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Comment on "Observation of two-dimensional Fermi contour of a reconstructed Au(111) surface using Fourier transform scanning tunneling microscopy" by D. Fujita, K. Amemiya, T. Yakabe, H. Nejoh, T. Sato, M. Iwatsuki [Surf. Sci. 423 (1999) 160]

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In a recent paper, Fujita and co-workers report on the observation of the two-dimensional (2D) Fermi contour of the s–p derived surface state on the reconstructed Au(111) surface [1]. This is done by Fourier transforming scanning tunneling microscopy (STM) constant-current images of standing wave patterns obtained at low bias voltage and low temperature.

The s–p surface-state electrons on noble metal (111) surfaces constitute a quasi-2D free-electron-like gas. Standing waves in the electronic local density of states (LDOS) are the result of scattering of surface-state electrons from the potentials associated with step edges and impurities. Electrons with energy E set up quantum interference patterns with a wave vector $q=2k_E$, where k_E is dictated by the dispersion relation $E(k)$.

At low bias voltage, a constant-current STM image can be interpreted as a picture of the LDOS at the Fermi level (E_F) and, consequently, standing waves with wave vector $q=2k_F$ are visible in such images. A 2D Fourier transform of a standing wave image produces a map of the k-vectors contributing to the wave pattern. The wave vectors for electrons with energy close to E_F are confined to lie on the Fermi contour and, thus, the Fourier transform will display the Fermi contour scaled by a factor of two, as we have previously pointed out [2,3].

An advantage of this method to determine surface Fermi contours is that one obtains information about the *local* electronic structure in the area scanned by STM [2,3]. This is in contrast to a photoemission experiment, for example, which averages over macroscopic areas of the surface. Fujita et al. [1] have studied whether there is any local influence of a specific domain of the Au(111) herringbone reconstruction [4] on the Fermi contour. They claim that the local Fermi contour has

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an elliptical shape, with the minor axis of the ellipse oriented in the direction perpendicular to the local partial dislocation lines of the herringbone reconstruction. The minor axis is found to be approximately 10% smaller than the major axis [1].

We have previously published Fourier transform STM measurements of the Au(111) Fermi contour performed at $T=150$ K. When thermal drift could be excluded, we did not see any indication of an elliptical Fermi contour [5]. Here we present similar measurements performed with a 4 K STM, which is particularly stable against thermal drift [6]. In contrast to the report of Fujita et al. [1], we have only observed isotropic surface Fermi contours on Au(111), and found no influence of the reconstruction on the shape of the Fermi contour. A typical example of the standing waves is shown in Fig. 1a. A standing wave pattern is created by the step edge on the right-hand side of the image as well as by point defects. The corresponding Fourier transform is shown in Fig. 1b. As is evident, the Fermi contour is circular and not elliptical (compare with Fig. 9 in Ref. [1]). Measuring the diameter of the ring in different directions proves that it is indeed circular to within $\sim 2\%$. This residual experimental uncertainty is either due to uncertainty in the relative piezo calibration or piezo creep, which can hardly be avoided completely. The spots arranged in an 'X' are caused by the periodic nature of the reconstruction lines and, thus, represent structural rather than electronic information. The spots are located at a distance $d=n(2\pi/L)$ from the centre of the Fourier transform ($n=1, 2, \ldots$), where $L\simeq 63$ Å is the distance between neighbouring pairs of reconstruction lines.

To further support that the local electronic structure on Au(111) is isotropic, we show the Fourier transform of a $\mathrm{d}I/\mathrm{d}V$ image obtained by means of a lock-in amplifier at $V=100$ mV (Fig. 2). To a first approximation, $\mathrm{d}I/\mathrm{d}V(V)$ represents the LDOS at energy $E=E_F+eV$. Fig. 2b shows that the surface state is isotropic 100 mV above the Fermi level as well. Notice that the image in Fig. 2a contains only one single domain of the reconstruction, so that any effects on the isotropy of the electronic structure should have been easily detectable.

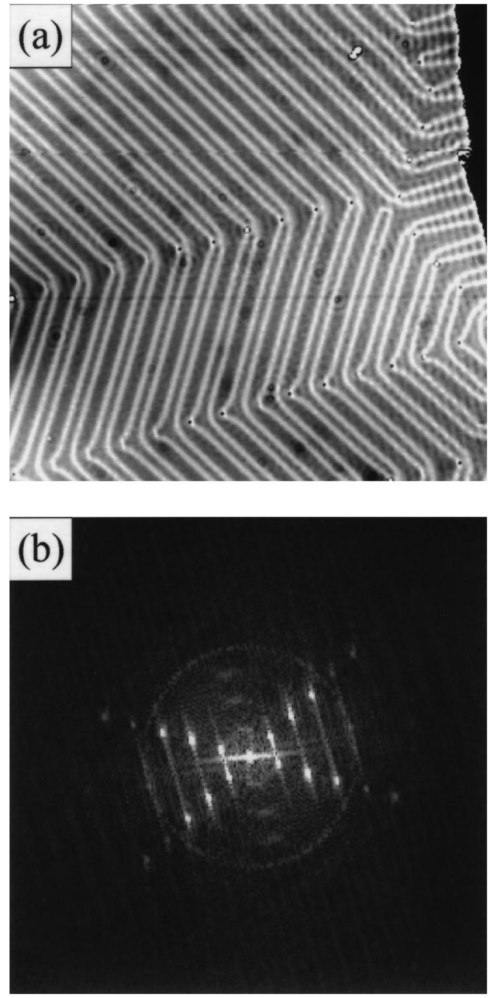

Fig. 1. (a) Constant-current STM image of Au(111) at 5 K ($V=10$ mV, $I=0.5$ nA, 1042 Å × 1042 Å). Standing waves are seen emanating from the step edge to the right and from point defects. The image has been processed slightly (by adding 50% of a Laplace transform of the original image) to enhance the visibility of the standing waves as compared with the reconstruction lines. (b) Power spectrum of the Fourier transform of the unprocessed image corresponding to (a).

Although Fujita et al. [1] claim that their elliptical Fermi contour "should not be an experimental artifact such as a drift effect", we speculate that this, nevertheless, might be the case. Effects such as temperature drift, wrong calibration of the piezos or piezo creep could all lead to distorted

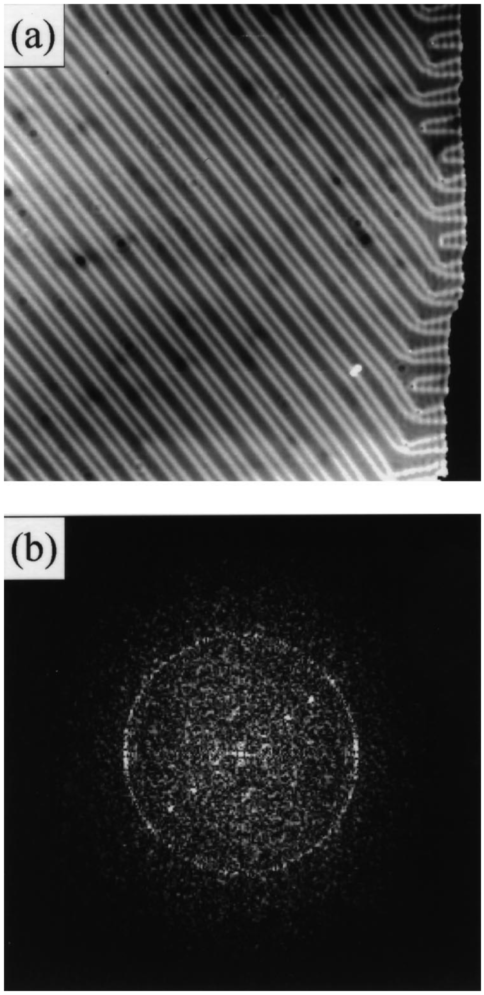

Fig. 2. (a) Constant-current STM image of Au(111) at 5 K (V= 100 mV, I=2.1 nA, 1141 Å × 1141 Å). Standing waves are seen, especially close to the step edge in the right-hand side of the image. Notice that there is only one single domain of the reconstruction present. (b) Power spectrum of the Fourier transform of a dI/dV image ($\Delta V_{RMS}=5$ mV) obtained simultaneously with (a).

images and consequently distorted Fourier transforms. If one inspects the Fourier transforms of atomically resolved images shown in Figs. 5b and 7 of Ref. [1], the atomic spots form a hexagon which is distorted by up to 15%. For an fcc (111) surface, a perfect hexagon is to be expected. In Fourier transforms of our atomically resolved images, the atomic spots indeed form a perfect hexagon (taking into account the unidirectional contraction caused by the reconstruction). This strongly indicates that the elliptical Fermi contour published by Fujita and co-workers is an experimental artifact.

Finally, we would like to mention that, in order to obtain the best accuracy in the calibration of the Fourier transforms, one should record a low-bias image showing both standing wave patterns and atomic resolution. The Fermi contour as well as the atomic spots would then be visible in the Fourier transform, allowing for an internal calibration of that particular image. To some extent, this is already possible by the use of the reconstruction spots. However, the atomic positions and thus the corresponding reciprocal vectors are known with a higher precision.

In conclusion, the surface Fermi contour on Au(111) observed by us is isotropic (circular), in contrast to the findings of Fujita et al. [1]. Thus, we cannot support the idea that the potential associated with the reconstruction (see Ref. [7]) makes the Fermi contour elliptical.

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