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L_3VV Auger electron spectra

The influence of crystal-field splitting and electron diffraction on the spin polarization of Fe L_3VV Auger electron spectra

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Abstract. The spin polarization of Auger electrons escaping from the Fe(100) surface has been calculated. All possible sources giving rise to spin polarization are discussed. It has been shown that taking account of different orbital symmetries of the valence d states, and including the electron diffraction by the surrounding atoms can significantly affect the value of the Auger electron spin polarization. The ratio of the T_{2g} and E_g contributions to the Auger electron intensity also determines the shape of the Fe L_3VV spectrum.

1. Introduction

Recently the magnetic behaviour of metallic surfaces, adlayers, and thin films has been intensively studied by means of spin-resolved spectroscopic techniques [1–7]. It has been shown [8] that spin-polarized Auger electron spectroscopy is a powerful probe of local magnetic properties of surfaces. In the case where the valence electrons are involved in the Auger transition, the local spin polarization of valence states should be reflected in the spin polarization of the Auger spectrum. However, the question of the relationship of these two quantities requires more detailed investigations. Sinković *et al* [9] have measured the spin polarization of the $L_3M_{45}M_{45}$ Auger transition in iron. They have obtained values for the integrated spin polarization which differ from the spin polarization of Fe valence electrons. These results have been discussed in terms of the density of states (DOS) for spin-up and spin-down valence electrons. From the experimental data, the ratio of the Auger transition probability for the valence electrons with parallel spins to that for the electrons with antiparallel spins has been estimated to be about 2:3. This consideration seems to be very simplified, in view of the many other factors which could also influence the value of the Auger electron spin polarization, and the process of the Auger transition should be studied more carefully.

   In particular, it was shown [10] that a single-band description, and a self-convolution of the single-particle d DOS only gives a very poor description of the Auger spectrum. Presilla and Sacchetti [10] have suggested using a many-band Hubbard Hamiltonian to calculate the shape of the Auger spectra of transition metals. They succeeded in explaining the shape of the M_1VV Auger rate for copper, introducing different parameters for the valence states of s, d(T_{2g}) and d(E_g) symmetry. In contrast to the atomic-like Cu CVV spectra, the Auger

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spectra of Fe retain a band-like shape, and the energy structure of the valence subbands would be even more important for the formation of the Auger electron distribution than in the case of Cu.

The aim of our paper is to discuss the formation process of the Fe L_3VV Auger spectrum in more detail, and to analyse the factors that can contribute to the spin polarization of the escaping Auger electrons. The theoretical description of the Auger process, and the details of calculations are presented in sections 2 and 3. The effect of the spin-dependent matrix elements is discussed in section 4. In section 5 we discuss the convoluted DOS for different subband–spin combinations. Conclusions are drawn in section 6.

2. Basic equations

The theoretical model and the main approximations used for the description of the Auger process have been given in [11]. Here we present the general expressions used for the calculation of the spin-polarized Auger electron intensity.

Let us consider the electron states involved in the core–valence–valence Auger transition: a core state c (quantum numbers j_c, l_c, μ_c) and two valence states i_1, i_2 (quantum numbers $l_{1,2}, m_{1,2}, \sigma_{1,2}$). The escaping Auger electron (final state, energy E) is described by a sum over spherical waves characterized by quantum numbers $L\ (=l, m)$ and σ. An initial excited state for the Auger decay (core hole c) could be created by photoionization. Then the core holes μ_c have different weights determined by the dipole transition probability and especially by the polarization of the light. Hole states $|j_c l_c \mu_c\rangle$ are created, where the spinors χ_+ and χ_- have different factors; furthermore, they are connected with different spherical harmonics. This is a source of the spin polarization of the photoelectron. It is usual (but not exact) to say that the core hole has a preferred spin. The spin polarization of the hole states is transferred to the Auger electron via the matrix element M of the Auger process:

$$M(L\sigma, c|i_1, i_2) = \langle f_{L\sigma}, c|V|i_1, i_2\rangle - \langle f_{L\sigma}, c|V|i_2, i_1\rangle. \tag{1}$$

It contains the expectation value of the Coulomb interaction, and the corresponding exchange integral.

If we assume that the matrix elements are independent of the energy of the valence states [12], then after integration over the Brillouin zone we can write the expression for the spin-polarized intensity of the Auger electrons in a direction e ($e = r/r$, $k = ke$, $k = \sqrt{E}$) in the form

$$I_\sigma(E, k) = \sum_{g_1 g_2} \langle M_\sigma^2 \rangle_{g_1 g_2} \int D_{g_1}(E + E_c - \varepsilon)\, D_{g_2}(\varepsilon)\, \mathrm{d}\varepsilon \tag{2}$$

where $D_g(\varepsilon)$ is the local partial DOS of the valence state (g denotes a set of quantum numbers characterizing the valence electron state). In magnetic systems like iron, the valence states are spin polarized. They can also contribute to the Auger electron spin polarization due to the different fractions of majority- and minority-spin states in the DOS convolution.

The Auger transition probabilities $\langle M_\sigma^2 \rangle_{g_1 g_2}$ can be expressed as

$$\langle M_\sigma^2 \rangle_{g_1 g_2} = \sum_{\mu_c} w_{\mu_c}(\epsilon, \hbar\omega) \left| \sum_L B_{L\sigma}(k)\, M(L\sigma, c|i_1, i_2) \right|^2. \tag{3}$$

$w_{\mu_c}(\epsilon, \hbar\omega)$ is the photoionization probability for the electron state μ_c in the core shell c. It depends on the polarization ϵ and on the energy $\hbar\omega$ of incoming photons. $B_{L\sigma}(k)$ is the scattering path operator. This expression is the same as the one that describes the electron

scattering in LEED and photoelectron diffraction [13–19]. It contains the expressions for the direct wave, and the single- and multiple-scattering contributions. In magnetic systems the spin polarization of the outgoing Auger electrons may be changed due to the spin dependence of the surrounding scattering potentials [20–22], which is reflected in the spin dependence of the scattering phase shifts involved in B. The effect of the electron diffraction on the Auger electron spin polarization depends also on the position R of the atom emitting the Auger electron in the crystal lattice with respect to the surface. Thus, B depends on R, and the Auger intensity is a sum over contributions (2) for different sites R.

In order to obtain the integral intensity of the core–valence–valence transition considered, we have to integrate the spectral intensity (2) over the region of Auger electron energies E. This gives

$$I_\sigma(\mathbf{k}) = \int I_\sigma(E, \mathbf{k}) \, \mathrm{d}E = \sum_{g_1 g_2} n_{g_1} n_{g_2} \langle M_\sigma^2 \rangle_{g_1 g_2} \tag{4}$$

where n_g is the occupation number for the corresponding valence subband. The spin polarization of the Auger electrons is obtained from the calculated spin-polarized intensities (2) as

$$P_{\text{AES}} = \frac{I_\uparrow - I_\downarrow}{I_\uparrow + I_\downarrow}. \tag{5}$$

For the integral spin polarization, the corresponding integral intensities (4) should be inserted into expression (5).

If we consider the spin polarization of the Auger electron intensity (2), we have to fix the axis of quantization. In magnetic systems we have a preferred direction due to the direction of the magnetization M. This axis is usually used for the evaluation of the matrix elements (1), and for the scattering path operator B. But, in an experiment, the spin polarization of the escaping Auger electron can also be measured with respect to the electron wave vector $\mathbf{k}$ or—for photoionization—with respect to the photon wave vector. The degree of the spin polarization depends on this choice, but the values could be recast for another coordinate system by means of spinor rotation. We note that in what follows the coordinate system is used in which the direction of the z-axis (the axis of quantization) coincides with that of the magnetization M.

3. Details of the calculation

For our calculations we consider a geometry similar to the one used in the experiment performed by Sinković *et al* [9]. Auger electron emission was excited from the Fe(100) surface by photoionization with linearly polarized soft x-ray photons. We consider the off-resonance case where the photon energy of 820 eV was used. The photons were incident at 45° with respect to the surface normal; the polarization ϵ lies in the plane given by the surface normal and the photon wave vector. The Auger electrons were collected along the surface normal. The core holes created by the linearly polarized photons are non-polarized. Thus, for this case the spin polarization of Auger electrons will be caused by the polarized valence states. A further source of the spin polarization is the Auger electron diffraction.

The iron surface has an in-plane magnetization M directed along the [001] axis of the cubic lattice. We choose the x-axis of the coordinate system antiparallel to the surface normal, and the y-axis in the surface plane.

We simulate the Fe(100) surface with a system of muffin-tin potentials. The spherically symmetric spin-polarized potential in the muffin-tin spheres was calculated using the

Mattheiss construction [23]. For the exchange and correlation part of the potential, the von Barth–Hedin approximation [24] was used. The dipole matrix elements and the Auger matrix elements were calculated using scalar relativistic wave functions. Taking into account the relaxation of electron states by the core hole, the Auger matrix elements (1) were obtained using the wave functions calculated including the core-hole potential, whereas for the dipole matrix elements the wave functions of the ground state were used.

The local partial densities of states, and the occupation numbers for the valence subbands were calculated by means of the recursion method [25], using tight-binding parameters published by Papaconstantopoulos [26]. The magnetic moments of the iron atoms in the bulk were chosen to be equal to 2.2 μ_B. The recursion method allows us to calculate local DOS at a surface site. At this site we get a magnetic moment of 2.6 μ_B. The magnetic moment caused by the valence d electrons only is to some extent higher, because the s, p subband has a small negative magnetic moment.

The partial contributions to the DOS from the electron states of different symmetries— s, p, d(T_{2g}), d(E_g)—were also calculated. Furthermore, we could include the breaking of the cubic symmetry at the surface. Thus, for example, the local (yz) DOS differs from the (xy) or (xz) DOS.

4. Auger transition probabilities

If we consider the Fe L_3VV spectrum, it should be noted that the Auger electron intensity is mainly determined by the transitions involving two valence d electrons. The calculated Auger matrix elements (1) for the final-state configuration with one s and one d hole in the valence band or with two s holes are about ten times smaller than that for the configuration with two valence d holes. Taking into account the occupations of the s and d subbands (or the partial DOS), the contributions to the Auger electron intensity differ by three orders of magnitude. Thus, the effect of the s subband on the intensity and, consequently, on the spin polarization of the Auger electrons is negligible, and in the following consideration it is not taken into account (but is always included in the numerical evaluation). In this case it is possible to talk about $L_3M_{45}M_{45}$ spectra.

4.1. A simple model: the degenerate d band

In order to compare our results with those of reference [9], we consider a simplified picture: two degenerate d subbands which are split by the exchange interaction. Furthermore, we assume for the Auger transition probabilities (3) that

$$\langle M_\uparrow^2 \rangle_{\uparrow\uparrow} = \langle M_\downarrow^2 \rangle_{\downarrow\downarrow} = T$$
$$\langle M_\uparrow^2 \rangle_{\uparrow\downarrow} = \langle M_\downarrow^2 \rangle_{\downarrow\uparrow} = S. \tag{6}$$

It follows directly from equations (4) and (5) that, for the given occupation of the spin-up and spin-down subbands, the integral spin polarization of Auger electrons depends only on the ratio S/T of the singlet and triplet transition probabilities:

$$P_{\mathrm{AES}} = P_{\mathrm{VB}}\left[1 + 2\frac{n_\uparrow n_\downarrow}{n^2}\left(\frac{S}{T} - 1\right)\right]^{-1} = P_{\mathrm{VB}}\left[1 + \frac{1}{2}(1 - P_{\mathrm{VB}})^2\left(\frac{S}{T} - 1\right)\right]^{-1} \tag{7}$$

where $n = n_\uparrow + n_\downarrow$ is the total d-electron number, and $P_{\mathrm{VB}} = (n_\uparrow - n_\downarrow)/n$ is the spin polarization of the d band.

Even in this simple model, it can be seen that P_{AES} is equal to P_{VB} only for the case where $S/T = 1$ (or where $P_{\mathrm{VB}} = 1$). Other values of the S/T ratio could lead to quite

different values of the Auger electron spin polarization: from $P_{AES} = 0$ for $S \gg T$ to $P_{AES} = (n_\uparrow^2 - n_\downarrow^2)/(n_\uparrow^2 + n_\downarrow^2) > P_{VB}$ for $S \ll T$. This simplified picture has already been discussed in [9]. It should be noted however that P_{VB} in (7) is referred to the number of valence d electrons, and not to the total number of valence electrons as is the case in [9].

Table 1. Calculated Auger transition probabilities $\langle M_\sigma^2 \rangle_{\sigma_1 \sigma_2}$ and integral intensities $I_\sigma(\mathbf{k})$ for normal emission (averaged over all d orbitals; all values are multiplied by a factor of 10^6). Partial contributions of p and f waves to the transition probabilities are also shown. The data were obtained for the bulk emitter position in the fifth atomic layer from the surface; only the direct Auger wave was included in the scattering path operator B.

Auger electron spin	$\sigma = \uparrow$		$\sigma = \downarrow$	
Final hole configuration	$(d\uparrow, d\uparrow)$	$(d\uparrow, d\downarrow)$	$(d\downarrow, d\uparrow)$	$(d\downarrow, d\downarrow)$
$\langle M_\sigma^2 \rangle_{\sigma_1 \sigma_2}$	0.156	0.741	0.749	0.152
p + f	0.156	0.721	0.729	0.152
p	0.011	0.033	0.033	0.011
I_σ	11.130		8.726	

According to our calculations for the iron atom in the bulk, the occupation of d subbands is 4.6 electrons for the spin-up states and 2.3 electrons for the spin-down states; therefore we have $P_{VB} = 0.333$. The calculated Auger transition probabilities (3) averaged over all d orbitals, and the integral intensities (4) are presented in table 1.

It follows from Auger transition selection rules that the $L_3 M_{45} M_{45}$ transition creates outgoing Auger electron waves with $l = 1, 3, 5$. However, it can be seen from table 1 that the fraction of the f wave dominates; its contribution to the Auger electron emission is over 90%.

Furthermore, one can see that the assumption (6) is accurate only for the matrix elements calculated with non-spin-polarized wave functions. The differences between the radial parts of the spin-up and spin-down functions calculated in the spin-polarized potential cause differences of a few per cent in the transition probability values, as shown in table 1. Nevertheless, we can estimate the singlet–triplet ratio as $S/T \approx 4.8$. It has already been shown that for $S > T$ we have $P_{AES} < P_{VB}$. From the intensity values given in table 1, one can obtain the spin polarization of Auger electrons of 0.121 in this simplified consideration.

For the surface atoms, the calculated results differ from those for atoms in the bulk. The differences in the transition matrix elements are not substantial ($S/T \approx 4.9$ for surface atoms), and the main effect on the spin polarization of Auger electrons arises from the higher magnetic moment of the surface atoms. As a result, we have for the Auger emission from the surface layer $P_{AES} = 0.136$, again in this simplified model.

4.2. Symmetrized cubic orbitals

Let us improve the theoretical model of section 4.1 in order to distinguish separate d states which have a different spatial orientation. We consider the symmetrized combinations of the d orbitals that belong to the irreducible representations E_g and T_{2g} of the cubic symmetry group. Both the energy distribution over the valence band and the spin polarization are different for the electron states of E_g and T_{2g} symmetry [26]: the Fe T_{2g} subband has 2.7 and 1.6 electrons in spin-up and spin-down states, respectively, whereas the E_g subband has 1.9 and 0.7 electrons correspondingly. The different orientations of orbitals could be

important for the angular dependence of the intensity and the spin polarization of the Auger electron emission.

Table 2. Calculated Auger transition probabilities $\langle M_\sigma^2 \rangle_{g_1 g_2}$ (g is a symmetry–spin parameter, the d-orbital indices are $(1, 2, 3, 4, 5) = (xy, yz, xz, x^2 - y^2, 3z^2 - r^2)$, and all values are multiplied by a factor of 10^6). The emitter position is as for table 1.

g_1	$1\uparrow$	$2\uparrow$	$3\uparrow$	$4\uparrow$	$5\uparrow$	$1\downarrow$	$2\downarrow$	$3\downarrow$	$4\downarrow$	$5\downarrow$
					g_2					
$1\uparrow$	$\times$	0.756	0.0	0.075	1.102	0.958	1.579	0.0	1.844	0.405
$2\uparrow$	—	$\times$	0.722	0.0	0.0	0.156	0.150	0.150	0.0	0.0
$3\uparrow$	—	—	$\times$	1.015	0.218	0.0	1.511	0.958	0.020	2.331
$4\uparrow$	—	—	—	$\times$	0.0	2.138	0.0	1.236	1.795	0.928
$5\uparrow$	—	—	—	—	$\times$	0.176	0.0	1.182	0.928	0.079
$1\downarrow$	0.968	1.598	0.0	1.861	0.409	$\times$	—	—	—	—
$2\downarrow$	0.158	0.151	0.151	0.0	0.0	0.741	$\times$	—	—	—
$3\downarrow$	0.0	1.525	0.968	0.020	2.359	0.0	0.709	$\times$	—	—
$4\downarrow$	2.158	0.0	1.250	1.809	0.937	0.072	0.0	0.990	$\times$	—
$5\downarrow$	0.176	0.0	1.197	0.937	0.079	1.080	0.0	0.214	0.0	$\times$

In table 2 the calculated Auger transition probabilities for different symmetry–spin combinations of the valence d states for the Fe atom in a cubic lattice can be found. It should be noted that these values were calculated according to (3), but only the direct Auger electron wave was included in the scattering path operator B. Above the diagonal the values for the spin-up Auger electrons ($\sigma = \uparrow$) are given, whereas under the diagonal the values for spin-down states ($\sigma = \downarrow$) can be found. One can see that only half of the different d-orbital combinations could create a configuration contributing to the Auger electron intensity. Except for certain combinations where the Pauli principle applies (the corresponding cells are denoted by $\times$ in table 2) or where spin conservation holds (these cells are denoted by —), the angular integration involved in the Auger transition matrix elements (1) provides zero contribution (0.0 appears in the corresponding cells). It should be noted that for directions of escaping Auger electrons other than that of the surface normal, these disappearing contributions retain their zero value, whereas the non-zero values of the Auger transition probabilities (3) can be different, due to the dependence of the scattering path operator $B_{L\sigma}(\mathbf{k})$ on the Auger electron moment $\mathbf{k}$. Owing to the radial integration over wave functions which are solutions in the spin-polarized potential, assumption (6) is valid only approximately. For example, the Auger transition probability for the symmetry–spin combination $(xy\downarrow, yz\uparrow)$, 1.598, differs by a few per cent from that for $(xy\uparrow, yz\downarrow)$, 1.579.

It can be seen from table 2 that the calculated Auger transition probabilities have quite different values. The differences can exceed an order of magnitude. This means that for the given geometry of the Auger emission measurements, some of the d orbitals provide a dominant contribution. This can however affect the Auger electron intensity (and consequently, spin polarization) only insignificantly, if the increasing contribution of any orbital configuration is compensated by decreasing contributions from other orbitals belonging to the same irreducible representation of the cubic symmetry group. Another situation is seen in the case of decreased symmetry at the surface, where the energy degeneracy of the subbands is removed. Owing to the occupation numbers being different for separate subbands, the spin polarization of the Auger emission from the surface layer increases to $P_{\text{AES}} = 0.154$. For the atom in the bulk we have the same occupation numbers

for the three T_{2g} orbitals, and this is the case for the two E_g orbitals too. In spite of the difference in occupation of the T_{2g} and E_g orbitals, the intensity values are very close to those calculated for the same occupation for all d states. As a result, the value of the spin polarization is practically unchanged (0.120) from that for the case where we do not distinguish the separate d orbitals.

4.3. The effect of the electron diffraction

The role of the spatial orientation of the d orbitals in the formation of the spin-polarized Auger electron distribution increases if in the calculations the scattering of escaping electrons by the surrounding atoms is taken into account. Without Auger electron diffraction, the contributions to the intensity decrease smoothly in going from the surface layer to the inside of the crystal. Diffraction effects change the situation considerably, increasing the contributions from the deep layers. It could be concluded that in Fe, for energies of about 700 eV, the forward scattering seems to be important.
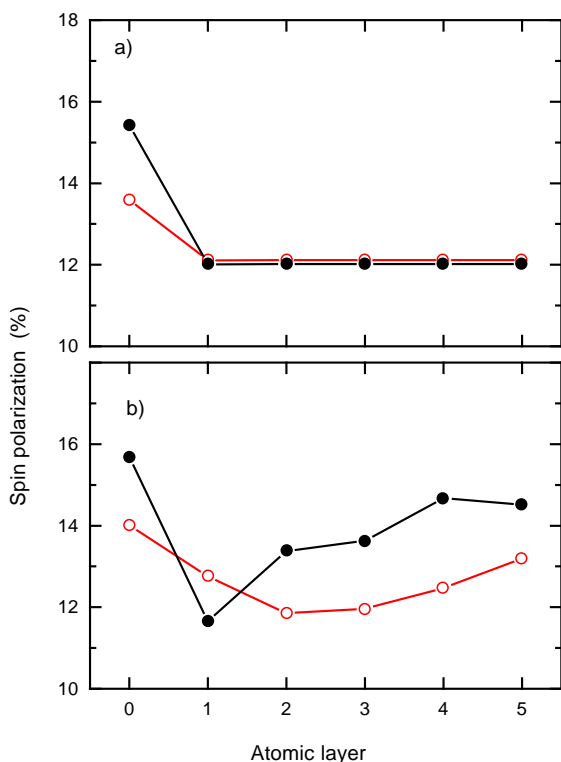

Figure 1. The spin polarization of Auger electrons emitted from different atomic layers (the surface layer is numbered 0). The calculations are performed (a) without and (b) with electron diffraction taken into account. Open symbols denote the results obtained with the same occupation numbers for all five d orbitals, while solid symbols denote those for different occupations of the T_{2g} and E_g orbitals.

It was already pointed out in the preceding subsection that the effect of different occupations for the d orbitals having different orientations is noticeable only for the surface layer, where the cubic symmetry is broken. Including the electron scattering leads to

calculated results which are very sensitive to the occupation numbers of the orbitals. From figure 1 one can see the changes to the Auger electron spin polarization that occur if the scattering is included in the calculations. For most positions of the emitters, the crystal-field splitting *and* the electron diffraction lead to increasing spin polarization of the Auger electrons. For the surface layer emission, we obtain $P_{\text{AES}} = 0.157$, whereas the average value after summation over emitter positions in six atomic layers is equal to 0.141.

5. The convoluted density of states

In section 4 we have discussed the integral spin polarization of the Auger spectrum. It seems interesting to study the spectral distribution of the polarized intensities (2) of Auger electrons. Indeed, the intensity (2) is determined by the convoluted valence DOS, and should reflect the energy distribution of the valence electron states. Moreover, the orientation of a special d orbital could determine the angular distribution of the Auger electrons at any energy if this orbital dominates in the Auger intensity at this energy.
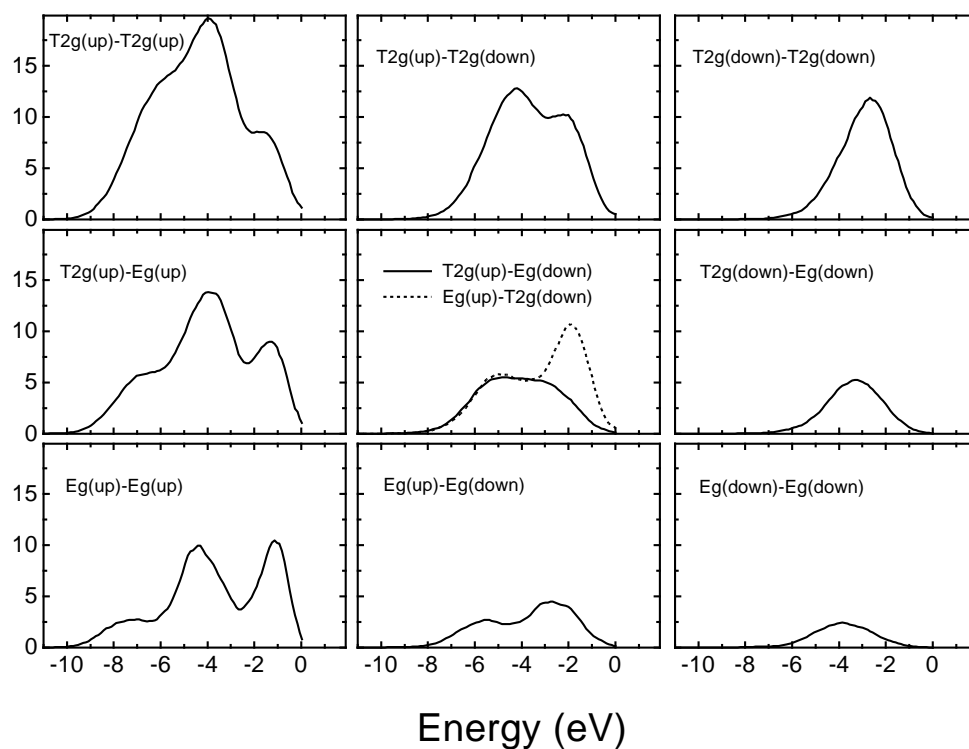

Figure 2. The convoluted Fe partial DOS (arbitrary units).

The convoluted partial DOS are presented in figure 2. One can see that due to the highest occupation the $T_{2g}\uparrow$–$T_{2g}\uparrow$ convolution has the highest intensity. The intensity decreases in going from T_{2g} to E_g, from spin-up to spin-down states, according to the subband occupation numbers. Different combinations of the partial DOS produce convolutions giving different energy distribution curves. However, it is possible to find general features determined by the energy distributions of the valence states. For example, the peak at the energies of

−1 to −2 eV is caused mostly by the $E_g\uparrow$ states, whereas $T_{2g}\uparrow$ states give the dominant contribution to the peak at −4 to −5 eV. Only the triplet $\uparrow$–$\uparrow$ combinations contribute to the shoulder at −7 to −8 eV, whereas the $\downarrow$–$\downarrow$ contributions are localized at −3 to −4 eV.
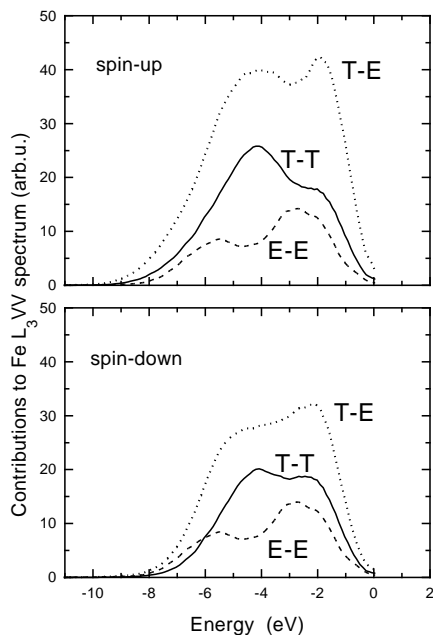

Figure 3. Contributions to the Fe L_3VV spectrum from different orbital combinations: T_{2g}–T_{2g}—solid line; E_g–E_g—dashed line; T_{2g}–E_g—dotted line.

6. Discussion and conclusions

Using expression (2) we can calculate the contributions to the Auger spectrum intensity as separate terms in the sum over g_1g_2. If we compare the convoluted partial DOS (figure 2) with these contributions, which are presented in figure 3, the effect of the Auger transition probabilities $\langle M_\sigma^2 \rangle_{g_1g_2}$ becomes clear. First, the most intense T_{2g}–T_{2g} DOS convolutions do not dominate in the Auger spectrum. The biggest contribution comes from the T_{2g}–E_g combinations, producing almost half of the spectral intensity. Second, the form of the spectral line is determined mostly by singlet transitions. One can see from table 2 that there are no triplet contributions to the spectrum from the E_g–E_g combinations. The shape of the T_{2g}–T_{2g} contribution is the $T_{2g}\uparrow$–$T_{2g}\downarrow$ DOS convolution only slightly modified by $\uparrow$–$\uparrow$ or $\downarrow$–$\downarrow$ terms: for the spin-up Auger electrons, the triplet transitions enhance the peak at the energy −4 eV, whereas for the spin-down Auger electrons, they contribute to the intensity at −2 eV.

The calculated Fe L_3VV spectrum is presented in figure 4. The majority-spin contribution has a two-peak structure: the high-energy peak at −2 eV and the wide peak at −4.5 eV. The maximum of the minority-spin intensity is located between these energies, at −2.5 eV. The energy positions of the spectral features are in very good agreement with the experimental results [9].

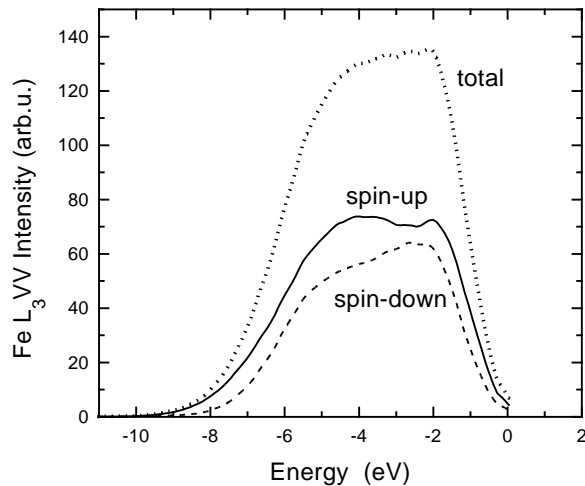It can be seen from figure 4 that the spin polarization of the Fe L_3VV Auger electrons

Figure 4. The Fe L_3VV spectrum, and the majority-spin (solid line) and minority-spin (dashed line) contributions.

is positive over the whole energy range of the spectrum. The spin polarization is higher on the low-energy side of the maximal value of the intensity; in this energy region the spin polarization exceeds the averaged-over-the-spectrum—or integral—value of the spin polarization. The experimental results [9] show the maximal value of $P_{AES} = 0.27$ at 2 eV lower kinetic energy than the intensity maximum, i.e. at -6.5 eV on our energy scale. The calculations give for this energy $P_{AES} = 0.23$, and the spin polarization increases even more for lower energies (with decreasing intensities).

Thus, the calculated results show that, in the case of a non-polarized initial core hole, the spin polarization of the Auger electrons is set essentially by the polarization of the valence band. It should be noted however that, due to the values of the singlet transition probabilities being higher than those of triplet ones, the value of P_{AES} should be always smaller than P_{VB} (see equation (7)). The calculated value of P_{AES} is modified if we take into account the orientation of the d orbitals, and include the breaking of the cubic symmetry at the surface. Involving the spin-dependent scattering of the escaping Auger electrons leads to an increase in P_{AES} in the case considered.

In the experiment described in [9], the integral value $P_{AES} = 0.2$ has been obtained, whereas our calculations give a smaller value of about 0.15. In order to explain this difference we have to consider other factors which could also affect the spin polarization of the Auger electrons.

First, in the case of the off-resonance Fe L_3VV spectrum, there are two channels for creating the L_3 core hole: direct photoionization, and the $L_2L_3M_{45}$ super-Coster–Kronig Auger process. In [9], it is pointed out that the latter contributes less than 8% to the intensity, and could not change the spin polarization significantly. Nevertheless, the L_3 core hole created as a result of the super-Coster–Kronig transition is polarized, and consequently an increase in P_{AES} of a few per cent would be possible.

Second, the dependence of the Auger transition matrix elements on the energy of the valence states [27, 28] could influence the integral spin polarization. In fact, if the electron states at the bottom of the valence band were to contribute to the Auger intensity with higher weight, the integral spin polarization could be enhanced. Finding a way to include

the energy-dependent matrix elements in our theoretical model seems to be a very important problem, which should be considered in our further work.

It seems interesting to study in more detail the Auger electron distribution for different energies in the spectral energy range. Indeed, it follows from figure 3 that the ratio of the E_g and T_{2g} contributions and their contributions in the formation of the Auger electron intensity are different at the energies of -2 eV and of -4.5 eV. These differences could be manifested in the angle-resolved Auger spectra. The theoretical study of this question is in progress now.

Acknowledgments

References

[1] Schneider C M and Kirschner J 1995 *Crit. Rev. Solid State Mater. Sci.* **20** 179
[2] Hermsmeier B, Osterwalder J, Friedman D J and Fadley C S 1989 *Phys. Rev. Lett.* **62** 478
[3] Clarke A, Brookes N B, Johnson P D, Weinert M, Sinković B and Smith N V 1990 *Phys. Rev.* B **41** 9659
[4] Sinković B, Johnson P D, Brookes N B, Clarke A and Smith N V 1995 *Phys. Rev.* B **52** R6955
[5] Stoppmanns P, David R, Müller N, Heinzmann U, Grieb H and Noffke J 1994 *J. Phys.: Condens. Matter* **6** 4225
[6] Müller N, David R, Snell G, Kuntze R, Drescher M, Böwering N, Stoppmanns P, Yu S-W, Heinzmann U, Viefhaus J, Hergenhahn U and Becker U 1995 *J. Electron Spectrosc. Relat. Phenom.* **72** 187
[7] Fuchs P, Totland K and Landolt M 1996 *Phys. Rev.* B **53** 9123
[8] Landolt M 1985 *Polarized Electrons in Surface Physics* ed R Feder (Singapore: World Scientific) ch 9
[9] Sinković B, Shekel E and Hulbert S L 1995 *Phys. Rev.* B **52** R15703
[10] Presilla C and Sacchetti F 1987 *J. Phys. F: Met. Phys.* **17** 779
[11] Rennert P and Kucherenko Yu 1995 *J. Electron Spectrosc. Relat. Phenom.* **76** 157
[12] In spite of the fact that this assumption is widely used for the interpretation of Auger spectra of solids, it is not correct, and has to be improved. The matrix elements may vary by a factor of two over the range of the valence band (see, for example, [28]).
[13] Pendry J B 1974 *Low-Energy Electron Diffraction* (London: Academic)
[14] Lee P A and Pendry J B 1975 *Phys. Rev.* B **11** 2795
[15] Fadley C S 1984 *Prog. Surf. Sci.* **16** 275
[16] Rennert P and Chassé A 1987 *Exp. Tech. Phys.* **35** 27
[17] Speder O, Rennert P and Chassé A 1995 *Surf. Sci.* **331–333** 1383
[18] Marre K, Neddermeyer H, Chassé A and Rennert P 1996 *Surf. Sci.* **357+358** 233
[19] Rennert P, Mück W and Chassé A 1996 *Surf. Sci.* **357+358** 260
[20] Hillebrecht F U, Rose H B, Roth C and Kisker E 1995 *J. Magn. Magn. Mater.* **148** 49
[21] Rose H B, Hillebrecht F U, Kisker E, Denecke R and Ley L 1995 *J. Magn. Magn. Mater.* **148** 62
[22] Rennert P, Mück W and Chassé A 1996 *Phys. Rev.* B **53** 14 262
[23] Mattheiss L F 1964 *Phys. Rev.* **133A** 1399
Mattheiss L F 1964 *Phys. Rev.* **134** A970
[24] von Barth U and Hedin L 1972 *J. Phys. C: Solid State Phys.* **5** 1629
[25] Haydock R 1980 *Solid State Physics* vol 35, ed H Ehrenreich, F Seitz and D Turnbull (New York: Academic) p 215
[26] Papaconstantopoulos D A 1986 *Handbook of the Band Structure of Elemental Solids* (New York: Plenum)
[27] Fowles P S, Inglesfield J E and Weightman P 1991 *J. Phys.: Condens. Matter* **3** 641
[28] Kucherenko Yu N 1995 *J. Electron Spectrosc. Relat. Phenom.* **72** 181