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SPIN POLARIZED SECONDARY ELECTRONS; THEORY

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We show that the spin polarization of the secondary electrons, $P(E)$, yields useful information about the electron–electron interaction. The ratio of majority to minority spin lifetimes is related to the measured values of $P(E)$ by $\tau_\uparrow(E)/\tau_\downarrow(E) = [(1-p_B)/(1+p_B)][(1+P(E))/(1-P(E))]$, where p_B is the bulk magnetization.

The spin polarization of secondary electrons has been measured in Fe [1], Co [1], Ni [2,3] and related glasses such as $Fe_{81.5}B_{14.5}Si_4$ [4]. In all cases the polarization is close to the bulk value at energies greater than a few eV above the vacuum level but exceeds it by a factor of two or three at zero energy (figs. 1 and 2). The first theory of the spin polarization distribution of the secondaries is reported here, We show that experiment provides direct information about the electron–electron interaction and we explain the large spin polarization at low energies.

The electron cascade process is expected to produce secondaries with the bulk magnetization as the vast majority of secondaries are scattered out of the ground state. However there is an excess of unfilled minority over unfilled majority spin d states into which excited minority spin electrons can scatter. Thus, a net majority polarization arises due to the difference in mean free paths. This effect increases at low energies where the ratio of empty d states to free electron states is largest. The role of the empty d states has been discussed qualitatively [1,2].

We generalize Wolff's theory [5] of the cascade process to include spin. At low energies the electron distribution in the solid is homogeneous and isotropic. Our extension of Wolff's theory takes the form

$$\psi(E\sigma) = S(E\sigma) + \sum_{\sigma'} \int_E^\infty \mathrm{d}E'\, \psi(E'\sigma') F(E'\sigma', E\sigma), \tag{1a}$$

$$\psi(E\sigma) = N(E\sigma)/\tau(E\sigma), \tag{1b}$$

where $N(E\sigma)$, $\tau(E\sigma)$, $S(E\sigma)$ are the number of electrons, the lifetime and the source function. $F(E'\sigma', E\sigma)$ is the probability that when an electron in the state $E'\sigma'$ is scattered, an electron is produced in the state $E\sigma$. It satisfies the sum rule [5] ${}_\sigma\int^{E'}\mathrm{d}E\; F(E'\sigma', E\sigma) = 2$. The polarization of the secondary electrons at energy E is

$$P(E) = \frac{N(E\uparrow) - N(E\downarrow)}{N(E\uparrow) + N(E\downarrow)} = \frac{(\psi^-/\psi^+) + (\tau^-/\tau^+)}{1 + (\psi^-/\psi^+)(\tau^-/\tau^+)}, \tag{2}$$

where $\psi^\pm(E) = \psi(E\uparrow) \pm \psi(E\downarrow)$ and $\tau^\pm(E) = \tau(E\uparrow) \pm \tau(E\downarrow)$.

We require the probability that an electron in the state $p'\sigma'$ scatters and produces an electron in the state $p\sigma$, $\omega(p'\sigma', p\sigma)$. For example, in the case $\sigma' = \bar{\sigma}$, where $\bar{\sigma}$ is the spin state opposite to σ

$$\begin{aligned} \omega(p'\sigma, p\bar{\sigma}) = \frac{2\pi}{h} \sum_{kk'} & f(E_{k\sigma})(1 - f(E_{k'\sigma})) \\ & \times |M^{p'\sigma,k\bar{\sigma}}_{k'\sigma,p\bar{\sigma}}|^2 \delta(E_{p'\sigma} + E_{k\bar{\sigma}} - E_{k'\sigma} - E_{p\bar{\sigma}}) \\ & \times \delta(E - E_{p\bar{\sigma}}), \end{aligned} \tag{3}$$

where $M^{p'\sigma,k\sigma'}_{p\sigma,k'\sigma'} = \langle p'\sigma k\sigma' |\mathrm{V}| p\sigma k'\sigma' \rangle$ and where V the electron–electron interaction. In the semi-classical case [5], p, p' etc. stand for momenta $\boldsymbol{p}$, $\boldsymbol{p}'$ and

$$F(E'\sigma', E\sigma) = W(E'\sigma', E\sigma)\tau(E'\sigma'), \tag{4}$$

where $E' = (h^2/2m)p'^2$, $E = (h^2/2m)p^2$ and W is the angular average of ω. τ is obtained by use of eq. (4) in the sum rule. $M^{p'\sigma,k\sigma'}_{p\sigma,k'\sigma'}$ is replaced by its average value which we characterize by the energy transfer and the nature of the states p', p, k, and k'; whether they are free electron-like (denoted by ϵ), or d-like (denoted by d). The small number the occupied s–p states will not be distinguished from the d's. It is assumed that only

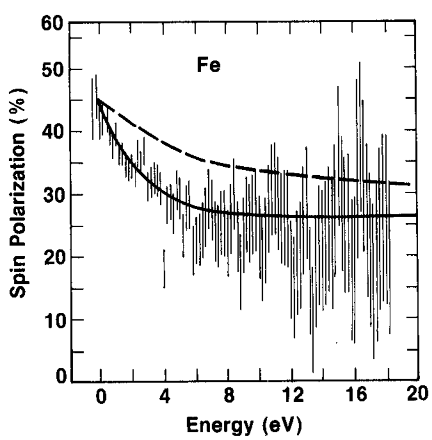

Fig. 1. Spin polarization of the secondary electrons in Fe. Dashed line is calculated spin polarization with constant matrix elements. Solid curve is calculated spin polarization with M_4 given by eq. (6).

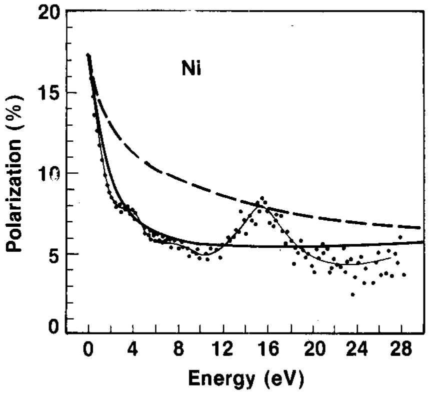

Fig. 2. Same as fig. 1 but for Ni.

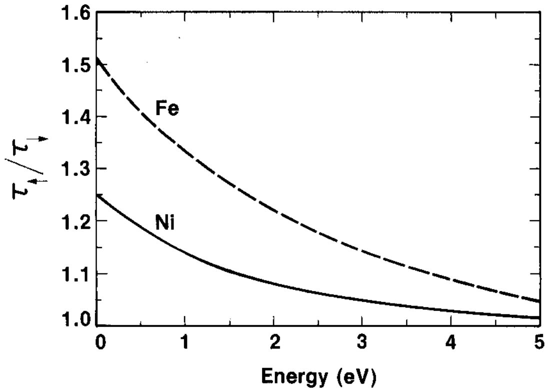

Fig. 3. Ratio of spin dependent lifetimes for Fe and Ni (eq. (7)).

the minority spin band contains unfilled d states (true for Ni and Co and approximately true for Fe). One obtains for E', $E > 0$,

$$F(E'\sigma,\ E\sigma) = A_\sigma\Big[\,|M_1|^2(\bar{\rho}_{\downarrow,\epsilon} + \bar{\rho}_{\uparrow,\epsilon}) + |M_3|^2\bar{\rho}_{\downarrow,d} + |M_2|^2\bar{\rho}_{\sigma,\epsilon} + \delta_{\sigma,\downarrow}|M_4|^2\bar{\rho}_{\downarrow,d}\Big], \qquad (5a)$$

$$F(E'\sigma,\ E\bar{\sigma}) = A_\sigma\Big[\,|M_2|^2\bar{\rho}_{\bar{\sigma},\epsilon} + \delta_{\sigma,\downarrow}|M_4|^2\bar{\rho}_{\uparrow,d}\Big], \qquad (5b)$$

where $A_\sigma = (2\pi/h)\tau(E'\sigma)\rho_\epsilon(E)$ and ρ_l is the density of states with orbital character $l = \epsilon$ or d. The elements M_i are $M_1 = M^{\epsilon,d}_{\epsilon,\epsilon}(E' - E)$, $M_2 = M^{\epsilon,d}_{\epsilon,\epsilon}(E - \epsilon_f)$, $M_3 = M^{\epsilon,d}_{\epsilon,d}(E' - E)$, and $M_4 = M^{\epsilon,d}_{d,\epsilon}(E' - \epsilon_f)$, where $M^{\epsilon,d}_{l,l'}(\omega)$ describes the scattering of a free electron into a state of type l with energy loss ω while a ground state d electron is scattered into a state of type l', and $\bar{\rho}_{\sigma,l}$ is the joint density of states for a ground state spinσ electron and an unoccupied state of orbitral character l.

The densities of states in eq. (5) are taken from band structure calculations. M_1 and M_2 are taken to be energy independent, in which case $M_1 = M_2$ and the polarization depends on $|M_3/M_1|$ and $|M_4/M_1|$. The polarization is very insensitive to the choice of $|M_3/M_1|$ (which we set equal to 0.3) but depends directly on $|M_4/M_1|$, see eq. (5). If M_4 is also energy independent, the choices $|M_4/M_1|^2 = 0.13$ (for Fe) and 0.19 (for Ni) result in the dashed lines in figs (1) and (2). Clearly the exchange matrix element M_4 must be taken as energy dependent. M_4 is extremely difficult to calculate because of screening and correlation effects, and we parameterized M_4 by:

$$|M_4(\omega)M_1|^2 = A^2\big/\big((\omega - \epsilon_f)^2 + B^2\big). \qquad (6)$$

For Fe and Ni, the choices $A = 1.8$ and 2.9 eV and B = 3.2 and 3.5 eV, respectively, result in the solid curves in figs. 1 and 2.

The ratio $\tau_\uparrow(E)/\tau_\downarrow(E)$ can be obtained from eq. (2) using the experimental values for $P(E)$ and the calculated values for $\psi^-(E)/\psi^+(E)$ (which is quite insensitive to the choice of matrix elements). In fact, we find that for energies greater than zero, $\psi^-/\psi^+ \approx p_B$, where p_B is the bulk magnetization. This result obtains for $|M_4/M_1|^2 \ll 1$ which is satisfied here. Eq. (2) yields

$$\tau_\uparrow(E)/\tau_\downarrow(E) = \frac{1 - p_B}{1 + p_B}\,\frac{1 + P(E)}{1 - P(E)}. \qquad (7)$$

Thus $\tau_\uparrow/\tau_\downarrow$ can be obtained directly from the experimental measurements without model calculations. $\tau_\uparrow/\tau_\downarrow$ versus energy is shown in fig. 3 for Fe and Ni. This ratio is larger for Fe because its ratio of unfilled d states to free electron states is larger. If $\tau_\uparrow \neq \tau_\downarrow$ the internal spin polarization will differ from that measured due to spin selective bulk scattering and the interpretation of many experiments would be affected. Fig. 3 shows this is important only at very low energies where it is difficult to carry out experiments due to strong fields.

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