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The relation of electron diffraction to surface magnetism—spin-polarised LEED from nickel (110)

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Abstract. Calculations for SPLEED from the nickel (110) surface, with an angle of incidence of 45°, are compared with experiment in the energy range 5–30 eV: strong azimuthal dependence in the exchange asymmetry is predicted. An optimisation of the geometrical, vibrational, and magnetic parameters, both surface and bulk, is presented. The comparison gives insight into the factors affecting spin-polarised electron scattering from ferromagnetic surfaces, but shows that there is no simple, unambiguous relation between spin asymmetry and surface magnetism.

When electrons scatter from ferromagnetic surfaces a number of spin-dependent processes may occur—spin–orbit and exchange-induced asymmetries in scattering intensity and spin-flip scattering. In an elegant experiment incorporating both spin-polarised and incident electrons and spin analysis of scattered electrons Abraham and Hopster [1] showed that spin-flip scattering was relatively unimportant for scattering of 5–30 eV electrons from Ni(110) and Ni(110) O(2 × 1). Furthermore, they were able to separate the spin–orbit and exchange asymmetries by magnetic field reversal. This distinction was reinforced by the observation of a radical reduction in the exchange asymmetry component on oxygen chemisorption.

In this paper we wish to give a theoretical interpretation of the observed exchange intensity asymmetry A_{exch} in terms of electron scattering from spin-dependent potentials at the surface; these are based on differences in the exchange interaction between the incident electrons and the 3d electrons within the muffin-tin spheres of the Ni atoms according to whether the incident spin is parallel or antiparallel to the magnetisation direction.

$$A_{\mathrm{exch}}(E_{\mathrm{p}}) = (I_{\uparrow\uparrow} - I_{\uparrow\downarrow})/(I_{\uparrow\uparrow} + I_{\uparrow\downarrow}) \tag{1}$$

where $I_{\uparrow\uparrow(\downarrow\downarrow)}$ represents the intensity in the (00) channel for electrons parallel (antiparallel) to the magnetisation direction, spin–orbit effects having been removed by averaging results from opposite fields. Electrons with spins parallel to the magnetisation direction of the Ni surface see larger parallel spin density, a more attractive potential and correspondingly modified scattering amplitudes. We consider two exchange–correlation potentials:

(i) the conventional Hartree–Fock–Slater exchange correlation potential ($\sim\alpha\rho^{1/3}$);

(ii) an energy-dependent Hara exchange potential [2] accompanied by an energy-independent Perdew–Zunger correlation potential [3]. The model is similar to those

Table 1. Scattering parameters for SPLEED on Ni(100).

	Range considered	Optimum
Surface relaxation		
first layer	−0–10%	−7 ± 2%
second layer	0–4%	0.5 ± 1%
Muffin-tin zero	−10→ −15 eV	−12.5 ± 0.5 eV
Imaginary component of inner potential	AE_p^β	$\beta = \frac{1}{3}, A = 0.8$
Angle of incidence	45 ± 2°	45 ± 0.5°
Azimuth	0 ± 2°	0 ± 0.5°
θ_D	290–390 K	355 ± 30 K
Surface θ_D	$(0.6–1)\theta_D$	$(0.7 \pm 0.1)\theta_D$
Bulk magnetisation	$(0.55 \pm 0.1)\mu_B$	$(0.55 \pm 0.05)\mu_B$
Surface magnetisation	$(0.5–2)\mu_B$	$(0.6 \pm 0.1)\mu_B$

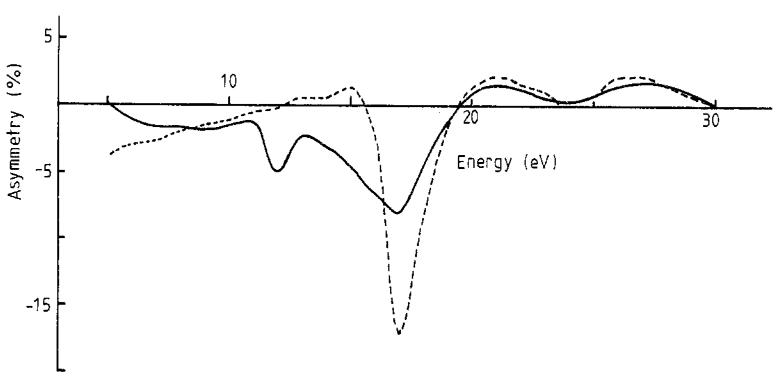

Figure 1. A comparison of the theoretical prediction of $A_{exch}(E_p)$ for Slater exchange (——) and that for Hara exchange (----) coupled with Perdew–Zunger correlation. (Ni(110) geometry, (00) beam, (45, 0) geometry.)

used in [4], [5], and [6] (see [7]), but here comparison is made with the new data of Abraham and Hopster [1] in the low-energy range $5 < E_p < 30$ eV where large asymmetry effects are anticipated and observed; correlation effects as well as exchange must be included explicitly in this energy regime.

Before embarking on the spin-dependent calculation our CAVLEED program provided by the Daresbury Laboratory, CCP3 library, was validated in the $30 < E_p < 100$ eV range by comparing with the theory from [8, 9] for 46° incidence angle on Ni(110). The program was modified to include energy-dependent real and imaginary inner potentials and a surface barrier half a lattice spacing above the top layer. Table 1 outlines the range of geometrical and potential parameters considered in the calculations—these reflect either experimental or theoretical uncertainties in the specification of the system. The variations imply mild ambiguity in some areas through to considerable ignorance in others. Firstly the optimum *spin-independent* parameters are consistent with those required to fit conventional LEED data. Secondly potential is important. Figure 1 compares Slater exchange with the Hara potential—no amount of parameter variation leads to the correct shape of $A_{exch}(E_p)$ for a Slater potential, adequate though such a potential

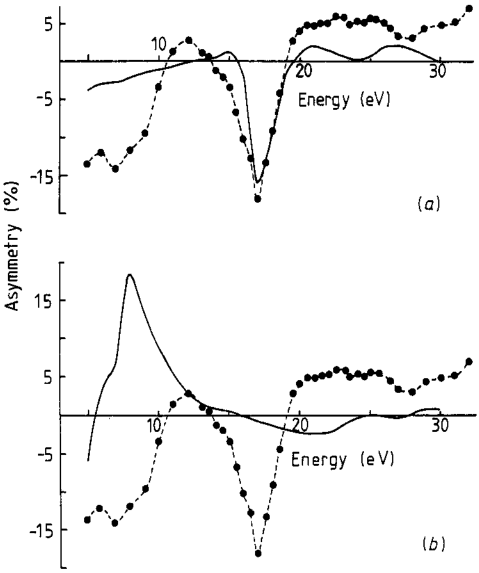

Figure 2. A comparison of theoretical $A_{exch}(E_p)$ (——) with the experiment of Abraham and Hopster (--●--) for an optimised theory at 45° incidence ((00) beam) on Ni(110) (*a*) for azimuth (001)—the correct experimental azimuth; (*b*) for azimuth (1$\bar{1}$0).

is for spin-averaged LEED at higher primary energy E_p. Thirdly the spin exchange is very sensitive to azimuth: figures 2(*a*) and 2(*b*) compare the predicted $A_{exch}(E_p)$ for 45° incidence on Ni(110) for a scattering plane along (001) (0° azimuth) and (1$\bar{1}$0) (90° azimuth) with the experiment of Abraham and Hopster [1] for (001). No parameter pattern for (1$\bar{1}$0) can reproduce even vague agreement, while quite good theory–experiment correspondence can be achieved along (001) with physically sensible parameters. Happily this was the experimental condition!

Surface relaxation is also significant. Substantial inward relaxation of FCC 110 surfaces is widely predicted by LEED, and this feature appears to be consistent wiht the requirements of $A_{exch}(E_p)$. Results are much less sensitive to surface and bulk Debye temperature, but the assumed muffin-tin zero is important in influencing the position of the main negative excursion of A_{exch}—no appreciable improvement was achieved by introducing energy dependence in the muffin-tin zero, but there was some evidence that the AE_p^{β} variation in the imaginary potential suggested in [8, 9] has some significance.

Amid this glalaxy of parameters it is the specification of magnetisation that is primarily of interest. The system was described by a bulk magnetisation (implying a net spin imbalance in the second and further layers) and by a surface layer magnetisation (both in Bohr magnetons per atom). The general scale of A_{exch} increases with increasing magnetisation, but A_{exch} is the result of spin dependence of a *multiple*-scattering process, so there is not a strict linear relation between them. If the surface magnetisation differs from the bulk, the changes in surface layer scattering will very directly affect the overall scattering amplitude and so the phenomenon is very sensitive to magnetisation anomalies at the surface. Here a surface magnetisation similar to that of the bulk appears to be consistent with the present results. However, words of caution are required. It is important to examine closely what A_{exch} represents. From equation (1) it is clear that A_{exch} will be large if $I_{\uparrow\uparrow} + I_{\uparrow\downarrow}$ is small with $I_{\uparrow\uparrow} - I_{\uparrow\downarrow}$ of reasonable magnitude. This implies that SPLEED tends to emphasise conditions of destructive interference in LEED (a very difficult task), and so results will be exceptionally sensitive to the quality of the scattering model. The tolerance limits on optimum parameters therefore represent

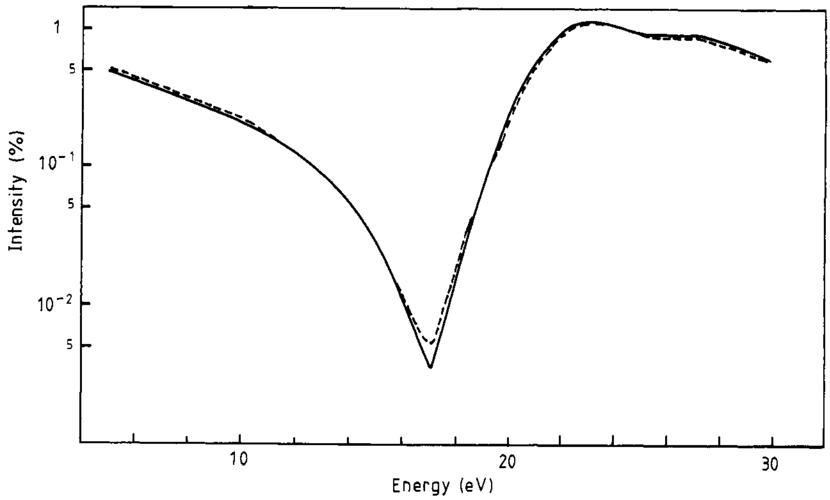

Figure 3. A theoretical comparison of $I_{\uparrow\uparrow}$ and $I_{\uparrow\downarrow}$ against energy for optimised scattering parameters at 45° incidence on Ni(110) along the (001) azimuth (——, spin up; ----, spin down).

parameter changes that produce significant deterioration in comparison with experiment *within the present model* rather than definitive error estimates. This is illustrated in figure 3 which compares $I_{\uparrow\uparrow}$ and $I_{\uparrow\downarrow}$ for optimised parameters. It is attractive to concentrate on fitting the main negative excursion in A_{exch} at 17 eV, which has been achieved with some success, but the model used does not guarantee specification of the *true* magnetisation parameters. Clearly a wider range of experimental data is required for definitive magnetic information to emerge, but the comprehensive parameter variation considered here for SPLEED on Ni(110) gives insight into the strengths and limitations of the technique in probing magnetic surfaces.

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