Selection rules in (e, 2e) spectroscopy from ferromagnetic surfaces

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Abstract
Electron pair emission from ferromagnetic crystalline surfaces, which occurs due to the collision of an incident low-energy electron with a valence electron, is shown to be governed by spatial and spin selection rules. Valence electron states with spatial parts antisymmetric with respect to the reaction plane are not observable for any spin configuration. If there is a spatial symmetry plane normal to the reaction plane, spin-polarized primary electrons selectively probe equal and opposite spin valence electrons. These analytical findings are further elaborated for ferromagnetic cubic (110) surfaces and illustrated by numerical results for Fe(110).

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The interaction of low-energy electrons with solid surface systems (clean and adsorbate-covered surfaces) comprises in particular the so-called (e, 2e) process, which involves a single collision event with a valence electron and the subsequent emission of an electron pair. Over the past half-decade, the energy- and momentum-resolved investigation of these pairs of time-correlated electrons has significantly advanced both experimentally and theoretically and is now established as a valuable method for studying spin-dependent electron collision dynamics and electronic structure in the topmost atomic layers of surface systems (see [1–9] and references therein).

Recently, spin-polarized primary electrons have fruitfully been applied in (e, 2e) spectroscopy from ferromagnetic surfaces [4, 7–9]. In order to extract from measured spectra information on the spin-split electronic structure of the target, it is essential to understand in detail the collision dynamics and its exchange-induced spin-dependence (see [8]). In the present paper we approach this problem with an emphasis on the symmetry properties of the spatial part of the valence state, which is involved in the (e, 2e) process. We obtain spin- and spatial-symmetry-dependent selection rules, and elucidate the relationship between the observable spin asymmetry of the reaction cross section and the valence electron spin polarization in the vicinity of the surface.

In section 2 we analytically show that spin-dependent (e, 2e) reaction cross sections from ferromagnetic crystalline surface systems are subject to selection rules due to spatial symmetries of the valence electron states involved. In section 3 we demonstrate this first analytically for cubic (110) surfaces and second computationally for Fe(110) by comparing numerically calculated (e, 2e) spectra with the underlying spin- and symmetry-resolved valence electron band structure and layer-resolved density of states.

2. Symmetry analysis of the spin-dependent cross section

The (e, 2e) process from ferromagnetic crystalline surface systems is treated within a theoretical framework, which has been presented in detail in earlier work (see [1, 2, 9]). We briefly recall the set-up and an expression obtained for the spin-dependent reaction cross section. From this expression we then deduce spin and spatial selection rules.

A primary electron with energy E_1, surface-parallel momentum component $\vec{k}_1^{\parallel}$ and spin orientation σ_1 relative to an axis $\vec{e}$ (i.e. spin polarization vector $\vec{P}_1 = \sigma_1 \vec{e}$ at the electron gun) collides with a valence electron with energy E_2, surface-parallel momentum component $\vec{k}_2^{\parallel}$ and spin orientation σ_2, and two outgoing electrons with $(E_3, \vec{k}_3^{\parallel}, \sigma_3)$ and $(E_4, \vec{k}_4^{\parallel}, \sigma_4)$ are detected. The primary electron and the valence electron are described by solutions $\psi_1^{\sigma_1}(\vec{r})$ and $\psi_2^{n\sigma_2}(\vec{r})$ of an effective-potential one-electron Dirac equation, where the quantum numbers E_i and $\vec{k}_i^{\parallel}$ are comprised in the respective subscripts 1 and 2, and the index n accounts for degeneracies of the valence electron state. If the Coulomb correlation between the two outgoing electrons is either neglected or incorporated in effective one-electron potentials (see [3]), these electrons are also described by one-electron four-spinors: $\psi_3^{\sigma_3}(\vec{r})$ and $\psi_4^{\sigma_4}(\vec{r})$. Due to spin–orbit coupling, the σ_i are strictly speaking only labels for degenerate pairs of solutions, which are chosen such as to match to plane waves with definite spins (as dictated by the source and by the detectors) in the vacuum region.

Using an antisymmetrized product of ψ_1 and ψ_2 and of ψ_3 and ψ_4 in a golden rule matrix element with the screened Coulomb interaction $U(\vec{r}, \vec{r}')$, one obtains the following expression for the (e, 2e) reaction cross section ('intensity'):

$$I_{\sigma_3,\sigma_4}^{\sigma_1}(E_3, E_4) = (k_3 k_4 / k_1) \sum_{E_2, \vec{k}_2^{\parallel}, n\sigma_2} |f_{\sigma_1, n\sigma_2, \sigma_3, \sigma_4} - g_{\sigma_1, n\sigma_2, \sigma_3, \sigma_4}|^2 \delta(E) \delta(\vec{k}^{\parallel}), \quad (1)$$

where

$$\delta(E) = \delta(E_1 + E_2 - E_3 - E_4) \qquad \text{and} \qquad \delta(\vec{k}^{\parallel}) = \delta(\vec{k}_1^{\parallel} + \vec{k}_2^{\parallel} - \vec{k}_3^{\parallel} - \vec{k}_4^{\parallel}) \qquad (2)$$

account for the conservation of energy and surface-parallel momentum; f and g are direct and exchange scattering amplitudes:

$$f_{\sigma_1, n\sigma_2, \sigma_3, \sigma_4} = \int \psi_3^{\sigma_3 *}(\vec{r}) \psi_4^{\sigma_4 *}(\vec{r}') U(\vec{r}, \vec{r}') \psi_1^{\sigma_1}(\vec{r}) \psi_2^{n\sigma_2}(\vec{r}') \, \mathrm{d}\vec{r} \, \mathrm{d}\vec{r}'; \qquad (3)$$

the expression for g is the same except for $\vec{r}$ and $\vec{r}'$ interchanged in the first product term. Equation (1) relates to a 'complete experiment' from a ferromagnetic surface with a spin-polarized source and detection of the spins of the two outgoing electrons. If the detectors do not resolve spin, one has to sum over σ_3 and σ_4. If the primary beam is unpolarized, one has to sum over $\sigma_1 = \pm$.

In order to make the following analysis more transparent, we now adopt a non-relativistic (two-component) approximation and neglect spin–orbit coupling. The four-component spinors $\psi_i^{\sigma_i}$ then reduce to $\varphi_i^{\sigma_i} |\sigma_i\rangle$, where $|\sigma_i\rangle$ with $\sigma_i = \pm$ are the basis spinors $(1, 0)$ and $(0, 1)$, and $\varphi_i^{\sigma_i}$ are scalar wavefunctions. It is important to note that in the ferromagnetic case the latter

actually depend on the spin orientation σ_i. Non-vanishing amplitudes f and g are then easily seen to exist only for a very reduced number of the sets $(\sigma_1, \sigma_2, \sigma_3, \sigma_4)$.

If the spin of the primary electron is parallel to the spins of the valence electrons of spatial degeneracy type n, i.e. $\sigma_1 = \sigma_2 =: \sigma$, we have only

$$f_{\sigma,n\sigma,\sigma,\sigma} = \int \varphi_3^{\sigma*}(\vec{r})\varphi_4^{\sigma*}(\vec{r}')U(\vec{r},\vec{r}')\varphi_1^{\sigma}(\vec{r})\varphi_2^{n\sigma}(\vec{r}')\,\mathrm{d}\vec{r}\,\mathrm{d}\vec{r}' =: f_n^{\sigma\sigma} \tag{4}$$

and

$$g_{\sigma,n\sigma,\sigma,\sigma} = \int \varphi_3^{\sigma*}(\vec{r}')\varphi_4^{\sigma*}(\vec{r})U(\vec{r},\vec{r}')\varphi_1^{\sigma}(\vec{r})\varphi_2^{n\sigma}(\vec{r}')\,\mathrm{d}\vec{r}\,\mathrm{d}\vec{r}' =: g_n^{\sigma\sigma}. \tag{5}$$

For primary spin σ, the cross section for detecting a parallel-spin σ electron pair is then

$$I_{\sigma,\sigma}^{\sigma}(E_3, E_4) = (k_3 k_4/k_1) \sum_{E_2,\vec{k}_2^{\parallel},n} |f_n^{\sigma\sigma} - g_n^{\sigma\sigma}|^2 \delta(E)\delta(\vec{k}^{\parallel}) =: \sum_n I_n^{\sigma\sigma} =: I^{\sigma\sigma}. \tag{6}$$

The partial intensity $I_n^{\sigma\sigma}$ defined in equation (6) can be regarded as the scattering cross section of the spin σ primary electron with a spin σ valence electron of spatial degeneracy type n.

If the spins of the primary electron and the valence electrons are anti-parallel, i.e. $\sigma_2 = -\sigma_1 = -\sigma = \bar{\sigma}$, the only non-vanishing scattering amplitudes are

$$f_{\sigma,n\bar{\sigma},\sigma,\bar{\sigma}} =: f_n^{\sigma\bar{\sigma}}, \qquad g_{\sigma,n\bar{\sigma},\bar{\sigma},\sigma} =: g_n^{\sigma\bar{\sigma}}, \tag{7}$$

which are given by matrix element expressions analogous to those in equations (4) and (5). For primary spin σ, the cross section for detecting an antiparallel-spin pair is then

$$I_{\sigma,\bar{\sigma}}^{\sigma} + I_{\bar{\sigma},\sigma}^{\sigma} = (k_3 k_4/k_1) \sum_{E_2,\vec{k}_2^{\parallel},n} (|f_n^{\sigma\bar{\sigma}}|^2 + |g_n^{\sigma\bar{\sigma}}|^2)\delta(E)\delta(\vec{k}^{\parallel}) =: \sum_n I_n^{\sigma\bar{\sigma}} =: I^{\sigma\bar{\sigma}}. \tag{8}$$

The partial intensity $I_n^{\sigma\bar{\sigma}}$ defined in equation (8) is the scattering cross section of the spin σ primary electron with an opposite-spin $\bar{\sigma}$ valence electron of spatial degeneracy type n. In experiments with a polarized electron gun (spin $\sigma = \pm$) and without detection of the spins of the outgoing electrons, the observed scattering cross section is

$$I^{\sigma} := I^{\sigma\sigma} + I^{\sigma\bar{\sigma}} \qquad \text{with } \sigma = \pm. \tag{9}$$

In the general case of arbitrary directions of the incident electron and of the two outgoing electrons, all the cross sections $I_n^{\sigma\sigma}$ and $I_n^{\sigma\bar{\sigma}}$ (see equations (6) and (8)) are usually non-zero. If by virtue of energy conservation (see equation (2)) the valence electron energy E_2 happens to lie in a majority spin energy gap (e.g. just below E_F for a strong ferromagnet like Ni), it is obvious that I_n^{++} and I_n^{-+} are zero.

In the following, we show that in more symmetrical geometries the spatial symmetries of the wavefunctions can cause some of the above partial cross sections to vanish, i.e. give rise to selection rules. We focus on coplanar setups, in which the incident and outgoing electrons move in a mirror plane of the semi-infinite crystal, which is perpendicular to the surface. The wavefunctions $\varphi_1^{\sigma_1}$, $\varphi_3^{\sigma_3}$ and $\varphi_4^{\sigma_4}$, which are plane waves at the source and at the detectors, are then symmetric with respect to the mirror operation at that plane, while the valence electron wavefunctions $\varphi_2^{n\sigma_2}$ generally comprise one symmetric and one antisymmetric function. For the latter, which we characterize by the index $n = a$, the scattering amplitudes $f_n^{\sigma\sigma'}$ and $g_n^{\sigma\sigma'}$, as defined in equations (4), (5) and (7), are identically zero. This is easily seen by, e.g., choosing the mirror plane as (x, z) and applying the transformation $(y, y') \to (-y, -y')$ to the integrals in equations (4) and (5), which by virtue of $\varphi_2^{a\sigma_2}(x, -y, z) = -\varphi_2^{a\sigma_2}(x, y, z)$ yields $f_a^{\sigma\sigma'} = -f_a^{\sigma\sigma'}$ and $g_a^{\sigma\sigma'} = -g_a^{\sigma\sigma'}$. Consequently, the contributions to the cross sections $I^{\sigma\sigma}$ (equation (6)) and $I^{\sigma\bar{\sigma}}$ (equation (8)) are identically zero. We thus have the selection rule

that valence electron states, which are antisymmetric with respect to the reaction plane, do not manifest themselves in (e, 2e) reaction cross sections.

A second selection rule can be derived for coplanar geometry in the more special case of normal incidence of the primary beam and of equal energies ($E_3 = E_4$) and oppositely equal parallel-momenta of the detected electrons ($\vec{k}_3^{\parallel} = -\vec{k}_4^{\parallel}$). From parallel-momentum conservation (see equation (2)) this implies that one selects valence electron states with $\vec{k}_2^{\parallel} = 0$, i.e. at the centre of the surface Brillouin zone. Let (x, z) be the reaction plane and (y, z) a mirror plane of the semi-infinite crystalline system with the surface (clean or covered with an ultrathin film) in the (x, y) plane. The valence electron wavefunctions are then either symmetric or antisymmetric with respect to the (y, z) plane. For parallel spins $\sigma_3 = \sigma_4 =: \sigma$, the wavefunctions of the two outgoing electrons are related as $\varphi_4^{\sigma}(x, y, z) = \varphi_3^{\sigma}(-x, y, z)$. Applying the transformation $(x, x') \rightarrow (-x, -x')$ to the integral in equation (5) and comparing with (4) reveals that $g_n^{\sigma\sigma} = f_n^{\sigma\sigma}$ if $\varphi_2^{n\sigma}$ is symmetric, and $g_n^{\sigma\sigma} = -f_n^{\sigma\sigma}$ if $\varphi_2^{n\sigma}$ is antisymmetric. The cross section contribution $I_n^{\sigma\sigma}$ (equation (6)) for the production of parallel-spin pairs therefore vanishes in the former case, whereas in the latter it is non-zero and determined by $4|f_n^{\sigma\sigma}|^2$. $I^{\sigma\sigma}$ (equation (6)), the scattering cross section of a spin σ primary electron with a spin σ valence electron, thus selectively reflects collisions involving valence electron states, which are antisymmetric with respect to a mirror plane perpendicular to the reaction plane.

The above-derived two selection rules are strictly speaking valid only in the absence of spin–orbit coupling. If the latter is taken into account, they are relaxed due to hybridization of different spatial symmetry types, but can still be expected to be useful in a large number of situations in which the valence electron spinor is dominated by a particular spatial symmetry type.

3. Ferromagnetic cubic (110) surfaces

In the following we apply the above-derived spin-dependent (e, 2e) selection rules analytically to ferromagnetic crystalline surface systems, which in the non-magnetic limit have a two-fold rotation axis and two mirror planes normal to the surface (i.e. spatial symmetry group $2mm$), and subsequently illustrate them quantitatively for the case of the (110) surface of bcc Fe by means of numerically calculated spectra.

For the present purpose, the most interesting set-up is the symmetric coplanar geometry with normal incidence of the primary beam and equal energies of the two detected electrons. Due to parallel-momentum conservation (see equation (2)) the relevant valence electrons then have $\vec{k}_2^{\parallel} = 0$ and their (crystal half-space plus vacuum-half-space) wavefunctions $\varphi_2^{n\sigma}(\vec{r})$ (with $\sigma = \pm$) can be classified according to the spatial symmetry types Σ_n with $n = 1, 2, 3, 4$. For a coordinate system with z along the surface normal [110] and x and y in the surface plane (chosen along [1$\bar{1}$0] and [001], respectively, for cubic (110) surfaces), the two surface-perpendicular mirror planes are (x, z) and (y, z). The valence electron wavefunctions then behave as follows under reflection at the two mirror planes: $\varphi_2^{1\sigma}$ is symmetric with respect to both, $\varphi_2^{2\sigma}$ is antisymmetric with respect to both, $\varphi_2^{3\sigma}$ is antisymmetric with respect to (x, z) and symmetric with respect to (y, z), and $\varphi_2^{4\sigma}$ is symmetric with respect to (x, z) and antisymmetric with respect to (y, z).

As the (e, 2e) reaction plane we choose first the (x, z) and second the (y, z) plane. From the results of section 2 we then easily obtain the (e, 2e) intensity contributions $I_n^{\sigma\sigma}$ (see equation (6)) and $I_n^{\sigma\bar{\sigma}}$ (see equation (8)), which are summarized in table 1. Valence electron states of Σ_1 symmetry contribute to $I^{\sigma\bar{\sigma}}$, but not to $I^{\sigma\sigma}$ due to their symmetry with respect to the (y, z) plane and consequently $g_1 = f_1$ (second selection rule). Valence electron states of Σ_2 symmetry cannot be 'seen' in the (e, 2e) spectra for both reaction planes.

Table 1. (e, 2e) selection rules in coplanar symmetric equal-energy set-up from ferromagnetic crystalline surface systems with a two-fold rotation axis and two mirror planes normal to the surface (spatial symmetry group $2mm$). For valence states with spatial symmetry types Σ_1, Σ_2, Σ_3, Σ_4, the first two rows indicate the even and odd mirror symmetry (+ and −) of the state with respect to the (x, z) and (y, z) planes, where z is normal to the surface. For bcc and fcc(110) surfaces, the in-surface-plane coordinates x and y are chosen along $[1\bar{1}0]$ and $[001]$, respectively. The subsequent rows give the contributions to the anti-parallel-spin cross section $I^{\sigma\bar{\sigma}}$ (equation (8)) and the parallel-spin cross section $I^{\sigma\sigma}$ (equation (6)), for the reaction plane chosen firstly as (x, z) and secondly as (y, z).

	Valence electron mirror symmetry plane		(e, 2e) in (x, z) plane contributions to		(e, 2e) in (y, z) plane contributions to	
	(x, z)	(y, z)	$I^{\sigma\bar{\sigma}}$	$I^{\sigma\sigma}$	$I^{\sigma\bar{\sigma}}$	$I^{\sigma\sigma}$
Σ_1	+	+	$2|f_1^{\sigma\bar{\sigma}}|^2$	0	$2|f_1^{\sigma\bar{\sigma}}|^2$	0
Σ_2	−	−	0	0	0	0
Σ_3	−	+	0	0	$2|f_3^{\sigma\bar{\sigma}}|^2$	$4|f_3^{\sigma\sigma}|^2$
Σ_4	+	−	$2|f_4^{\sigma\bar{\sigma}}|^2$	$4|f_4^{\sigma\sigma}|^2$	0	0

For the (x, z) reaction plane, there is no contribution from Σ_3 states on the grounds of our first selection rule, but Σ_4 states do contribute, most notably also to $I^{\sigma\sigma}$, since their antisymmetry with respect to reflection at the (y, z) plane entails $g_4 = -f_4$ (see equation (6)). The scattering cross section of a spin σ primary electron with a spin σ valence electron stems thus exclusively from valence electrons of Σ_4 symmetry. For the (x, z) reaction plane, the results are analogous, with Σ_3 and Σ_4 interchanged.

In view of studying quantitatively the allowed (e, 2e) spectra and their relation to the spin-polarized bulk band structure and the spin- and layer-resolved density of states, we have performed numerical calculations for the ferromagnetic Fe(110) surface by means of a layer-KKR code [10], in which an equivalent of the original expression equation (1) in terms of the valence electron spectral function has been implemented. The real part of the effective one-electron potential was obtained from a nine-layer-film self-consistent GGA-FLAPW [11] charge density. For the imaginary part of the potential we chose -0.05 eV for the valence electrons—which is not energy-dependent and rather small in order to make our symmetry analysis more transparent—and $-0.07(E_i - E_F)$ with $i = 1$ for the incident and $i = 3, 4$ for the emitted electrons. The screened Coulomb interaction $U(\vec{r}, \vec{r}')$ in equation (1) was approximated by the form $\exp((|\vec{r}-\vec{r}'|)/\lambda)/|\vec{r}-\vec{r}'|$, with the parameter λ chosen as the Thomas–Fermi screening length $\lambda = (4\pi n(E_F))^{-1/2}$, where $n(E_F)$ is the total density of states per unit volume at the Fermi energy as obtained in our self-consistent GGA-FLAPW calculation [11]. In accordance with previous computational experience we note that a variation of λ within a physically reasonable range affects the absolute magnitudes of the calculated spectra but leaves the relative magnitudes of individual features within the spectra essentially unchanged.

In figure 1 we show the spin-resolved bulk band structure of Fe along $\Gamma(\Sigma)N$ and the spin- and spatial-symmetry-resolved bulk and surfaces layer densities of states (LDOS) of the Fe(110) surface for $\vec{k}^{\parallel} = 0$. For each symmetry type Σ_i the bulk LDOS features are seen to be associated with the bands in the usual way. The surface LDOS (topmost atomic layer) is significantly different. In particular, there are sizeable surface state or resonance peaks of Σ_1 symmetry for both spin directions and of Σ_4 symmetry for majority spin.

In figure 2(a) we present, for fixed emission angles in the (x, z) reaction plane, a typical set of equal-energy-sharing (e, 2e) cross sections from Fe(110) as functions of the valence electron energy relative to the Fermi energy. The solid and dashed spectra in the topmost panel result
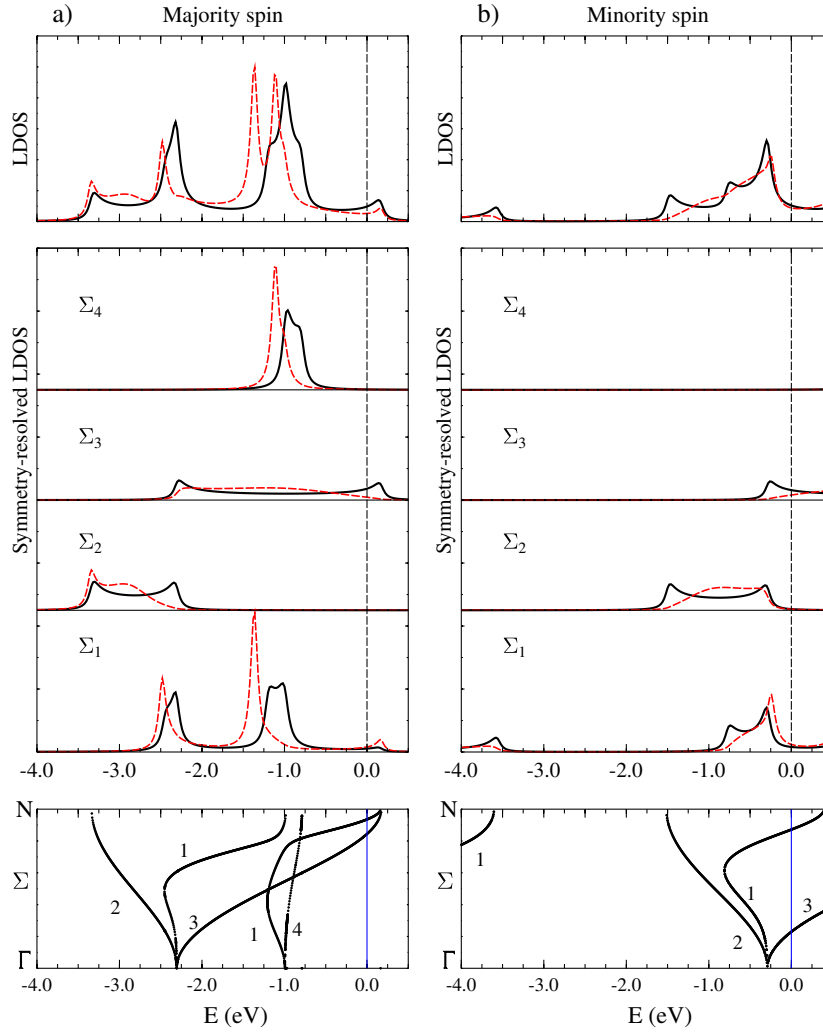
Figure 1. Valence electron states (without spin–orbit coupling) of ferromagnetic Fe(110): (a) for majority spin; bottom panel: bulk band structure along $\Gamma(\Sigma)N$ with the symbols 1–4 indicating the spatial symmetry types Σ_1, Σ_2, Σ_3, Σ_4 of the individual bands. Top panels: bulk (solid curves) and surface (broken curves) layer-resolved densities of states (LDOS) for the four symmetry types Σ_i and their sum (in the uppermost panel). (b) As (a), but for minority spin. (The Σ_4-LDOS is negligible in the present plotting range.)

from spin-up and spin-down primary electrons, respectively, without detection of the spins of the two emitted electrons. With this spin analysis, the top-panel spectra decompose into those shown in the lower two panels. Comparison of these partial spectra with the symmetry- and spin-resolved valence electron LDOS in figure 1 reveals their detailed origin as indicated by the symbols 1^+, 1^- and 4^+ above the respective peaks. The locations of the peaks are seen to coincide with the corresponding features of the surface LDOS rather than those of the bulk LDOS. This demonstrates, in line with earlier findings [5] that (e, 2e) spectroscopy is extremely surface-sensitive. In accordance with table 1, Σ_2 and Σ_3 valence electrons do not manifest themselves in the spectra at all.
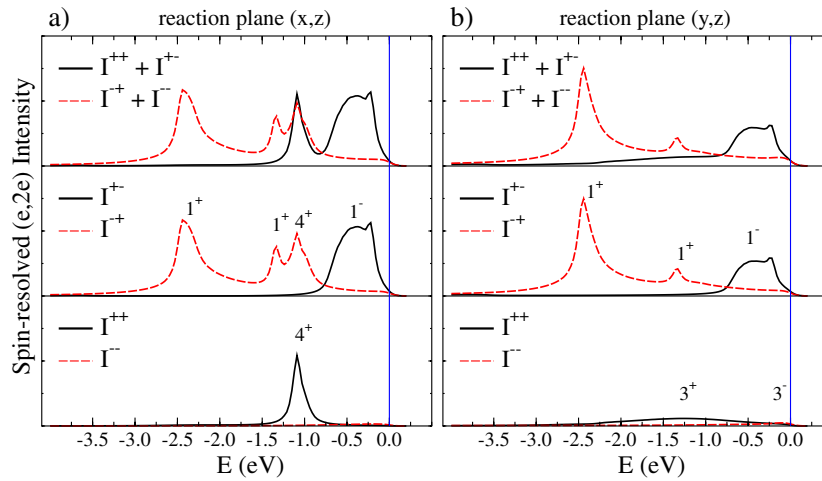
Figure 2. (a) Calculated (e, 2e) intensity spectra $I^{\sigma\sigma}$ (equation (6)), $I^{\sigma\bar\sigma}$ (equation (8)) and their sums from Fe(110) surface in symmetric coplanar geometry with reaction plane (x, z) (intersecting the surface along $[1\bar{1}0]$) for normally incident primary electrons with energy $E_1 = 22.7$ eV and spin polarization along the majority (solid curves) and minority (dashed curves) spin directions. The two emitted electrons have equal energies $E_3 = E_4$ and propagate at fixed polar angles $\theta_3 = \theta_4 = 40°$ relative to the surface normal (z-axis). The intensities are thus functions of $E_3 = E_4$ and can, because of energy conservation $E_2 = 2E_3 - E_1$, also be regarded as functions of the valence electron energy $E_2 =: E$, which we take (relative to the Fermi energy) as the abscissa. In the lower two panels, the symbols 1^+, 1^- and 4^+ above individual peaks indicate their origin from majority (+) and minority (−) valence electron states of Σ_1 and Σ_4 symmetry. (b) Same as (a) but for reaction plane (y, z) (intersecting the surface along [001]) and the symbols 3^+ and 3^- indicating that the respective peaks originate from Σ_3 majority and minority spin valence electrons.

Analogous results obtained for the (y, z) reaction plane are shown in figure 2(b). In this case, Σ_2 and Σ_4 valence electrons do not contribute, whereas the majority spin Σ_3 surface density of states (see figure 1(a)) is seen to be reflected in the cross section for collisions with spin-up primary electrons in the bottom panel of figure 2(b). The Σ_1-derived features in the central panel are at the same energies as in the case of the (x, z) reaction plane, but their relative heights are significantly different. The latter result is due to the fact that the off-normal time-reversed LEED states ψ_3 and ψ_4, and consequently the matrix elements, are quite different in the two cases.

In table 1 and figure 2 transitions involving Σ_2 valence states are forbidden by the first selection rule, since the (e, 2e) reaction plane has been chosen parallel to a mirror plane of the crystalline system. If, however, the reaction plane is rotated about the surface normal by some arbitrary angle, Σ_2 valence states will manifest themselves—together with states of the other three symmetry types—in the (e, 2e) cross sections.

4. Conclusion

We have analytically derived two selection rules for (e, 2e) spectroscopy from ferromagnetic surface systems, which arise from spatial symmetries of the valence electron states for coplanar geometries, i.e. momenta of the incident electron and of the two detected electrons in a plane. If this reaction plane is a mirror plane of a semi-infinite crystalline system normal to the surface, the *first selection rule* entails that valence electron states, which are antisymmetric

with respect to the reaction plane, do not manifest themselves in (e, 2e) scattering cross sections at all. This holds irrespective of whether the primary electrons are spin polarized or the detected electrons are spin-analysed. The *second selection rule* has been obtained for coplanar symmetric geometries with normal incidence of the primary electron and equal energies and oppositely equal parallel momenta of the two detected electrons, in which the plane normal to the reaction plane and to the surface plane is a mirror plane of the crystalline system. In this case, the cross section for the detection of a parallel-spin pair arises exclusively from valence electron states, which are antisymmetric with respect to this plane. In contrast, the cross section for the detection of an antiparallel-spin pair contains contributions due to both antisymmetric and symmetric valence electron states.

Although these two selection rules are strictly speaking valid only in the absence of spin–orbit coupling, they will hold in good approximation and be useful over wide energy and momentum ranges, in which the valence electron spinor is dominated by a particular spatial symmetry type.

For (e, 2e) spectroscopy from ferromagnets by spin-polarized primary electrons (see [8] and references therein) the second selection rule has important consequences for the interpretation of equal energy sharing spectra in terms of the spin-split valence electron structure. The spin-up (spin-down) spectra reflect not only spin-down (spin-up) valence states, but also spin-up (spin-down) valence states. In favourable cases, like for Fe(110), the solid curves in figure 2(a), the peaks arising from valence electrons of opposite spins are well separated in energy. In less favourable cases, they can be resolved by theory and possibly by future experiments with spin analysis of the detected electrons.

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