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INELASTIC ELECTRON SCATTERING AND ELECTRON-HOLE EXCITATIONS IN IRON AND NICKEL

J. A. Blackman (1) and J. F. Cooke (2)

(1) Dept. of Physics, University of Reading, Whiteknights, PO Box 220, Reading RG6 2AF, G.B.
(2) Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, U.S.A.

Abstract. – Spin-flip and non-spin-flip mechanisms have been proposed to explain polarization asymmetry in inelastic electron scattering from iron and nickel. A maximum in the asymmetry near 2 eV in iron can occur by both mechanisms. The 300 meV maximum in nickel is unlikely to occur by non-spin-flip transitions.

Spin-resolved electron-energy loss spectroscopy has been used to study electron-hole excitations in the itinerant ferromagnets nickel [1] and iron [2]. A key feature of the experiments was the observation that electrons with polarization antiparallel to the magnetic vector display greater inelastic scattering than those with parallel polarization. Furthermore the asymmetry in polarization dependent scattering is at a maximum for energy losses near 300 meV in nickel and 2 eV in iron. Because the values are roughly the exchange splitting energies it was concluded that Stoner excitations play an important role. Specularly scattered \( q \sim 0 \) electrons were analysed in [1], while in [2], where full polarization analysis was used, off-specular scattering (finite \( q \)) was studied. More recent experiments [3] on iron have been interpreted in terms of spin-flip and non-spin-flip processes for both specular and off-specular scattering.

Scattering can take place via dipolar fields in the region above the surface. These are generated by electron-hole pairs within the metal. This is a direct process and is important only near the specular direction. The alternative process, impact scattering, takes place in the metal, and the interaction can be either of a direct or exchange type. Multiple elastic scattering off the ion cores is assumed to be responsible for the electrons reemergence from the surface.

Polarization dependent effects can occur within the impact regime due to exchange processes either with or without a spin-flip. The spin-flip case, which dominates away from specular [3], is associated with Stoner excitations [4].

An alternative mechanism that produces polarization asymmetry is possible for scattering near to the specular direction. The direct dipolar scattering and the non-spin-flip part of the exchange scattering can both occur with the same initial and final states. Hence a “cross-term” can occur between the two, the sign of which depends on the incident electron polarization. This was first proposed by Mills [5] in the context of nickel. He also suggested that the maximum in the asymmetry near 300 meV could arise from this mechanism rather than from Stoner excitations.

The purpose of the present paper is to address this point and to calculate the energy dependence of the cross-term for both nickel and iron. It is important to use realistic electronic energy bands in theoretical work. This has already been demonstrated in the context of inelastic neutron scattering [6-8].

The asymmetry due to the cross-term can be expressed [5] in terms of the energy and wave-vector transforms of the correlation function \( \langle \rho(t) S_z \rangle \) where \( \rho \) is the charge density and \( S_z \) is the spin component of the itinerant electron system. The appropriate wavevector \( q \) is related to the wavevector of the incident electron. A value of the order of the Brillouin zone boundary is suitable. A Slater-Koster empirical band structure is used with 9 spin-up and 9 spin-down bands (based on s, p, and d orbitals). The calculation proceeds along the lines described earlier [6-8] except that electron-electron effects are not expected to be important for large momentum transfers and are ignored.

The correlation function for iron for \( q = \left( \frac{1}{2}, \frac{1}{2}, 0 \right) \) is shown in figure 1. This has to be multi-

![Fig. 1. Asymmetry in the polarization dependent scattering for iron at q = \( \left( \frac{1}{2}, \frac{1}{2}, 0 \right) \). q is in units of 2\( \pi /a \); asymmetry is in arbitrary units.](image-url)
plied by various factors [5] that have only weak energy dependence to get the asymmetry in absolute units. The asymmetry changes sign between 1.0 and 1.5 eV and is peaked between 2.5 and 3.0 eV. The peak is fairly close to the exchange splitting energy but has no connection with it. Rather, it is roughly the centre of the bandwidth for non-spin-flip excitations. This describes the behaviour for a wide range of q values in the (110) direction.

Similar correlation functions for nickel for two values of σ are shown in figures 2 and 3. Here there is no change in the sign of the asymmetry except near 5 eV in figure 2, but there is considerable variation with q. At $\left(\frac{1}{4}, \frac{1}{4}, 0\right)$ there is a very pronounced peak around 300 meV, while at $\left(\frac{3}{4}, \frac{3}{4}, 0\right)$ there is a broad structure reminiscent of iron with only a relatively minor feature at 300 meV. The $\left(\frac{3}{4}, \frac{3}{4}, 0\right)$ behaviour is the more typical over a wide range of q.

It would be very interesting to see a full polarization analysis for nickel as has been done for iron [3]. If the Mills mechanism is important, it would be expected from our calculations that the asymmetry would show considerable variation with the incident electron energy. Furthermore the dependence on energy loss should in most cases extend over a similar range to that occurring in iron.

A comparison between figure 1 and the experimental results for iron [3] does not provide strong evidence for the Mills mechanism. It should be noted, however, that even realistic calculations of the Stoner joint densities of states do not relate closely to the spin-flip part of the asymmetry. Calculations show a much stronger peaking at the exchange splitting energy than is observed experimentally. Furthermore, even though Vignale and Singwi [9] have shown why spin waves do not completely dominate the scattering, their total absence remains surprising.

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Fig. 2. - Asymmetry for nickel at $q = \left(\frac{1}{4}, \frac{1}{4}, 0\right)$.

Fig. 3. - Asymmetry for nickel at $q = \left(\frac{3}{4}, \frac{3}{4}, 0\right)$.