Comment on "Real Space Investigation of the Roughening and Deconstruction Transitions of Au(110)"

Sturmat, Koch, and Rieder (SKR) describe in [1] scanning tunneling microscopic (STM) observations of steps along the $[1\bar{1}0]$ direction on the missing-row reconstructed Au(110) surface. The images of noncompact step structures (step meandering) as well as the increase of the meandering amplitude with temperatures are interpreted by SKR as the initial stages of a combined roughening and deconstruction transition. By contrast, our measurements clearly show compact steps ([2,3] and this paper). In the following we point out that SKR's conclusion is based on a misinterpretation of their experimental data, caused by the fast dynamics of the surface, in spite of their own remark that *Au atoms located at kink sites are quite mobile even at room temperature.*

As already shown in [3], the high mobility of kinks makes the steps only *seem* rough. Consider, for example, Fig. 2(b) in [1]. This image of steps at 420 K spans 140×140 Å^2. From Ref. [3] we see that the root-mean-square displacement of a kink along a step at 421 K reaches a value of 140 Å in 117 s. In order for this motion not to have affected Fig. 2(b) in [1], the image should have been recorded in a time orders of magnitude shorter than 117 s. In fact, for a typical image (300×300 pixels, 2.88 Å/pixel), the total imaging time must be shorter than 2.4 s to avoid atomic-scale step displacements between subsequent scan lines under these conditions (<0.008 s/scan line). Similarly, the images at 550, 620, and 700 K should have been taken within 25, 4, and 1 ms. Scan speeds are not mentioned in [1], but we assume them to have been substantially longer than 2.4 s. On these grounds, one should seriously doubt the *fjordlike shapes* in Figs. 2 and 3 of [1]. To further substantiate our point, we have performed STM measurements on Au(110) at 384 K (Fig. 1 upper panels) and 479 K (lower panels). The fast direction in our STM images is displayed horizontally. By rotating the scan, we easily vary the time resolution on the step shape by a factor of 300. The two left panels are in an orientation similar to that in Ref. [1], and have a low time resolution on the steps. The two right panels were obtained by a simple rotation of the scans without changing the location on the surface, to improve the time resolution. As expected the left panels are very similar to those in Figs. 2(b) and 2(c) of [1], and show seemingly rough steps. The very smooth configurations in the two right panels demonstrate that the roughness in the left panels simply results from a lack of time resolution. The modest smearing of the kink positions in the lower right panel indicates that even for this optimized scan orientation and short imaging time of 5 s, it is not possible to obtain a real STM *snapshot* of the steps.

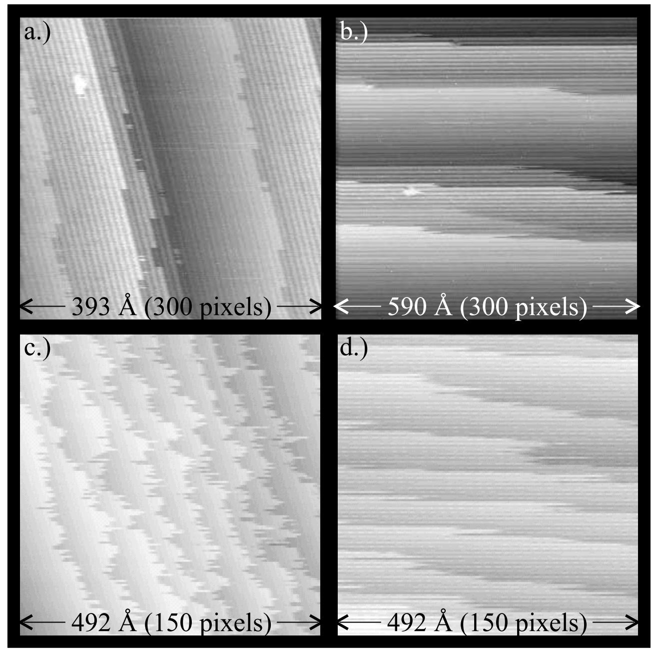

FIG. 1. STM images (tunneling parameter: $V = -0.7$ V, $I < 0.1$ nA) of Au(110), taken at 384 K (upper panels), 479 K (lower panels). The two left panels were measured in 31 s (a) and 21 s (c) in a scan orientation comparable to SKR. In the two right panels, 31 s (b) and 5 s (d), the scans were repeated at the same location, with an orientation roughly parallel to the steps, to optimize the time resolution on the steps. The rough structures in the two left panels are not *real* but merely result from rapid kink motion along the steps.

On the basis of these observations, we conclude that SKR have not observed the roughening and deconstruction transition of the Au(110) surface. The atomic-scale mechanism of the transition still remains to be observed in real space.

This work is financially supported by FOM and NWO.

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Received 31 October 2000; published 28 June 2001
DOI: 10.1103/PhysRevLett.87.039603
PACS numbers: 61.50.Ks, 68.35.Bs, 68.35.Fx, 68.35.Md

[1] M. Sturmat *et al.,* Phys. Rev. Lett. **77**, 5071 (1996).
[2] M. Rost *et al.,* Phys. Rev. Lett. **84**, 1966 (2000).
[3] L. Kuipers *et al.,* Phys. Rev. B **52**, 11 387 (1995).

Koch and Schulz Reply: When investigating surfaces with the STM (scanning tunneling microscope) one has to be aware of two crucial problems which may deteriorate imaging of the *real* structure: (i) Is the scanning speed fast enough and (ii) is the tip/surface interaction small enough, so that the structure of interest essentially remains unchanged while scanning the image? The Comment of Rost and Frenken (RF) [1] addresses the first problem in connection with the step roughness found in our high temperature STM study of Au(110) [2]. RF argue that the high mobility of kinks makes the steps only seem rough and, in particular, doubt the fjordlike structures found in our previous study. To substantiate their point, RF provide STM images at 384 and 479 K, which reveal rough steps at arbitrary scanning directions and a compact step morphology when scanning parallel to the close-packed atom rows. Since the scanning direction is related to time resolution, their results suggest that the rough morphology is mainly the result of an undersampling by the STM.

Recently we have shown that the degree of step roughness on Au(110) depends severely on the density of preexisting kinks (Fig. 6 in [3]). Whereas ideal $[1\bar{1}0]$ steps are straight over large distances even at 500 K, arbitrarily oriented steps are stable only at 300 K, where kink movement is almost frozen out. With increasing step edge diffusion at elevated temperatures kinked steps are imaged rough, the more the larger the misalignment of the steps against $[1\bar{1}0]$ (see Fig. 1). In order to increase time resolution, we recorded STM images from the forward and backward scans. In Fig. 1 the time interval between corresponding data points of the left and the right image is smaller than 0.2 s compared to about 1 min for consecutively taken images. Nevertheless, single kinks are still too mobile to appear at the same position in forth and back scans. More extended units, however, which are divided by broad atom-free regions (e.g., "fjords" marked by arrows), are easily identified at the same place in both images, thus supporting their interim existence. This interpretation is further corroborated by the deep fjord in the upper terrace of Fig. 2(a), which separates a region close to a [001] step. RF's assumption of permanently compact step profiles leads to the following scenario: Initially the upper terrace is entirely filled up to the right side, where scanning started. It broadens and shrinks during scanning according to the imaged step corrugation. At the large fjord the region on its right necessarily has dissolved. Figure 2(b), which includes the same surface area (confined by dashed lines), was recorded ~3 min later. The upper terrace still extends to the very right and exhibits similar features as in Fig. 2(a) with a nearly equal data point coverage. The large and highly coordinated mass flow necessary for draining and refilling of the upper terrace clearly doubts the hypothesis of permanently compact steps and favors the occurrence of fjords in rough steps. We remark that in parallel scans the real step profile may be concealed by tip-induced atom movement — similar to our recent findings on Ag(110) [4].

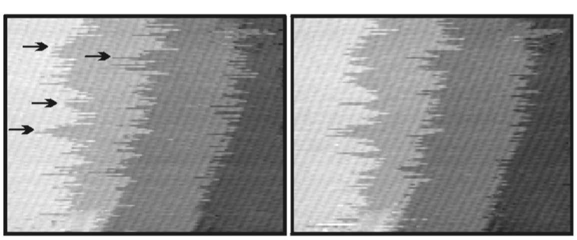

FIG. 1. STM image sections [160×125 data points (dp) of 256×256] of the same Au(110) area taken at 460 ± 20 K obtained from forward (left) and backward scans (right); $U_T = 688$ mV, $I_T = 0.2$ nA; scanning speed: 2330 dp/s.

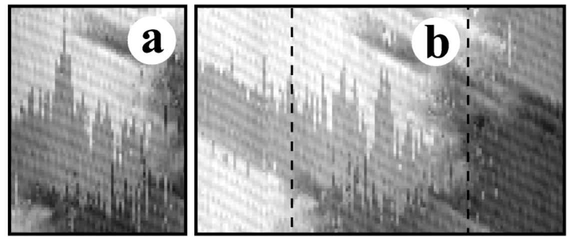

FIG. 2. Subsequent STM images of Au(110): the area displayed in (a) is included in (b) marked by dashed lines; tunneling conditions as in Fig. 1, fast scanning direction vertical.

We agree with RF that the atomic scale mechanism of the roughening transition of Au(110) remains an open question. The main topic of our previous study was to demonstrate that extended (110) terraces — the experimental counterpart to the infinite model surfaces of theoretical studies — are flat and (1×2) reconstructed until the 3D roughening sets in, in contrast to existing theoretical models. The results presented here confirm the increased roughness of preexisting steps above 300 K, whereby the typical scanning speed is sufficient to detect larger units. Therefore our previous presumption that the 2D step roughening is responsible for the weakening of the half order spots in diffraction patterns remains a valid explanation.

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Received 29 November 2000; published 28 June 2001
DOI: 10.1103/PhysRevLett.87.039604
PACS numbers: 61.50.Ks, 61.18.–j, 68.35.Bs, 68.35.Fx

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