Elastic and magnon-inelastic differential cross sections of spin-polarized low-energy electrons in magnetic nickel and iron*

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Scattering experiments with spin-polarized electron beams of 100–1000 eV on magnetic materials are now feasible. In view of this the spin-dependent part of the scattering cross section is calculated in the Born approximation for a ferromagnet in the spin-wave regime. It is evaluated as a function of momentum transfer for Ni and Fe using self-consistent potentials.

INTRODUCTION

When low-energy primary electrons (100–1000 eV) strike a metal, several scattering processes happen. There is elastic scattering, and also inelastic scattering due to the excitation of single electrons (inter- and intraband transitions) and of collective modes (plasmons, spin waves). The inelastic scattering gives rise to a characteristic energy-loss spectrum whose peaks correspond to the characteristic electronic excitation energies of the metal.

The interection potential between the primary electrons and the electrons of the target contains a spin-dependent exchange interaction—which is small compared with the total potential. In nonmagnetic metals it is impossible to observe the exchange interaction separately since there is no distinction between electrons with spins up and down. However, in magnetic metals it would be in principle possible to observe this effect by using a beam of spin-polarized primary electrons. In this case the exchange interaction would lead to different cross sections depending on the relative orientation of the primary beam polarization with respect to the magnetization of the metal.

This type of experiments can now be performed due to the availability of intense sources of polarized electrons whose spin orientation can be reversed at a high rate.[1] Thus, the difference between the cross sections for any scattering process produced by a successively spin-up and spin-down polarized primary beam can be measured by a lock-in-technique. At present this technique can reach a sensitivity of 10^{-5}. This experiment would provide direct evidence of the role played by the exchange interaction on the elastic and inelastic scattering processes and allow the determination of exchange coupling constants. In this paper we estimate the exchange interaction effect to be expected on the spin-polarized low-energy-electron elastic cross section and on the inelastic cross section resulting from the interaction with magnons in Ni and Fe.

Let us consider the following experimental setup: The target consists of a ring-shaped Ni crystal (Fig. 1). The domains are oriented by means of a small coil. This special shape is chosen to avoid stray fields. A beam of low-energy electrons, whose polarization is modulated at about 10^3 rpm, is directed against the border of the ring. The outcoming primary electrons, selected in a given energy interval, are detected through a lock-in technique that picks up only the 10^3-rpm component of the current. The amplitude of the current is a measure of the differential effect due to the spin-dependent part of the interaction between the primary electrons and the Ni crystal.

MODEL

The interaction Hamiltonian between the primary electron and the target is

$$H_i = H_{em} + V \quad . \tag{1}$$

Here $V = \sum_j v(\vec{r} - \vec{R}_j)$ describes the spin-independent part of the primary electron interaction with each atom in the target. $\vec{R}_j$ is the position of the atom j.

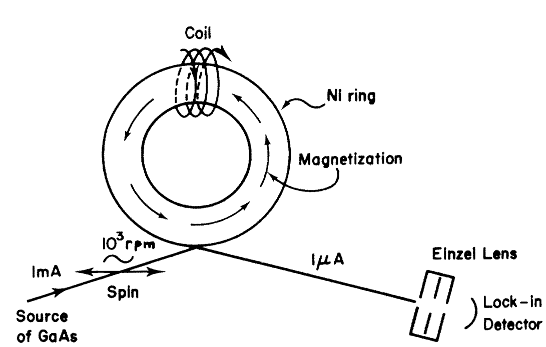

FIG. 1. Experimental setup.

$$H_{em}=\sum_j J(\vec{r}-\vec{R}_j)\vec{s}\cdot\vec{S}_j \qquad (2)$$

describes the exchange interaction between the spin $\vec{s}$ of the primary electron and the spin $\vec{S}_j$ of the magnetic metal ion at $\vec{R}_j$. $J(\vec{r}-\vec{R}_j)$ is the exchange coupling constant. We use a localized spin model for the magnetic metal, although its validity may be doubtful for the transition metals under consideration.

In second-quantized formalism and in the spin-wave region ($T \ll T_c$) H_i can be written in the form[2]

$$H_i=\frac{1}{\Omega}\sum_j\sum_{\vec{k}}\sum_{\vec{k}'}e^{i\vec{Q}\cdot\vec{R}_j}\Bigg\{v_{\vec{Q}}(a^\dagger_{\vec{k}'\uparrow}a_{\vec{k}\uparrow}+a^\dagger_{\vec{k}'\downarrow}a_{\vec{k}\downarrow}) -\tfrac{1}{2}J_{\vec{Q}}\Bigg[\left(\frac{2S}{N}\right)^{1/2}\sum_{\vec{q}}(e^{-i\vec{q}\cdot\vec{R}_j}a^\dagger_{\vec{k}'\uparrow}a_{\vec{k}\downarrow}b^\dagger_{\vec{q}}+e^{i\vec{q}\cdot\vec{R}_j}a^\dagger_{\vec{k}'\downarrow}a_{\vec{k}\uparrow}b_{\vec{q}}) +\left(S-\frac{1}{N}\sum_{\vec{q}}\sum_{\vec{q}'}e^{i(\vec{q}'-\vec{q})\cdot\vec{R}_j}b^\dagger_{\vec{q}}b_{\vec{q}'}\right)(a^\dagger_{\vec{k}'\uparrow}a_{\vec{k}\uparrow}-a^\dagger_{\vec{k}'\downarrow}a_{\vec{k}\downarrow})\Bigg]\Bigg\}, \qquad (3)$$

where

$$v_{\vec{Q}}=\int d^3r\,v(r)e^{-i\vec{Q}\cdot\vec{r}} \qquad (4)$$

and

$$J_{\vec{Q}}=\int d^3r\,J(r)e^{-i\vec{Q}\cdot\vec{r}}. \qquad (5)$$

$a^\dagger_{\vec{k}\sigma}$ and $a_{\vec{k}\sigma}$ are the creation and destruction electron operators, respectively. $b^\dagger_{\vec{q}}$ and $b_{\vec{q}}$ are the creation and destruction magnon operators. $\vec{Q}=\vec{k}-\vec{k}'$ and Ω is a normalization volume.

DIFFERENTIAL CROSS SECTIONS

The matrix element for the transition of an electron from the state $|\vec{K}_0\uparrow\rangle$ to the state $|\vec{K}_0'\uparrow\rangle$, within the one-magnon approximation, is

$$\langle\vec{K}_0'\uparrow\phi_m|H_i|\phi_m\vec{K}_0\uparrow\rangle =\frac{1}{\Omega}\sum_j e^{i\vec{Q}\cdot\vec{R}_j}\left[v_{\vec{Q}}-\tfrac{1}{2}J_{\vec{Q}}\left(S-\frac{1}{N}\sum_{\vec{q}}n_{\vec{q}}\right)\right], \qquad (6)$$

where $n_{\vec{q}}$ is the number of magnons with momentum $\vec{q}$ in the magnetic state ϕ_m.

The matrix element for the transition of an electron from the state $|\vec{K}_0\uparrow\rangle$ to the state $|\vec{K}_0'\downarrow\rangle$ is

$$\langle\vec{K}_0'\downarrow\phi_m'|H_i|\phi_m\vec{K}_0\uparrow\rangle =\frac{1}{\Omega}\sum_j e^{i\vec{Q}\cdot\vec{R}_j}\left(-\tfrac{1}{2}J_{\vec{Q}}\sum_{\vec{q}}e^{i\vec{q}\cdot\vec{R}_j}\sqrt{n_{\vec{q}}}\right). \qquad (7)$$

Analogously, the matrix elements for the transitions from the electron state $|\vec{K}_0\downarrow\rangle$ to $|\vec{K}_0'\uparrow\rangle$ and $|\vec{K}_0'\downarrow\rangle$ are

$$\langle\vec{K}_0'\uparrow\phi_m'|H_i|\phi_m\vec{K}_0\downarrow\rangle =\frac{1}{\Omega}\sum_j e^{i\vec{Q}\cdot\vec{R}_j}\left(-\tfrac{1}{2}J_{\vec{Q}}\sum_{\vec{q}}e^{i\vec{q}\cdot\vec{R}_j}\sqrt{n_{\vec{q}}+1}\right) \qquad (8)$$

and

$$\langle\vec{K}_0'\downarrow\phi_m|H_i|\phi_m\vec{K}_0\downarrow\rangle =\frac{1}{\Omega}\sum_j e^{i\vec{Q}\cdot\vec{R}_j}\left[v_{\vec{Q}}+\tfrac{1}{2}J_{\vec{Q}}\left(S-\frac{1}{N}\sum_{\vec{q}}n_{\vec{q}}\right)\right], \qquad (9)$$

respectively.

In the following we disregard the energy of the magnon absorbed or emitted during the scattering process as compared with the energy of the scattered electron. That is, all scattering processes are considered to be elastic. This approximation is consistent with the experimental conditions, in the sense that the energy resolution of the present day detectors is smaller than the energy difference between the elastic peak and the inelastic peaks corresponding to absorption and emission of magnons. Thus, the differential cross section for scattering of electrons with spin up is given by

$$\frac{d\sigma_\uparrow}{d\omega}=\left(\frac{m^*}{2\pi}\right)^2\frac{\Omega^2}{\hbar^4}(\langle|\langle\vec{K}_0'\uparrow\phi_m|H_i|\phi_m\vec{K}_0\uparrow\rangle|^2+|\langle\vec{K}_0'\downarrow\phi_m'|H_i|\phi_m\vec{K}_0\uparrow\rangle|^2\rangle_T)$$

$$=\left(\frac{m^*}{2\pi}\right)^2\frac{1}{\hbar^4}\left\{S(\vec{Q})[|v_{\vec{Q}}|^2-\tfrac{1}{2}(v_{\vec{Q}}J_{\vec{Q}}^*+v_{\vec{Q}}^*J_{\vec{Q}})m+\tfrac{1}{4}|J_{\vec{Q}}|^2m^2]+|J_{\vec{Q}}|^2\frac{S}{2N}\sum_{\vec{q}}n_{\vec{q}}S(\vec{Q}+\vec{q})\right\}, \qquad (10)$$

where $\langle \cdots \rangle_T$ denotes a thermodynamical average over the magnetic states of the system, m denotes the magnetization at temperature T and m^* is the electron mass

$$S(\vec{Q}) = \left\langle \sum_j \sum_l e^{i\vec{Q}\cdot(\vec{R}_l - \vec{R}_j)} \right\rangle \quad (11)$$

is the static structure factor of the target. Here $\langle \cdots \rangle$ denotes a thermodynamic average over the positions of the atoms of the target.

Analogously, the differential cross section for the scattering of electrons with spin down, is

$$\frac{d\sigma_\downarrow}{d\omega} = \left(\frac{m^*}{2\pi}\right)^2 \frac{1}{\hbar^4} \left(S(\vec{Q}) [|v_{\vec{Q}}|^2 + \tfrac{1}{2}(v_{\vec{Q}} J_{\vec{Q}}^* + v_{\vec{Q}}^* J_{\vec{Q}}) m + \tfrac{1}{4} |J_{\vec{Q}}|^2 m^2] + |J_{\vec{Q}}|^2 \frac{S}{2N} \sum_{\vec{q}} (n_{\vec{q}} + 1) S(\vec{Q} - \vec{q}) \right) . \quad (12)$$

The relative current P measured with the experimental setup described above is given by

$$P_Q = \left(\frac{d\sigma_\downarrow}{d\omega} - \frac{d\sigma_\downarrow}{d\omega} \right) \Big/ \frac{1}{2} \left(\frac{d\sigma_\uparrow}{d\omega} + \frac{d\sigma_\downarrow}{d\omega} \right) . \quad (13)$$

Here $Q = |\vec{Q}| = 2K_0 \sin\frac{1}{2}\theta$, where θ is the scattering angle.

The main contribution to P_Q comes from processes in which the spin of the electron is conserved. The processes involving the emission or absorption of magnons are of the order $|J|^2$. If we neglect terms of the order $|J|^2$ we are left with

$$P_Q = -[(v_Q J_Q^* + v_Q^* J_Q)/|v_Q|^2] m . \quad (14)$$

In this approximation the structure factor drops out and the result depends only on the interaction between the electron and a single atom.

The self-consistent Hartree-Fock-Slater potentials for fully polarized Ni ($0.6\mu_B$ per atom) and Fe ($1.72\mu_B$ per atom) have been calculated by Wakoh.[3] The results for the self-consistent potential for spin-up electrons $V_\uparrow(r)$ and for spin-down electrons $V_\downarrow(r)$ are tabulated.

We can write $v(r)$ and $J(r)$ in terms of Wakoh's potential as follows

$$v(r) = \tfrac{1}{2}[V_\uparrow(r) + V_\downarrow(r)] , \quad (15)$$

$$J(r) = V_\downarrow(r) - V_\uparrow(r) . \quad (16)$$

We calculated numerically

$$v_Q = \frac{4\pi}{Q} \int_0^\infty dr\, r v(r) \sin Qr \quad (17)$$

and

$$J_Q = \frac{4\pi}{Q} \int_0^\infty dr\, r J(r) \sin Qr . \quad (18)$$

Since v_Q and J_Q are real Eq. (14) reduces to

$$P_Q = -(2J_Q/v_Q)(m/m_s) , \quad (19)$$

where m_s is the saturation magnetization. P_Q as a function of Q for $m = m_s$ is shown in Fig. 2 for Ni and Fe.

DISCUSSION

Wakoh's self-consistent potentials are calculated for fully polarized Ni and Fe ($T = 0$ K). The evaluation of P_Q at a finite temperature T would require the calculation of the self-consistent potentials corresponding to a magnetization $m(T)$. This information is not available at present. At low temperatures ($T << T_c$), the behavior of $P_Q(T)$ can be estimated using the spin-wave approximation together with Wakoh's potentials [Eq. (19)]. However, the validity of this extension to finite temperatures is doubtful because it is based on a spin localized model for the d electrons.

In the experimental setup described above the primary electrons may penetrate only a few angstroms in the metal, therefore in Eq. (19) one should use the surface rather than the bulk magnetization. On the other hand, the dependence of the electron penetration on the primary energy could be used to measure the magnetization profile near the surface. Depolariz-

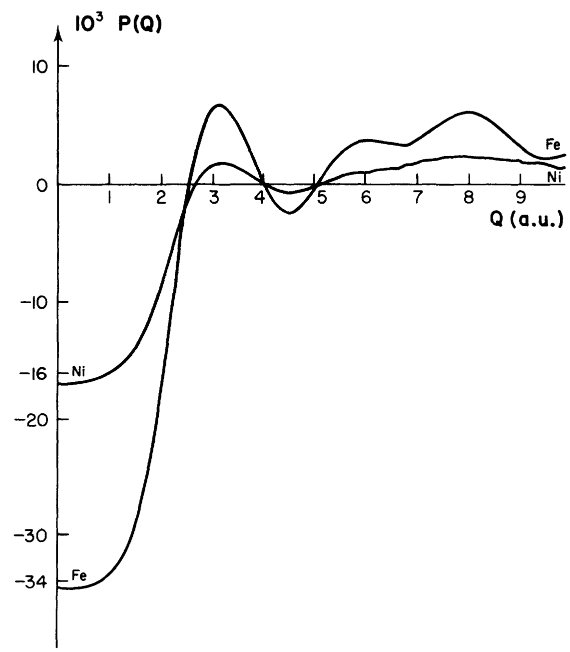

FIG. 2. P_Q as a function of the momentum transfer Q.

ing effects due to multiple scattering should not be important, since the penetration of the scattered electrons is small. A more rigorous treatment of the low-energy-electron diffraction by the surface could be carried out along the lines of the work by Kerre and Phariseau[4] by incorporating the spin-dependent exchange interaction into the electron-ion interaction.

SUMMARY

The spin-dependent part of the interaction potential between an electron and a magnetized Ni or Fe target should have an easily observable effect on the differential cross section when measured by the technique described in this paper. We expect $P_Q(m)$ to behave like

$$P_Q(m) = P(m_s)[m(T)/m_s] \ ,$$

where $P(m_s)$ is plotted in Fig. 2. The effect is largest for small momentum transfer. Furthermore, within the approximations used, P_Q does not depend explicitly on the energy of the primary electrons.

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