magnitude for Fe and Ni and was followed by further work on the theory of magneto-optical Kerr effect by Cooper⁶ and Bennet and Stern.⁷ The inherent difficulty in performing sufficiently accurate band-structure calculations limited these early attempts to a simple perturbational approach and fitting to experimental data. Subsequently, Wang and Callaway⁸ calculated the absorptive part of the off-diagonal optical conductivity for Ni and achieved fair agreement with experiment. Given the problems involved, these pioneering results were very encouraging.

More recently, there have been several calculations of the absorptive part of the off-diagonal dielectric function using modern band-structure techniques. Ebert⁹ studied Fe and Ni with poor and good agreement, respectively, for the off-diagonal dielectric function. Cooper *et al.*¹⁰ calculated the off-diagonal optical conductivity for Fe, achieving good

agreement with measurements, and various complex itinerant *f* electron systems where agreement with experiment was poor. Cooper *et al.*¹⁰ suggested that the deficiencies in the latter case were due to many-body effects. Halilov and Uspenskii¹¹ have also calculated the off-diagonal optical conductivity for Fe, Co, and Ni and achieved reasonable results for all three metals.

The above-mentioned papers addressed themselves to the absorptive part of the off-diagonal dielectric function. The response part is obtained, in principle, by a Kramers-Kronig transformation, but the final step was not taken and the Kerr angle itself—which is a function of both real and imaginary parts of the off-diagonal optical conductivity—was not calculated.

In a more recent paper, Halilov¹² considered the effect of different orientations upon the magneto-optical Kerr effect (MOKE) for Ni. More specifically, he calculated the difference in light intensity change, δ between the equatorial and longitudinal Kerr configurations: Orientation MOKE = $\delta^{\text{equat}} - \delta^{\text{long}}$. The equatorial (longitudinal) orientations are given with the magnetization vector perpendicular to the surface and normal (perpendicular) to the light incident plane. Agreement with measurements was not outstanding but it was difficult to draw any conclusions due to the complexity of the evaluated formula.

Until recently, the only available calculations for the Kerr angle were by Daalderop *et al.*¹³ for UNiSn and Oppeneer *et al.*,^{14,15} for Fe, Co, and Ni. The latter obtained good agreement with measurements but there was no experimental data for the former. This situation has now changed and, in the last year, several groups have calculated the Kerr effect^{16,17} for various elements and compounds. Some of these papers have gone beyond the simplest expression for the evaluation of the matrix elements [Eq. (11) of this paper], including relativistic effects in their calculation of the matrix elements. However, as shown by Wang and Callaway,⁸ the effect of

this is negligible for the cases studied here.

Halilov's¹² paper raises the problem of the different possible orientations of magnetic moment and incident wave vector. In the following, we shall consider only the polar Kerr effect, where both incident wave vector and magnetization vector are perpendicular to the surface of the material, lying along the [001] direction (referred to as the z axis). For Fe and Co this is not a problem as their easy axes lie in the z axis. Ni has its easy axis in the [111] direction. Fortunately, the magnetocrystalline anisotropy energy is small and the magnetic moment may be aligned along the [001] direction relatively easily.¹⁸ This is not the case for actinide compounds such as US,^{19,20} which we have discussed in another paper.²¹

This paper is organized as follows. We first outline the theory of the magneto-optical Kerr effect for both cubic and hcp structures. We then compare our results for bcc Fe and fcc Ni with those of other authors and measurements to confirm the accuracy of the method. We focus upon hcp Co, calculating the Kerr effect from first principles. This is of special interest as many compounds with high Kerr values form in hexagonal structures and not in the simpler cubic structures. We also comment upon the relative merits of the Kramers-Kronig transformation to obtain the real part of the off-diagonal dielectric function and direct calculation of the entire response function by treating the energy as a complex variable.

II. THEORY

Our summary of the macroscopic theory of magneto-optical Kerr effect, follows the paper by Kahn *et al.*²² and our treatment of the microscopic theory of the optical conductivity and dielectric constants follows the work of Callaway and collaborators.^{8,23}

For a crystal with at least threefold rotational symmetry (hexagonal, tetragonal, trigonal or cubic), with a magnetic field along the z axis, the dielectric tensor ϵ reduces to

$$\epsilon = \begin{pmatrix} \epsilon_0 & i\epsilon_1 & 0 \\ -i\epsilon_1 & \epsilon_0 & 0 \\ 0 & 0 & \epsilon_z \end{pmatrix}, \quad (1)$$

where ϵ is complex, $\epsilon = \epsilon' + i\epsilon''$. The coordinate axes lie along the principle axes of the crystal which are the z axis and two orthogonal axes perpendicular to z but otherwise arbitrary, which we denote by x and y . The normal modes of light propagation are the eigenvectors of ϵ . The eigenvalues of ϵ are $\epsilon_{\pm} = n_{\pm}^2 = \epsilon_0 \pm \epsilon_1$, and the normal modes for light propagating with $\mathbf{q} \parallel z$ are circularly polarized

$$\begin{aligned} \hat{\phi}_+ &= \frac{-i}{\sqrt{2}}(\hat{\mathbf{x}} + i\hat{\mathbf{y}}), \\ \hat{\phi}_- &= \frac{1}{\sqrt{2}}(\hat{\mathbf{x}} - i\hat{\mathbf{y}}). \end{aligned} \quad (2)$$

If the incoming beam is taken to be linearly polarized at an angle, α , measured counterclockwise to $\hat{\mathbf{x}}$ then $\mathbf{E}_{\text{in}} = E_0(\hat{\mathbf{x}} \cos\alpha + \hat{\mathbf{y}} \sin\alpha) = E_0 \hat{\mathbf{r}}_{\alpha}$ is expressed, in terms of

normal modes by $\mathbf{E}_{\text{in}} = E_+ \hat{\phi}_+ + E_- \hat{\phi}_-$, and the reflected beam will be $\mathbf{E}_{\text{out}} = r_+ E_+ \hat{\phi}_+ + r_- E_- \hat{\phi}_-$ where r_{\pm} are the reflection coefficients for left and right circularly polarized light

$$r_{\pm} = \frac{1 - \sqrt{\epsilon_{\pm}}}{1 + \sqrt{\epsilon_{\pm}}}. \quad (3)$$

The direction of polarization perpendicular to $\hat{\mathbf{r}}_{\alpha}$ is $\hat{\mathbf{r}}_{\bar{\alpha}} = -\hat{\mathbf{x}} \sin\alpha + \hat{\mathbf{y}} \cos\alpha$ in terms of which the reflected beam is

$$\mathbf{E}_{\text{out}} = \frac{1}{2}(r_+ + r_-) \left[\hat{\mathbf{r}}_{\alpha} + \frac{i(r_+ - r_-)}{(r_+ + r_-)} \hat{\mathbf{r}}_{\bar{\alpha}} \right]. \quad (4)$$

The complex Kerr rotation is therefore

$$\Psi = i \frac{(r_+ - r_-)}{(r_+ + r_-)} = i \frac{(\sqrt{\epsilon_+} - \sqrt{\epsilon_-})}{(\sqrt{\epsilon_+} + \sqrt{\epsilon_-} - 1)}, \quad (5)$$

where the complex Kerr rotation Ψ is comprised of the Kerr angle θ and an ellipticity $i\psi$. For small rotations, we may finally write

$$\Psi = \theta + i\psi \approx \frac{i\epsilon_1}{\sqrt{\epsilon_0}(\epsilon_0 - 1)}, \quad (6)$$

which is the expression normally evaluated.

The macroscopic quantities entering Eqs. (5) and (6) are obtained from linear response of the microscopic current to the applied field.²⁴ An element of the conductivity tensor is

$$\begin{aligned} \sigma_{ij}(\mathbf{q}, \omega) &= \left(\frac{iNe^2}{m\omega} \right) \\ &+ \frac{1}{\hbar\omega} \int_{-\infty}^0 dt \langle [j_j(\mathbf{q}, 0), j_j(-\mathbf{q}, t)] \rangle \exp^{-i\omega t} \end{aligned} \quad (7)$$

and, for optical properties, the $q=0$ limit is appropriate. The conductivity and dielectric tensors are related by

$$\epsilon_{ij}(\omega) = \delta_{ij} + \left[\frac{4\pi i \sigma_{ij}(0, \omega)}{\omega} \right]. \quad (8)$$

When equation (8) is evaluated over the set of single-particle energy band states, the diagonal elements of the *interband* dielectric function become

$$\begin{aligned} \epsilon_0(\omega) &= 1 - \frac{2\pi}{\hbar\omega} \sum_{\mathbf{k}} \sum_l \sum_n \frac{1}{\omega_{nl}(\mathbf{k})} [|\mathbf{j}_+^{nl}(\mathbf{k})|^2 + |\mathbf{j}_-^{nl}(\mathbf{k})|^2] \\ &\times \left[\frac{1}{\omega - \omega_{nl}(\mathbf{k}) + i\delta} + \frac{1}{\omega + \omega_{nl}(\mathbf{k}) + i\delta} \right] \\ &\times [f_l(\mathbf{k}) - f_n(\mathbf{k})] \end{aligned} \quad (9)$$

and the off-diagonal elements are

$$\begin{aligned} \varepsilon_1(\omega) = & \frac{2\pi i}{\hbar\omega} \sum_{\mathbf{k}} \sum_l \sum_n \frac{1}{\omega_{nl}(\mathbf{k})} [|\mathbf{j}_+^{nl}(\mathbf{k})|^2 - |\mathbf{j}_-^{nl}(\mathbf{k})|^2] \\ & \times \left[\frac{1}{\omega - \omega_{nl}(\mathbf{k}) + i\delta} + \frac{1}{\omega + \omega_{nl}(\mathbf{k}) + i\delta} \right] \\ & \times [f_l(\mathbf{k}) - f_n(\mathbf{k})], \end{aligned} \quad (10)$$

where $f_n(\mathbf{k})$ is the Fermi distribution function and l and n label initial and final energy band states, respectively. Here the energies of transitions between energy band states are $\hbar\omega_{nl}(\mathbf{k}) = \hbar\omega_n(\mathbf{k}) - \hbar\omega_l(\mathbf{k})$ and $\mathbf{j}_\alpha^{nl}(\mathbf{k})$ is a matrix element of the circularly polarized components of the current operator between the branches n and l at the wave vector \mathbf{k}

$$j_\alpha^{nl}(\mathbf{k}) = \frac{i\hbar e}{m} \langle \phi_{\mathbf{k}n} | \nabla_\alpha | \phi_{\mathbf{k}l} \rangle, \quad (11)$$

where $\alpha = \pm$ corresponds to $x \pm iy$. The matrix elements of the current operator are easily evaluated and factor to a product of a radial component and an angular component.²⁵ The angular component is evaluated from the Wigner-Eckart theorem, leading directly to the optical selection rules $\Delta l = \pm 1, \Delta m_l = \pm 1$. The radial component is evaluated by direct differentiation of the radial wave functions followed by integration.¹⁶

The imaginary part of Eq. (9) and the real part of Eq. (10) may be evaluated directly from a normal band-structure calculation. The real part of Eq. (9) and the imaginary part of Eq. (10) are normally then obtained by a Kramers-Kronig transformation, required by causality. For example, the real part of Eq. (9) is obtained from

$$\varepsilon'(\omega) = 1 + \frac{2}{\pi} \wp \int_0^\infty \frac{\omega' \varepsilon''(\omega')}{\omega'^2 - \omega^2} d\omega', \quad (12)$$

if the imaginary part is known over a sufficient range with sufficient accuracy. Measurements only stretch over a certain energy window and they must be sensibly extrapolated to allow a meaningful Kramers-Kronig transformation. Once the bulk of the structure in the optical spectrum has been passed, the form of extrapolation does not have a great effect on the calculated peak positions or intensities. This Kramers-Kronig transformation has then been used in many theoretical works on the diagonal part of the dielectric function, and has been shown to work across the periodic table.²⁶

The situation was different for the off-diagonal term, until recently no theoretical Kramers-Kronig transformation had been performed that could be compared to experiment. One possible reason had been put forward. These calculations all suffer from the same problem. The further a state lies from the Fermi energy, the less accurately it is given and thus the matrix elements, Eq. (11), become less accurate with increasing ω . It could then be thought that ε''_1 , which still has appreciable character at 6 eV, is too inaccurate to allow the Kramers-Kronig transformation to work. Furthermore, due to its oscillatory nature it is difficult to give a good extrapolation to higher energies, unlike the generally decreasing ε_0 and thus difficult to converge. In an attempt to circumvent this problem, Oppeneer *et al.*¹⁴ evaluated Eqs. (9) and (10) directly, in the complex energy plane. They claim that this then avoids the inaccuracies induced by performing the

Kramers-Kronig transformation on the (less accurate) high-energy transitions to yield their contribution to the low energy ε'_1 . However, a closer analysis of Eq. (10) shows that the high-energy transitions contribute to ε'_1 in the direct (complex energy) evaluation. Various calculations have recently used the Kramers-Kronig transformation to calculate ε'_1 , we have verified numerically that the two methods yield identical results.¹⁶ The difficulty with the Kramers-Kronig transformation is that it requires a dense mesh in the energy grid. To achieve satisfactory convergence an energy mesh of 1 mRy is required for a double Kramers-Kronig transformation test.²⁷ This test confirms the convergence of the Kramers-Kronig transformation but not the accuracy of ε'_1 . Compared to this, the complex energy integration requires much fewer points (50 mRy gives an acceptable graph) but the time involved in the integration is much greater per energy point. We find that the results from the two methods are identical but that the Kramers-Kronig transformation must be checked for convergence and is therefore less pleasing from a computational point of view. Further, evaluating Eqs. (9) and (10) directly allows a broadening to be included in a physical manner. There are many prescriptions for such a broadening function. We choose a broadening that corresponds to many optical and photoemission experiments in that it is proportional to the excitation energy squared, being 2 eV at 1 Ry energy.

III. RESULTS

We have calculated the band structure self-consistently for Fe, Co, and Ni, using the linear muffin-tin orbital (LMTO) method,²⁸ with the von Barth and Hedin²⁹ exchange-correlation term in the local-spin-density approximation.³⁰ The calculation was scalar relativistic for the wave functions and spin-orbit interaction was added to the Hamiltonian matrix. Both the orbital moment and the magneto-optical Kerr effect were found to be zero with zero spin-orbit interaction, as expected by general arguments (both are broken time-reversal symmetry effects). Spin-orbit coupling was also included for the p states. Exclusion of the latter has the effect of reducing the calculated Kerr effect by approximately 10%. A fuller discussion of these effects can be found in Ref. 16.

As was pointed out by Söderlind *et al.*,³¹ the calculated orbital moments tend to be underestimated in this procedure, akin to the much more serious underestimation that occurs for actinide intermetallics.³² A proposed solution to this is the inclusion of an ‘‘orbital polarization’’ term; a shift in the eigenvalues given by

$$\Delta \epsilon_{m_l} = -BL_Z^\sigma m_l, \quad (13)$$

where B is the Racah parameter (for d states) and L_Z^σ is the total orbital momentum *per spin channel*. A result of this is that the splitting is different for spin-up and spin-down states. Interestingly, this has a form similar to that required by relativistic density-functional theory, that is that the energy functional has an L dependence (see the discussion by Jansen³³), although the motivation for this shift is given by an analysis of Hartree-Fock theory.^{34,35} With this shift, Söderlind *et al.* found much improved agreement with ex-

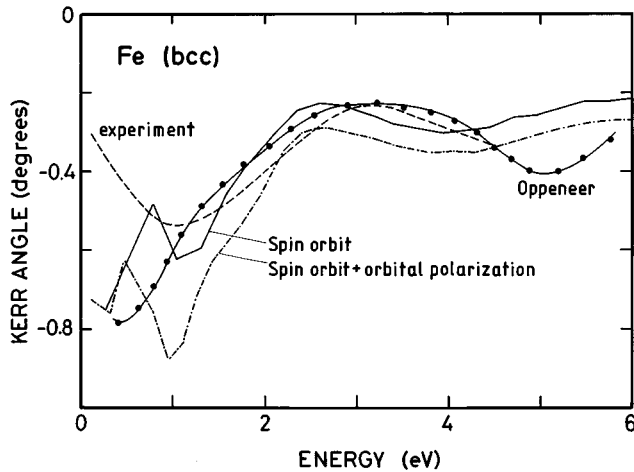


FIG. 1. Calculated Kerr angle for Fe: calculated with spin-orbit coupling (full line), and orbital polarization (dotted line) compared with Oppeneer's calculation (Ref. 14) (with points) and experiment (Ref. 3) (dashed line).

periment for the calculated moments. The exact implementation of such an orbital polarization scheme can be questioned due to its non *ab initio* form but a more rigorous derivation gives similar results for the transition metals.³⁵ Clearly, an accurate description of the ground-state properties is required before we can attempt to calculate the optical spectra; we have therefore included this term in our calculations in order to illustrate its effects.

In Figs. 1–3 we present the calculated magneto-optical Kerr rotation for Fe, Co, and Ni in their correct crystal structure. We have compared with other calculations, those of Oppeneer *et al.*^{14,15} For Fe we have good agreement for the spin-orbit coupling calculation except that the minimum occurs at too low energy. Orbital polarization enhances the magneto-optical Kerr rotation by approximately 20%. For Co we have very good agreement from 0.5 to 3 eV, above this the calculation diverges from experiment. At higher energies, the calculation of Oppeneer is in better agreement

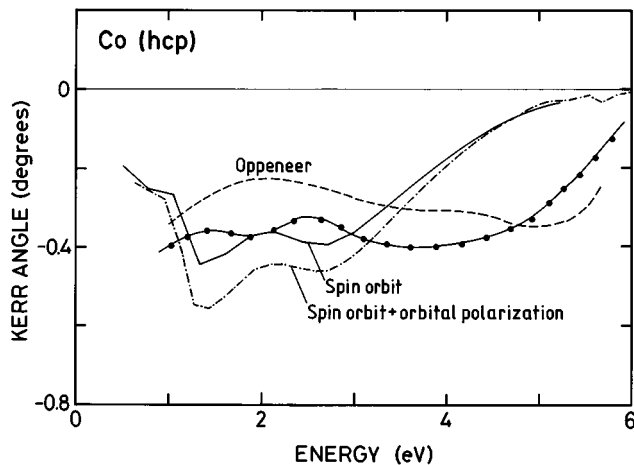


FIG. 2. Calculated Kerr angle for Co: calculated with spin-orbit coupling (full line), and orbital polarization (dotted line) compared with Oppeneer's calculation (Ref. 15) and experiment (Ref. 37) (with points).

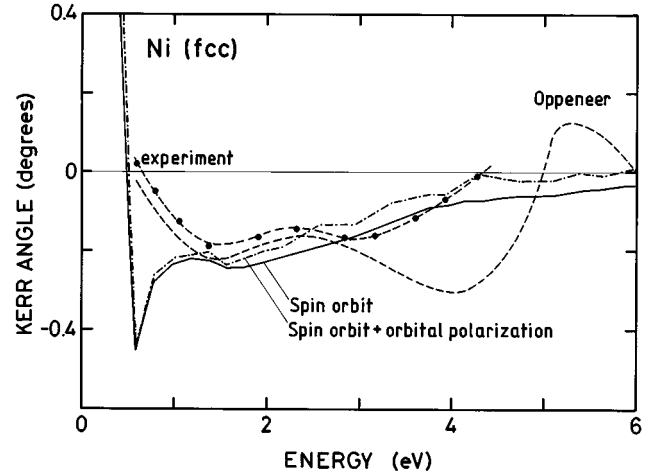


FIG. 3. Calculated Kerr angle for Ni: calculated with spin-orbit coupling (full line), and orbital polarization (dotted line) compared with Oppeneer's calculation (Ref. 14) (dashed line) and experiment (Ref. 3) (with points).

with experiment than ours. Orbital polarization has a small effect, increasing magneto-optical Kerr rotation by 30% at 1.5 eV, this decreases almost linearly to no enhancement at 5 eV. For Ni we have good agreement with experiment whereas Oppeneer's calculation deviates from experiment above 3 eV. Orbital polarization has no effect at 1 eV, at 2 eV and higher it tends to decrease the magneto-optical Kerr effect slightly. At low energy the calculation shows a strange behavior, this is due to our choice of broadening function which is only 0.01 Ry at 1 eV and our neglect of the intra-band contribution to the optical conductivity.

Recently, a sample of fcc Co has been stabilized as a 1000 Å thick overlayer.³⁶ Careful measurements of the Kerr effect have been carried out on these "single-crystal" fcc and also single-crystal hcp samples.³⁷ Similar data has also presented by Weller *et al.*³⁸ The fcc lattice parameter was found to be 3.54 Å,³⁹ which is the same atomic volume as hcp Co. In Fig. 4 we present the calculated and experimental Kerr angle for the fcc structure. The penetration depth is of the order of

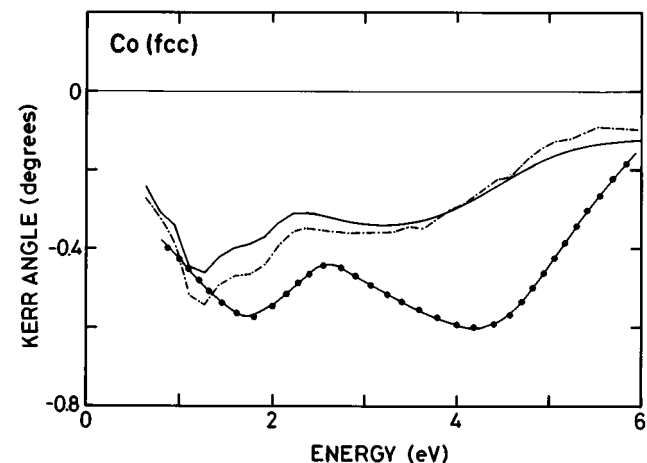


FIG. 4. Calculated Kerr angle for Co in the fcc structure: calculated with spin-orbit coupling (full line) and orbital polarization (dotted line) compared with experiment (Ref. 37) (with points).

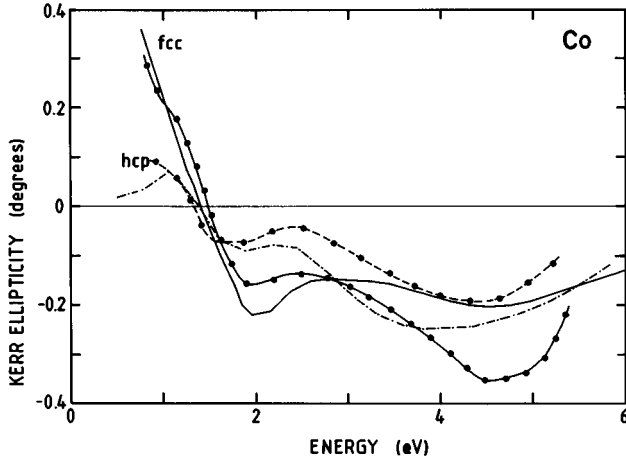


FIG. 5. Calculated Kerr ellipticity for Co in hcp (dashed line) and fcc (full line) structures: compared with experiment (Ref. 37) (with points).

100 Å and we therefore can apply bulk calculations directly. The first peak, just over 1 eV is well reproduced but above 3 eV, the magnitude of the magneto-optical Kerr effect is not reproduced. The second peak, at 4 eV, is not found, although a trough can be discerned at 3.5 eV. By expanding the lattice by 6% we find that this trough develops into a second peak but that it shifts to lower energy.

The ellipticity for fcc and hcp Co is plotted in Fig. 5. As for the Kerr angle, agreement with measurements is fair, the peaks are reproduced but the intensity is out by up to a factor of 2.

One of the reasons for theoretical research into the magneto-optical Kerr effect is a wish to explain and then predict these effects. The obvious starting point is the transition metals Fe, Co, and Ni. It is understood that spin-orbit coupling is responsible for the magneto-optical Kerr effect and yet the spin-orbit parameters are almost identical for these three metals. This leads to the conclusion that the band structure is important in determining the magneto-optical Kerr effect as these three metals have different structures. Now that measurements are available on fcc Co, we can extend the analysis to look at the effect of changing structure for the same element (Co) and changing element in the same structure (Co, Ni in the fcc structure). Experimentally, both fcc Co and Ni have a low-energy peak at 1.5 eV but their high-energy behavior diverges. The difference in intensities is well reproduced by theory. A major factor in the difference between fcc Co and Ni is band filling which reduces the spin splitting as more spin down bands are filled.

Comparing fcc and hcp Co, we find that theory reproduces the experimental curves well up to 3 eV, after which agreement becomes worse. Both systems have a measured second peak at 3 eV (hcp), 4 eV (fcc), which is not well reproduced in the calculation. The origin of the magnitude of the Co fcc magneto-optical Kerr effect is still not explained. Although the spin-orbit coupling is the same, the actual moment may vary in different structures. In Table I we present the calculated moments for these two structures. The orbital moment is $\approx 10\%$ smaller for fcc than hcp, whereas the magneto-optical Kerr effect is larger. Furthermore, the effect of orbital polarization on the orbital moment is an increase of

TABLE I. Calculated spin and orbital moments for Co (μ_B /atom).

	Spin-orbit coupling			S-O + orbital polarization		
	Spin	Orbital	Total	Spin	Orbital	Total
Fcc	1.595	0.079	1.674	1.596	0.122	1.718
Hcp	1.567	0.086	1.655	1.571	0.132	1.703

50% while the effect on the magneto-optical Kerr effect varies between an increase of 20% to a decrease of 10%. Thus neither the size of the orbital moment nor the effect of orbital polarization can explain the difference in the two spectra.

The role of orbital polarization (OP) appears, at first sight, a little strange. Although it gives an increase in the orbital moment, it can yield a decrease in the Kerr angle. This difference in behavior may be explained by considering the differences between the optical spectra and magnetic moments. The magnetic moments are integrated quantities, given by an integral over all occupied states, whereas the optical spectra are given by considering transitions from all occupied to all unoccupied states. We would expect that an increase in the splitting of the $\pm m_l$ degenerate bands around the fermi level (such that part of one of the bands were forced above the fermi level) would result in an increase in the orbital moment. This is what we observe; the increased splitting [Eq. (13)] yields a larger moment. It has previously been shown that an increase (or decrease) in the spin-orbit coupling gives a corresponding scaling of the Kerr effect.¹⁵ This scaling is not observed here as orbital polarization does not give a uniform increase to the splitting. An easy, and appealing, way to view the origin of ε_1 is to treat the problem in a pure $|ls\rangle$ basis set, with spin-orbit coupling treated as a perturbation to the band structure only. Then, ε_1 is simply given as proportional to the difference between the expectation values of the step-up and step-down operators for angular momentum (with the selection rules $\Delta m_l = \pm 1$, respectively) see Eqs. (10) and (11), also Ref. 16. The actual value of ε_1 depends on the delicate cancellation between the step-up ($\Delta m_l = +1$) and step-down ($\Delta m_l = -1$) transitions. Using this idea we can now understand the reason for the role of orbital polarization. OP tends to increase the splitting between $\pm m_l$ states in one spin channel more than in the other. This alters the cancellation effects and it is possible to construct simple models where ε_1 would either increase or decrease. Thus, although OP tends to increase the Kerr effect, its role is much more complicated than expected from simple considerations of the orbital moment. The complexity of the actual band structure makes it impossible to accurately predict the effect of OP, and it is only a full calculation that can actually yield the final result.

IV. CONCLUSIONS

We have presented first-principles calculations of the magneto-optical Kerr effect for Fe, Co, and Ni in their ground-state crystal structures and fcc Co. Our results are in good agreement with measurements for Fe and Ni and fair agreement for Co in both structures. These results, using the

LMTO method, are very similar to those of Oppeneer *et al.*¹⁴ who also used density-functional theory but with the ASW method.

The effect of orbital polarization on the optical spectra is found to be much smaller than the effect on the magnetic moments. For hcp Co it worsens agreement with experiment, for fcc Co there is a slight improvement. There is no simple correlation between either crystal structure or magnetic moment (spin or orbital) and the size of the Kerr effect. Most importantly, the magneto-optical Kerr effect is calculated correctly for Fe and Ni and for Co up to 3 eV and we have

confirmed, similar to Refs. 14 and 17, that it is possible to calculate the magneto-optical Kerr effect from first principles.

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