Spin-polarized LEED from Xe-Pt(111)

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($\sqrt{3} \times \sqrt{3}$)-R30° Xe layers on Pt(111) were studied by spin-polarized LEED. Spin-polarized photoelectrons from a GaAs source were diffracted and the spin-dependent intensities of the adsorbate-induced beams were measured. Different adsorbate-induced beams not equivalent by symmetry in the system Xe-Pt(111) but equivalent in an isolated Xe layer show identical spin-dependent scattering asymmetries indicating a diminishing interlayer scattering and thus a diminishing influence of the substrate. Thus the adsorbate-induced beams are not suitable for structure determination. Spin-dependent scattering asymmetries measured in spin-polarized LEED of adsorbed Xe show a structure similar to one in asymmetry profiles of free Xe known in the literature.

1. Introduction and experimental setup

Adsorbed layers of Xe atoms have been studied by photoemission[1-6], by elastic atom scattering (TEAS)[7] and by LEED[8-11]. In this paper we report spin-polarized LEED data from Xe-Pt(111).

In our experiment, a spin-polarized incident electron beam with spin-polarization vector **P** normal to the scattering plane is scattered at the surface and the spin-dependent intensity of the diffracted beams is measured (Figure 1).

The spin-polarized photoelectrons are emitted from NEA-GaAs[12-14] using light of 830 nm from a laserdiode circularly polarized by a pockels-cell. The electrons are deflected by 90° electrostatically and transported to the sample by electron optics. The intensities of the diffracted electron beams are measured by a movable faraday cup with retarding grids to suppress inelastically scattered electrons.

The direction of **P** is switched from ↑ to ↓ by switching the helicity of the incident light giving the two corresponding measured intensities $I\uparrow$ and $I\downarrow$. The scattering asymmetry $A_\perp$ is defined as:

$$A_\perp := \frac{1}{|\mathbf{P}|} \frac{I\uparrow - I\downarrow}{I\uparrow + I\downarrow}.$$

The Pt(111) crystal can be rotated about its surface normal and about a polar axis lying on the surface and perpendicular to the scattering plane.

The substrate was cleaned by sputtering (2.5 keV Ne$^+$) and heating in oxygen (400 °C)[16]. The ($\sqrt{3} \times \sqrt{3}$)-R30° Xe layer was prepared at 70 K. The pressure in the uhv chamber was in the 10^{-11} mbar regime.

The GaAs crystal was cleaned by heating (620 °C, 30 min) and was activated to NEA in cycles of alternating cesiation and oxidation[12-14]. The maximum emitted electron current is about 10 μA. The spin polarization of the beam was determined to be $28 + 2/ - 3\%$ by using spin-polarized LEED of the clean Pt(111) crystal as a polarization analyser based on reference data[15].

2. Results and discussion

Figure 2 shows schematically a normal incidence LEED pattern of ($\sqrt{3} \times \sqrt{3}$)-R30° Xe-Pt(111) with the mirror planes of the system Xe-Pt(111) and the additional mirror planes of the isolated Xe layer. The beams studied (with varied angle of incidence) are denoted by P*I* and P*II* (clean Pt(111)), and I_1, I_2, II_1 and II_2 (adsorbate induced) corresponding to the scattering geometries *I* and *II*.

Figure 3 shows a series of asymmetry profiles of beam II_1. The asymmetry profiles depend significantly on the scattering angle and on the scattering energy. $|A_\perp|$ is less than 20%, while for free Xe values $|A_\perp|$ up to 50% have been observed[17].

Figure 2 also shows a series of symmetry operations to transform scattering geometry *I* into scattering geometry *II* and vice versa with fixed scattering plane. This series contains a time reversal, which leaves $A_\perp$ invariant if the scattering plane is a mirror plane of the scattering experiment[18-20].

The scattering processes causing diffraction into the adsorbate induced beams of type *I* and *II* contain two different contributions[21,22]:

(a) scattering events from the adsorbate layer only; the symmetry is determined by the six-fold symmetry of the isolated Xe layer. Thus the scattering plane is a mirror plane and
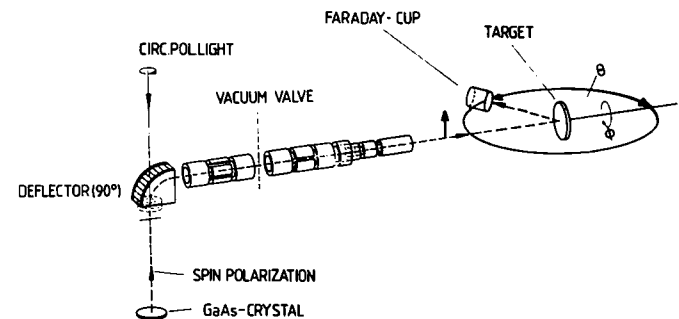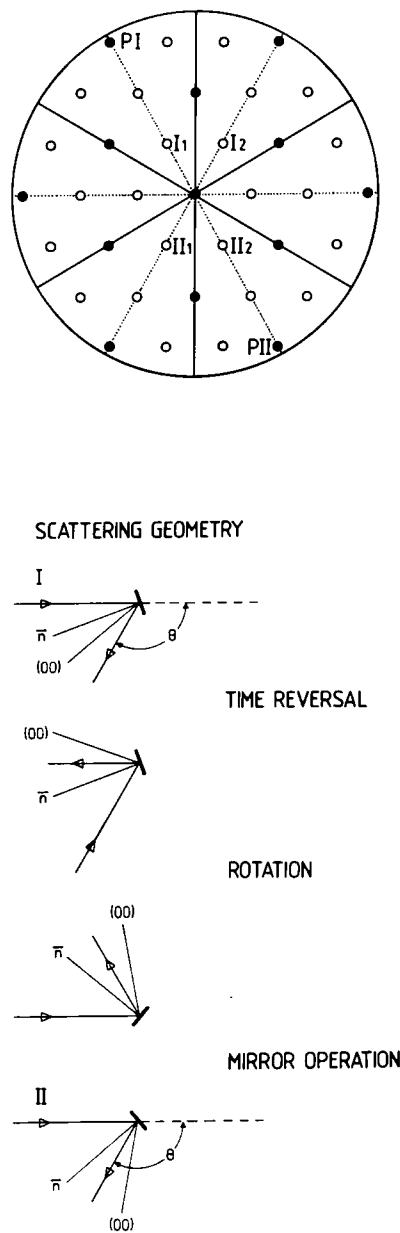

Figure 1. Scheme of the experimental setup.

SCATTERING GEOMETRY

I

TIME REVERSAL

ROTATION

MIRROR OPERATION

II

Figure 2. Upper part: schematic LEED pattern of $(\sqrt{3} \times \sqrt{3})$-R30° Xe-Pt(111) and scattering geometries of the studied beams I_1, I_2, II_1 II_2, PI and PII. (●: substrate beams, ○: adsorbate induced beams, solid lines: mirror planes of Xe-Pt(111), solid lines + dotted lines: mirror planes of the isolated Xe layer). Lower part: series of symmetry operations to transform geometry I into geometry II and vice versa.

therefore this contribution should be identical for the beams with different scattering geometries.

(b) multiple scattering between at least one Xe atom and the Pt substrate; the symmetry is determined by the three-fold symmetry of the system Xe-Pt(111)*. Here the scattering plane is not a mirror plane and therefore this contribution should generally be different for the beams with different scattering geometries.

In any case the two adsorbate induced beams with identical

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*It is assumed that the adsorbed Xe atoms occupy the three-fold hollow sites of the Pt(111) surface.
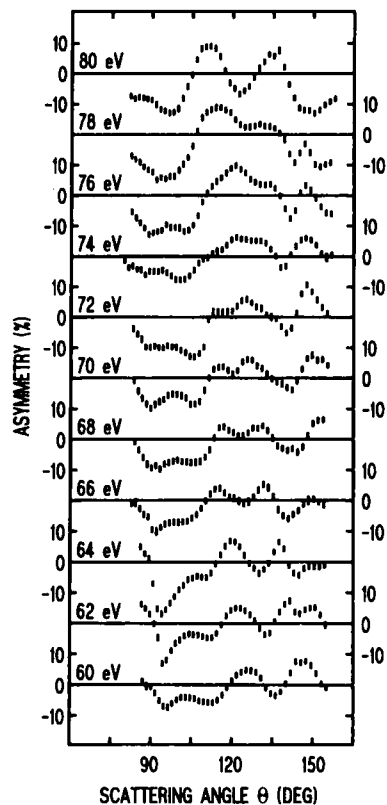
Figure 3. Series of asymmetry profiles of adsorbate-induced beam II_1 as function of the scattering angle.

scattering geometry have to reveal identical asymmetry profiles because of the symmetry of the system Xe-Pt(111) and of the isolated Xe layer as well.

Figure 4 shows the measured asymmetry profiles of the adsorbate-induced beams. The asymmetry profiles of the beams with identical scattering geometries reveal the required identity. However, the profiles of the beams with different scattering geometries are also identical.

For comparison, Figure 5 shows asymmetry profiles of the beams PI and PII (clean Pt(111)), which are of the same symmetry as the adsorbate-induced beams of types I and II. In contrast to those of the adsorbate, the asymmetry profiles of the substrate beams exhibit significant differences.

The six-fold symmetry found in our measurements at the adsorbate-induced beams indicates that here $A_\perp$ is mainly determined by the adsorbed Xe layer and that there are almost no contributions due to multiple scattering from the substrate.

For the determination of adsorbate structures it is necessary to investigate scattering processes with contributions of both adsorbate and substrate. Thus if the main interest lies in structure determination of adsorbates with weak interlayer scattering between adsorbate and substrate, one has to make use of the outgoing intensities in the position of beams of the clean substrate for commensurate adsorbates and the specular beam for incommensurate adsorbates.

It is known from LEED studies that electron scattering at adsorbed Xe layers shows an almost kinematic behaviour[9,10]. The asymmetry profiles of adsorbed Xe atoms are much too structured to allow the scattering to be described kinematically, but the influence of single scattering can be seen clearly: Figure 6 shows a comparison of asymmetry profiles of free Xe[17] and of
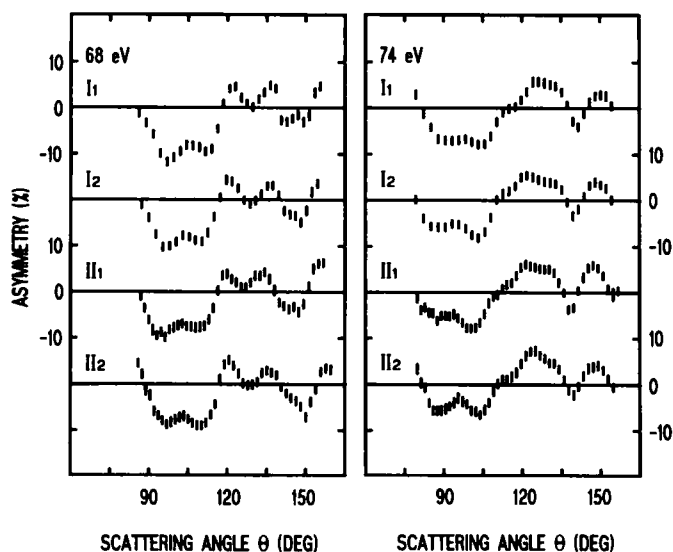
Figure 4. Comparison of the spin-dependent scattering asymmetry $A_\perp(\Theta)$ for different kinetic energies of adsorbate induced beams of type *I* with that of type *II* as function of the scattering angle Θ.
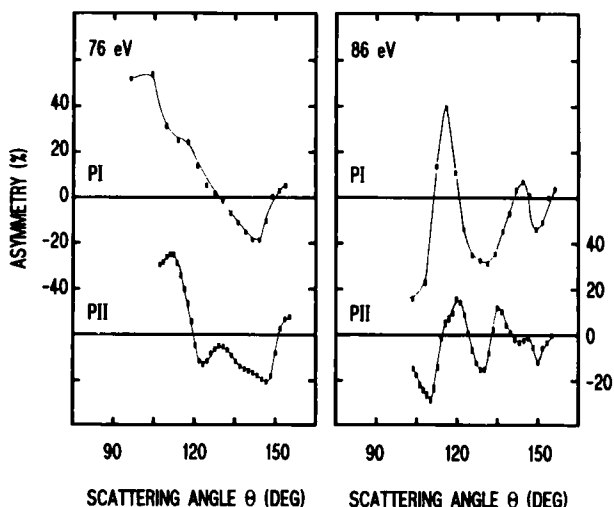

Figure 5. Spin-dependent scattering asymmetry $A_\perp(\Theta)$ of the beams P*I* and P*II* of the clean Pt(111) surface as function of the scattering angle Θ.
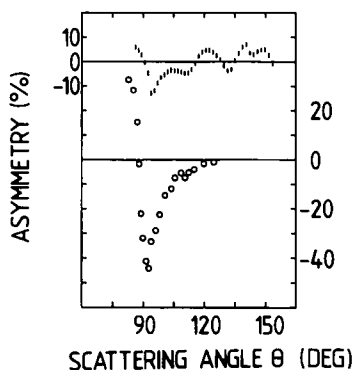

Figure 6. Comparison of asymmetry profiles of adsorbed Xe atoms (|) (beam II_1, scattering energy 62 eV) with those of free Xe atoms (○)[17] (scattering energy 60 eV). For energy correction see text.

adsorbed Xe. The position of the peak and of the zero crossing near $\Theta = 90°$ are almost identical. In contrast, the peak height is less pronounced for adsorbed Xe than for free Xe.

For free Xe atoms this structure is caused by a deep minimum in the direct scattering amplitude and a strong change in the phase shift difference between the direct scattering amplitude and the spin flip amplitude[17]. Because of the atomic nature of this structure the scattering energy for this comparison is lowered by 2 eV due to the -2 eV-shift[4] of the ionization threshold of adsorbed Xe with respect to the ionization threshold of free Xe instead of correcting the energy due to the inner potential of $V_0 = -4$ eV[1] of the adsorbed Xe layer.

3. Conclusion

Our measurements indicate that for scattering into the adsorbate induced beams the spin-dependent scattering asymmetry $A_\perp$ contains almost no contribution due to scattering from the substrate. Thus Xe–Pt(111) is a system with weak interlayer scattering between adsorbate and substrate. This may be caused by the relatively strong backscattering from the medium-Z Xe-atoms.

Furthermore, structures similar to those in asymmetry profiles of free Xe atoms can be found in the asymmetry profiles of adsorbed Xe atoms. This shows the influence of single scattering processes and makes an energy correction due to the shift of the ionization threshold likely instead of the inner potential of the adsorbate.

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