Simple theory for spin polarization of Auger electrons from ferromagnetic solids

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A simple theory is presented explaining some of the important features observed recently for spin polarization of Auger electrons from ferromagnetic solids.

Recently, spin polarization of Auger electrons from ferromagnetic $Fe_{83}B_{17}$ glass has been studied in detail.[1] Depending on the Auger process, positive as well as negative spin polarization was observed. The experimental results are summarized in Fig. 1. Also, one expects on general physical grounds similar behavior of Auger electrons from ferromagnetic solids. Since spin-dependent forces are of fundamental importance,[2] it is of general interest to understand these results. In the following we present a simple theory providing a first qualitative understanding of some of the significant experimental results. Why are Auger electrons from ferromagnetic solids spin polarized; why can this spin polarization $p(E)$ be positive as well as negative; and why is the peak in $p(E)$ shifted to lower-energy E with respect to the peak in the Auger-intensity curve $I(E)$?

It should be noted that spin polarization $p>0$ in Ni of the resonant Auger process $3p^5 3d^{10} \rightarrow 3p^6 3d^8$ after absorption $3p^6 3d^9 \rightarrow 3p^5 3d^{10}$ has been calculated previously by Feldkamp and Davis.[3] These authors obtained, however, almost no spin polarization for nonresonant Auger decay. Here we show that strong spin polarization and $p \gtrless 0$ may result for (nonresonant) $3p^5 3d^0$, etc., Auger decays.

First, we analyze the spin polarization of Auger electrons

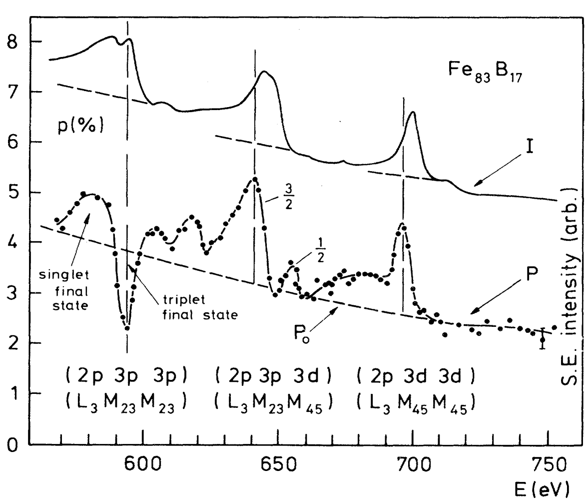

FIG. 1. Illustration of experimental results for the intensity I and spin polarization p (in %) of Auger electrons as a result of various processes at Fe sites. For the $(2p\ 3p\ 3p)$ process the assumed singlet and triplet two-hole final state is indicated. Note relative positions of peaks in $I(E)$ and $p(E)$. The contribution to $p(E)$ due to Auger electrons is given approximately by the deviations of p from the dashed curve p_0.

as a result of the process $(2p\ 3p\ 3p)$ involving a two-hole $3p$ final state and a $2p$-hole initial state. According to Hund's rule coupling Auger electrons associated with the singlet two-hole final $3p$ state $|\uparrow\downarrow\rangle$ should possess smaller kinetic energy than those associated with the triplet two-hole final $3p$ states $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, or $|(\uparrow\downarrow+\downarrow\uparrow)\rangle$. Assuming for the intra-atomic Coulomb interaction energy a value U between 5 and 10 eV, one expects in $I(E)$ a splitting reflecting singlet and triplet two-hole final states, as is observed. Thus we identify in Fig. 1 the peak in $I(E)$ which lies at lower energy E as a result of Auger-electron emission associated with a singlet two-hole final state. The spin polarization[1,2] $p=(I_\uparrow - I_\downarrow)/(I_\uparrow + I_\downarrow)$, where $I_{\uparrow(\downarrow)}$ denotes the intensity of Auger electrons with spin $\uparrow(\downarrow)$ can now be estimated as follows. We assume[4]

$$I_\uparrow \propto |\langle C_\uparrow 2p_\downarrow | V_{\text{Coul}} | 3p_\uparrow 3p_\downarrow \rangle|^2 \ ,$$

where C refers to the emitted Auger electron. $I_\downarrow$ is given correspondingly. Obviously,

$$I_\uparrow \propto m_{2p\downarrow} \ ,$$

where m_{2p} denotes the multiplicity of the $2p$-hole state which makes the $3p \rightarrow 2p$ transition spin selective and which is given by

$$m_{2p\downarrow(\uparrow)} = (2s+1)_d \pm 1 \ ,$$

depending on whether the net spin of the $2p$ shell with one hole is parallel or antiparallel to the net spin S_d of the d electrons. Here we assumed for simplicity an exchange coupling between the $3d$ and the $2p$ spins dominating other spin-dependent forces.[3] Note that the multiplicity of the two-hole final state is the same for C referring to a spin-up or spin-down emitted electron. Hence, for a singlet two-hole final state one obtains approximately

$$p_s \approx \frac{1}{(2s+1)_d} > 0 \ .$$

In the case of Fe one may use $2s_d = 1$ and then $p_s \approx 50\%$ maximally in reasonable agreement with experiment. Of course, configurational mixing[4] and spin-orbit coupling should somewhat modify our estimate for p_s. The spin polarization p_t of Auger electrons associated with the two-hole triplet final state is estimated similarly as p_s. Since the multiplicity m_{3p} of the two-hole $3p$ state is given by $m_{3p} = (2s+1)_d \mp 2$, if the net spin of the $3p$ shell is antiparallel or parallel to the net spin of the $3d$ electrons, and by $m_{3p} = (2s+1)_d$ for the other triplet state, we have now to use

$$I_{\uparrow(\downarrow)} \propto m_{2p} m_{3p} \ .$$

Thus, p_t is approximately given by

$$p_t \approx \frac{[(2s+1)_d - 2] - 3[(2s+1)_d + 2]}{I_1 + I_2 + I_3} < 0 \ ,$$

where I_1, I_2, and I_3 refer to the three triplet states, and for $2s_d = 1$, one estimates $p_t \approx -\frac{12}{14} \approx -80\%$ maximally. Again, this is in fair agreement with the experimental result.[1] Note, $|p_t| > p_s$. Clearly, it follows from our analysis that $p_s = p_t = 0$ if the magnetization of the $3d$ electrons is zero.

Next, we analyze the spin polarization observed for the $(2p\ 3d\ 3d)$-Auger process. Note, no two-peak structure is seen in $I(E)$. This is expected since U for $3d$ electrons should be somewhat smaller than for $3p$ electrons. Furthermore, as illustrated in Fig. 2, we expect that $p(E)$ peaks at an energy of the order of 5 eV below the energy at which one observes a peak for $I(E)$. This results from the exchange splitting of $3d$ spin-up and spin-down bands. The similar shift observed for the $(2p\ 3p\ 3d)$ process results for the same reason and should be of the same order. The width of $p(E)$ and $I(E)$ should be of the order of the d bandwidth. Again, p is estimated by assuming (m_{2p} is neglected for simplicity)

$$I_{\uparrow(\downarrow)} \propto \int d\epsilon N_{d\uparrow(\downarrow)}(\epsilon') N_{d\downarrow(\uparrow)}(\epsilon)$$

in the case of the singlet two-hole d-electron final state, and

$$I_{\uparrow(\downarrow)} \propto \int d\epsilon N_{d\uparrow(\downarrow)}(\epsilon') N_{d\uparrow(\downarrow)}(\epsilon)$$

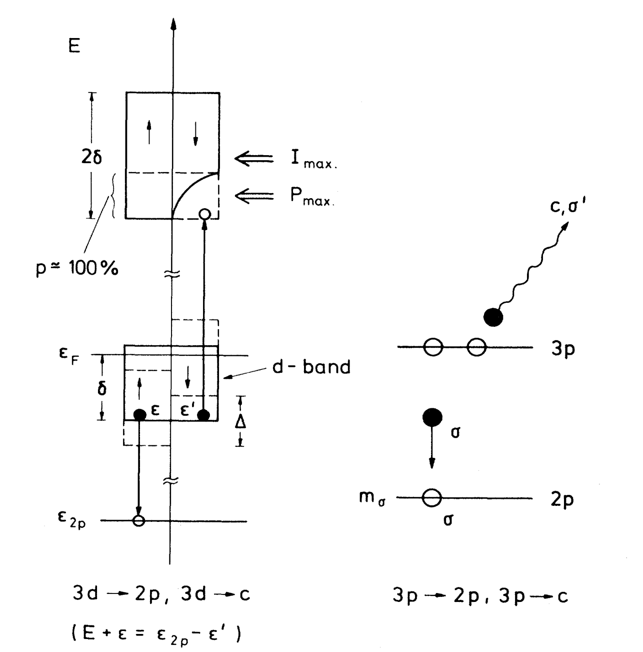

FIG. 2. Illustration of behavior of $I(E)$ and $p(E)$ as a result of the $(2p\ 3d\ 3d)$-Auger process. For Fe we use for the exchange splitting $\Delta \simeq 2$ eV and $\delta \approx 5$ eV in view of the d bandwidth of the order of 5 eV. ϵ_F is the Fermi energy. Then, as indicated, one obtains that the peaks in $I(E)$ and $p(E)$ are split by about 5 eV. Also, we illustrate the $(2p\ 3p\ 3p)$ process. Note the spin dependence of the multiplicity m_σ of the $2p$ state with one hole causes the spin selectivity of the $3p \rightarrow 2p$ transition.

in the case of the two-hole triplet final state. Here, $N_{d\sigma}(\epsilon)$ is the density of states for d electrons with spin σ. The energy ϵ' of the emitted Auger electron can be simply expressed by ϵ with use of energy conservation. Approximating for simplicity $N_{d\sigma}(\epsilon)$ by rectangularly shaped density-of-states curves, it is easy to see how $p_s > 0$ and $p_t > 0$ since there are simply more d electrons with spin up than with spin down. Assuming overlapping singlet and triplet two-hold final states, we estimate a total spin polarization

$$p \propto \sum_\sigma \int N_{d\sigma}(\epsilon)[N_{d\uparrow}(\epsilon') - N_{d\downarrow}(\epsilon')] d\epsilon \ .$$

Thus, approximately $p \propto M$, $p > 0$, where M denotes the d-electron magnetization and p is estimated to be of the order of 25% in excellent agreement with experiment. Since approximately $p \propto M$, we predict a smaller spin polarization, for example, if Fe is replaced by Ni.

Note, applying our analysis also to the $(3p\ 3d\ 3d)$ process, we find similar results for p_s, p_t, or p as in the case of the $(2p\ 3d\ 3d)$ process. This explains the observed large peak in $p(E)$, but not the smaller satellite peak.[1]

Finally, we analyze the spin polarization of Auger electrons as a result of the $(2p\ 3p\ 3d)$ process. The singlet-triplet splitting in $I(E)$ is smaller than for $(2p\ 3p\ 3d)$ since U between $3p$ and $3d$ electrons is expected to be somewhat smaller than U between $3p$ electrons. For p_s and p_t one expects, on general physical grounds, a behavior in-between that one for the $(2p\ 3p\ 3p)$- and $(2p\ 3d+3d)$-Auger process. As is obvious from Fig. 2, as a result of the exchange splitting of the $3d\sigma$ bands, the peak in $p(E)$ is shifted by about 2–3 eV to lower energy as compared with the peak in $I(E)$. Then, neglecting for simplicity spin-orbit coupling, one obtains for the Auger process $3p \rightarrow 2p$ and $3d \rightarrow c$ for the emitted electrons c a spin polarization which is approximately given by

$$p \approx \frac{N_{d\uparrow}(\epsilon) - N_{d\downarrow}(\epsilon)}{N_{d\uparrow}(\epsilon) + N_{d\downarrow}(\epsilon)} > 0 \ .$$

$(E - \epsilon = \epsilon_{3p} - \epsilon_{2p}.)$ Here we used

$$I_{\uparrow(\downarrow)} \propto \sum_\sigma m_{2p\sigma} N_{d\uparrow(\downarrow)}(\epsilon) \ .$$

This yields a maximal spin polarization of about 100% for such E where $N_{d\downarrow}(\epsilon)$ is zero. Furthermore, the total spin polarization of the $(2p\ 3p\ 3d)$ process is about 25% which compares well with the experimental estimate 16%.[1] If one takes into account spin-orbit coupling, implying a different coupling between $2p$ and $3d$ spins and configurational mixing will, of course, modify our estimate of p. Also note that we neglected the contribution to p resulting from the transitions $3d \rightarrow 2p$ and $3p \rightarrow c$ and which we expect to be very small since there are as many $3p$ electrons with spin up as with spin down.

In conclusion, we have shown that the spin polarization of Auger electrons from ferromagnetic solids can be understood qualitatively as resulting from the exchange coupling between the net spin of the $3d$ electrons and inner-core electrons. The analysis presented here simply extends arguments previously used by Fadley and Shirley[4] to explain the multiplet splitting observed by x-ray photoelectron spectroscopy in ferromagnetic transition metals. It could be useful to extend our analysis more qualitatively to treat more carefully many-body effects.[5] Such effects, for example, are clearly reflected by the broad low-energy shoulder in $p(E)$ for the $(2p\ 3d\ 3d)$ process.

It is interesting that Landolt and Mauri[1] observed a two-peak structure for $p(E)$ for $M_{23}M_{45}M_{45}$. The two peaks in $p(E)$ are, however, separated by about 10 eV. Our simple analysis seems not to explain this two-peak structure. It would be worthwhile to study other mechanisms to explain the large separation of the two peaks in $p(E)$. The resonance mechanism involving $3p\downarrow \rightarrow 3d\downarrow$ as the driving force for $p(E)$[3] could presumably not easily explain a 10-eV splitting.

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