Electron spin polarisation in LEED from Au (110)

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Abstract. A special LEED system was combined with a Mott polarisation detector. For various beams diffracted from a Au (110) surface, the electron spin polarisation was measured as a function of scattering angle, of energy and of temperature. Up to 80% polarisation was observed. Dependence on temperature is of particular interest for the Au (110) surface, since a structural phase transition occurs, which can be monitored by spin polarisation measurements. For the high-temperature phase, experimental data are compared with theoretical model predictions. Our results suggest that analysis of spin polarisation in LEED could provide information on surface properties not obtainable by currently used intensity analysis only.

The 50th anniversary of the discovery of the wave properties of electrons is a suitable occasion to recall that the existence of electron spin had been postulated around the same time (Uhlenbeck and Goudsmit 1925). Initial experiments for detecting spin polarisation of electron waves (in analogy with the polarisation of light waves) by double diffraction seemed, however, to yield negative results (Davisson and Germer 1928, 1929). Progress was achieved only fairly recently: both theory and experiment provided definite evidence of polarisation effects in electron diffraction from crystal surfaces (Jennings 1970, Feder 1971, 1976, O'Neill *et al* 1975, Müller and Wolf 1976). In the present work, we report measurements and calculations on the Au (110) surface, which demonstrate that spin-polarised low-energy electron diffraction (SPLEED) is suited for the investigation of geometric, electronic and vibronic structures of crystal surfaces.

A schematic drawing of the apparatus is given in figure 1. Its essential feature is the combination of a two-grid LEED system with movable electron gun and a fixed polarisation detector. The angle of incidence can be varied and every LEED reflex can be extracted to determine the polarisation. The detection itself is performed by Mott scattering in a four-counter arrangement (van Klinken 1966, Kessler 1976).

The Au (110) surface was chosen because of its special structural properties. At room temperature, the clean surface exhibits a (1 × 2) superstructure. At temperatures of about 720 K, LEED pictures show the transition from a (1 × 2) pattern to a (1 × 1) bulk-type pattern (Fedak and Gjostein 1967, Wolf 1972). This transition is correlated with an essential disorder of the close-packed chains in the [110] direction (Wolf 1972, Wolf *et al* 1978, Jagodzinski 1977).

Firstly, we made measurements on the low-temperature phase characterised by the (1 × 2) LEED pattern. Figure 2 shows, for the specular beam at several fixed energies,

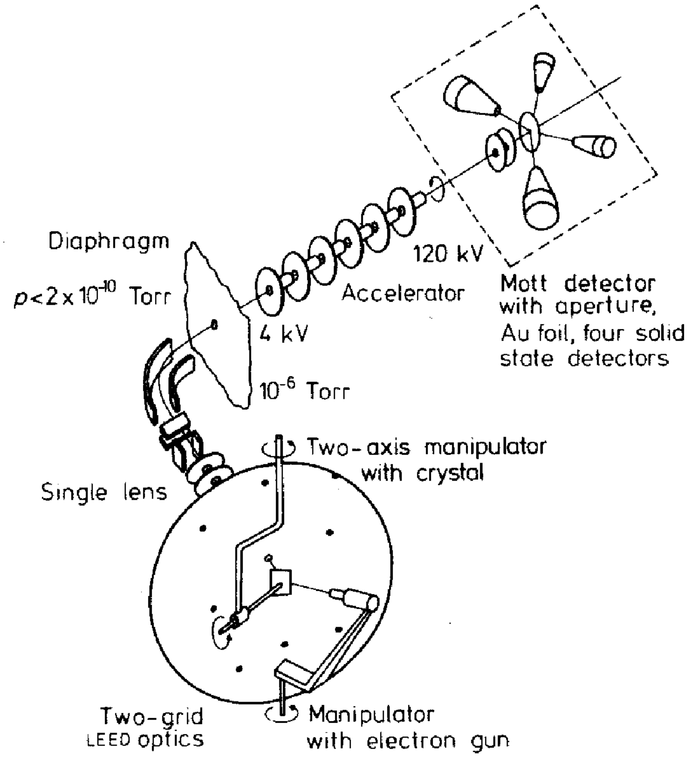

Figure 1. Experimental set-up for SPLEED. (The cylindrical condenser, which was essential in an earlier design for field emission work, prevents gas atoms from getting directly from the detector section to the crystal. It does not affect a polarisation vector normal to the scattering plane.)

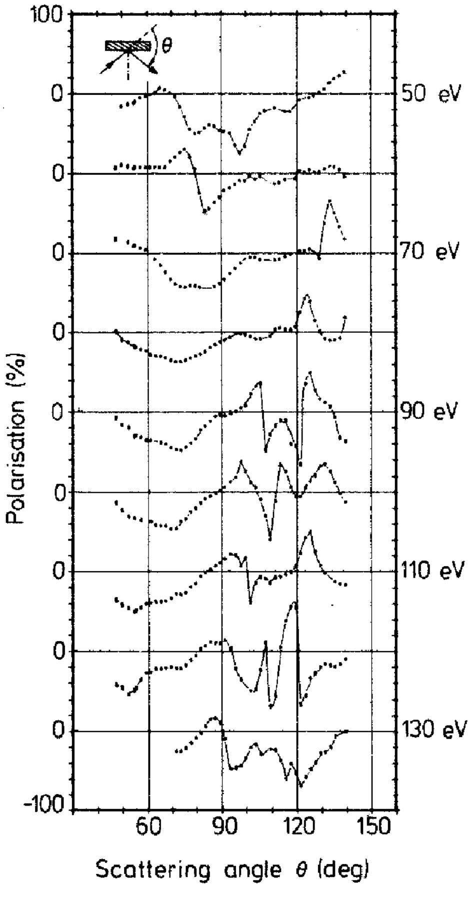

Figure 2. Spin polarisation of the 00 beam against scattering angle θ (see inset) for energies 50, 60 . . . 130 eV. The scattering plane is normal to the $1\bar{1}0$ direction. The crystal temperature is 320 K. The error bars indicate the statistical errors. (Additional experimental uncertainties: scattering angle ± 2°, polarisation zero ± 0·5%, polarisation calibration ± 5% of given values, energy ± 1 eV.)

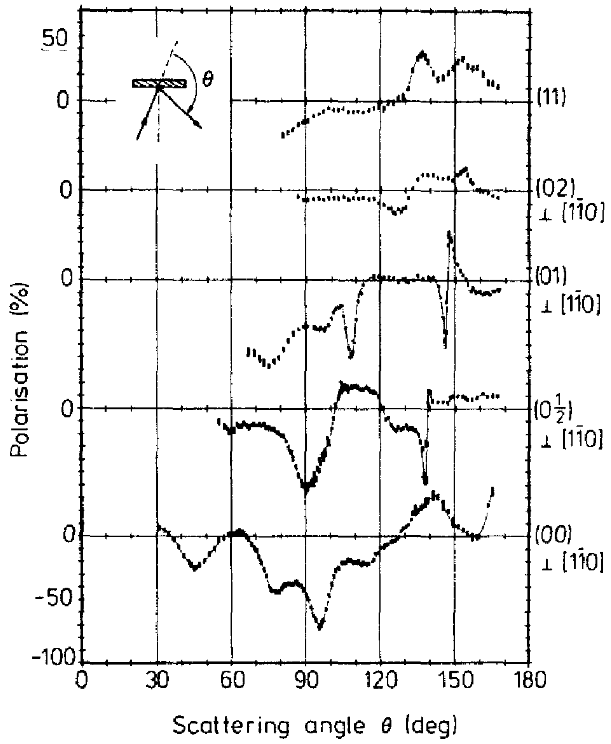

Figure 3. Spin polarisation against scattering angle for different beams for a primary beam energy of 50 eV and a crystal temperature of 320 K. (For experimental uncertainties see caption to figure 2.)

the dependence of spin polarisation on the scattering angle θ, which is defined as the angle between the primary beam and the diffracted beam under consideration. The polarisation profiles exhibit large peak values and sharp structural features. The latter are clearly due to multiple scattering effects, since a kinematic LEED theory would predict the comparatively smooth profiles of electron–atom scattering (Kessler 1976). The influence of dynamic effects is even more impressive in figure 3, the different profiles of which would be identical on kinematic grounds. The same applies to figure 4, where polarisation–θ profiles are shown for various temperatures. The relative heights of the negative polarisation maxima near $\theta = 78°$ and $\theta = 96°$ can be seen to change drastically with increasing temperature, spin polarisation thus monitoring the structural phase transition.

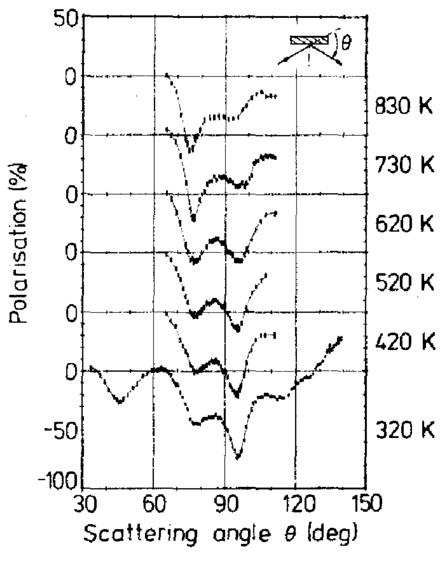

Figure 4. Spin polarisation of the 00 beam against scattering angle at 50 eV for crystal temperatures of 320, 420 . . . 830 K. The scattering plane is normal to the $1\bar{1}0$ direction. (For experimental uncertainties see caption to figure 2.)

In order to obtain quantitative information on surface properties, experimental spin polarisation data have to be compared to theoretical results calculated — by means of a dynamic relativistic LEED formalism (Feder 1972, 1976) — for assumed model surfaces. For reasons of computational convenience, we chose profiles in the high-temperature regime, in which the (1 × 1) LEED pattern exists. Measurements were made at crystal temperatures between 710 and 750 K, calculations for a crystal temperature of 723 K and Debye temperatures of 111 K and 170 K, which correspond to the limits of dominant diffraction by the surface atomic layer and deeper layers respectively. The top-layer spacing was assumed as contracted by 0–10% of the bulk interlayer spacing. The surface barrier was taken either as non-reflecting or as an exponential-type smooth function.

In figure 5, we present polarisation–energy profiles for the 11 beam, calculated for normal incidence and measured, by virtue of the reciprocity theorem, for normal exit. Assuming an inner potential of 14 eV, good agreement between theory and experiment is found around 50 eV. Near 90 eV, a somewhat smaller inner potential is more appropriate. For the specular beam, for which polarisation–scattering angle profiles at 50 eV are shown in figure 6, the surface barrier is quite important. Contrary to naive expectation, a non-reflecting barrier yields results closer to the experimental data. In comparing experiment and theory, three angular regimes should be distinguished

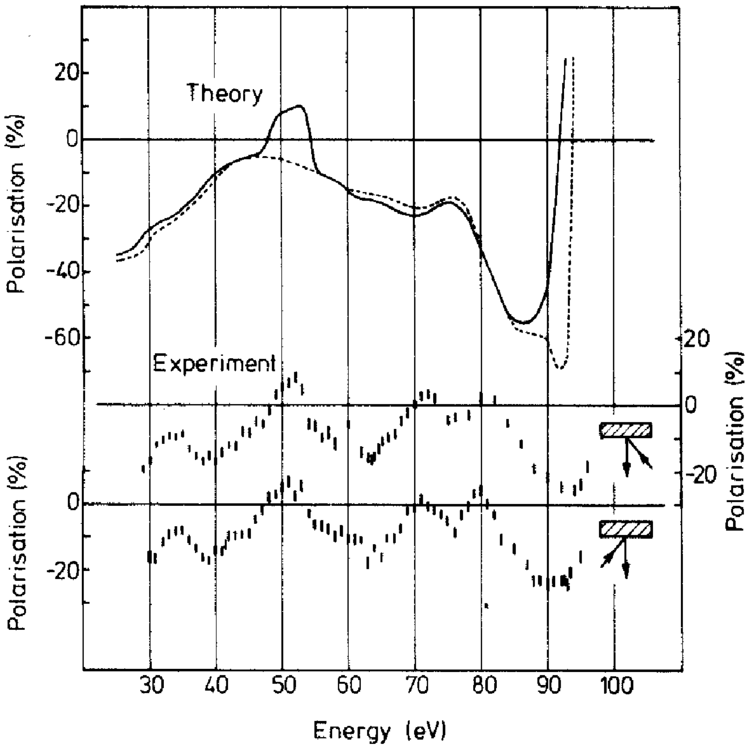

Figure 5. Spin polarisation of the 11 beam against energy. The theoretical results (—— for no contraction of the top layer spacing; ----- for 5% contraction) were obtained for a normally incident primary beam for a crystal temperature of 723 K and a bulk Debye temperature of 170 K. The experimental results were obtained via reciprocity for normal exit (see insets) for a crystal temperature between 710 and 750 K. (For experimental uncertainties see caption to figure 2.)

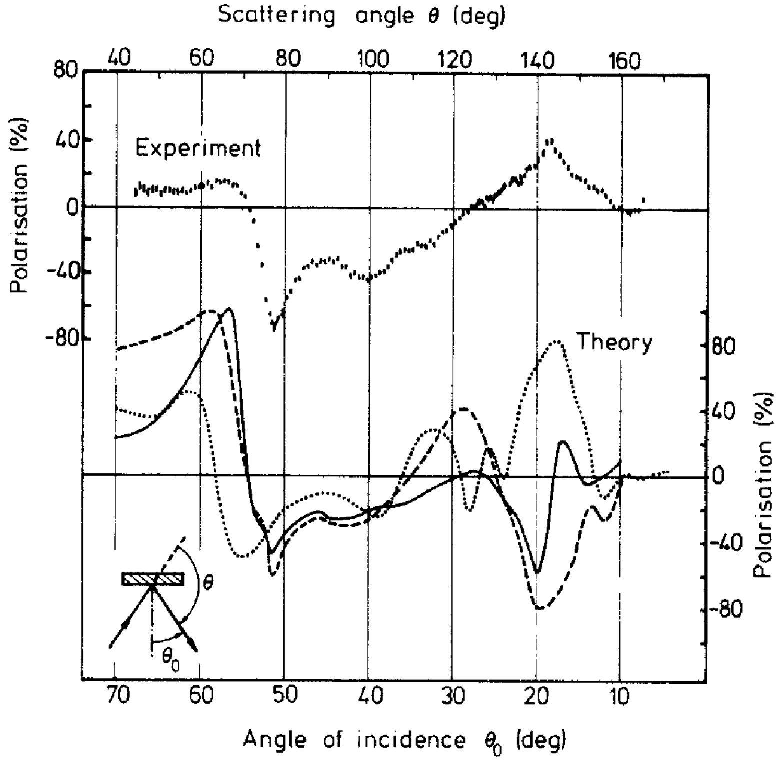

Figure 6. Spin polarisation of the 00 beam against scattering angle at 50 eV. Theory (no-reflection barrier): —— $T_{\mathrm{Deb}} = 111$ K and 10% contraction of the top layer spacing; ----- $T_{\mathrm{Deb}} = 111$ K and no contraction; ····· $T_{\mathrm{Deb}} = 170$ K and no contraction. The temperatures are the same as in figure 5. The scattering plane is normal to the $1\bar{1}0$ direction. (For experimental uncertainties see caption to figure 2.)

in figure 6. For $\theta > 130°$ (i.e. small angles of incidence) the theoretical results obtained with the bulk Debye temperature are preferred. For $70° < \theta < 130°$, a lower Debye temperature leads to good agreement. For $\theta < 70°$ (i.e. an angle of incidence greater than 55°) the agreement is poor. The fact that the angle of 55° almost coincides with the inclination of the (111) facets of the (110) surface suggests that surface roughness could be responsible for the discrepancy. In comparing theory and experiment, it should be borne in mind that the former assumes an ideal perfect surface, whilst the latter is dealing with the real surface, which exhibits (at the rather high temperature) considerable roughness and disorder.

In conclusion, the present work shows that large effects can be found in SPLEED. Comparison between theory and experiment appears encouraging, and there is hope that SPLEED can yield information on surface properties which is not obtainable by LEED intensity analysis alone.

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