Magnetic dichroism and electron spin polarization in photoemission: analytical results

1996 J. Phys.: Condens. Matter 8 47

(http://iopscience.iop.org/0953-8984/8/1/007)

J. Phys.: Condens. Matter **8** (1996) 47–65. Printed in the UK

Magnetic dichroism and electron spin polarization in photoemission: analytical results

J Henk, T Scheunemann, S V Halilov and R Feder
Theoretische Festkörperphysik, Universität Duisburg, D-47048 Duisburg, Germany

Received 21 June 1995, in final form 26 October 1995

Abstract. For cubic (001), (110) and (111) surface systems with in-plane or perpendicular magnetization, valence-band photoemission along the surface normal is studied analytically by evaluating electric dipole transition matrix elements between half-space initial and final states of the appropriate double-group symmetry. Explicit expressions are obtained for the spin-polarization vector of the photoelectrons, and the spin-averaged intensity and its change upon reversal of the magnetization direction, i.e. magnetic dichroism, for circularly and linearly polarized incident light. These results firstly elucidate the origin of spin polarization and dichroism in terms of an interplay between spin–orbit coupling and exchange, and secondly provide a systematic overview of possible effects. In particular, we predict new types of magnetic linear dichroism for s-polarized light in the case of magnetization perpendicular to surfaces with a twofold rotation axis and in the case of in-plane magnetization of fcc (111) or hcp (0001) surfaces.

1. Introduction

Spin-resolved photoemission is well established as a powerful tool for studying magnetic properties of surfaces and ultrathin films (see, e.g., monographs by Feder (1985) and Kevan (1992), recent original articles by Hartmann *et al* (1993a, b), Carbone *et al* (1993), Rader *et al* (1994), Smith *et al* (1994), Wu *et al* (1994), and references therein). The traditional analysis of the photoelectron spin-polarization component along the magnetization direction has recently been complemented by asymmetries in the spin-averaged photocurrent produced by circularly or linearly polarized radiation upon reversal of the magnetization. This so-called magnetic circular dichroism (MCD) and linear dichroism (MLD) in photoemission was first experimentally observed from core levels (Baumgarten *et al* 1990, Roth *et al* 1993a, b). Its potential relevance for magnetic storage technology was recently highlighted by the successful element-specific imaging of magnetic domains (Schneider *et al* 1994). There is also experimental evidence of MCD and MLD in valence-band photoemission (Schneider *et al* 1991a, b, Bansmann *et al* 1992, Rose *et al* 1994). A systematic overview and classification of the rather wide variety of magnetic dichroism effects have been provided by Venus (1993, 1994) (see also Venus *et al* 1993). On the theoretical side, there have been a series of many-body-type studies (see Thole and van der Laan (1994) and references therein), which are however in practice restricted to an atomic approximation not quantitatively valid for crystalline systems. Quantitative explanations of MCD and MLD in photoemission from core levels have been obtained by means of relativistic multiple-scattering formalisms, treating the final state as bulk-like (Ebert *et al* 1991) and as a time-reversed LEED state

0953-8984/96/010047+19$19.50

(Tamura *et al* 1994). As regards valence-band photoemission, a relativistic multiple-scattering formalism (Halilov *et al* 1993) has recently been applied to Ni(001), yielding prototype numerical results on MCD for magnetization normal to the surface (Scheunemann *et al* 1994) and on two types of MLD due to s-polarized and p-polarized light in the case of in-plane magnetization (Henk *et al* 1994). While this type of numerical calculation is indispensable for a detailed quantitative analysis of experimental results, more information on general features and insight into the underlying physical mechanisms might be gained by analytical calculations.

In this paper, we therefore present an analytical study of spin-polarization and magnetic dichroic effects in valence-band photoemission. For the sake of transparency, we focus on highly symmetric set-ups: normal emission, i.e. with $\boldsymbol{k}_{\|} = 0$, from low-index surfaces with a perpendicular fourfold, threefold or twofold rotational axis. In line with experimental reality, the magnetization is assumed normal to the surface or parallel to it along a high-symmetry direction. Within a relativistic single-particle framework, we calculate the photoelectron spin-density matrix by evaluating electric dipole transition matrix elements produced by s-, p- and circularly polarized radiation between initial and final half-space states, which are constructed from symmetry-adapted basis functions. From this density matrix, we obtain explicit expressions for the photoelectron spin-polarization vector, the spin-averaged intensity and its asymmetry upon magnetization reversal, i.e. magnetic dichroism. Firstly, we thus derive general relations, which are valid both in valence-band and in core-level photoemission. Apart from their fundamental interest, they might be useful in checking the reliability of experimental and of numerically calculated spectra. Secondly, the origin of the components of the electron spin-polarization (ESP) vector is elucidated by explicitly expressing them in terms of spin–orbit- and exchange-derived contributions. The occurrence of the two contributions in a component is generally associated with magnetic dichroism. Comparison of our results for ferromagnetic surface systems with their nonmagnetic limit reveals an intimate connection between MLD and spin-polarization effects, which are produced by linearly polarized light from nonmagnetic surfaces due to SOC. If such a 'linear spin-polarization effect' (LSPE) involves an ESP component parallel to the magnetization, MLD is found. The situation is analogous in the case of MCD, where the purely spin–orbit-induced ESP component is due to optical orientation (Fano effect) by circularly polarized light. We thus reach a unified understanding of both MCD and MLD.

This paper is organized as follows. In section 2 we give some basic properties of relativistic electronic states in connection with photoemission. In section 3 we present analytical results for normal photoemission from systems with magnetization normal to the surface, before turning to the case of in-plane magnetization in section 4. In section 5 we discuss the connection between magnetic dichroism and spin-polarization effects. Some concluding remarks are made in section 6.

2. Symmetry-adapted electronic states and photoemission

The general framework of a fully relativistic one-step theory of photoemission from semi-infinite crystalline systems, which incorporates both spin–orbit coupling and a ferromagnetic ground state, and simpler spin-dependent approximations have been presented in chapter 4.5 in a monograph by Feder (1985). It may therefore suffice here to briefly specify the approach used in the present work. Whilst a relativistic Green function formulation, like the one worked out in detail by Halilov *et al* (1993), should be employed in numerical calculations aiming at a quantitative comparison with experimental spectra, analytical expressions are more transparent and instructive if one firstly replaces the initial-state Green function by its spectral representation in terms of states $|i\rangle$ (solutions of the Dirac equation without an imaginary potential part), and secondly approximates the initial- and final-state four-component spinors with two-component spinors $|i_s\rangle$ and $|f_s\rangle$, with $s = \pm$, which are eigenfunctions of a Pauli-like Hamiltonian retaining of course spin–orbit coupling (see, e.g., Feder (1985), p 131). One thus obtains a golden rule form for the spin-density matrix of the photocurrent with elements

$$\varrho_{ss'}(E_f) = \sum_{i,s''} \langle f_s|H'|i_{s''}\rangle\langle i_{s''}|H'|f_{s'}\rangle \; \delta(E_f - \hbar\omega - E_{i_{s''}}). \tag{1}$$

The final states $|f_+\rangle$ and $|f_-\rangle$ both have the energy E_f, and only initial states with energy $E_f - \hbar\omega$ contribute. As a consequence of lattice periodicity parallel to the surface, all states have the same surface-parallel wave vector $\boldsymbol{k}_\parallel$. The photon–electron interaction H' is $\boldsymbol{E}\cdot\boldsymbol{r}$ with a spatially constant electric field vector $\boldsymbol{E}$ of the incident light, i.e. we adopt the electric dipole approximation, which is adequate for valence-band photoemission by radiation in the vacuum–ultraviolet regime. With a view to explicitly evaluating equation (1) for highly symmetrical set-ups, we now introduce symmetry-adapted forms of the initial and final states.

Consider two sets of basis functions, $\{|g_n^+\rangle\}$ and $\{|g_n^-\rangle\}$—consisting of an angular part and a Pauli spinor (Rose 1961)—of an extra irreducible representation of the double group associated with some point group, which transform under time reversal $\widetilde{T}$ as $\widetilde{T}|g_n^+\rangle = |g_n^-\rangle$ and $\widetilde{T}|g_n^-\rangle = -|g_n^+\rangle$. The basis function sets are not unique, but the results presented below do not depend on the particular choice. Electronic eigenstates of the Pauli Hamiltonian of a *nonmagnetic* semi-infinite system can be expressed as $|\Psi_s\rangle = \sum_n \alpha_n|R_n\rangle|g_n^s\rangle$, $s = \pm$, where $|R_n\rangle$ are normalized radial functions and α_n are real coefficients. These states obviously transform under time reversal like their respective basis sets. Both have the same α_n and $|R_n\rangle$ as well as the same energy, i.e. Kramers' degeneracy. For *magnetic* systems, Kramers' degeneracy is lifted and we have

$$|\Psi_s\rangle = \sum_n \; \alpha_n^{(s)}|R_n^s\rangle|g_n^s\rangle \qquad s = \pm \tag{2}$$

with $\alpha_n^{(+)} \neq \alpha_n^{(-)}$ and $|R_n^+\rangle \neq |R_n^-\rangle$ and exchange-split energy eigenvalues. As a consequence of spin–orbit coupling, the spin-polarization expectation value $\boldsymbol{P}$ of $|\Psi_s\rangle$ generally has an absolute value less than unity and may change sign with energy. But it is still meaningful to refer to 'majority' and 'minority' states according to the direction of their $\boldsymbol{P}$.

We now use the above for further evaluating the photocurrent-density matrix ϱ. The final states $|f_s\rangle$ at energy E_f are the time-reversed LEED spinors with electron spin s (relative to some fixed direction) at the detector. They are expressed in the form of equation (2) with complex coefficients $\beta_m^{(s)}$:

$$|f_s\rangle = \sum_m \beta_m^{(s)}|\tilde{R}_m^s\rangle|g_m^s\rangle \qquad s = \pm. \tag{3}$$

As is evident from group theory, the set of conceivable initial states (with energy $E_f - \hbar\omega$) decomposes into pairs of initial states $|i_+^r\rangle$ and $|i_-^r\rangle$, where r denotes the relevant representations (cf. Falicov and Ruvalds 1968). The total photocurrent is thence the sum of the photocurrents obtained for each pair. We note that in many practical cases only one pair or even only one of its partners actually contributes, and therefore focus on these partial photocurrents, drop the symmetry index l and express the initial states $|i_s\rangle$ as in equation (2). The dipole transition matrix elements

$$W_{ss'} = \langle f_s|\boldsymbol{E}\cdot\boldsymbol{r}|i_{s'}\rangle \qquad s, s' = \pm \tag{4}$$

then become linear combinations of matrix elements between the basis functions. The (spatially uniform) electric field vector $\boldsymbol{E}$ of the incident light is decomposed into $E_\parallel$ and $E_\perp$ parallel and normal to the plane of incidence. Defining

$$H_\perp(\varphi) = \frac{\mathrm{i}}{\sqrt{2}}\left(\exp(\mathrm{i}\varphi)Y_1^{-1} + \exp(-\mathrm{i}\varphi)Y_1^1\right) \tag{5a}$$

$$H_\parallel(\varphi) = \frac{1}{\sqrt{2}}\left(\exp(\mathrm{i}\varphi)Y_1^{-1} - \exp(-\mathrm{i}\varphi)Y_1^1\right) \tag{5b}$$

$$H_z = Y_1^0 \tag{5c}$$

where Y_l^m are the usual spherical harmonics, we obtain for the electric dipole operator

$$\boldsymbol{E}\cdot\boldsymbol{r} = \sqrt{\frac{4\pi}{3}}\,r\left(E_\parallel(-\sin\vartheta\;\; H_z + \cos\vartheta\;\; H_\parallel(\varphi)) + E_\perp H_\perp(\varphi)\right). \tag{6}$$

The polar and azimuthal angles ϑ and φ refer to the direction of light incidence. For s- and p-polarized light we have $(E_\parallel, E_\perp) = (0, E)$ and $(E, 0)$, and for left- (right-) handed circularly polarized light $(E_\parallel, E_\perp) = E(\pm\mathrm{i}, 1)/\sqrt{2}$. Equation (6) and the state expansion equations (2) and (3) are then used to evaluate the matrix elements $W_{ss'}$. The resulting expressions are employed in the photoelectron spin-density matrix

$$\varrho = \begin{pmatrix} |W_{++}|^2 + |W_{+-}|^2 & W_{++}W_{-+}^\star + W_{+-}W_{--}^\star \\ W_{++}^\star W_{-+} + W_{+-}^\star W_{--} & |W_{-+}|^2 + |W_{--}|^2 \end{pmatrix}. \tag{7}$$

The (not spin-resolved) intensity $I(\varphi, \vartheta)$ and the electron spin-polarization (ESP) vector $\boldsymbol{P}(\varphi, \vartheta)$ of the energy- and angle-resolved symmetry-specific photocurrent are then easily obtained as $I(\varphi, \vartheta) = \mathrm{tr}(\varrho)$ and $\boldsymbol{P}(\varphi, \vartheta) = \mathrm{tr}(\boldsymbol{\sigma}\varrho)/I(\varphi, \vartheta)$. Magnetic dichroism can be characterized by the (not normalized) asymmetry $A(\varphi, \vartheta) = I(\varphi, \vartheta, \boldsymbol{M}) - I(\varphi, \vartheta, -\boldsymbol{M})$, i.e. the intensity change upon magnetization reversal.

3. Results for magnetization normal to the surface

We now evaluate the above expressions for normal emission from surface systems with two-, three-, and fourfold rotational axes and with magnetization $\boldsymbol{M}$ normal to the surface. The underlying nonmagnetic point groups are $2mm$, $3m$, and $4mm$, i.e. C_{2v}, C_{3v}, and C_{4v} in the Schönflies notation. Taking into account $\boldsymbol{M}$, the surface normal remains an n-fold rotation axis, but the mirror operations m are no longer symmetry operations, since they reverse $\boldsymbol{M}$. We thus have a *reduction of symmetry* with respect to the nonmagnetic case. Instead of applying magnetic double-group theory (Falicov and Ruvalds 1968, Ruvalds and Falicov 1968), we adopt a more transparent approach, which facilitates contact with the nonmagnetic case and reveals easily the roles played by the spin–orbit and by the exchange interaction in producing the photoelectron spin-polarization vector and magnetic dichroism. The essential idea is to express initial and final states in terms of the basis functions of the irreducible representations of the *nonmagnetic double groups*, but with Kramers' degeneracy lifted. We then use these forms to evaluate the dipole transition matrix elements $W_{ss'}$ (cf. equation (4)). Details of this approach are given in the case of twofold rotation symmetry, to which we now turn.

3.1. The twofold rotational axis

Spin–orbit coupling mixes the four one-dimensional representations $\Sigma^1, \ldots, \Sigma^4$ of the single group $2mm$ into one representation Σ_5 of the corresponding double group (see, for example, Inui *et al* 1990). Initial and final states can then be written in the form

$$|\Psi_s\rangle = c_1^{(s)}|\Sigma_5^{1s}\rangle|s\rangle + c_2^{(s)}|\Sigma_5^{2s}\rangle|s\rangle + c_3^{(s)}|\Sigma_5^{3s}\rangle|-s\rangle + c_4^{(s)}|\Sigma_5^{4s}\rangle|-s\rangle. \tag{8}$$

The $|s\rangle$ are the Pauli spinors (aligned with respect to $\boldsymbol{M}$) and the $|\Sigma_5^{is}\rangle$ (with $i = 1, \ldots, 4$) are normalized spatial parts of the single-group symmetry Σ^i; the weight coefficients $c_n^{(s)}$ directly reflect the spin–orbit coupling. The upper index $s = \pm$ is needed because of the absence of Kramers' degeneracy due to the exchange interaction. Without magnetization, $|\Sigma_5^{n+}\rangle = |\Sigma_5^{n-}\rangle$. Dipole matrix elements between states of the form of equation (8) are easily evaluated, since the dipole operator does not affect the Pauli spinors and couples the spatial parts according to the usual nonrelativistic dipole selection rules. As the final states have pure Σ_5^1 spatial symmetry outside the crystal and still predominantly so inside, we approximate them in the following as $|f_s\rangle = |\Sigma_5^{1s}\rangle|s\rangle$, i.e. we neglect SOC in the final state. The nonvanishing partial matrix elements involving final-state spatial parts Σ_5^{1s} and initial-state parts $\Sigma_5^{is'}$ are denoted by $M^{iss'}$. The dipole matrix elements then become

$$W_{++} = -\sin\vartheta\ E_\parallel M_\perp^{(1++)} \tag{9a}$$

$$\begin{aligned} W_{+-} = E_\perp &\left\{-\sin\varphi\ M_\parallel^{(3+-)} + \mathrm{i}\cos\varphi\ M_\parallel^{(4+-)}\right\} \\ &+E_\parallel \cos\vartheta \left\{\cos\varphi\ M_\parallel^{(3+-)} + \mathrm{i}\sin\varphi\ M_\parallel^{(4+-)}\right\} \end{aligned} \tag{9b}$$

$$\begin{aligned} W_{-+} = E_\perp &\left\{\sin\varphi\ M_\parallel^{(3-+)} + \mathrm{i}\cos\varphi\ M_\parallel^{(4-+)}\right\} \\ &+E_\parallel \cos\vartheta \left\{-\cos\varphi\ M_\parallel^{(3-+)} + \mathrm{i}\sin\varphi\ M_\parallel^{(4-+)}\right\} \end{aligned} \tag{9c}$$

$$W_{--} = -\sin\vartheta\ E_\parallel M_\perp^{(1--)}. \tag{9d}$$

The corresponding results for a nonmagnetic system are easily recovered from the above by noting that for vanishing exchange splitting $M^{i+-} = M^{i-+} = M^i$.

For *s-polarized light*, i.e. $E_\perp = E$ and $E_\parallel = 0$, we obtain upon substitution of equation (8) into equation (7)

$$\begin{aligned} I(\varphi) = \sin^2\varphi &\left(|M_\parallel^{(3+-)}|^2 + |M_\parallel^{(3-+)}|^2\right) + \cos^2\varphi \left(|M_\parallel^{(4+-)}|^2 + |M_\parallel^{(4-+)}|^2\right) \\ &+ \sin 2\varphi \left(\mathrm{Im}(M_\parallel^{(3-+)} M_\parallel^{(4-+)\star}) - \mathrm{Im}(M_\parallel^{(3+-)} M_\parallel^{(4+-)\star})\right) \end{aligned} \tag{10}$$

and

$$\begin{aligned} P_z(\varphi) = \Big\{\sin^2\varphi &\left(|M_\parallel^{(3+-)}|^2 - |M_\parallel^{(3-+)}|^2\right) + \cos^2\varphi \left(|M_\parallel^{(4+-)}|^2 - |M_\parallel^{(4-+)}|^2\right) \\ &- \sin 2\varphi \left(\mathrm{Im}(M_\parallel^{(3-+)} M_\parallel^{(4-+)\star}) + \mathrm{Im}(M_\parallel^{(3+-)} M_\parallel^{(4+-)\star})\right)\Big\} \Big/ I(\varphi). \end{aligned} \tag{11}$$

The surface-parallel spin-polarization components P_x and P_y are zero. Since reversal of the magnetization interchanges $M_\parallel^{(i+-)}$ with $M_\parallel^{(i-+)}$, the asymmetry, which constitutes the MLD, is obtained from equation (10) as

$$A(\varphi) = 2\sin 2\varphi \left(\mathrm{Im}(M_\parallel^{(3-+)} M_\parallel^{(4-+)\star}) - \mathrm{Im}(M_\parallel^{(3+-)} M_\parallel^{(4+-)\star})\right). \tag{12}$$

This expression directly reveals spin–orbit coupling as the physical origin of this type of MLD: the products $M_\parallel^{(3-+)} M_\parallel^{(4-+)\star}$ arise from the simultaneous presence of symmetry types Σ_5^3 and Σ_5^4 in the initial state, equation (8), which is brought about by SOC. In the nonmagnetic limit, $A(\varphi)$ is seen to be identically zero, as it should be. Also, there is no

MLD if the electric field vector lies in a mirror plane ($\varphi = 0$ or $\pi/2$). The spin–orbit-induced product terms also occur in the above expression for P_z in addition to the first two terms, which are due to exchange interaction. If $\boldsymbol{M}$ equals zero, this expression becomes

$$P_z(\varphi) = 2\sin 2\varphi \; \mathrm{Im}(M_\parallel^{(3)} M_\parallel^{(4)\star}) \Big/ I(\varphi) \tag{13}$$

i.e. the 'linear spin-polarization effect' predicted by Henk and Feder (1994) for $2mm$-symmetry nonmagnetic surfaces.

Our above analytical expressions are in line with what follows from general symmetry arguments. The reflection operations m_1 and m_2 at the (x, z)- and (y, z)-plane do not leave the total set-up invariant, but their combination $m_1 m_2$ does. The latter dictates that P_x and P_y are zero, since it reverses their signs, but does not impose any restriction on P_z. Reflection m_1 implies the relations $I(\varphi, \boldsymbol{M}) = I(-\varphi, -\boldsymbol{M})$ and $P_z(\varphi, \boldsymbol{M}) = -P_z(-\varphi, -\boldsymbol{M})$, which can also be seen directly from our above formulae.

For off-normally incident *p-polarized light*, we obtain for the intensity

$$\begin{aligned} I(\vartheta, \varphi) = {} & \sin^2\vartheta \left(|M_\perp^{(1++)}|^2 + |M_\perp^{(1--)}|^2 \right) + \cos^2\vartheta \cos^2\varphi \left(|M_\parallel^{(3+-)}|^2 + |M_\parallel^{(3-+)}|^2 \right) \\ & + \cos^2\vartheta \sin^2\varphi \left(|M_\parallel^{(4+-)}|^2 + |M_\parallel^{(4-+)}|^2 \right) \\ & + \cos^2\vartheta \sin 2\varphi \left(\mathrm{Im}(M_\parallel^{(3+-)} M_\parallel^{(4+-)\star}) - \mathrm{Im}(M_\parallel^{(3-+)} M_\parallel^{(4-+)\star}) \right) \end{aligned} \tag{14}$$

and three nonzero ESP components

$$\begin{aligned} P_z(\vartheta, \varphi) = {} & \frac{1}{I(\vartheta, \varphi)} \Big[\sin^2\vartheta \left(|M_\perp^{(1++)}|^2 - |M_\perp^{(1--)}|^2 \right) \\ & + \cos^2\vartheta \cos^2\varphi \left(|M_\parallel^{(3+-)}|^2 - |M_\parallel^{(3-+)}|^2 \right) \\ & + \cos^2\vartheta \sin^2\varphi \left(|M_\parallel^{(4+-)}|^2 - |M_\parallel^{(4-+)}|^2 \right) \\ & + \cos^2\vartheta \sin 2\varphi \left(\mathrm{Im}(M_\parallel^{(3+-)} M_\parallel^{(4+-)\star}) + \mathrm{Im}(M_\parallel^{(3-+)} M_\parallel^{(4-+)\star}) \right) \Big] \end{aligned} \tag{15a}$$

$$\begin{aligned} P_x(\vartheta, \varphi) = {} & \frac{\sin 2\vartheta}{I(\vartheta, \varphi)} \Big[\cos\varphi \left(\mathrm{Re}(M_\perp^{(1++)} M_\parallel^{(3-+)\star}) - \mathrm{Re}(M_\perp^{(1--)} M_\parallel^{(3+-)\star}) \right) \\ & - \sin\varphi \left(\mathrm{Im}(M_\perp^{(1++)} M_\parallel^{(4-+)\star}) + \mathrm{Im}(M_\perp^{(1--)} M_\parallel^{(4+-)\star}) \right) \Big] \end{aligned} \tag{15b}$$

$$\begin{aligned} P_y(\vartheta, \varphi) = {} & -\frac{\sin 2\vartheta}{I(\vartheta, \varphi)} \Big[\cos\varphi \left(\mathrm{Im}(M_\perp^{(1++)} M_\parallel^{(3-+)\star}) + \mathrm{Im}(M_\perp^{(1--)} M_\parallel^{(3+-)\star}) \right) \\ & - \sin\varphi \left(\mathrm{Re}(M_\perp^{(1++)} M_\parallel^{(4-+)\star}) - \mathrm{Re}(M_\perp^{(1--)} M_\parallel^{(4+-)\star}) \right) \Big]. \end{aligned} \tag{15c}$$

The asymmetry $A(\vartheta, \varphi)$ is the same as for s-polarized light (equation (12)) but multiplied by $\cos^2\vartheta$, i.e. there is again MLD, which is due to SOC between Σ_5^3 and Σ_5^4 symmetry initial-state parts.

P_z again consists of an exchange-induced part (the first three terms in equation (15*a*)) and a spin–orbit-induced part (the last term in equation (15*a*)), which in the nonmagnetic limit again becomes the recently predicted LSPE (Henk and Feder 1994). P_x and P_y also do not vanish in the nonmagnetic case, but reproduce the LSPE due to p-polarized light, with $\boldsymbol{P}$ normal to the reaction plane, which was predicted by Tamura and Feder (1991a, b) and experimentally verified by Heinzmann's group (Schmiedeskamp *et al* 1991, Irmer *et al* 1992).

The intensity and ESP fulfil the symmetry relation

$$(I, P_x, P_y, P_z) \overset{\varphi\to-\varphi, \boldsymbol{M}\to-\boldsymbol{M}}{\longrightarrow} (I, -P_x, P_y, -P_z). \tag{16}$$

The relations for P_x and P_y follow immediately from the symmetry operation $2 \circ m_1 \circ m_2$. Furthermore,

$$(I, P_x, P_y, P_z) \overset{\vartheta\to-\vartheta}{\longrightarrow} (I, -P_x, -P_y, P_z) \tag{17}$$

as is obvious from the twofold rotational symmetry. Note that the transformation $\vartheta \to -\vartheta$ is identical to $\varphi \to \varphi + \pi$. The results for s-polarized light can be easily obtained from equations (14) and (15*c*) by setting $\vartheta = 0$ and $\varphi \to \varphi + \pi/2$.

For *circularly polarized light*, we confine ourselves (in this paper) to the case of normal incidence, i.e. $\vartheta = 0$. The intensity and ESP are given by

$$\begin{aligned} I(\sigma_\pm) = \frac{1}{2} \Big(&|M_\parallel^{(3+-)}|^2 + |M_\parallel^{(3-+)}|^2 + |M_\parallel^{(4+-)}|^2 + |M_\parallel^{(4-+)}|^2 \\ &\mp \Big(\mathrm{Re}(M_\parallel^{(3+-)} M_\parallel^{(4+-)\star}) - \mathrm{Re}(M_\parallel^{(3-+)} M_\parallel^{(4-+)\star}) \Big) \Big) \end{aligned} \tag{18}$$

and

$$\begin{aligned} P_z(\sigma_\pm) = \frac{1}{2I(\sigma_\pm)} \Big(&|M_\parallel^{(3+-)}|^2 - |M_\parallel^{(3-+)}|^2 + |M_\parallel^{(4+-)}|^2 - |M_\parallel^{(4-+)}|^2 \\ &\mp \Big(\mathrm{Re}(M_\parallel^{(3+-)} M_\parallel^{(4+-)\star}) + \mathrm{Re}(M_\parallel^{(3-+)} M_\parallel^{(4-+)\star}) \Big) \Big) \end{aligned} \tag{19}$$

where the two signs correspond to the two helicities of the light $(\sigma_\pm)$. The asymmetry, i.e. the MCD, is immediately obtained as

$$A(\sigma_\pm) = \mp 2 \Big(\mathrm{Re}(M_\parallel^{(3+-)} M_\parallel^{(4+-)\star}) - \mathrm{Re}(M_\parallel^{(3-+)} M_\parallel^{(4-+)\star}) \Big). \tag{20}$$

Obviously, it requires for its existence SOC between initial-state parts of Σ_5^3 and Σ_5^4 symmetry as well as exchange splitting. It is interesting to note that MCD (equation (20)) involves the real part of the matrix element product, whereas MLD (cf. equation (12)) is described by its imaginary part. By measuring, in addition to the intensity, the asymmetries for circularly and linearly polarized light, one can therefore obtain information not only about the modulus of the transition matrix elements, but also about their real and imaginary parts, i.e. their phase.

The intensity and ESP obey the relations $I(\sigma_\pm, \boldsymbol{M}) = I(\sigma_\mp, -\boldsymbol{M})$, and $P_z(\sigma_\pm, \boldsymbol{M}) = -P_z(\sigma_\mp, -\boldsymbol{M})$. Furthermore, the intensity is closely related to that for s-polarized light,

$$I(s, \varphi = 0) + I(s, \varphi = \pi/2) = I(\sigma_+) + I(\sigma_-). \tag{21}$$

3.2. The fourfold rotational axis

Electronic states of surface systems with 4*mm* symmetry, i.e. C_{4v} in Schönflies notation, can be classified according to two irreducible representations, Δ_6 and Δ_7, of the (nonmagnetic) double group. For magnetization normal to the surface, this classification still holds except for the lifting of Kramers' degeneracy. We recall that in the case of Δ_6 SOC mixes spatial parts of Δ_6^1 and Δ_6^5 spatial symmetry. The final states have Δ_6 symmetry, and we restrict ourselves again to the dominant part, Δ_6^1.

Let us first consider photoemission from Δ_6 initial states. Proceeding analogously to the above method for twofold rotational symmetry, we obtain for s-polarized light the intensity

$$I = |M_\parallel^{(5+-)}|^2 + |M_\parallel^{(5-+)}|^2 \tag{22}$$

and for the ESP, which only has a component normal to the surface,

$$P_z = \left(|M_{\parallel}^{(5+-)}|^2 - |M_{\parallel}^{(5-+)}|^2\right) \Big/ I. \tag{23}$$

In contrast to our above findings for surfaces with twofold rotational axes, both the intensity and the ESP are independent of the azimuth φ, and there is no MLD. This is easily understood from our previous results: going from $2mm$ to $4mm$ symmetry we get $M_{\parallel}^{(3+-)} = M_{\parallel}^{(4+-)}$ and $M_{\parallel}^{(3-+)} = M_{\parallel}^{(4-+)}$. Further we obtain, in accordance with symmetry arguments, the following (rather trivial) relations: $I(\boldsymbol{M}) = I(-\boldsymbol{M})$ and $P_z(\boldsymbol{M}) = -P_z(-\boldsymbol{M})$.

We now turn to p-polarized light. In this case, the intensity is obtained as

$$I(\vartheta) = \sin^2\vartheta \left(|M_{\perp}^{(1++)}|^2 + |M_{\perp}^{(1--)}|^2\right) + \cos^2\vartheta \left(|M_{\parallel}^{(5+-)}|^2 + |M_{\parallel}^{(5-+)}|^2\right). \tag{24}$$

All three components of the ESP are nonzero:

$$P_z(\vartheta) = \left\{\sin^2\vartheta \left(|M_{\perp}^{(1++)}|^2 - |M_{\perp}^{(1--)}|^2\right) + \cos^2\vartheta \left(|M_{\parallel}^{(5+-)}|^2 - |M_{\parallel}^{(5-+)}|^2\right)\right\} \Big/ I(\vartheta) \tag{25a}$$

$$\begin{aligned} P_x(\vartheta,\varphi) = -\sin 2\vartheta \Big\{&\cos\varphi \left(\mathrm{Re}(M_{\perp}^{(1++)} M_{\parallel}^{(5-+)\star}) - \mathrm{Re}(M_{\perp}^{(1--)} M_{\parallel}^{(5+-)\star})\right) \\ &- \sin\varphi \left(\mathrm{Im}(M_{\perp}^{(1++)} M_{\parallel}^{(5-+)\star}) + \mathrm{Im}(M_{\perp}^{(1--)} M_{\parallel}^{(5+-)\star})\right)\Big\} \Big/ I(\vartheta) \end{aligned} \tag{25b}$$

$$\begin{aligned} P_y(\vartheta,\varphi) = \sin 2\vartheta \Big\{&\cos\varphi \left(\mathrm{Im}(M_{\perp}^{(1++)} M_{\parallel}^{(5-+)\star}) + \mathrm{Im}(M_{\perp}^{(1--)} M_{\parallel}^{(5+-)\star})\right) \\ &- \sin\varphi \left(\mathrm{Re}(M_{\perp}^{(1++)} M_{\parallel}^{(5-+)\star}) - \mathrm{Re}(M_{\perp}^{(1--)} M_{\parallel}^{(5+-)\star})\right)\Big\} \Big/ I(\vartheta). \end{aligned} \tag{25c}$$

There is no MLD. Reflection at the (x, z)-plane implies

$$(I, P_x, P_y, P_z) \overset{\varphi\to-\varphi, \boldsymbol{M}\to-\boldsymbol{M}}{\longrightarrow} (I, -P_x, P_y, -P_z). \tag{26}$$

Furthermore, we have

$$P_x(\vartheta,\varphi) = \cos\varphi \; P_x(\vartheta,0) - \sin\varphi \; P_y(\vartheta,0) \tag{27a}$$

$$P_y(\vartheta,\varphi) = \sin\varphi \; P_x(\vartheta,0) + \cos\varphi \; P_y(\vartheta,0). \tag{27b}$$

For right-handed (σ_+) and left-handed (σ_-) circular light, we obtain

$$I(\sigma_+) = 2|M_{\parallel}^{(5+-)}|^2 \qquad \text{and} \qquad I(\sigma_-) = 2|M_{\parallel}^{(5-+)}|^2. \tag{28}$$

In the first case (σ_+), only transitions from initial states of symmetry Δ_6^5 of the function class $|f_n^-\rangle$ into the final state of the function class $|f_m^+\rangle$ can take place. In the latter case, the two function classes are interchanged. In general, this may lead to a pronounced MCD (Scheunemann *et al* 1994). The photoelectrons are completely polarized, $P_z(\sigma_\pm) = \pm 1$. But note that the ESP given here is in fact a partial polarization, in the sense that the complete intensity (due to both Δ_6 and Δ_7 initial states) is replaced by that arising only from Δ_6 initial states. The intensity asymmetry (MCD) can be obtained by reversing the magnetization or by reversing the photon helicity, $I(\sigma_\pm, \boldsymbol{M}) = I(\sigma_\mp, -\boldsymbol{M})$ and $P_z(\sigma_\pm, \boldsymbol{M}) = -P_z(\sigma_\mp, \boldsymbol{M})$. Furthermore, the intensity is closely related to that for s-polarized light, $I(s) = (I(\sigma_+) + I(\sigma_-))/2$.

Now we consider emission from initial states with Δ_7 symmetry. Because W_{11} and W_{22} are equal to zero, only P_z is nonzero. For s-polarized light, we obtain the same result as for Δ_6 initial states (see equation (22) and subsequent equations).

In contrast to Δ_6 initial states (where Δ_6^1 couples to the electric field vector component normal to surface), Δ_7 initial states couple only to the electric field vector component parallel to the surface. Therefore, the intensity and ESP for p-polarized light are very closely related to those for s-polarized light, carrying an additional (geometrical) factor:

$$I(p) = \cos^2\vartheta \left(|M_\parallel^{(5+-)}|^2 + |M_\parallel^{(5-+)}|^2\right) = \cos^2\vartheta\, I(s) \tag{29}$$

and $P_z(p) = P_z(s)$.

For circularly polarized light, the intensity and ESP are given by

$$I(\sigma_+) = 2|M_\parallel^{(5-+)}|^2 \qquad \text{and} \qquad I(\sigma_-) = 2|M_\parallel^{(5+-)}|^2 \tag{30}$$

and $P_z(\sigma_\pm) = \mp 1$. Note that the ESP is reversed with respect to that for Δ_6 initial states (compare, e.g., equation (28)) (Wöhlecke and Borstel 1984) and both the intensity and the ESP obey the same symmetry relations as for Δ_6 initial states.

3.3. *The threefold rotational axis*

Electronic states at surfaces with 3*m* symmetry, i.e. C_{3v} in Schönflies notation, may be classified according to two irreducible representations of the respective double group, Λ_6 and $\Lambda_{4,5}$. The final state has Λ_6^1 symmetry.

First, consider transitions from Λ_6 initial states. Comparing the transition matrix elements with those obtained for Δ_6 initial states (4*mm* symmetry), we note that $M_\parallel^{(3+-)}$ corresponds to $M_\parallel^{(5+-)}$ and $M_\parallel^{(3-+)}$ to $M_\parallel^{(5-+)}$. Therefore, we get the same results as given in equations (22)–(28), but with $M_\parallel^{(5ss')}$ replaced by $M_\parallel^{(3ss')}$. In particular, there is also no MLD.

We now turn to photoemission from $\Lambda_{4,5}$ initial states. For s-polarized light we obtain the intensity

$$I = \frac{1}{2}\left(|M_\parallel^{(3++)}|^2 + |M_\parallel^{(3+-)}|^2 + |M_\parallel^{(3-+)}|^2 + |M_\parallel^{(3--)}|^2\right). \tag{31}$$

The z-component of the ESP is exclusively due to exchange splitting and is given by

$$P_z = \frac{1}{2I}\left(|M_\parallel^{(3++)}|^2 + |M_\parallel^{(3+-)}|^2 - |M_\parallel^{(3-+)}|^2 - |M_\parallel^{(3--)}|^2\right). \tag{32}$$

The components parallel to the surface are due to both exchange and SOC, i.e.

$$P_x(\varphi) = \frac{1}{I}\Big[-\sin 2\varphi\left(\mathrm{Re}(M_\parallel^{(3++)}M_\parallel^{(3-+)\star}) - \mathrm{Re}(M_\parallel^{(3--)}M_\parallel^{(3+-)\star})\right)$$
$$- \cos 2\varphi\left(\mathrm{Im}(M_\parallel^{(3++)}M_\parallel^{(3-+)\star}) + \mathrm{Im}(M_\parallel^{(3--)}M_\parallel^{(3+-)\star})\right)\Big] \tag{33a}$$

$$P_y(\varphi) = \frac{-1}{I}\Big[-\cos 2\varphi\left(\mathrm{Re}(M_\parallel^{(3++)}M_\parallel^{(3-+)\star}) - \mathrm{Re}(M_\parallel^{(3--)}M_\parallel^{(3+-)\star})\right)$$
$$- \sin 2\varphi\left(\mathrm{Im}(M_\parallel^{(3++)}M_\parallel^{(3-+)\star}) + \mathrm{Im}(M_\parallel^{(3--)}M_\parallel^{(3+-)\star})\right)\Big]. \tag{33b}$$

Without exchange splitting, we have $M_\parallel^{(3++)} = M_\parallel^{(3--)}$ and $M_\parallel^{(3+-)} = M_\parallel^{(3-+)}$. This leads to the intensity

$$I = \left(|M_\parallel^{(3++)}|^2 + |M_\parallel^{(3+-)}|^2\right) \tag{34}$$

and to

$$P_z = 0 \tag{35a}$$

$$P_x(\varphi) = \frac{-2}{I}\cos 2\varphi\ \mathrm{Im}(M_\parallel^{(3++)}M_\parallel^{(3-+)\star}) \tag{35b}$$

$$P_y(\varphi) = \frac{2}{I}\sin 2\varphi\ \mathrm{Im}(M_\parallel^{(3++)}M_\parallel^{(3-+)\star}) \tag{35c}$$

which may be expressed as

$$P_x(\varphi) = \cos 2\varphi \ P_x(0) \qquad \text{and} \qquad P_y(\varphi) = -\sin 2\varphi \ P_x(0). \tag{36}$$

We thus retrieve the result for the LSPE of $3m$ surfaces (Tamura *et al* 1987), where s-polarized light produces an in-plane spin polarization.

We obtain the (typical) symmetry relations for the intensity and the normal component of the ESP,

$$(I, P_x, P_y, P_z) \stackrel{\varphi\to-\varphi, M\to -M}{\longrightarrow} (I, P_x, -P_y, -P_z) \tag{37}$$

and

$$P_x(\varphi) = \cos 2\varphi \ P_x(0) - \sin 2\varphi \ P_y(0) \tag{38a}$$

$$P_y(\varphi) = -\sin 2\varphi \ P_x(0) + \cos 2\varphi \ P_y(0). \tag{38b}$$

Analogously to the case for $4mm$ symmetry, $\Lambda_{4,5}$ initial states couple only to the components of the electric field vector parallel to the surface. Therefore, results for p-polarized light are like those for s-polarized light except for the geometrical factor $\cos^2\vartheta$ (cf. equation (29)).

For circularly polarized light we find

$$I(\sigma_+) = |M_\parallel^{(3-+)}|^2 + |M_\parallel^{(3--)}|^2 \qquad \text{and} \qquad I(\sigma_-) = |M_\parallel^{(3+-)}|^2 + |M_\parallel^{(3++)}|^2 \tag{39}$$

and $P_z(\sigma_\pm) = \mp 1$. The (partial) polarization is complete and reversed with respect to that of Λ_6 initial states.

Table 1. Magnetic dichroic effects and photoelectron spin-polarization components for magnetization $\boldsymbol{M}$ normal to surfaces (parallel to the z-axis) with twofold, threefold, or fourfold rotational axes, i.e. with spatial symmetry groups $2mm$, $3m$, and $4mm$ in the nonmagnetic limit. s, p, and circ. stand for s-, p-, and normally incident circularly polarized light. The signs in brackets indicate whether the respective ESP component occurs (+ sign) or does not occur (− sign) if only SOC (first sign), only exchange (second sign), or both (third sign) are present. MLD and MCD occur if a spin-polarization component parallel to $\boldsymbol{M}$ is produced by SOC in the nonmagnetic case.

$2mm$ light	P_x	P_y	P_z	I
s	(−, −, −)	(−, −, −)	(+, +, +)	MLD
p	(+, −, +)	(+, −, +)	(+, +, +)	MLD
circ.	(−, −, −)	(−, −, −)	(+, +, +)	MCD
$4mm$ light	P_x	P_y	P_z	I
s	(−, −, −)	(−, −, −)	(−, +, +)	
p	(+, −, +)	(+, −, +)	(−, +, +)	
circ.	(−, −, −)	(−, −, −)	(+, +, +)	MCD
$3m$ light	P_x	P_y	P_z	I
s	(+, −, +)	(+, −, +)	(−, +, +)	
p	(+, −, +)	(+, −, +)	(−, +, +)	
circ.	(−, −, −)	(−, −, −)	(+, +, +)	MCD

In table 1 we summarize our findings for photoemission from systems with magnetization normal to the surface. For systems with twofold rotational axes, we observe both MLD and MCD, whereas for surfaces with three- or fourfold rotational symmetry we find only MCD but no MLD.

4. Results for magnetization parallel to the surface

We now address surface systems with in-plane magnetization $\boldsymbol{M}$. Irrespective of whether the corresponding nonmagnetic system has $2mm$, $3m$ or $4mm$ symmetry, the magnetic system in this case has no rotational symmetry axis and at most one mirror plane. Nevertheless, the photoemission intensity and ESP expressions and in particular the occurrence of magnetic dichroism depend on the specific mirror symmetries of the corresponding nonmagnetic system and on the orientation of $\boldsymbol{M}$ relative to these mirror planes. We can distinguish three practically important cases. (i) The nonmagnetic system has two mirror planes (perpendicular to each other and to the surface plane) and $\boldsymbol{M}$ is parallel to one of them, for example the (yz)-plane. This is a typical for cubic (001) and (110) surfaces, where $\boldsymbol{M}$ points from an atom to one of its nearest neighbours. The other two cases involve only one mirror plane (chosen as the (xz)-plane), like (111) surfaces of cubic crystals and (0001) surfaces of hcp crystals. (ii) $\boldsymbol{M}$ is perpendicular to the mirror plane (pointing to a nearest-neighbour atom) or (iii) $\boldsymbol{M}$ is not perpendicular to the mirror plane. In the first two cases, the system is characterized by the spatial symmetry group m (i.e. C_s in the Schönflies notation). In the third case there is no nontrivial symmetry operation.

Table 2. Symmetry-adapted basis functions for systems with two mirror planes—(x, z) and (y, z)—(in the nonmagnetic limit) and $\boldsymbol{M}$ parallel to the x-axis, i.e. parallel to the surface and to the (y, z) mirror plane. The angular-momentum-quantization axis is normal to the surface; the spin-quantization axis is parallel to the magnetization (Pauli spinors $|\alpha\rangle$ and $|\beta\rangle$). l and m denote the quantum numbers of the angular momentum and its projection onto the z-axis.

	$\lvert g_n^+\rangle$	$\lvert g_n^-\rangle$	
S_1	$Y_l^0\lvert\alpha\rangle$	$Y_l^0\lvert\beta\rangle$	$l \geqslant 0$
	$(1/\sqrt{2})\left(Y_l^m + Y_l^{-m}\right)\lvert\alpha\rangle$	$[(-1)^m/\sqrt{2}]\left(Y_l^m + Y_l^{-m}\right)\lvert\beta\rangle$	$l \geqslant 1, -l \leqslant m \leqslant l$
S_2	$(1\sqrt{2})\left(Y_l^m - Y_l^{-m}\right)\lvert\beta\rangle$	$[-(-1)^m/\sqrt{2}]\left(Y_l^m - Y_l^{-m}\right)\lvert\alpha\rangle$	$l \geqslant 1, -l \leqslant m \leqslant l$

Table 3. The connection of single-group representations of the symmetry-adapted basis functions given in table 2 and those for $2mm$ and $4mm$ symmetry.

	S_1	S_2
$2mm$	Σ_1, Σ_4	Σ_2, Σ_3
$4mm$	$\Delta_1, \Delta_2, \Delta_5$	$\Delta_1', \Delta_2', \Delta_5$

4.1. *Cubic (001) and (110) surfaces*

We are now dealing with case (i), with $\boldsymbol{M}$ chosen along the x-axis. It is convenient to introduce symmetry-adapted basis functions (see table 2), the angular-momentum-quantization axis of which is normal to the surface, whereas the spin-quantization axis is parallel to the magnetization. These are closely related to those for $2mm$ symmetry (Inui *et al* 1990). In table 3 we give the connection between spatial parts of basis functions for $2mm$ and $4mm$ symmetry and the symmetry-adapted basis functions. Because the quantization axes for angular momentum and spin differ, a unitary transformation has to be applied to the spin-density matrix (Kessler 1985). Initial and final states then have the form

$$|\Psi_s\rangle = c_1^{(s)}|S^{1s}\rangle|s\rangle + c_2^{(s)}|S^{2s}\rangle|-s\rangle \qquad s = \pm \tag{40}$$

where the notation is analogous to what we used in equation (8) and again explicitly displays SOC. The evaluation of the photoelectron spin-density matrix proceeds in the same way as described in subsection 3.1. It should be noted, however, that now there are two types of matrix element involving initial-state parts of S^1 spatial symmetry: $M_{\parallel}^{(1ss)}$ is due to the dipole operator part $H_{\parallel}$ and $M_{\perp}^{(1ss)}$ to H_z (cf. equations (5*c*) and (6)).

For *p-polarized light* we obtain

$$\begin{aligned}
I(\vartheta,\varphi) = {} & \sin^2\vartheta\left(|M_{\perp}^{(1++)}|^2 + |M_{\perp}^{(1--)}|^2\right) + \cos^2\vartheta\ \sin^2\varphi\left(|M_{\parallel}^{(1++)}|^2 + |M_{\parallel}^{(1--)}|^2\right) \\
& + \cos^2\vartheta\ \cos^2\varphi\left(|M_{\parallel}^{(2+-)}|^2 + |M_{\parallel}^{(2-+)}|^2\right) \\
& + \sin 2\vartheta\ \sin\varphi\left(\mathrm{Im}(M_{\perp}^{(1++)\star} M_{\parallel}^{(1++)}) - \mathrm{Im}(M_{\perp}^{(1--)\star} M_{\parallel}^{(1--)})\right)
\end{aligned} \tag{41}$$

and

$$\begin{aligned}
P_x(\vartheta,\varphi) = {} & \Big\{\sin^2\vartheta\left(|M_{\perp}^{(1++)}|^2 - |M_{\perp}^{(1--)}|^2\right) + \cos^2\vartheta\ \sin^2\varphi\left(|M_{\parallel}^{(1++)}|^2 - |M_{\parallel}^{(1--)}|^2\right) \\
& + \cos^2\vartheta\ \cos^2\varphi\left(|M_{\parallel}^{(2+-)}|^2 - |M_{\parallel}^{(2-+)}|^2\right) \\
& + \sin 2\vartheta\ \sin\varphi\left(\mathrm{Im}(M_{\perp}^{(1++)\star} M_{\parallel}^{(1++)}) + \mathrm{Im}(M_{\perp}^{(1--)\star} M_{\parallel}^{(1--)})\right)\Big\} \Big/ I
\end{aligned} \tag{42a}$$

$$\begin{aligned}
P_z(\vartheta,\varphi) = {} & -\Big\{\sin 2\vartheta\ \cos\varphi\left(\mathrm{Re}(M_{\perp}^{(1++)} M_{\parallel}^{(2-+)\star}) - \mathrm{Re}(M_{\perp}^{(1--)} M_{\parallel}^{(2+-)\star})\right) \\
& + \cos^2\vartheta\ \sin 2\varphi\left(\mathrm{Im}(M_{\parallel}^{(1++)} M_{\parallel}^{(2-+)\star}) + \mathrm{Im}(M_{\parallel}^{(1--)} M_{\parallel}^{(2+-)\star})\right)\Big\}
\end{aligned} \tag{42b}$$

$$\begin{aligned}
P_y(\vartheta,\varphi) = {} & -\Big\{\sin 2\vartheta\ \cos\varphi\left(\mathrm{Im}(M_{\perp}^{(1++)} M_{\parallel}^{(2-+)\star}) + \mathrm{Im}(M_{\perp}^{(1--)} M_{\parallel}^{(2+-)\star})\right) \\
& - \cos^2\vartheta\ \sin 2\varphi\left(\mathrm{Re}(M_{\parallel}^{(1++)} M_{\parallel}^{(2-+)\star}) - \mathrm{Re}(M_{\parallel}^{(1--)} M_{\parallel}^{(2+-)\star})\right)\Big\}.
\end{aligned} \tag{42c}$$

Since the last term in the above intensity expression reverses sign upon reversal of $\boldsymbol{M}$, there is an MLD, which is maximal for the azimuthal angle of photon incidence $\varphi = \pi/2$ and vanishes for $\varphi = 0$. In the first case, the reaction plane is the (y, z)-plane, i.e. perpendicular to $\boldsymbol{M}$ (aligned along the x-axis). From the above expressions, the ESP components P_y and P_z are seen to vanish, and the nonzero P_x is composed of two exchange-induced terms, which change sign upon reversal of $\boldsymbol{M}$, and a third spin–orbit-induced term, which does not change sign and survives in the nonmagnetic limit, retrieving the 'linear spin-polarization effect' predicted by Tamura and Feder (1991a, b). We thus find again, as above in the case of twofold symmetry with magnetization normal to the surface, that the occurrence of both an exchange- and a spin–orbit-induced additive contribution in one of the ESP components is associated with MLD. This connection is explicit in our above formulae: the last term in I, which is responsible for MLD, and the last term in P_x, the spin–orbit contribution, involve the same matrix element combinations $\mathrm{Im}(M_{\perp}^{(1ss)\star} M_{\parallel}^{(1ss)})$ (with $s = \pm$).

In the case where $\varphi = 0$, in which $\boldsymbol{M}$ is parallel to the reaction plane, equation (41) shows that there is no MLD, but all three ESP components are nonzero. P_x is seen to be due to exchange only, reversing its sign upon reversal of $\boldsymbol{M}$, and P_y due to SOC only, whereas P_z involves both interactions in such a way that it would vanish if one or the other were absent. This interplay between exchange interaction and SOC is clearly different from the additive one in forming P_x in the previously discussed case where $\varphi = \pi/2$.

For general φ, our formulae yield the relation

$$(I, P_x, P_y, P_z) \xrightarrow{\varphi\to-\varphi,\, \boldsymbol{M}\to-\boldsymbol{M}} (I, -P_x, P_y, -P_z). \tag{43}$$

This also follows directly by considering reflection of the total set-up at the (x, z)-plane (which is, however, not a symmetry operation).

The results for *s-polarized light* incident at azimuth φ can very easily be obtained from the above ones for p-polarized light by setting $\vartheta = 0$ (i.e. normal incidence) and replacing φ by $\varphi + \pi/2$. Intensity and ESP components are then seen to obey the relations

$$(I, P_x, P_y, P_z) \stackrel{M\to -M}{\longrightarrow} (I, -P_x, -P_y, P_z) \tag{44a}$$

$$(I, P_x, P_y, P_z) \stackrel{\varphi\to-\varphi, M\to -M}{\longrightarrow} (I, P_x, -P_y, -P_z). \tag{44b}$$

In particular, there is no MLD in the sense of an intensity asymmetry upon reversal of $\boldsymbol{M}$. There is, however, a difference between the intensities for $\varphi = 0$ and $\varphi = \pi/2$, i.e. for normally incident s- and p-polarized light. If one defines dichroism as an intensity asymmetry occurring for two orthogonal states of photon polarization, one can therefore identify a MLD.

For off-normally incident *circularly polarized light* of helicity σ_+ or σ_-, the intensity is

$$\begin{aligned} I(\vartheta, \varphi, \sigma_\pm) = \frac{1}{2}\Big\{ & \sin^2\vartheta \ \left(|M_\perp^{(1++)}|^2 + |M_\perp^{(1--)}|^2\right) \\ & \pm 2\sin\vartheta \ \cos\varphi \ \left(\mathrm{Re}(M_\perp^{(1++)} M_\parallel^{(1++)\star}) - \mathrm{Re}(M_\perp^{(1--)} M_\parallel^{(1--)\star})\right) \\ & - \sin 2\vartheta \ \sin\varphi \ \left(\mathrm{Im}(M_\perp^{(1++)} M_\parallel^{(1++)\star}) - \mathrm{Im}(M_\perp^{(1--)} M_\parallel^{(1--)\star})\right) \\ & + (1 - \sin^2\vartheta \ \sin^2\varphi)\left(|M_\parallel^{(1++)}|^2 + |M_\parallel^{(1--)}|^2\right) \\ & + (1 - \sin^2\vartheta \ \cos^2\varphi)\left(|M_\parallel^{(2+-)}|^2 + |M_\parallel^{(2-+)}|^2\right)\Big\}. \end{aligned} \tag{45}$$

The two terms involving real and imaginary parts of M-products imply two different types of MCD. The second one is associated with the MLD for p-polarized light—cf. the last term in equation (41)—which vanishes for $\varphi = 0$, i.e. for $\boldsymbol{M}$ in the plane of incidence. This MCD is independent of the helicity of the incident radiation. The first MCD arises if $\boldsymbol{M}$ is not perpendicular to the plane of incidence. It further shows the symmetry relation $I(\sigma_+, +\boldsymbol{M}) = I(\sigma_-, -\boldsymbol{M})$. Since the ESP expressions are rather lengthy, it may suffice to say that all three components are generally nonzero.

For normally incident *circularly polarized light* ($\vartheta = 0$ and arbitrary φ) the above intensity formula reduces to

$$I(\sigma_\pm) = \left(|M_\parallel^{(1++)}|^2 + |M_\parallel^{(1--)}|^2 + |M_\parallel^{(2+-)}|^2 + |M_\parallel^{(2-+)}|^2\right)\Big/ 2 \tag{46}$$

and the ESP is given by

$$P_x(\sigma_\pm) = \frac{1}{2I}\left(|M_\parallel^{(1++)}|^2 - |M_\parallel^{(1--)}|^2 + |M_\parallel^{(2+-)}|^2 - |M_\parallel^{(2-+)}|^2\right) \tag{47a}$$

$$P_y(\sigma_\pm) = \pm\left(\mathrm{Im}(M_\parallel^{(1++)} M_\parallel^{(2-+)\star}) - \mathrm{Im}(M_\parallel^{(1--)} M_\parallel^{(2+-)\star})\right)\Big/ I \tag{47b}$$

$$P_z(\sigma_\pm) = \mp\left(\mathrm{Re}(M_\parallel^{(1++)} M_\parallel^{(2-+)\star}) + \mathrm{Re}(M_\parallel^{(1--)} M_\parallel^{(2+-)\star})\right)\Big/ I. \tag{47c}$$

Evidently, there is no MCD and all three components of the ESP are generally nonzero, in contrast to the case '$\boldsymbol{M}$ normal to the surface' treated above. P_x (along the direction of $\boldsymbol{M}$) is seen to be exchange induced, reversing its sign upon reversal of $\boldsymbol{M}$, whereas P_z can be produced by SOC alone, reducing to the usual optical orientation (Fano) effect in the nonmagnetic limit. P_y requires the simultaneous presence of magnetic exchange and SOC. This situation is analogous to the above-discussed case of p-polarized light for $\varphi = 0$.

On the grounds of our results it may appear surprising that in a recent photoemission experiment using normally incident circularly polarized light (Schneider *et al* 1991b), no ESP component P_z normal to the surface was detected. This finding was interpreted as follows. First, the spin-quantization axis is predominantly defined by $\boldsymbol{M}$, which should lead to vanishing ESP components normal to the magnetization. Second, because of the exchange splitting and the reduced symmetry (with respect to the nonmagnetic solid) the electronic wave functions change symmetry and the dipole selection rules leading to optical orientation do not hold. We therefore wish to point out that our above analytical results are supported by numerical calculations for Ni(001) (Henk *et al* 1994), which yield not only a strong ESP in the direction of $\boldsymbol{M}$ but also two ESP components normal to $\boldsymbol{M}$. The latter are, however, much smaller with values within the statistical error of the above experiment.

Reversing the photon helicity or $\boldsymbol{M}$, we obtain the relations

$$(I, P_x, P_y, P_z) \xrightarrow{\sigma_\pm \to \sigma_\mp} (I, P_x, -P_y, -P_z) \tag{48a}$$

$$(I, P_x, P_y, P_z) \xrightarrow{\boldsymbol{M} \to -\boldsymbol{M}} (I, -P_x, -P_y, P_z). \tag{48b}$$

Dichroic effects and spin polarizations for magnetization parallel to the surface are summarized in table 5. Prototype numerical results for Ni(001) with a single photon energy (Henk *et al* 1994) fully confirm the present qualitative predictions.

4.2. The fcc (111) and hcp (0001) surfaces

We now turn to the above-defined cases (ii) and (iii) relating to magnetic surfaces with in-plane magnetization, which in the nonmagnetic limit have threefold rotational symmetry and three mirror planes (symmetry 3*m*), e.g. (111) surfaces of fcc or (0001) surfaces of hcp systems. We recall that for 3*m* symmetry the irreducible representations of the double group consist of the two-dimensional one, Λ_6, and two one-dimensional ones degenerate by time-reversal symmetry, Λ_4 and Λ_5.

Table 4. Symmetry-adapted basis functions for systems with one mirror plane—(x, z)—and $\boldsymbol{M}$ along the y-axis, i.e. parallel to the surface and perpendicular to the mirror plane. The spin- and angular-momentum-quantization axes are chosen normal to the surface (Pauli spinors χ^+ and χ^-). l and m denote the quantum numbers of the angular momentum and its projection onto the z-axis.

	$\lvert g_n^+\rangle$	$\lvert g_n^-\rangle$	
γ_1	$Y_l^{-m}\chi^- + \mathrm{i}Y_l^m\chi^+$	$Y_l^m\chi^+ + \mathrm{i}Y_l^{-m}\chi^-$	m odd
γ_2	$-Y_l^{-m}\chi^- + \mathrm{i}Y_l^m\chi^+$	$Y_l^m\chi^+ - \mathrm{i}Y_l^{-m}\chi^-$	m even

Let us now specialize to case (ii), i.e. where $\boldsymbol{M}$ is perpendicular to a mirror plane, for example the (xz)-plane, with $\boldsymbol{M}$ pointing in nearest-neighbour directions. There remains one nontrivial symmetry operation, the reflection at this plane, i.e. we are concerned with the double group m. In the magnetic case there are only two one-dimensional representations, γ_1 and γ_2, which are connected to the former by $\Lambda_4 \to \gamma_1$, $\Lambda_5 \to \gamma_2$, and $\Lambda_6 \to \gamma_1 + \gamma_2$ (Falicov and Ruvalds 1968). Furthermore, γ_1 and γ_2 are degenerate by time-reversal symmetry. Their spin-angular basis functions are given in table 4.

For s-polarized light with the azimuthal angle φ of the electric field vector $\boldsymbol{E}$, we obtain the following expression for the photoemission intensity:

$$I(\varphi) = 2\sin^2\varphi \left(|M_1^{(++)}|^2 + |M_2^{(--)}|^2\right) + 2\cos^2\varphi \left(|M_1^{(-+)}|^2 + |M_2^{(+-)}|^2\right) \tag{49}$$

and for the ESP

$$P_x = -\frac{2}{I} \sin 2\varphi \left(\mathrm{Re}(M_1^{(++)} M_1^{(-+)\star}) - \mathrm{Re}(M_2^{(--)} M_2^{(+-)\star}) \right) \tag{50a}$$

$$P_y = \frac{2}{I} \left\{ \sin^2 \varphi \left(|M_1^{(++)}|^2 - |M_2^{(--)}|^2 \right) - \cos^2 \varphi \ \left(|M_1^{(-+)}|^2 - |M_2^{(+-)}|^2 \right) \right\} \tag{50b}$$

$$P_z = -\frac{2}{I} \sin 2\varphi \left(\mathrm{Im}(M_1^{(++)} M_1^{(-+)\star}) + \mathrm{Im}(M_2^{(--)} M_2^{(+-)\star}) \right) \tag{50c}$$

where $M_1^{(s+)}$ ($M_2^{(s-)}$) denotes a transition matrix element from initial state $|i_+\rangle$ ($|i_-\rangle$) with complex expansion coefficients α_n^+ (α_n^-), cf. equation (2), into final state $|f_s\rangle$. It is important to note that in the present case the expansion coefficients cannot be chosen as real because the basis functions behave differently under time reversal and mirror operations. Thus, in M_2 the complex conjugate expansion coefficients of the respective initial state appear, in contrast to the case for M_1.

The above expressions evidently obey the symmetry relation

$$(I, P_x, P_y, P_z) \xrightarrow{\varphi \to -\varphi} (I, -P_x, P_y, -P_z). \tag{51}$$

Since the matrix elements M_1 and M_2 differ from each other, the intensity $I(\varphi)$ changes upon reversal of the magnetization, i.e. there is MLD. This MLD is closely related to the 'linear spin-polarization effect', which occurs in photoemission by s-polarized light from nonmagnetic surfaces with $3m$ symmetry (Tamura *et al* 1987). In the nonmagnetic limit we have $M_1^{(++)} = M_1^{(-+)}$ and $M_2^{(--)} = M_2^{(+-)}$. Equations (49) and (50*c*) thus become

$$I(\varphi) = 2 \left(|M_1|^2 + |M_2|^2 \right) \tag{52a}$$

$$P_x = -\frac{2}{I} \sin 2\varphi \left(|M_1|^2 - |M_2|^2 \right) \tag{52b}$$

$$P_y = -\frac{2}{I} \cos 2\varphi \left(|M_1|^2 - |M_2|^2 \right) \tag{52c}$$

$$P_z = 0 \tag{52d}$$

where M_1 and M_2 denote matrix elements of transitions from a linear combination of initial states with Λ_4 and Λ_5 double-group symmetry into Λ_6^1 final states. In the rather complicated derivation of the last equations from those for the magnetic case one has to employ the fact that the final state is of Λ_6^1 spatial symmetry. The photoemission intensity and the modulus of the ESP vector are independent of the azimuth φ. For $\varphi = \pi/4$ no ESP component parallel to the y-axis, i.e. parallel to the magnetization, is brought about by SOC and there is no MLD in this case.

If $\boldsymbol{M}$ is not perpendicular to a mirror plane of the nonmagnetic system, i.e. our case (iii), there is no spatial symmetry operation except the trivial one. Our analytical results (not shown here) indicate that for general $\boldsymbol{M}$ and general azimuthal angles φ of the surface-parallel electric field vector $\boldsymbol{E}$ there is always MLD. It is absent, however, in the special cases where $\boldsymbol{M}$ is in the mirror plane and $\boldsymbol{E}$ is either parallel or perpendicular to $\boldsymbol{M}$. From the 'nonmagnetic' expressions (52) we see that in these special cases P_x, the (SOC-induced) ESP component parallel to $\boldsymbol{M}$, vanishes.

The above MLDs for *s-polarized* light and the ESP symmetry relations are confirmed by numerical relativistic layer KKR photoemission calculations, which we have carried out for ferromagnetic Ni(111). At photon energies around 28 eV these new types of MLD are so strong that they should be easily detectable in experiments.

For *circularly polarized* light at *normal* incidence, which is a coherent superposition of s-polarized light with φ and $\varphi + \pi/2$, the above impressions imply that there is no intensity asymmetry, i.e. no MCD, and all three ESP components are generally nonzero.

For *p-polarized* light the analytical expressions get rather lengthy. Suffice it to say that one generally obtains three nonzero ESP components and a MLD, which is a superposition of the MLD found for s-polarized light with a new one, which is akin to the one found in section 4.2. For *circularly polarized* light at *off-normal* incidence, we obtain MCD, if $\boldsymbol{M}$ is parallel to the plane of incidence.

5. The connection between magnetic dichroism and nonmagnetic spin-polarization effects

From the various specific cases which we have analysed above, a general picture emerges of the interplay of exchange interaction and spin–orbit coupling (SOC) producing photoelectron spin polarization and magnetic dichroism.

Since the spin-polarization effects, which occur in *nonmagnetic* systems as a consequence of SOC, are an essential ingredient for understanding the results from magnetic systems, we first briefly summarize these effects. *Circularly polarized light* produces an electron spin-polarization (ESP) vector $\boldsymbol{P}$ aligned with the helicity of the light, which is well known as the Fano effect or optical orientation (cf., e.g., Wöhlecke and Borstel 1984, and references therein). In the case of normal incidence, there is thus $\boldsymbol{P}$ normal to the surface. Contrary to a long-held common belief, ESP also occurs for *linearly polarized light* in three different ways. The first such 'linear spin-polarization effect' (LSPE) was theoretically predicted by Tamura *et al* (1987) and experimentally confirmed by Heinzmann's group (Schmiedeskamp *et al* 1988) for surfaces with threefold rotational symmetry: s-polarized light produces an in-plane $\boldsymbol{P}$ because of a peculiarity of the double-group symmetry $\Lambda_{4,5}$. A second LSPE was found theoretically (Tamura and Feder 1991a, b) and experimentally (Schmiedeskamp *et al* 1991, Irmer *et al* 1992) for off-normally incident p-polarized light for surfaces with two-, three- and fourfold rotational symmetry. It consists in an ESP component perpendicular to the reaction plane. Thirdly, for surfaces with twofold rotational symmetry, s-polarized light was recently predicted to produce an ESP component normal to the surface (Henk and Feder 1994). This effect is due to spin–orbit coupling between states with Σ^3 and Σ^4 spatial symmetry. It was recently verified by experiment (Irmer *et al* 1995).

Now consider light of arbitrary polarization incident on a *magnetic* semi-infinite system with magnetization $\boldsymbol{M}$. If there was no spin–orbit coupling, the exchange interaction would produce only a photoelectron spin-polarization vector $\boldsymbol{P}_{\mathrm{ex}}$ aligned parallel to $\boldsymbol{M}$. Upon reversal of $\boldsymbol{M}$, $\boldsymbol{P}_{\mathrm{ex}}$ is reversed and the intensity does not change. Taking into account spin–orbit coupling and going to the limit of vanishing exchange splitting, one retrieves the above-described ESP exclusively due to SOC, which we may call $\boldsymbol{P}_{\mathrm{so}}$. Naturally it does not change sign with $\boldsymbol{M}$. The phenomena observed for magnetic systems depend on the relative orientation of $\boldsymbol{P}_{\mathrm{so}}$ and $\boldsymbol{M}$. If $\boldsymbol{P}_{\mathrm{so}}$ is perpendicular to $\boldsymbol{M}$, the $\boldsymbol{P}$ of the photoelectrons has three components: an exchange-induced one along $\boldsymbol{M}$, a SOC-induced one along $\boldsymbol{P}_{\mathrm{so}}$, and a third one which requires the simultaneous presence of exchange and SOC. In this case, the intensity does not depend on the direction of $\boldsymbol{M}$, i.e. there is no magnetic (circular or linear) dichroism. If $\boldsymbol{P}_{\mathrm{so}}$ is parallel to $\boldsymbol{M}$, $\boldsymbol{P}$ consists of two additive terms, an exchange-induced one, which changes sign with $\boldsymbol{M}$, and a SOC-induced one, which does not. The matrix element combinations, which occur in the latter, also provide an additive contribution to the total intensity, which changes sign with $\boldsymbol{M}$. Consequently, the intensity changes upon reversal of $\boldsymbol{M}$, i.e. there is *magnetic dichroism*. We would like to emphasize that these findings are quite general and hold for both MCD and for the various types of MLD associated with the above spin–orbit-induced 'linear spin-polarization effects'.

Table 5. Magnetic dichroic effects and photoelectron spin-polarization components for magnetization $\boldsymbol{M}$ parallel to the surface (x-axis) and linearly polarized (s, p) as well as circularly polarized light. The signs in brackets indicate whether the respective ESP component occurs (+ sign) or does not occur (− sign) if only SOC (first sign), only exchange (second sign), or both (third sign) are present. MLD and MCD arise if a spin-polarization component P_x parallel to $\boldsymbol{M}$ is produced by SOC in the nonmagnetic limit. For circularly polarized light, ϑ denotes the polar angle of incidence, and the azimuthal angle φ is taken as arbitrary.

Light	Group	P_x	P_y	P_z	I
					Linear
s	$2mm$	$(-,+,+)$	$(-,-,+)$	$(+,-,+)$	
	$4mm$	$(-,+,+)$	$(-,-,+)$	$(-,-,+)$	
	$3m$	$(+,+,+)$	$(+,-,+)$	$(-,-,+)$	MLD
p	$2mm$	$(+,+,+)$	$(+,-,+)$	$(+,-,+)$	MLD
	$4mm$	$(+,+,+)$	$(+,-,+)$	$(-,-,+)$	MLD
	$3m$	$(+,+,+)$	$(+,-,+)$	$(-,-,+)$	MLD
					Circular
$\vartheta = 0$		$(-,+,+)$	$(-,-,+)$	$(+,-,+)$	
$\vartheta \neq 0$		$(+,+,+)$	$(+,-,+)$	$(+,-,+)$	MCD

Our main results are summarized in tables 1 and 5. In the case of 'magnetization $\boldsymbol{M}$ normal to the surface', $2mm$ surfaces exhibit both MLD and MCD, whereas for $3m$ and $4mm$ no MLD occurs, because the nonmagnetic LSPEs produce no ESP component normal to the surface, i.e. in the direction of $\boldsymbol{M}$. In all three cases, MCD occurs. If $\boldsymbol{M}$ is parallel to the surface (see table 5), p-polarized light produces MLD for all surfaces, and s-polarized light produces MLD for $3m$ surfaces. Circularly polarized light generally produces MCD except in the special case of normal incidence.

6. Concluding remarks

Our analytical results explicitly confirm findings from general symmetry arguments. Moreover, however, they reveal in detail the physical origin of the various magnetic dichroisms and spin-polarization effects in terms of an interplay between spin–orbit coupling and exchange. In the limit of vanishing magnetization we retrieve purely spin–orbit-induced spin-polarization effects, which occur for circularly and for linearly polarized light on nonmagnetic surfaces. This connection provides a deeper understanding of MCD and several types of MLD. As our dichroism and spin-polarization expressions contain terms involving single-group initial states mixed by spin–orbit coupling, they can be employed to infer from experimental data the types of initial states and their hybridization underlying individual spectral features.

Experimentally, in addition to MCD for various cases, MLD has so far been observed for *p-polarized* light and magnetization parallel to the surface, which is in line with our analytical results. Beyond this we predict, for surfaces with a twofold normal rotation axis and magnetization normal to the surface, a new type of *s-polarized-light* MLD associated with a photoelectron spin polarization normal to the surface. Since clean surfaces usually have an in-plane magnetization, we would like to emphasize that our results are also valid for ultrathin magnetic films (i.e. in the monolayer regime). Further, we predict another MLD for surfaces with a threefold rotational axis (in the nonmagnetic limit) and magnetization parallel to the surface. This MLD is associated with the spin–orbit effect for *s-polarized* light, which for nonmagnetic surfaces is known to produce an in-plane component of the photoelectron spin polarization.

Since our analytical expressions rely on an effective one-electron picture, which provides a good approximation for valence-band photoemission, their applicability to core-state photoemission, where many-body effects like multiplet and satellite structure are important (cf., e.g., Thole and van der Laan (1994) and references therein), is restricted to special cases for which a modified one-electron picture may still lead to reasonable results (cf., e.g., Tamura *et al* 1994).

The formulae derived in this paper could be computationally implemented and applied to specific crystalline surface systems. This would, however, have two drawbacks: firstly, stationary initial states of a semi-infinite system imply the neglect of hole lifetime effects, which are well known to be important; secondly, the present two-component approximation is presumably not sufficiently accurate. Quantitatively realistic calculations should therefore rather be based on our relativistic Green function formalism (Halilov *et al* 1993). The results of such calculations for Ni(001) with M normal and parallel to the surface (see, Scheunemann *et al* (1994) and Henk *et al* (1994), respectively) and for ultrathin Co films on Cu(001) (Henk *et al* 1995) are fully in line with the present analytical findings.

Acknowledgment

This work was funded by the German Ministry for Research and Technology under Contracts 055PGABB7 and 05621PGA.

References

Bansmann J, Westphal C, Getzlaff M, Fegel F and Schönhense G 1992 *J. Magn. Magn. Mater.* **104** 1691
Baumgarten L, Schneider C M, Petersen H, Schäfers F and Kirschner J 1990 *Phys. Rev. Lett.* **65** 492
Carbone C, Vescovo E, Rader O, Gudat W and Eberhardt W 1993 *Phys. Rev. Lett.* **71** 280
Ebert H, Baumgarten L, Schneider C M and Kirschner J 1991 *Phys. Rev.* B **44** 4406
Falicov L M and Ruvalds J 1968 *Phys. Rev.* **172** 498
Feder R 1985 (ed) *Polarized Electrons in Surface Physics* (Singapore: World Scientific)
Halilov S V, Tamura E, Gollisch H, Meinert D and Feder R 1993 *J. Phys.: Condens. Matter* **5** 3859
Hartmann D, Weber W, Wesner D A, Popovic S and Güntherodt G 1993a *J. Magn. Magn. Mater.* **121** 160
——1993b *Phys. Rev.* B **48** 16837
Henk J and Feder R 1994 *Europhys. Lett.* **28** 609
Henk J, Halilov S V, Scheunemann T and Feder R 1994 *Phys. Rev.* B **50** 8130
Henk J, Scheunemann T, Halilov S V and Feder R 1995 *Phys. Status Solidi* b **192**
Inui T, Tanabe Y and Onodera Y 1990 *Group Theory and Its Applications in Physics (Springer Series in Solid State Sciences 78)* (Berlin: Springer)
Irmer N, David R, Schmiedeskamp B and Heinzmann U 1992 *Phys. Rev.* B **45** 3849
Irmer N, Frentzen F, Yu S W, Schmiedeskamp B and Heinzmann U 1995 *Verh. Deutsch. Phys. Ges.* **7** 1573
Kessler J 1985 *Polarized Electrons (Springer Series on Atoms and Plasmas 1)* 2nd edn (Berlin: Springer)
Kevan S V (ed) 1992 *Angle-resolved Photoemission: Theory and Current Applications* (Amsterdam: Elsevier)
Rader O, Vescovo E, Redinger J, Blügel S, Carbone C, Eberhardt W and Gudat W 1994 *Phys. Rev. Lett.* **72** 2247
Rose M E 1961 *Relativistic Electron Theory* (New York: Wiley)
Rose H B, Roth C, Hillebrecht F U and Kisker E 1994 *Solid State Commun.* **91** 129
Roth C, Hillebrecht F U, Rose H B and Kisker E 1993a *Phys. Rev. Lett.* **70** 3479
Roth C, Rose H B, Hillebrecht F U and Kisker E 1993b *Solid State Commun.* **86** 147
Ruvalds J and Falicov L M 1968 *Phys. Rev.* **172** 508
Scheunemann T, Halilov S V, Henk J and Feder R 1994 *Solid State Commun.* **91** 487
Schmiedeskamp B, Irmer N, David R and Heinzmann U 1991 *Appl. Phys.* A **53** 418
Schmiedeskamp B, Vogt B and Heinzmann U 1988 *Phys. Rev. Lett.* **60** 651
Schneider C M, Celinski Z, Neuber M, Wilde C, Grunze M, Meinel K and Kirschner J 1994 *J. Phys.: Condens. Matter* **6** 1177

Schneider C M, Hammond M S, Schuster P, Cebollada A, Miranda R and Kirschner J 1991a *Phys. Rev.* B **44** 12 066

Schneider C M, Schuster P, Hammond M S and Kirschner J 1991b *Europhys. Lett.* **16** 689

Smith N V, Brookes N B, Chang Y and Johnson P D 1994 *Phys. Rev.* B **49** 332

Tamura E and Feder R 1991a *Solid State Commun.* **79** 989

Tamura E, Piepke W and Feder R 1987 *Phys. Rev. Lett.* **59** 934

——1991b *Europhys. Lett.* **16** 695

Tamura E, Waddill G D, Tobin J G and Sterne P A 1994 *Phys. Rev. Lett.* **73** 1533

Thole B T and van der Laan G 1994 *Phys. Rev.* B **50** 11 474

Venus D 1993 *Phys. Rev.* B **48** 6144

——1994 *Phys. Rev.* B **49** 8821

Venus D, Baumgarten L, Schneider C M, Boeglin C and Kirschner J 1993 *J. Phys.: Condens. Matter* **5** 1239

Wöhlecke M and Borstel G 1984 *Optical Orientation* ed F Meier and B P Zakharchenya (Amsterdam: North-Holland)

Wu S C, Garrison K, Begley A M, Jona F and Johnson P D 1994 *Phys. Rev.* B **49** 14 081