

SURFACE SCIENCE LETTERS

**SPIN POLARIZATION IN LOW-ENERGY ELECTRON DIFFRACTION FROM
Pt(111): EXPERIMENT AND THEORY**

Peter BAUER *

Max-Planck-Institut für Plasmaphysik, Euratom Association, SFB 128, D-8046 Garching bei München, Germany

Roland FEDER

Theoretische Festkörperphysik, FB 10, Universität Duisburg GH, D-4100 Duisburg, Germany

and

Norbert MÜLLER **

Max-Planck-Institut für Plasmaphysik, Euratom Association, and Institut für Kristallographie der Universität München, SFB 128, D-8000 München, Germany

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Spin polarization in low-energy electron diffraction from the (111) surface of platinum, which is geometrically unreconstructed, was measured by means of a Mott detector. Corresponding relativistic calculations yield mostly excellent agreement with the data and clearly favour an ion-core scattering potential model containing an energy-dependent exchange approximation.

Spin polarization effects in low-energy electron diffraction (LEED) from large- Z materials, for which spin-orbit coupling is strong, have so far been studied experimentally and theoretically only for surfaces of Au(110) [1,2] and W(001) [3–5] which exhibit geometrical reconstruction and disorder or at least a contraction of the topmost interlayer spacing with respect to the bulk interlayer spacing. Since spin polarization versus energy or angle profiles were found to be very sensitive both to changes in surface geometry [6,2] and to details of the scattering potential [7] used in the calculations, it is essential for the use of spin-polarized LEED (SPLEED) for surface structure analysis to disentangle structural and nonstructural effects. It is the aim of this investigation to focus on the latter by choosing a surface, the geom-

* Present address: Institut für Experimentalphysik, Universität Linz, A-4040 Linz-Auhof, Austria.

** Present address: Fachbereich 4, Festkörper und Festkörpertechnologie, Universität Osnabrück, D-4500 Osnabrück, Germany.

etry of which is known to be a simple termination of the bulk lattice. This is, with a margin of possibly 1% dilatation, the case for Pt(111), as is evidenced independently by LEED intensity analysis [8,9] and ion scattering [10].

The apparatus used in the experiment is based on the apparatus described in refs. [1] and [2]. The following modifications were made. The pumping system is improved in order to minimize crystal-surface contaminations. The pressure in the Mott detector is now less than 10^{-7} mbar and in the UHV system it is about 6×10^{-11} mbar. A third spherical grid is introduced in the LEED optics and a glancing incidence 3 keV electron gun is mounted in the system, so the surface can be characterized also by Auger electron spectroscopy. The Pt crystal was sparkcut from a single crystal rod, oriented to the (111) plane by means of an X-ray diffractometer within 0.1° and mechanically polished with diamond paste down to $0.25 \mu\text{m}$. After cleaning it was mounted on a new high-precision crystal manipulator which permits the rotation of the crystal about two axes: one in the crystal surface plane (variation of the polar angle) and one perpendicular to the crystal surface (within 0.15°) (azimuthal angle). The crystal was further cleaned in vacuo by alternate heating to about 1100 K at 10^{-6} – 10^{-7} mbar O_2 and bombardment with 1–3 keV argon ions at 300–400 K for several days. During the measurements the crystal was kept clean by repeated heating to 600 K and, about once a week, by bombardment with 1–2 keV neon ions. The experimental data are given with error bars which only contain the statistical errors due to the counting in the Mott detector. In addition, the following experimental uncertainties have to be considered: for changes in energy ± 0.1 eV, for absolute values of energy ± 1 eV, for changes in polar angle $\pm 0.1^\circ$, for absolute values of polar angle at most $\pm 0.5^\circ$, for changes in azimuthal angle $\pm 0.2^\circ$, for absolute values of azimuthal angle $\pm 0.4^\circ$, for reproducibility of polarization values $\pm 3\%$ and for absolute values of polarization $\pm 7\%$ of the measured values.

Spin polarization profiles were calculated by means of the relativistic LEED theory described previously [6]. The following specific model assumptions were made. The real part V_r of the inner potential was chosen as 14 eV for the normal incidence calculations and subsequently found, via comparison with the experimental data, to be 12 eV, which was then used in the offnormal incidence calculations. For the imaginary part V_i , the standard values 4 and 5 eV were taken. The surface barrier models used were nonreflecting and, more realistically, exponentially smooth in order to check for possible surface-sensitive features. For the effective ion-core scattering potential, representatives of two different classes were employed, which were previously found to lead to substantial differences in both intensity [11] and spin polarization [7]: firstly a band structure potential [12], which implies a constant exchange approximation, and secondly a potential constructed from a self-consistent charge density [13] with an energy-dependent exchange contribution [14,15]. The resulting phase shifts (up to $l=7$) were corrected for room temperature using a Debye temperature of 178 K. For computational reasons, the present study neglects the reduction of the Debye temperature in the topmost layers, although this may have a noticeable effect on the spin polarization [1].

Spin polarization [16] as a function of energy, polar and azimuthal angle of incidence has been measured and calculated for the specular beam and various non-specular beams. In the following, some typical polarization results are shown to illustrate the general conclusions reached.

The normal incidence data in fig. 1 are strongly structured with large peak values. The agreement between the experimental profiles of two beams, which should be identical due to the three-fold rotation symmetry about the surface normal, demonstrates the accuracy of the experimental geometry. The theoretical profiles obtained for the two different ion-core potentials are seen to differ strongly from each other, the energy-dependent exchange potential producing significantly better agreement with experiment above about 70 eV [17]. The extreme sensitivity of the spin polarization near 60 eV to the potential approximation indicates the

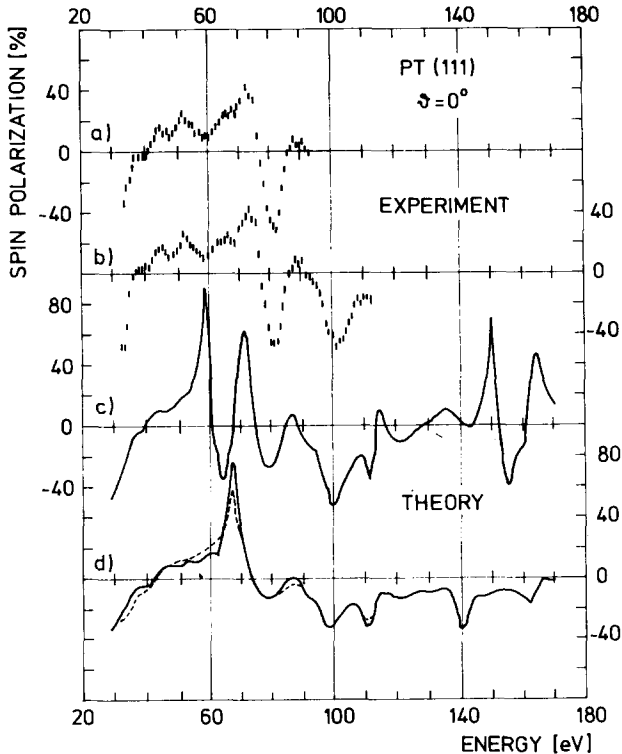


Fig. 1. Spin polarization versus energy for normal incidence on Pt(111). Experimental (10) beam (a) and (01) beam (b) measured for normal exit by virtue of time reversal symmetry [1]; theoretical (10) beam obtained for potential with energy-dependent exchange (c) and band structure potential (d); the imaginary inner potential was 4 eV (—) and 5 eV (---), the real inner potential 14 eV [17], the surface barrier exponentially smooth.

need for refinement of the exchange-correlation contribution to the potential and provides a crucial test. Curves (d) of fig. 1 show that a physically reasonable change of the imaginary part of the inner potential has a comparatively small influence. Results for the two barrier models were found to be practically identical.

At constant primary beam energies, spin polarization is found to vary rapidly with polar angle of incidence (see fig. 2). Agreement between experiment and theoretical results obtained for the energy-dependent exchange potential is generally very good not only with regard to peak positions and line shape but also in absolute polarization values. Again, the band structure potential leads to different results, which are at strong variance with the data. For each ion-core potential, polarization

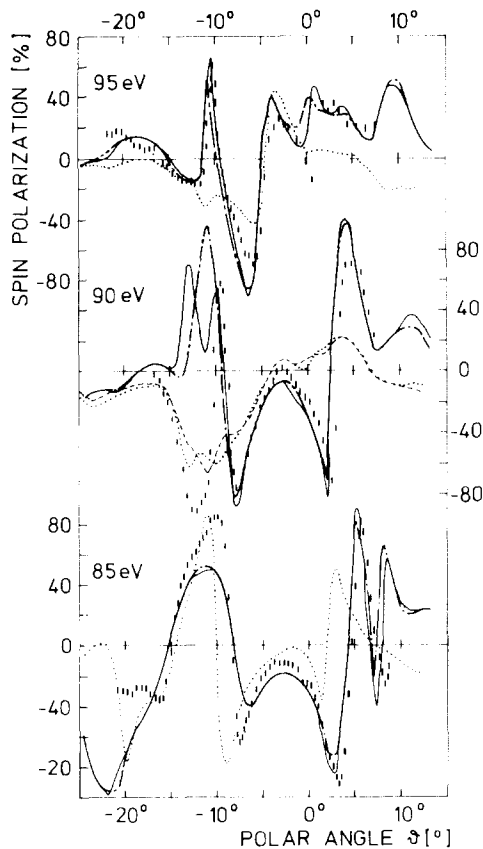


Fig. 2. Spin polarization of the (10) beam from Pt(111) at fixed energies as a function of the polar angle θ (defined with respect to the surface normal). The scattering plane is normal to the surface. Experiment (||||) and theory for $V_r = 12$ eV and $V_i = 4$ eV using band structure potential and nonreflecting (---) or exponential (.....) surface barrier and potential with energy-dependent exchange and nonreflecting (- · - ·) or exponential (——) barrier.

profiles obtained for the nonreflecting and the more realistic smooth surface barrier model are found to be generally very similar except for some angular and energy regions, e.g. at $E = 90$ eV near $\vartheta = -11^\circ$ (fig. 2), in which surface resonances occur. Since the nonreflecting barrier model is an unphysical artifact, results for different smooth barrier models can be expected to be even closer to each other. As for the discrepancy between experiment and theory at 90 eV near $\vartheta = -11^\circ$, the surface-sensitivity of the profiles is outweighed by their sensitivity to the exchange approximation in the ion-core potential. This region seems therefore also suitable to test refinements in the potential model. Calculations were also made for a 1% dilatation

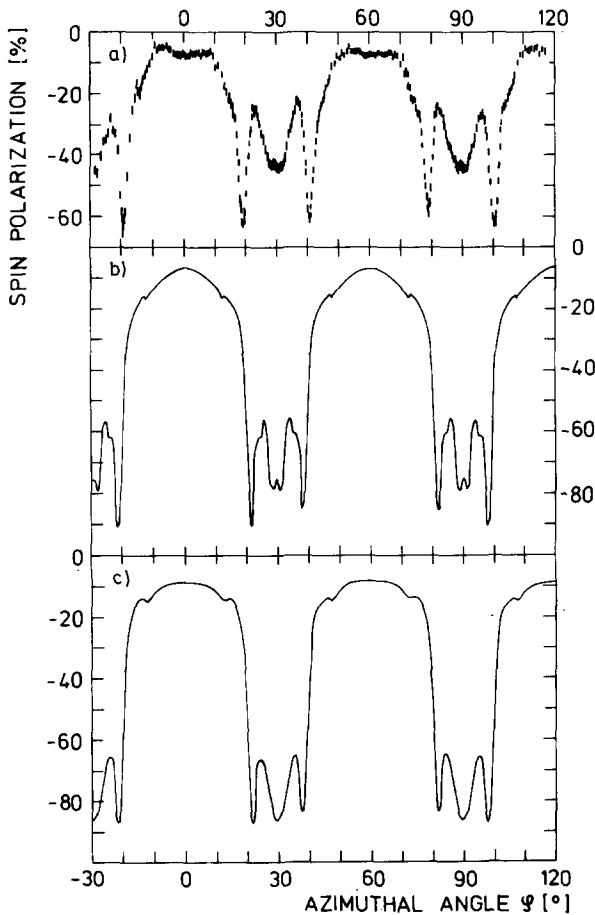


Fig. 3. Spin polarization of the (00) beam versus azimuthal angle of incidence φ (see ref. [18]) from Pt(111) for fixed energy $E = 60$ eV and fixed polar angle $\vartheta = 44^\circ$. Experiment (a) and theory with exponential (b) and nonreflecting (c) surface barrier.

of the top interlayer spacing. The results are almost identical to those for 0%.

Fig. 3 shows spin polarization [16] rotation diagrams [18] for the specular beam. The experimental diagram exhibits polarization peaks of about 60% with full width at half-maximum of only 3° . The calculated results are sensitive to the shape of the surface barrier, the exponential barrier yielding better agreement with the data. The mirror symmetry with respect to $\varphi = 0^\circ$ and 60° , which is present in the calculated rotation diagrams, also occurs in the experimental data taking into account an uncertainty of 3% of the measured polarization values. Deviations from mirror symmetry with respect to $\varphi = 30^\circ$ and 90° apparent in the theoretical results are of the order of the experimental uncertainty and require further investigation.

In conclusion, we have found very good agreement between experiment and theory for $P(E)$ and $P(\vartheta)$ of the nonspecular beams above 70 eV using an energy-dependent exchange potential. Since the exchange interaction does in fact decrease with increasing energy, the potential supported by our results is also of a physically more adequate type than a potential with constant exchange (like the band structure potential V_B).

The extreme sensitivity of the calculated results to the exchange approximation around 60 eV indicates that spin polarization can provide a crucial test for further refinements of the potential model. Attempts to optimize the potential via comparison with experimental data should, however, also take account of the fact that the surface Debye temperature is smaller than the bulk value, since this may produce noticeable effects on the spin polarization [1].

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- [15] The charge densities from which the two potentials were derived, are almost identical [13]. Consequently, differences in the scattering properties must be due to the different exchange approximations used.
- [16] By "spin polarization", we mean in the present context the projection of the spin polarization vector normal to the scattering plane, i.e. the plane defined by the incident beam and the diffracted beam under consideration. As a consequence of multiple scattering, the spin polarization vector in LEED is in general not normal to the scattering plane (cf. ref. [6b]) except when this plane is a mirror symmetry plane.
- [17] Since a shift of the calculated profiles by 2 eV towards higher energies produces better alignment with the data, the appropriate inner potential V_r is 12 eV rather than 14 eV.
- [18] The angle φ is defined such that $\varphi = 0$ corresponds to the scattering plane parallel to the $(\bar{1}10)$ mirror plane (normal to the surface).