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## **In-situ X-Ray Surface Scattering Studies of the Potential-induced Reconstruction of Ultrathin Au Films on Pt(111) Electrodes**

Beamline(s): X22A

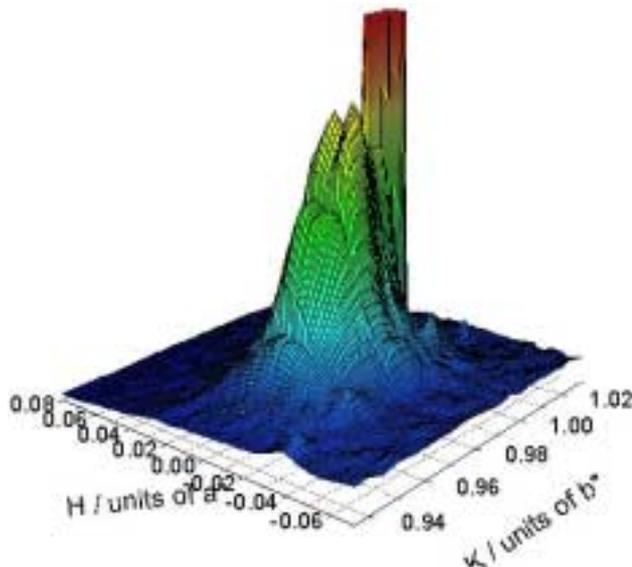
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The structure of ultrathin epitaxial metal film on foreign metal substrates results from a subtle interplay between the interface energy, favoring a pseudomorphic arrangement, and the energetic contribution due to strain of the film, favoring film relaxation. In studies under ultrahigh vacuum conditions a general scheme of film relaxation was found where with increasing film thickness the structure changes from pseudomorphic, to one-dimensional dislocation networks, two-dimensional, hexagonal dislocation networks, and finally to completely relaxed films. In an electrochemical environment film relaxation can be induced by the applied potential as we show here for the case of 1-2 ML thick Au films on Pt(111) electrodes in 0.1 M H<sub>2</sub>SO<sub>4</sub> solution. Starting from a pseudomorphic structure at potentials negative of 0.35 V<sub>Ag/AgCl</sub>, a sequence of transitions into various dislocation network structures was observed by *in-situ* scanning tunneling microscopy (STM) with increasing potential: (1x1) → “striped” phase in the Au bilayer, (1x1) → “striped” phase in the monolayer, and “striped” → “hex” phase in the bilayer [1].

To clarify the structure of these phases, *in-situ* surface x-ray scattering studies were carried out on thin Au films (1-2 monolayers thick) prepared on flame annealed Pt(111) crystals. Upon increasing the potential into the regime of the dislocation network phases, the diffracted intensity at the (0, 1) rods of the Pt substrate drastically decreased (to ¼ of the maximum intensity observed in the “striped” phase), in agreement with a loss of commensuration of the overlayer. Simultaneously, broad peaks emerge on the lower q<sub>||</sub> side of the (0, 1) rods. For the Au monolayer film a pair of peaks at (±q<sub>r</sub>/√3, 1-q<sub>r</sub>/√3) is found for potentials ≥ 0.70 V<sub>Ag/AgCl</sub>, in complete agreement with a uniaxial dislocation network structure of light domain walls, i.e. an expanded Au lattice (Fig. 1). For the Au bilayer the same type of structure is found at potentials ≥ 0.40 V<sub>Ag/AgCl</sub>, followed at potentials ≥ 0.75 V<sub>Ag/AgCl</sub> by a transition to a structure with a broad on-axis peak at (0, 1-q<sub>r</sub>/√3), characteristic for a hexagonal dislocation network. The substantial peak widths and the absence of satellite peaks indicate a high defect density in the dislocation pattern. In addition, measurements of the peak intensity along the surface normal direction indicate an oscillatory behavior in the Au bilayer, suggesting that both Au layers reconstruct.

The data are a direct, quantitative confirmation of the structural models derived from the dislocation patterns *in-situ* STM data. They can be rationalized by a stepwise relaxation of the Au surface layer(s) due to anion adsorption, resembling the potential-induced reconstruction of Au(111) and in good agreement with Frenkel-Kontorowa theory.

[1] E. Sibert, F. Ozanam, F. Maroun, O.M. Magnussen, R.J. Behm, submitted.



**Figure 1:** In-plane diffracted intensity at  $L=0.2 c_{Pt}^*$  for a Au monolayer on Pt(111) in 0.1 M H<sub>2</sub>SO<sub>4</sub> at 0.75 V<sub>Ag/AgCl</sub>, showing the sharp (0, 1) rod of the Pt(111) substrate (truncated) and a broad pair of peaks, corresponding to the uniaxial dislocation network.