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Xe-adlayers on Pt(111) and Pd(111): structure investigation by spin-polarized LEED

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$(\sqrt{3} \times \sqrt{3})$R30° Xe-layers on Pt(111) and Pd(111) are studied by spin-polarized LEED. In the experiment spin-polarized electrons from a GaAs photoemission source were scattered and the spin-dependent intensities are measured in different diffracted beams. Corresponding calculations were performed using a new relativistic LEED code. Measurements and calculations agree reasonably. They show strong contributions from multiple scattering between substrate and adlayer, and therefore spin-polarized LEED reveals strong sensitivity to structural parameters.

Spin-polarized low energy electrons are diffracted at the surface and the spin-dependent intensities of the diffracted beams are measured. The source of spin-polarized electrons is a negative electron affinity GaAs photoemission source [1–3] with a degree of polarization of 26% ±3%/2%. The surface normal is chosen to be in the scattering plane, which is defined by the incoming and outgoing beam. The spin-polarization vector $\boldsymbol{P}$ of the incident beam is aligned normal to the scattering plane. $\boldsymbol{P}$ is switched between the two normal directions (+, −) by switching the helicity of the circularly polarized light incident on the GaAs crystal. The resulting spin-dependent intensities I_+, I_- yield the scattering asymmetry $A_\perp$

$$A_\perp := \frac{1}{|\boldsymbol{P}|} \frac{I_+ - I_-}{I_+ + I_-} .$$

The target crystal can be rotated about its surface normal and about a polar axis lying on the surface and being perpendicular to the scattering plane. The asymmetry profiles were measured as a function of the scattering angle Θ. The $(\sqrt{3} \times \sqrt{3})$-R30° Xe-layer was prepared at 70 K for both Xe/Pt(111) and Xe/Pd(111).

Fig. 1 shows angular dependent asymmetry profiles of $A_\perp(\Theta)$ for identical adsorbate induced beams measured at Xe/Pt(111) and at Xe/Pd(111). The asymmetry profiles of Xe/Pd(111) are much smoother and are less structured than those of Xe/Pt(111). As the lattice constant of the $(\sqrt{3} \times \sqrt{3})$R30° Xe-layers on these two substrates is identical within 1% these differences clearly show the influence of the substrate.

Fig. 2 shows measured angular dependent asymmetry profiles in the specular beam of clean Pt(111) and $(\sqrt{3} \times \sqrt{3})$R30° Xe/Pt(111) at 52 eV. The asymmetry profiles of clean and Xe-covered Pt(111) are similar in their general structure. The adsorption of the Xe-layer leads to decreased heights and displaced positions of the asymmetry peaks and to a new peak around $\theta = 80°$.

The spin-dependent LEED calculations are performed in three steps. Firstly the scattering of the electrons at a single muffin-tin core is treated fully relativistically by solving the Dirac equation

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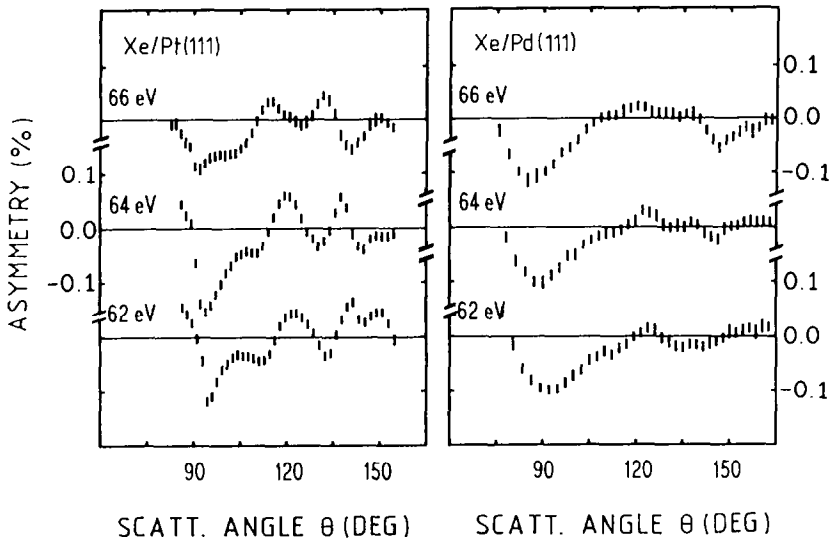

Fig. 1. Angular dependent asymmetry profiles of the adsorbate induced (1/3, 1/3)-beams measured at $(\sqrt{3} \times \sqrt{3})$R30° Xe/Pt(111) and $(\sqrt{3} \times \sqrt{3})$R30° Xe/Pd(111). The length of the error bars represents the statistical error. There is an additional scaling error of +12%/−8% of the given values due to the calibration of $|P|$.

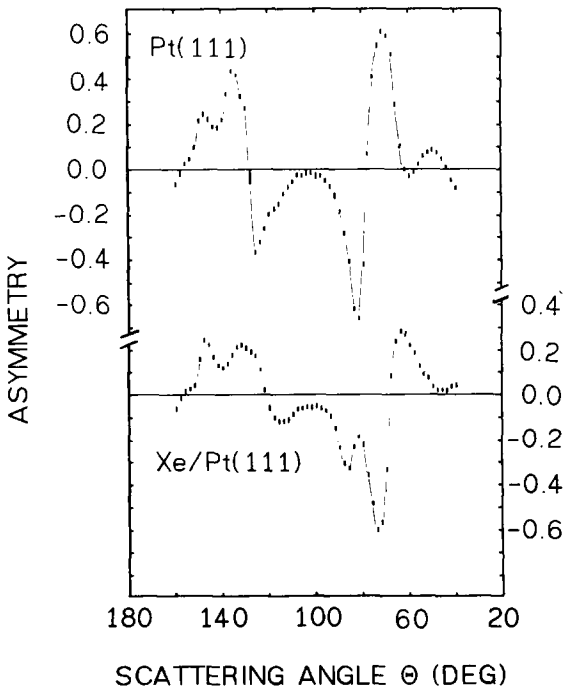

Fig. 2. Asymmetry profiles of the specular beam of clean Pt(111) and $(\sqrt{3} \times \sqrt{3})$R30° Xe/Pt(111) for 52 eV (errors: see fig. 1).

[4]. Secondly intra layer multiple scattering is taken into account by a two component analogue of the "layer-KKR"-formulation of Pendry [5–7]. Thirdly interlayer multiple scattering is treated by combining the scattering matrices of the bulklayers by layer doubling [5]. The reflection matrix of the whole system is constructed by combining the bulk reflection matrix with the scattering matrices of the adlayer.

The ion-core phase shifts are modified to approximate the effects of thermal lattice vibrations [6]. In the calculations the Debye temperatures of Pt and Xe are assumed to be 229 and 200 K, respectively. The inner potential of the Pt-bulk and of the Xe-adsorbate has been varied from 5.0 to 15.0 eV (real part) and from 1.0 to 5.0 eV (imaginary part). For an inner potential of the Pt-bulk of 12.5 eV (real part) and 3.4 eV (imaginary part) best agreement with measurements from clean Pt(111) is achieved and thus these values are taken for the presented calculations. The inner potential of the Xe-adlayer in the presented calculated data is 10.0 eV (real part) and 3.0 eV (imaginary part). At an electron energy of 64 eV typically 60 reciprocal lattice vectors are included,

and phase shifts up to $l_{max} = 7$ for Pt and up to $l_{max} = 10$ for Xe are taken into account.

Fig. 3 shows a series of calculated asymmetry profiles in comparision with the measured data for $(\sqrt{3} \times \sqrt{3})$R30° Xe/Pt(111). Peak positions are very sensitive to small variations in the layer spacing d. So an exact determination of this parameter is possible in principle. However, measurement and calculations show agreement for $d = 3.2$ Å and for $d = 4.2$ Å as well. The periodicity in calculated asymmetry profiles is observed also for higher values of the layer spacing. Further investigations are necessary to find out the right value. This includes studies at different energies and in different beams and in addition an R-factor analysis.

The value $d = 4.2$ Å corresponds to the value of 4.8 Å for the distance between Xe-atoms in the

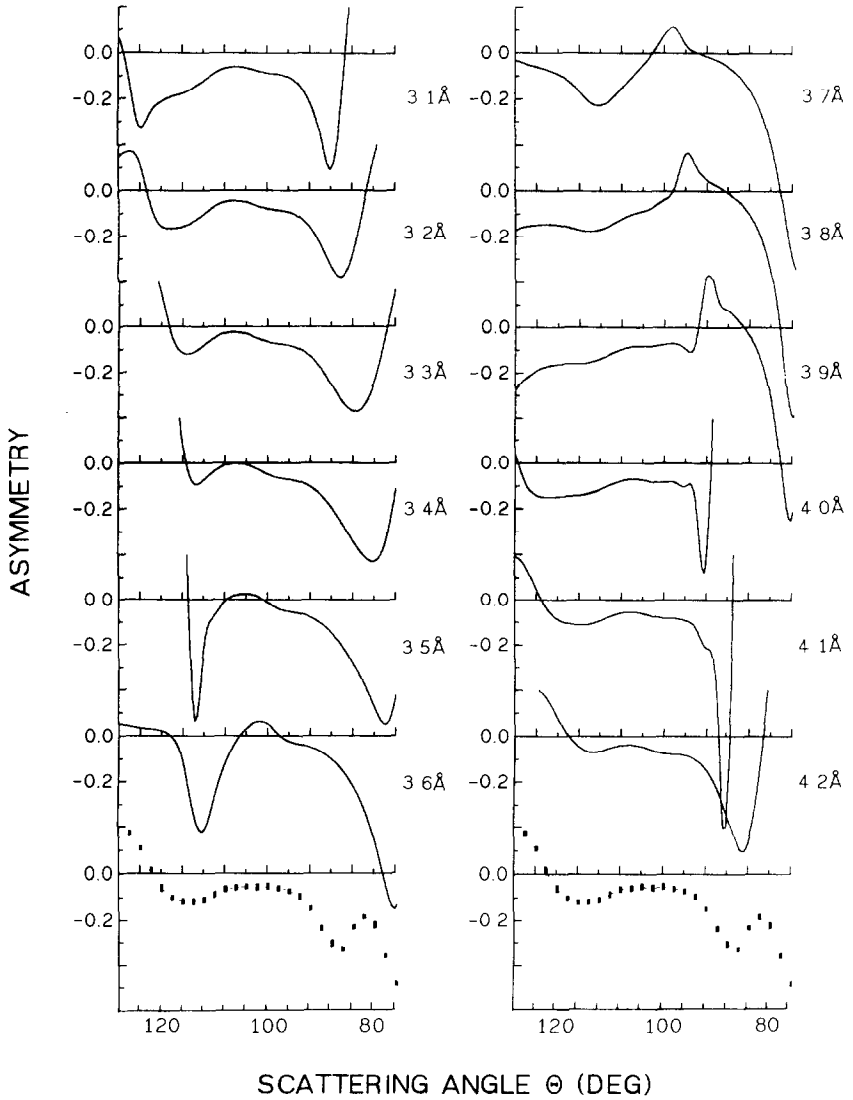

Fig. 3. Calculated asymmetry profiles of the specular beam for different layer spacings in comparison to experimental data of $(\sqrt{3} \times \sqrt{3})$R30° Xe/Pt(111) for 52 eV.

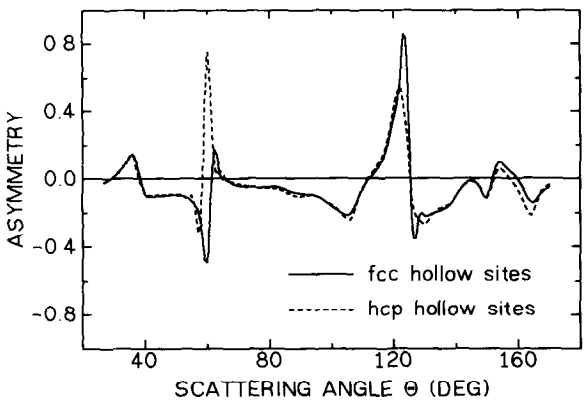

Fig. 4. Calculated asymmetry profiles of the specular beam for different adsorption sites of $(\sqrt{3} \times \sqrt{3})R30°$ Xe/Pt(111) for 70 eV.

overlayer and to the value of 4.4 Å of a xenon crystal. If hollow sites are assumed to be the adsorption sites, the value of 3.2 Å agrees with the minimum layer spacing resulting from the hard sphere radii of 2.2 Å for Xe and of 1.4 Å for Pt.

It is not yet possible to distinguish between fcc- and hcp hollow sites. Fig. 4 shows asymmetry profiles calculated for these two adsorption sites. Only peak heights differ significantly. These peak heights are connected with minima in the calculated intensity. The low intensity in these minima cannot be reproduced in the experiment because of a background due to disorder scattering. Thus it is not possible to get structural information from fig. 4.

In conclusion our investigations show spin-polarized LEED to be a powerful method to study adsorbate structures. The calculations show the spin-dependent scattering properties to be very sensitive to variations of structural parameters, and the general agreement between measurement and calculation allows us to evaluate these parameters.

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