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Surface X-Ray and Neutron Scattering

Proceedings of the 2nd International Conference, Physik Zentrum, Bad Honnef, Fed. Rep. of Germany, June 25–28, 1991

With 120 Figures

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Au Adsorption on Si(111) Studied by Grazing Incidence X-Ray Diffraction

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Abstract. The atomic arrangement in the three ordered structures of Au on Si(111) has been studied by in plane x-ray diffraction. The common feature in all three structures is the formation of small Au clusters and substantial distortions of the substrate. The (5x1) structure consists of a disordered (5x2) structure with partially occupied rows of Au clusters in low symmetric adsorption sites. For the ($\sqrt{3}$x$\sqrt{3}$) structure the trimer model could be confirmed. The (6x6) structure consists of trimer triplets located at different adsorption sites and is probably connected with a reconstruction of the top substrate layer.

In the range of monolayer coverages Au forms three ordered structures on Si(111). Between 0.2 and 0.8 monolayers (ML) a (5x1) structure is observed [1]. In agreement with the common usage in the literature the notation (5x1) is used here though this structure is in fact a disordered (5x2) structure as has been noticed already in earlier LEED studies [2]. Above 0.5 ML the ($\sqrt{3}$x$\sqrt{3}$)R30° structure occurs and above 1.5 ML the (6x6) structure exists [1]. 1 ML refers to one Au atom per (1x1) substrate unit cell. These structures have been subject of a number of studies with a variety of methods but the atomic arrangement has not become clear until now. Particularly, for the ($\sqrt{3}$x$\sqrt{3}$) structure two different structure models have been proposed. A honeycomb structure of Au occupying high symmetric adsorption sites at a coverage of 2/3 [3] and trimer model corresponding to 1 ML coverage [4]. The ($\sqrt{3}$x$\sqrt{3}$)R30° structure is also found in the related systems Ag/Si(111) [5] and Ag/Ge(111) [6] and the structure model presented here is closely related to these structures.

We present the structure models as determined from in-plane x-ray diffraction data. The details of the analysis are described in ref. [7,8]. All structure models are in agreement with recent scanning tunneling microscopy (STM) topographs [9-11]. Au was deposited on the clean Si(111)(7x7) surface at a rate of 0.3 ML/min and at a substrate temperature of 400° C. After preparation the sample was transferred under UHV conditions to a small x-ray diffraction chamber. X-ray diffraction data were measured at the wiggler beam line at the HASYLAB [12].

For the (5x1) structure 52 fractional order in plane structure factors were measured. Since the maxima of the patterson function do not agree with Si-Si distances Au atoms adsorb in low symmetric positions [7,12]. The Au sites 1-5 (fig. 1) follow directly from a Patterson map however, elongations of the Patterson

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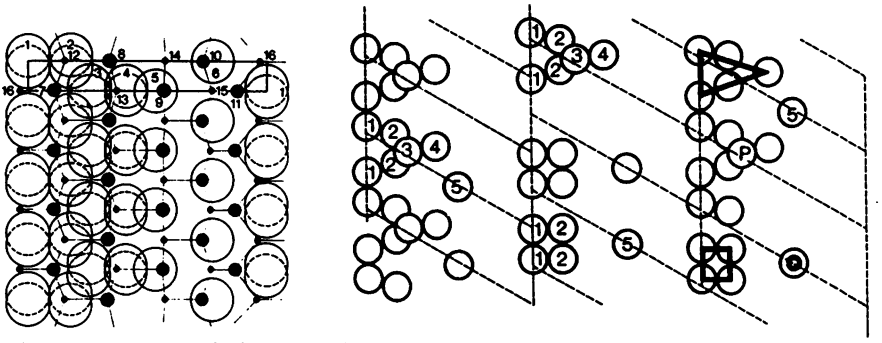

Fig. 1: Au- (large circles) and Si-positions in the first (large dots) and second (small dots) layer as obtained from the refinement of the (5x1) structure (left panel). A model taking account of a (5x2) unit cell and the partial occupation of the Au sites (right panel) explains protrutions (P), round, rectangular and triangular configurations as are observed in (STM) topographs [9].

maxima indicate a disorder in the [110] direction, which can be described by split positions corresponding to a statistical occupation of two different sites. Assuming the symmetry c1m1 the refinement of 25 free parameters, including 6 Au- and 10 Si positions, 5 occupation factors and an overall temperature factor gives a X^2 of 1.7 [7]. The distance of 2.9 Å between the Au sites 1 and 2 agrees with the nearest neighbour distance in the bulk Au. The split positions correspond to the superposition of the (5x2) unit cells into a single (5x1) unit cell. Two distances between Au atoms occur along the rows 1 and 2: 3.10 Å and 4.58 Å. The smaller value comes close to the bulk value of Au. In agreement with STM topographs [9] we find an irregular sequence of small Au clusters along the [110] direction (fig. 1).

14 fractional order structure intensities are used to elaborate the ($\sqrt{3}$x$\sqrt{3}$) structure including a substrate distortion (fig. 2). Only the trimer model [4] is consistent with the Patterson map as has been reported earlier [8]. The interatomic Au-Au distance of 2.7 Å is slightly smaller than the bulk value. Au Atoms are located near H3 sites, assuming that Si atoms of the top layer are shifted. The registry with the bulk remains uncertain because only superstructure reflections were evaluated. The deviation between the coverage for the ($\sqrt{3}$x$\sqrt{3}$)-structure found in experiments [1] and the coverage for the trimer model (1 ML) probably results from missing trimers.

The Patterson function for the (6x6) structure was calculated from 139 fractional order intensities (fig. 3). Two main features of the Patterson function have to be discussed. First, it is evident that all interatomic vectors of the ($\sqrt{3}$x$\sqrt{3}$) structure appear again in the (6x6) structure (peaks 1-3 in fig. 3). Consquently Au trimers remain the structural element of the (6x6) reconstruction. Secondly no peaks in the middle of the unit cell are observed (indicated by A and B in fig. 3). Therefore the double of a translation vector of the ($\sqrt{3}$x$\sqrt{3}$) unit cell in all directions is missing. This means that the (6x6) structure cannot be explained by a simple superstructure of the ($\sqrt{3}$x$\sqrt{3}$) reconstruction. Only an arrangement of trimers where the occurrence of three Au atoms in a row is avoided can explain the Patterson function. The structure (fig. 3) has a low symmetry leading necessarily to the existence of 6 twin domains [8]. The coverage of 0.75 ML is well below the experimentally observed coverage of 1

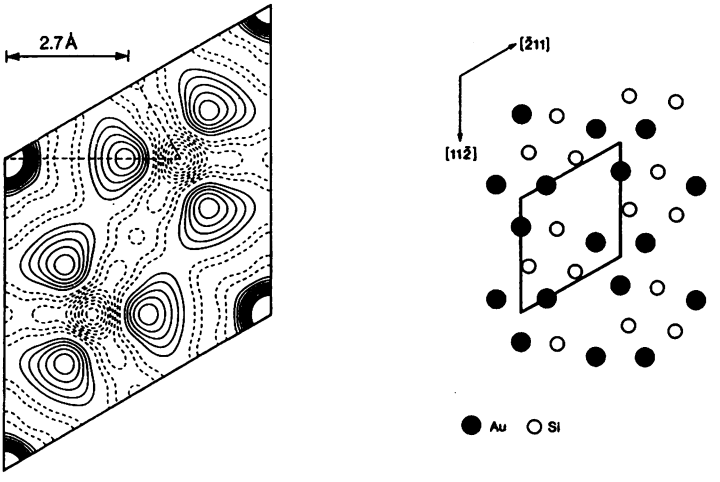

Fig. 2: Patterson function of the ($\sqrt{3}$x$\sqrt{3}$) structure (left panel). The irreducible unit cell is marked by dashed lines. In the right panel the trimer model with the 1st distorted Si layer is outlined. H3-like adsorption sites for the Au atoms are assumed.

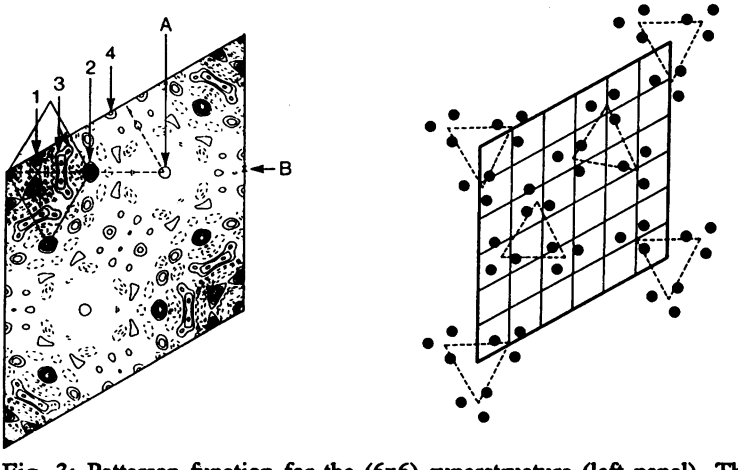

Fig. 3: Patterson function for the (6x6) superstructure (left panel). The shaded area corresponds to a ($\sqrt{3}$x$\sqrt{3}$) unit cell. The right panel illustrates a single twin domain of the (6x6) structure.

ML or above. We explain the discrepancy by additional Au atoms either adsorbed in sites between the trimers or diffused into subsurface sites. These Au sites could not be identified in the patterson map and have therefore been left out in the analysis.

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