Surface Science 131 (1983) L379–L384
North-Holland Publishing Company

SURFACE SCIENCE LETTERS

(111) FACETS AS THE ORIGIN OF RECONSTRUCTED Au(110) SURFACES

G. BINNIG, H. ROHRER, Ch. GERBER and E. WEIBEL

IBM Zurich Research Laboratory, CH-8803 Rüschlikon, Switzerland

Received 22 April 1983

The Au(110) surface has been investigated by scanning tunneling microscopy. The reconstructed surface consists of long ribbons of narrow (111) facets along the [1$\bar{1}$0] direction with maximum three free rows. Two-row facets give rise to the 1×2 reconstruction of the missing-row type, while three-row facets account for the 1×3 reconstruction. Disorder arises from locally random sequences of the two facets.

The surfaces of Au, Ir and Pt exhibit a variety of surface reconstructions of which the 1×2 structure of the (110) surface has attracted most attention. Of the various models proposed [1], an unrelaxed missing-row model was favored on the basis of LEED calculations for Ir(110) [2]. Controversial results have been reported for Au(110): While Noonan and Davis [3] found little agreement between measured LEED I–V profiles and calculations for the missing-row model, others [4] present good evidence for this model based on LEED analyses. An inherent difficulty with the missing-row model appears to be the surface mass transport. Atoms must move over several hundred Å to produce the ordered 1×2 reconstruction on a well-ordered 1×1 surface. Since the transition time from the 1×1 to the 1×2 structure on Pt(110) could not be reconciled with surface self-diffusion times, an asymmetric sawtooth model was recently proposed [1]. The large corrugation found in He-scattering experiments [5] on Au(110) and Pt(110) is compatible with either model, but intensity analysis [6] as well as Ne-scattering data [7] again favor the missing-row model. Finally, spin-polarized LEED experiments give conflicting evidence even as to the symmetry of the reconstruction [8].

In view of the simple unit cell, it is astonishing that the problem is still open. One of the reasons might be the nonlocal, averaging character of diffraction experiments. As shown recently, local information can be obtained by the scanning tunneling microscope (STM) [9–11]. Here, we present experimental evidence for the basic driving mechanism for the various reconstructions as well as the observed disorder, namely, the (111) facetting. A brief preliminary account of this experiment has already been presented [12].

The basic experimental procedure is the same as described in ref. [10]. There, misled by the sharpness of isolated atomic steps and adsorbate structures (believed to be responsible for the rough regions in fig. 3a of ref. [10]), we erroneously concluded that the 1×2 reconstruction should be smooth. In the meantime, we have learned that, for a given tip geometry, the resolution is not necessarily the same for adsorbates, isolated steps and short wavelength corrugations. This phenomenon is not yet understood and requires further study. In the present experiment, we achieved a considerably better resolution by sharpening the tip in situ, exposing it for some minutes to electric fields exceeding 10^8 V/cm. (Such sharpening probably occurred involuntarily before taking fig. 3b of ref. [10], another cause for a different resolution from that in fig. 3a.) Measurements were taken with +10 mV applied to the tip. The width of the vacuum gap is approximately 4 Å, as estimated from resonant tunneling observations [13].

Fig. 1 shows the topography of a section exhibiting various typical features of a Au(110) surface. It consists essentially of clearly separated parallel hills usually running several hundred Å along the $[1\bar{1}0]$ direction. Most of the hills are separated by 8 Å, thus forming 1×2 reconstructed ribbons. The latter are separated by steps and 1×3 channels causing considerably stronger disorder along the [001] than the $[1\bar{1}0]$ direction. An example for the weak disorder in the $[1\bar{1}0]$ direction is illustrated by the change of the hill structure at A to a different configuration at B. In fig. 2, an area with an increased density of 1×3 channels and a transition from a 1×4 channel to two 1×2 ones is observed with an even higher resolution. The mean corrugation amplitudes amount to 0.45 Å for the 1×2 and 1.4 Å for both 1×3 and 1×4 channels, respectively.

In general, the corrugation observed with the STM reflects qualitatively the topography of the surface. Essentially, it is closely related to the corrugation of the electron density near the Fermi level in the middle of the vacuum gap, folded with the instrumental resolution. Because of the smoothing effect of the conduction electrons, the corrugations of the core positions are considerably stronger than those observed. The limiting factors for the resolution obtainable by a given tip are not yet understood since they are determined by tunneling from small-scale non-planar features, for which a theory is still lacking. Nevertheless, we can make important statements on the nature of the Au(110) surface.

Before turning to the 1×2 reconstruction, we discuss first what we believe to be the basic characteristic of the Au(110) surface, its facetting. Our interpretation of the measured corrugation for the surface structure between A and B is shown in the inset on fig. 2. We arrive at this model by first considering the *deep and symmetric* 1×3 channel. From its depth it is obvious that rows are missing within the channel. Starting with the 1×1 structure and removing two top rows (two for symmetry) exposes a second-layer row in the

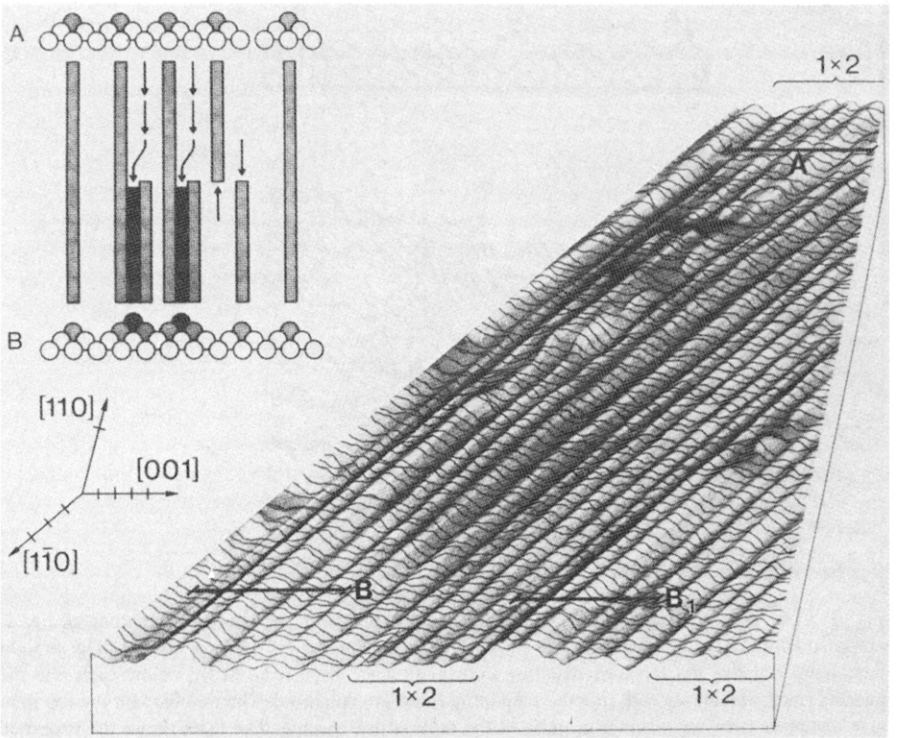

Fig. 1. Original recordings of an STM picture, showing 1×2 reconstructed ribbons interrupted by monolayer steps and 1×3 channels. The skewed directions of the [1$\bar{1}$0] and [110] axes are determined by thermal drift and crystal misalignment respectively. Divisions on all axes correspond to 5 Å. The disorder structure at B is repeated at B_1. The inset envisages a possible transition from the structure at A to that at B by shifting rows along the [1$\bar{1}$0] direction.

middle of the channel. Since this middle row is not resolved, be it for insufficient instrumental resolution and/or weak corrugation of the electron density (recall, that the STM tests the corrugation of the wave functions in the middle of the vacuum gap and not the core corrugation), the measured corrugation of 1.4 Å is too large for a fundamental core corrugation of 1.5 Å. Therefore, we conclude that second-layer rows are also missing. Removing the middle second-layer row retains the symmetry, a missing fourth row makes the corrugation asymmetric, removing more than four rows is unreasonable. Therefore, the proposed structure of a three-missing-row 1×3 channel, exposing two (111) facets with three free rows each (see inset of fig. 2) appears quite convincing. Next, consider such 1×3 channels together with a sequence of other channels and steps. (We define a step by a change in the vertical position

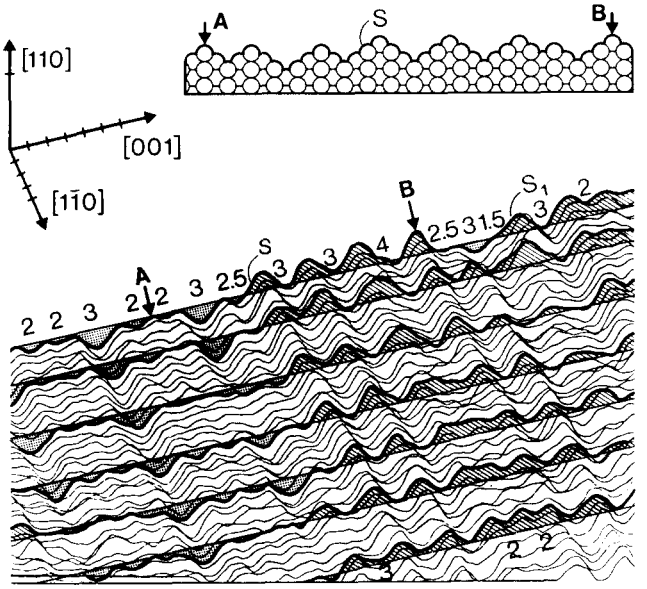

Fig. 2. STM picture of a section exhibiting considerably stronger disorder than that of fig. 1, obtained with increased resolution and stability. Divisions on the crystal axes are 5 Å. The straight lines help visualize the terraced structure with monolayer steps (e.g., at S); below each line the missing rows, and above each line the remaining rows, are enhanced. The numbers on the top scan give distances between maxima in units of the bulk lattice spacing. The inset shows the proposed structural model for the observed corrugation between A and B.

of the topmost atoms, i.e., the maxima.) Distances between maxima are always multiples of lattice spacings except at steps, e.g., at S or S_1, and in the 1×4 channels, where half-lattice spacings occur. We therefore conclude: (a) The 1×2 reconstruction cannot be of the asymmetric sawtooth or pairing-row type since they require half-integer lattice spacings between their maxima and those of adjacent 1×3 channels. (b) Monolayer steps (the only steps observed in both figures) are made out of (111) facets. Most steps involve three-row (111) facets, e.g., at S and the inset of fig. 1. Two-row steps, e.g., at S_1, are the exception. This is attributed to the fact that the latter always contain a single-row facet which can be viewed as a local 1×1 structure. Finally, the asymmetric 1×4 channel with the same depth as the 1×3 channel is reasonably well explained by a three-row (111) facet (the right side of the one shown in fig. 2 looks equivalent to that of a 1×3 channel) and two two-row facets. The latter include a one-row facet which again might be the reason for the rare observation of 1×4 channels. Corrugations deeper than those of 1×3 and 1×4 channels (plus monolayer steps) were never observed. All this strongly indicates that the surface of lowest energy consists of narrow ($\leq$ three

free rows) ribbons of (111) facets along the [1$\bar{1}$0] direction.

This basic characteristic is also believed to generate the 1×2 structure, resulting in the missing-row model. The considerations above already excluded other models except buckled-surface models. The latter contains no (111) facets and is also not favored by analysis of scattering experiments. Besides, spontaneous buckling does not provide any energy gain on Si(111) [14]; this is a fortiori expected for metal surfaces. Finally, for the missing-row model, the configuration changes from a 1×4 channel into two 1×2 channels (fig. 2), as well as that from A to B shown in the inset of fig. 1, appear quite natural.

The next point concerns the disorder along the [001] direction. Considerable disorder of this kind has been observed by Moritz and Wolf [15] while others have detected none. We also find an exponential statistical distribution of 1×2 terrace widths with a decay length somewhat smaller than that inferred by Moritz and Wolf [15]. This exponential decay might be a general feature with a mean terrace width depending on sample preparation; this appears quite plausible. Our observations demonstrate that all the disorder observed is caused by intermediate three-row (and much less frequently two-row) (111) facets. We could not find a physical process which would convert such ribbons into two-row facets (1×2 structure) without locally creating an intermediate 1×1 structure which acts as a potential barrier. Thus the disorder should be quite stable, i.e., initial growth conditions determine the mean terrace width.

Finally, the mass transfer problem still remains open. It is, however, quite uncertain that thermal surface self-diffusion provides the relevant time scale for the 1×1 to the 1×2 transition. A hint in this direction is given by the inset of fig. 1, suggesting that mass transport (i.e., via kinks) might occur in rows along the [1$\bar{1}$0] direction.

In conclusion, our experiments demonstrate the (111)-facetted nature of the Au(110) surface. This facetting is believed to be the basic driving mechanism for the reconstructions. In particular, (111) facets with two free rows generate the 1×2 reconstruction of the missing-row type. Three-row facets produce the 1×3 reconstruction, combinations of two- and three-row facets can give other local reconstructions and are the cause of disorder.

In the meantime, we have learned of two other experiments which strongly support the missing-row 1×2 reconstruction: direct TEM observation [16] and glancing angle X-ray diffraction [17]. Further, interpretation of our results with a new tunnel theory gives excellent agreement with the missing-row model [18].

Valuable discussions with K.H. Rieder, B. Reihl and A. Baratoff, and preprints from the authors of refs. [16–18], are gratefully acknowledged.

References

[1] For references, see H.P. Bonzel and S. Ferrer, Surface Sci. 118 (1982) L263. In this paper, the sawtooth model is proposed.
[2] C.M. Chan, M.A. Van Hove, W.H. Weinberg and E.D. Williams, Solid State Commun. 30 (1979) 47; Surface Sci. 91 (1980) 440.
[3] J.R. Noonan and H.L. Davis, J. Vacuum Sci. Technol. 16 (1979) 587.
[4] W. Moritz and D. Wolf, Surface Sci. 88 (1979) L29.
[5] K.H. Rieder, T. Engel and N. García, in: Proc. ECOSS-3, Cannes, 1980 [Suppl. Le Vide, Les Couches Minces 201 (1980) 861].
[6] M. Mannihen, Y.K. Nørskov and C. Umrigar, Surface Sci. 199 (1982) L393.
[7] C. Ocal, N. García, K.H. Rieder and T. Engel, to be published.
[8] B. Reihl and B.T. Dunlap, Appl. Phys. Letters 37 (1980) 941;
N. Müller, M. Erbüdak and D. Wolf, Solid State Commun. 39 (1981) L247.
[9] G. Binnig, H. Rohrer, Ch. Gerber and E. Weibel, Appl. Phys. Letters 40 (1982) 178; Physica 109/110B (1982) 2075.
[10] G. Binnig, H. Rohrer, Ch. Gerber and E. Weibel, Phys. Rev. Letters 49 (1982) 57.
[11] G. Binnig, H. Rohrer, Ch. Gerber and E. Weibel, Phys. Rev. Letters 50 (1983) 120.
[12] G. Binnig and H. Rohrer, Surface Sci. 126 (1983) 236; Physik. Blätter 39 (1983) 16;
G. Binnig and H. Rohrer, Meeting on Current Topics in Solid State Physics, Santander, Spain, 1982, unpublished;
G. Binnig and H. Rohrer, Ultramicroscopy 11 (1983) 157.
[13] G. Binnig and H. Rohrer, Spring Meeting of the German Physical Society, Münster, 1982, and of the European Physical Society, Manchester, 1982, unpublished;
G. Binnig and H. Rohrer, Helv. Phys. Acta, in press.
[14] K.C. Pandey, Phys. Rev. Letters 49 (1982) 223.
[15] W. Moritz and D. Wolf, preprint.
[16] D.J. Smith and L.D. Marks, Nature, in press.
[17] I.K. Robinson, Phys. Rev. Letters 50 (1983) 1145.
[18] J. Tersoff and D.R. Hamann, preprint.