

## Magnetic circular dichroism in photoemission by linear polarized light

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For light in a general state of polarization incident in a general direction on a ferromagnetic cubic (001) surface, magnetic dichroism and spin polarization in valence-band photoemission normal to the surface are investigated analytically and numerically, taking into account the optical response of the solid in the classical Fresnel approximation. Evaluation of relativistic dipole matrix elements leads to explicit expressions which reveal details of the underlying physical mechanisms and provide general semiquantitative results. Using a fully relativistic Green function method, numerical results have been obtained for fct Ni(001) with magnetization perpendicular and parallel to the surface. For perpendicular magnetization and linearly polarized light with the electric field vector rotated out of the incidence plane, the optical response leads to substantial magnetic dichroism, the spectral shape of which is the same as in the case of circular polarization of the incident light. [S0163-1829(97)08117-4]

### I. INTRODUCTION

In recent years, the power of photoemission for studying magnetic properties of surfaces and ultrathin films has been greatly enhanced by virtue of magnetic dichroism (MD), an asymmetry in the spin-averaged (not spin-resolved) photocurrent upon reversal of the magnetization direction. MD essentially arises from an interplay between the spin-orbit coupling (SOC) and exchange interaction in the initial state. It occurs quite generally if the geometry of surface, magnetization direction  $\vec{M}$ , photon incidence, and electron emission directions is such that in the nonmagnetic limit the photoelectrons have a spin-orbit-induced spin polarization component along  $\vec{M}$ . Since brief surveys of the development of MD and ample references to the original literature are contained in four recent articles,<sup>1-4</sup> it may suffice here to mention these articles dealing with MD in angle-resolved valence band photoemission. An overview of theoretical approaches and results has been given in Ref. 1, and analytical results for a variety of geometries were presented in Ref. 2. Joint experimental and theoretical MD investigations were performed on perpendicularly magnetized Ni films using normally incident circularly polarized light<sup>3</sup> and on in-plane magnetized Co films using *p*-polarized light.<sup>4</sup>

All of the above-mentioned theoretical work focused on MD produced by normally incident circularly polarized light and by off-normally incident *s*- and *p*-polarized light. The electric field inside the solid was approximated by the external field, which is valid for the first two cases of light polarization and still meaningful for *p*-polarized light. In the present work, we analytically and numerically investigate MD in valence-band photoemission by light in a general state of polarization incident at general polar and azimuthal angles. As one might expect and as our results confirm quantitatively, it is essential to take into account the modification of the radiation field by the optical response of the solid. A microscopic theory of the optical response being beyond the scope of this work, we approximate the internal radiation field by the classical field as described by Fresnel's formulas.

Our analytical expressions and numerical results show that this may strongly influence MD. A drastic effect is found for perpendicular magnetization and *linearly polarized light* with the electric-field vector rotated out of the incidence plane: While there is no MD in the external-field approximation, the optical response leads, via a circularly polarized field part inside the solid, to a substantial MD, the spectral shape of which is the same as in the case of *circular polarization* of the incident light. The usual classification of MD into "circular" (MCD) and "linear" (MLD) according to the polarization of the incident radiation thus becomes less meaningful.

This paper is organized as follows. In Sec. II we analytically derive expressions for the intensity, its asymmetry upon magnetization reversal (MD), and the spin polarization of photoelectrons emitted normally from cubic (001) surfaces with perpendicular and with in-plane magnetization by generally polarized light. In Sec. III we present corresponding numerical results, obtained by a relativistic Green function method, for Ni(001) for various light polarizations.

### II. ANALYTICAL INVESTIGATION

Analytical calculations of magnetic dichroism and spin polarization in photoemission have proved useful for revealing details of the underlying physical mechanisms and for obtaining qualitative predictions for specific surface and photoemission geometries.<sup>2</sup> In the following, we first outline the extension of this approach to general light polarization and to the inclusion of the optical response of the solid. Subsequently, we present explicit expressions for photoemission normal to cubic (001) surfaces with perpendicular and with in-plane magnetization.

#### A. Method

Within a fully relativistic one-step theory of photoemission from semi-infinite crystalline magnetic systems, the density matrix for the photocurrent at the detector is approximated by a golden-rule form (neglecting hole lifetime ef-

fects), as has been described in detail in Ref. 2. This form involves matrix elements of the electron-photon interaction  $H_{e-p} = \vec{E}' \cdot \vec{r}$  (in the electric dipole approximation) between relativistic initial and final states, where  $\vec{E}'$  is the electric vector of the radiation field inside the solid, assumed as spatially constant.

While in previous work  $\vec{E}'$  was simply taken as the external field  $\vec{E}$ , we now approximate it macroscopically according to classical electrodynamics (cf., e.g., Ref. 5). Strictly speaking, the magneto-optical response of the solid should then be described by a  $3 \times 3$  dielectric tensor. In the following, we neglect, however, its off-diagonal terms and assume the diagonal terms as equal, because (a) an *ab initio* calculation is beyond the scope of this paper and (b) interesting new effects arise already in this approximation. We thus represent the optical response by a dielectric constant  $\epsilon'$ , which is in general complex and related to the refractive index  $n'$  by  $n' = \sqrt{\epsilon'}$  where  $n'$  has positive real part. (In the following, quantities associated with the radiation field inside the solid are indicated by a prime.) The internal polar angle of incidence  $\vartheta'$  is related to the external one (vacuum side)  $\vartheta$  by Snell's law,

$$\sin \vartheta' = \sin \vartheta / n', \quad (1a)$$

$$\cos \vartheta' = -\sqrt{\epsilon' - \sin^2 \vartheta} / n'. \quad (1b)$$

Because  $\epsilon'$  is in general complex, these expressions and  $\vartheta'$  are also complex. The amplitudes of the internal electric field are given by Fresnel's formulas as

$$E'_\perp = \frac{2 \cos \vartheta E_\perp}{\cos \vartheta + \sqrt{\epsilon' - \sin^2 \vartheta}}, \quad (2a)$$

$$E'_\parallel = \frac{2 n' \cos \vartheta E_\parallel}{\epsilon' \cos \vartheta + \sqrt{\epsilon' - \sin^2 \vartheta}}, \quad (2b)$$

where  $E_\perp$  and  $E_\parallel$  are the amplitudes of the components of the external field  $\vec{E}$  parallel and perpendicular to the plane of incidence, respectively. These two amplitudes characterize the light polarization: *s*-polarized light is described by  $(E_\parallel, E_\perp) = (0, 1)$  and *p*-polarized light by  $(E_\parallel, E_\perp) = (1, 0)$ . For circularly polarized light, there is a phase shift of  $\pm i$  between the *s* and *p* components of  $\vec{E}$ , i.e.,  $(E_\parallel, E_\perp) = (1, \pm i) / \sqrt{2}$ . A particularly interesting special case of linearly polarized light, which for short we refer to as *sp*-polarized light, is characterized by  $(E_\parallel, E_\perp) = (1, \pm 1) / \sqrt{2}$ . From Eq. (2) it is evident that incident *s*- and *p*-polarized light remain so inside the solid, whereas for general linear polarized light and for circular polarized light the internal field becomes elliptically polarized.

## B. Results for perpendicular magnetization

First we consider the case  $\vec{M}$  along the surface normal (see, for example, Ref. 3). In normal emission electronic states can be classified with respect to four one-dimensional representations  $\Delta_6^\pm$  and  $\Delta_7^\pm$  (for details see Ref. 2). Note that the surface normal remains a fourfold rotational axis of the lattice.

For the pair of initial states with  $\Delta_6^\pm$  symmetry we obtain the intensity

$$I_6 = |\sin \vartheta'|^2 |E'_\parallel|^2 (|M_\perp^{(1++)}|^2 + |M_\perp^{(1--)}|^2) + (|E'_\perp|^2 + |\cos \vartheta'|^2 |E'_\parallel|^2) (|M_\parallel^{(5+-)}|^2 + |M_\parallel^{(5-+)}|^2) - 2 \operatorname{Im}(\cos \vartheta' E'_\parallel E'_\perp^*) (|M_\parallel^{(5+-)}|^2 - |M_\parallel^{(5-+)}|^2), \quad (3)$$

and the component of  $\vec{P}$  normal to the surface

$$P_{6z} = \frac{1}{I_6} [|\sin \vartheta'|^2 |E'_\parallel|^2 (|M_\perp^{(1++)}|^2 - |M_\perp^{(1--)}|^2) + (|E'_\perp|^2 + |\cos \vartheta'|^2 |E'_\parallel|^2) (|M_\parallel^{(5+-)}|^2 - |M_\parallel^{(5-+)}|^2) - 2 \operatorname{Im}(\cos \vartheta' E'_\parallel E'_\perp^*) (|M_\parallel^{(5+-)}|^2 + |M_\parallel^{(5-+)}|^2)], \quad (4)$$

where the dipole matrix elements  $M^{(iss')}$  are defined as in Ref. 2. We recall that  $i = 1, 5$  indicates the spatial symmetry  $\Delta^i$  of the relevant initial state part. The labels *s* and *s'* distinguish two pairs of initial and final states, respectively, with the partners in each pair belonging to the one-dimensional irreducible representations  $\Delta_6^+$  and  $\Delta_6^-$ , the basis functions of which are connected by the time-reversal operation. If the magnetization is reversed,  $M^{(iss')}$  in the above expressions is replaced by  $M^{(i,-s,-s')}$ . The spin polarization components  $P_{6x}$  and  $P_{6y}$  are also nonzero. Since for the present case of perpendicular magnetization they are not related to magnetic dichroism, their rather lengthy expressions are not shown here.

In the intensity expression, Eq. (3), reversal of the magnetization leaves the first two terms unchanged and reverses the sign of the third term. Magnetic dichroism therefore occurs if  $\operatorname{Im}(\cos \vartheta' E'_\parallel E'_\perp^*)$  is nonzero. This first requires that both components of  $\vec{E}'$  be nonzero. Here *p*-polarized light ( $E'_\perp = 0$ ) and *s*-polarized light ( $E'_\parallel = 0$ ) therefore produce no MD. If both components  $E_\parallel$  and  $E_\perp$  of the external field are nonzero,  $\operatorname{Im}(\cos \vartheta' E'_\parallel E'_\perp^*)$  is generally nonzero due to the dielectric constant, as can be seen from Eq. (2). In particular, linearly polarized light with  $\vec{E}$  rotated by a general angle out of the incidence plane (*sp*-polarized light) thus produces MD. If the optical response is ignored, i.e.,  $\epsilon = 1$ ,  $\cos \vartheta' = \cos \vartheta$  is real and the internal field components equal

the external ones  $E_{\parallel}$  and  $E_{\perp}$ . A phase shift between the latter is therefore required to obtain MD. This is especially the case for circular polarized light (with phase shift of  $\pm i$ ), but not for  $sp$ -polarized light.

The expression for  $P_{6z}$ , Eq. (4), is similar in structure to the intensity expression, but in each of the three additive terms the sign in front of the second matrix element is reversed. The first and second terms change sign upon magnetization reversal, whereas the third one does not. We thus have a decomposition of  $P_{6z}$  into an exchange-related and a spin-orbit-related part. Note that the latter contains the same factor  $\text{Im}(\cos\vartheta' E_{\parallel}' E_{\perp}'^*)$  as the third term in the intensity, which gives rise to MD. This explicitly shows the intimate connection between spin-orbit-induced photoelectron spin polarization and MD. In the limit of vanishing magnetization, we have  $M^{(iss')} = M^{(i,-s,-s')}$ . The MD-producing term in Eq. (3) then vanishes, as it should, but  $P_{6z}$  is nonzero if the imaginary part factor is nonzero. The above is in accordance with our general criterion for the existence of MD (cf. Refs. 1 and 2): If in the nonmagnetic limit SOC produces a component of  $\vec{P}$  in the direction of the magnetization, then there is MD.

For the pair of initial states with  $\Delta_7^{\pm}$  symmetry, the expressions for  $I_7$  and  $P_{7z}$  are obtained from those in Eqs. (3) and (4) by dropping the term involving the factor  $\sin\vartheta'$  and reversing the sign of the  $\text{Im}(\dots)$  term.  $P_{7x}$  and  $P_{7y}$  are identically zero. The above statements on MD for  $\Delta_6^{\pm}$  initial states remain valid. In the nonmagnetic limit,  $P_{6z}$  and  $P_{7z}$  have opposite sign, as it should for ‘‘optical orientation’’ (cf., e.g., Ref. 6).

Without performing a complete photoemission calculation, one can obtain qualitative and semiquantitative information on MD in the Fresnel-field approximation by evaluating the relevant term  $\text{Im}(\cos\vartheta' E_{\parallel}' E_{\perp}'^*)$  in Eq. (3). In Fig. 1 we show its dependence on the polar angle of incidence  $\vartheta$  for some typical vacuum ultraviolet (vuv) photon energies, with the dielectric function values of Ni taken from Ref. 7. At  $\vartheta=0^\circ$ , for circular polarized light this term and hence the MD is maximal, but there is no MD for  $sp$ -polarized light because there is no phase shift between  $E_{\parallel}'$  and  $E_{\perp}'$  and  $\cos\vartheta' = -1$  [cf. Eqs. (1) and (2)]. At grazing incidence, the MD term vanishes for any incident light polarization, since the light does not penetrate into the solid ( $E_{\parallel}' = E_{\perp}' = 0$ ). MD with  $sp$ -polarized light is sizable in the polar angle range from about  $35^\circ$  to about  $75^\circ$ . At  $\vartheta=45^\circ$  it is by a factor of about 3 smaller than for circular polarized light. For certain photon energies and polar angles, however, the MD with

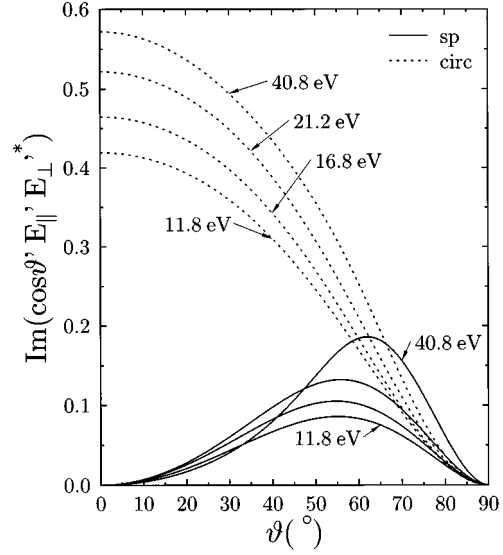


FIG. 1. Dependence of  $\text{Im}(\cos\vartheta' E_{\parallel}' E_{\perp}'^*)$  [cf. Eq. (3)] on the polar angle of incidence  $\vartheta$  of  $sp$ -polarized (solid) and circularly polarized (dotted) light with photon energies 11.8 eV, 16.8 eV, 21.2 eV, and 40.8 eV.

$sp$  polarized light may exceed the one with circular polarized light (cf., for example,  $\hbar\omega = 40.8$  eV and  $\vartheta > 67^\circ$ ).

### C. Results for in-plane magnetization

The rotational symmetry of the lattice about the surface normal is now broken. Taking  $\vec{M}$  along the  $x$  axis, there is one symmetry operation: reflection at the  $(y,z)$  plane. Electronic states can be classified with respect to two one-dimensional representations (for details see Ref. 2). In the mainly used standard geometry,  $p$ -polarized or unpolarized light is incident in the  $(y,z)$  plane, i.e., normal to  $\vec{M}$ . As has been shown in detail in Ref. 2 in the external-field approximation, there is a spin-orbit-induced spin polarization component along  $\vec{M}$  and consequently MD. Since this effect is produced by  $E_{\perp}$  alone, it persists, with some modification in size, for general light polarization and in the presence of optical response.

If, however,  $\vec{M}$  is parallel to the incidence plane, i.e., the  $(x,z)$  plane in our notation, the role of the light polarization is more crucial. Analytical calculations lead to the (spin-averaged) photoemission intensity

$$\begin{aligned}
I = & (|E_{\perp}'|^2 + |\sin\vartheta'|^2 |E_{\parallel}'|^2) (|M_{\perp}^{(1++)}|^2 + |M_{\perp}^{(1--)}|^2) + |\cos\vartheta'|^2 |E_{\parallel}'|^2 (|M_{\parallel}^{(2+-)}|^2 + |M_{\parallel}^{(2-+)}|^2) \\
& - 2 \text{Re}(\sin\vartheta' E_{\parallel}' E_{\perp}'^*) [\text{Im}(M_{\perp}^{(1++)} M_{\parallel}^{(1++)*}) - \text{Im}(M_{\perp}^{(1--)} M_{\parallel}^{(1--)*})] \\
& - 2 \text{Im}(\sin\vartheta' E_{\parallel}' E_{\perp}'^*) [\text{Re}(M_{\perp}^{(1++)} M_{\parallel}^{(1++)*}) - \text{Re}(M_{\perp}^{(1--)} M_{\parallel}^{(1--)*})].
\end{aligned} \tag{5}$$

The spin polarization component collinear with  $\vec{M}$  reads

$$\begin{aligned}
P_x = \frac{1}{7} & \{ (|E'_\perp|^2 + |\sin\vartheta'|^2 |E'_\parallel|^2) (|M_\perp^{(1++)}|^2 - |M_\perp^{(1--)}|^2) + |\cos\vartheta'|^2 |E'_\parallel|^2 (|M_\parallel^{(2+-)}|^2 - |M_\parallel^{(2-+)}|^2) \\
& - 2 \operatorname{Re}(\sin\vartheta' E'_\parallel E'_\perp^*) [\operatorname{Im}(M_\perp^{(1++)} M_\parallel^{(1++)*}) + \operatorname{Im}(M_\perp^{(1--)} M_\parallel^{(1--)*})] \\
& - 2 \operatorname{Im}(\sin\vartheta' E'_\parallel E'_\perp^*) [\operatorname{Re}(M_\perp^{(1++)} M_\parallel^{(1++)*}) + \operatorname{Re}(M_\perp^{(1--)} M_\parallel^{(1--)*})] \}. \tag{6}
\end{aligned}$$

These expressions are similar in structure to the above ones for perpendicular  $\vec{M}$  and can be discussed in an analogous manner. Most importantly, a SOC-induced  $P_x$  component and MD occur if  $\sin\vartheta' E'_\parallel E'_\perp^*$  is nonzero. As for perpendicular magnetization, both components of the electric field vector have therefore to be nonzero.  $p$ -polarized light ( $E'_\perp = 0$ ) and  $s$ -polarized light ( $E'_\parallel = 0$ ) produce no MD. The last two terms in Eq. (6) reveal a close connection between the MD's for  $sp$ -polarized and for circular polarized light. Since for complex  $z$  we have  $\operatorname{Re}(iz) = -\operatorname{Im}(z)$  and  $\operatorname{Im}(iz) = \operatorname{Re}(z)$ , a change of the phase of the incident light by  $i$  (e.g., turning  $sp$ -polarized into circular polarized light) interchanges the prefactors  $\operatorname{Re}(\sin\vartheta' E'_\parallel E'_\perp^*)$  and  $\operatorname{Im}(\sin\vartheta' E'_\parallel E'_\perp^*)$ .

These prefactors are shown in Fig. 2 as a function of the external incidence angle  $\vartheta$  for the special case of  $sp$ -polarized light for several photon energies and the dielectric function values of Ni. The imaginary parts are seen to be by far smaller than the real parts. This indicates that the main contribution to the MD should be produced by the terms involving  $\operatorname{Im}(M_\perp^{(1\pm\pm)} M_\parallel^{(1\pm\pm)*})$ . Consequently, for circular polarized light, the main contribution should come from the terms  $\operatorname{Re}(M_\perp^{(1\pm\pm)} M_\parallel^{(1\pm\pm)*})$ . In contrast to the above finding for perpendicular  $\vec{M}$ , the MD spectra for  $sp$ -polarized and circularly polarized light can therefore be expected to differ significantly from each other in shape (rather than only by a scaling factor).

In the nonmagnetic limit, the intensity expression (5) is

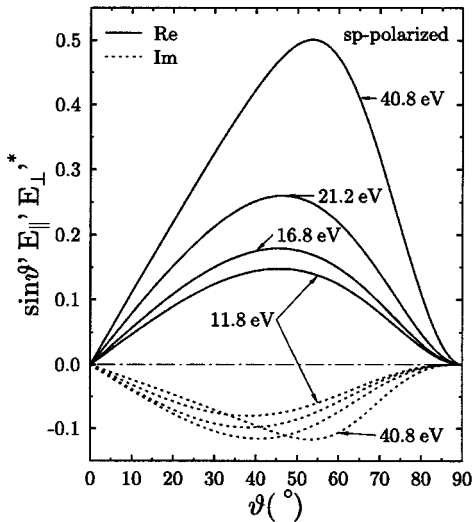


FIG. 2. Dependence of the real (dotted curves) and imaginary (solid curves) parts of  $\sin\vartheta' E'_\parallel E'_\perp^*$  [cf. Eq. (5)] on the polar angle of incidence  $\vartheta$  of  $sp$ -polarized light with photon energies 11.8 eV, 16.8 eV, 21.2 eV, and 40.8 eV.

reduced to the first two terms, and  $P_x$  consists only of the two terms involving  $\sin\vartheta' E'_\parallel E'_\perp^*$  which indicate ‘‘optical orientation.’’ We would like to emphasize that  $P_x$  is nonzero not only for circularly, but also for  $sp$ -polarized light, even in the absence of optical response.

### III. NUMERICAL RESULTS FOR fct Ni(001)

In order to illustrate the above in a quantitative way, we have performed numerical calculations using a relativistic one-step model Green function formalism of photoemission.<sup>8</sup> Since MCD with normally incident circular polarized light and perpendicular magnetization has recently been studied experimentally and theoretically for a 15 monolayer (ML) Ni film on Cu(001),<sup>3</sup> we chose the same system for the present purpose.

As reported in Ref. 3, an appropriate model for the geometrical structure of the Ni film is a tetragonal distorted fcc lattice (fct) with the in-plane lattice constant of bulk Cu, namely, 2.55 Å (compared to 2.49 Å for bulk Ni). Since experimentally no emission from the Cu substrate was found, it is adequate to use for the calculations a semi-infinite Ni crystal (with the above fct structure) instead of a 15-layer Ni slab on top of the Cu substrate. For the effective quasiparticle potential (in the muffin-tin shape approximation) we take the same as in Ref. 3. We recall that an *ad hoc* spin-dependent self-energy correction is employed to reduce the splitting between the majority- and the minority-spin potentials from the self-consistently calculated value of about 0.6 eV to an average value of 0.3 eV as observed in photoemission experiments.

As a basis for interpreting calculated normal photoemission spectra, we show in Fig. 3 the relativistic bulk band structure of perpendicular magnetized fct Ni(001) along  $\Gamma$ - $\Delta$ - $X$ , with the majority and minority character of the spin expectation value along the bands indicated by thick and thin lines, respectively. For normally incident circularly polarized 21.22 eV light, the spin-averaged spectra for  $+\vec{M}$  and  $-\vec{M}$  are almost identical to those obtained for 21.1 eV photon energy in Ref. 3, where a detailed interpretation of the peaks in terms of direct interband transitions has been given. As a particularly interesting finding we recall that peaks *b* and *c* in the  $+\vec{M}$  spectrum reflect a spin-orbit-induced gap in the initial state band structure near  $-0.5$  eV, with the two relativistic  $\Delta_7$  bands changing from majority to minority spin. Since in the  $-\vec{M}$  spectrum these two peaks are absent and a new peak (*d*) occurs, there is a pronounced MD in this energy range [see Fig. 3(c)]. For circularly polarized 21.22 eV light incident at  $\vartheta = 45^\circ$  in the  $(x, z)$  plane, the corresponding spectra—obtained in the external-field approximation—are seen to exhibit, with somewhat reduced intensity, the

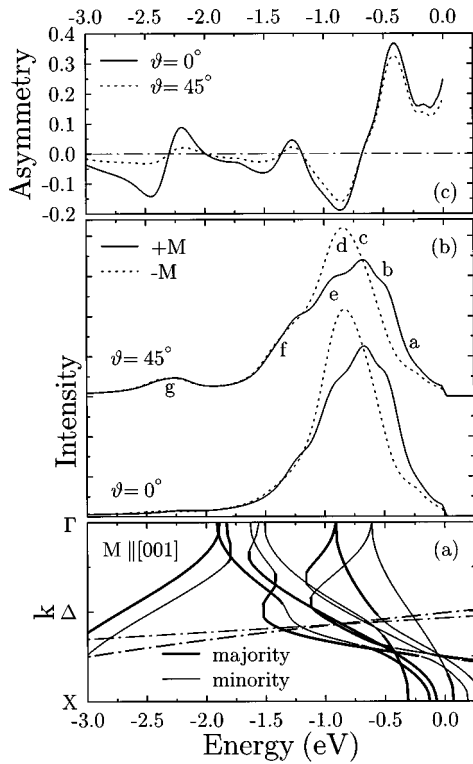


FIG. 3. (a) Fully relativistic bulk band structure of fct Ni along the  $\Delta$  axis with magnetization along the same axis ([001]), calculated with a real effective potential. Bands with majority (minority) spin expectation value are shown as thick (thin) solid lines. Final state bands with mainly  $\Delta^1$  spatial symmetry, shifted downwards by photon energy 21.22 eV, are shown as a dash-dotted line. (b) Spin-integrated normal photoemission spectra from fct Ni with magnetization vector  $\vec{M}$  along the surface normal (solid lines) and with  $-\vec{M}$  (dashed lines), produced by circularly polarized 21.22 eV light incident in the  $(x,z)$  plane at polar angles  $\vartheta=0^\circ$  and  $\vartheta=45^\circ$  as indicated. In the calculations the above potential was augmented by a uniform imaginary part describing the finite hole lifetime, and the internal radiation field was approximated by the external field. (c) Asymmetries  $[I(+\vec{M}) - I(-\vec{M})]/[I(+\vec{M}) + I(-\vec{M})]$  corresponding to the two pairs of spectra in panel (b), i.e., MD.

same peaks. In addition, there is a small peak (g) due to a transition from a mainly  $\Delta^1$  initial state by the  $z$  component of the electric field.

In Fig. 4 we show the influence of changing to linearly polarized light and of including the optical response in the Fresnel approximation. For circularly polarized light, the optical response is seen to hardly affect the intensity spectra. Consequently, asymmetry and  $P$  spectra are also almost identical. The spin polarization component  $P_z$  in the magnetization direction clearly reflects the majority- and minority-spin character of the initial states. However, there is a substantial difference between  $P_z(\vec{M})$  and  $P_z(-\vec{M})$ , which is due to SOC. We recall that SOC by itself (in the nonmagnetic limit) already produces a finite  $P_z$ . For linearly  $sp$ -polarized light in the external-field approximation, the intensity spectra for  $+\vec{M}$  and  $-\vec{M}$  coincide; i.e., there is no MD asymmetry, in accordance with our above analytical results. In the Fresnel approximation, however, there appears a substantial MD. As is seen in panel (b) of Fig. 4, the

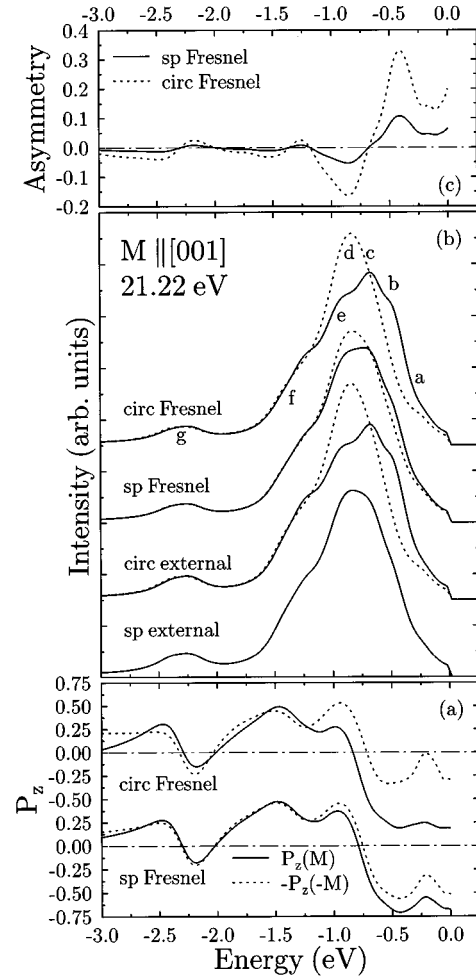


FIG. 4. Normal photoemission from perpendicularly magnetized fct Ni(001) by  $sp$ -polarized and circularly polarized 21.22 eV light incident at polar angle  $\vartheta=45^\circ$  in the  $(x,z)$  plane. (a) Spin polarization components  $P_z(\vec{M})$  and  $-P_z(-\vec{M})$  normal to the surface in the Fresnel approximation. (b) Spin-averaged intensity spectra for  $+\vec{M}$  (solid curves) and  $-\vec{M}$  (dotted curves) with the internal radiation field approximated by the external field and by the Fresnel field as indicated next to the curves. (c) Corresponding asymmetry  $[I(+\vec{M}) - I(-\vec{M})]/[I(+\vec{M}) + I(-\vec{M})]$ , i.e., MD.

$I(+\vec{M})$  and  $I(-\vec{M})$  spectra exhibit the same peaks as those for circularly polarized light, although somewhat less pronounced. This similarity manifests itself more clearly in the asymmetry spectra [panel (c) of Fig. 4]. In fact, the  $sp$ -light spectrum has the same shape as the circular-light spectrum and is simply reduced by a factor of 3. This is readily understood from Eq. (3): the last term, which is responsible for MD, consists of a matrix element part, which determines the spectral shape, and the light-dependent part  $\text{Im}(\cos \vartheta' E_{\parallel}^{\prime} E_{\perp}^{\prime *})$ . As we already found in Fig. 1, the latter is, for  $\vartheta=45^\circ$ , reduced by a factor of 3 for  $sp$ -polarized light compared to circularly polarized light. The above similarity implies that  $sp$ -polarized light is capable of yielding the same physical information as circularly polarized light.

To demonstrate typical effects for systems with in-plane magnetization, we have chosen the same fct Ni(001) as above, but with  $\vec{M}$  in the surface plane along the  $x$  axis.<sup>9</sup> We can thus compare directly with the above perpendicular-

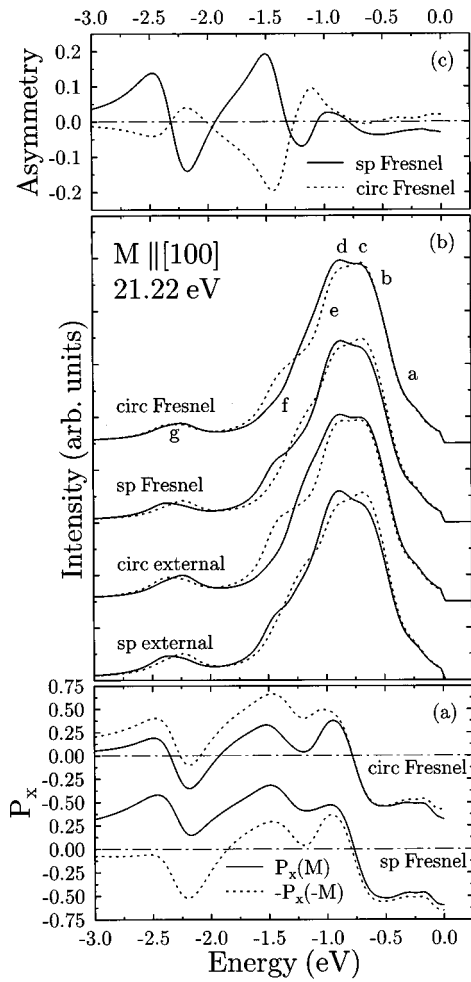


FIG. 5. As in Fig. 4, but with magnetization parallel to the surface (along [100], the  $x$  axis) and with  $P_x$  (instead of  $P_z$ ) in panel (a).

magnetization results. Differences to actually existing in-plane-magnetized fct films or fcc Ni(001) are rather minor. The spin-averaged photoemission intensity spectra in panel (b) of Fig. 5 are seen to be broadly similar to those for perpendicular  $\vec{M}$  in Fig. 4, but there are significant differences. Most notably,  $sp$ -polarized light produces MD already in the external-field approximation, with fairly little modification by the optical response. The latter also holds for circularly polarized light. In contrast to the perpendicular  $\vec{M}$  case, the asymmetry spectra for  $sp$ -polarized and circularly polarized light [panel (c) of Fig. 4] are now essentially different from each other, as has already been anticipated from our analytical result, Eq. (5).

Spectra from analogous calculations for different photon

energies (11.8 eV and 16.8 eV), while of course different in shape, exhibit the same relations between the various light polarization cases. In particular, the influence of the optical response is very similar, which is plausible from the values of the dielectric function:  $0.62+1.52i$ ,  $0.51+1.27i$ , and  $0.60+0.84i$  for  $h\nu=11.8$  eV, 16.8 eV, and 21.2 eV, respectively.

#### IV. CONCLUSION

Our analytical and numerical study of valence-band photoemission normal to a ferromagnetic surface demonstrates that—for light in a general state of polarization incident in a general direction—magnetic dichroism and spin polarization of the photocurrent can be strongly affected by the optical response of the solid. In particular, *linearly* polarized light with the electric-field vector rotated out of the incidence plane thus leads—via a circularly polarized field part inside the solid—to a substantial MD, the spectral shape of which is the same as in the case of *circular* polarization of the incident light. In addition to its intrinsic interest, this finding has a practical implication: Measurements, which are traditionally performed using the circularly polarized light of a synchrotron facility, can now (for selected photon energies) equivalently be carried out in the local laboratory using linearly polarized light.

For surfaces other than (001), our findings for  $sp$ -polarized light and the influence of optical response essentially remain valid, but there are some modifications, which are associated with special spin-orbit-induced spin polarization effects. For example, at twofold rotation symmetry surfaces [like cubic (110)] with perpendicular magnetization,  $s$ -polarized light can already produce MD. For  $sp$ -polarized light, this MD combines with the one found in the present work.

We recall that we have approximated the internal radiation field by the classical Fresnel field with the additional simplification of replacing the dielectric tensor by a scalar, thus neglecting magneto-optic effects. Further calculations, in which the optical response was treated in the hydrodynamic model (cf. Ref. 10) (i.e., with an additional longitudinal electric field component inside the crystal), produced, however, only very minor changes in our results at vuv photon energies, which are well above the plasmon energies of metals. The extent to which magneto-optic effects might modify our results still remains to be investigated.

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