Available online at www.sciencedirect.com
ScienceDirect
Applied Surface Science 253 (2007) 4715–4720
applied surface science
www.elsevier.com/locate/apsusc

STM studies of the reconstructed Au(1 1 1) thin-film at elevated temperatures

P. Kowalczyk [a,*], W. Kozlowski [a], Z. Klusek [a], W. Olejniczak [a], P.K. Datta [b]

[a] *Department of Solid State Physics, University of Lodz, Pomorska 149/153, 90-236 Lodz, Poland*
[b] *Advanced Materials Research Institute (AMRI), Northumbria University, Ellison Building, Ellison Place, Newcastle upon Tyne, NE1 8ST, United Kingdom*

Received 30 March 2006; received in revised form 16 October 2006; accepted 18 October 2006
Available online 28 November 2006

Abstract

High temperature scanning tunneling microscope (HT-STM) was used to investigate a reconstructed Au(1 1 1) film evaporated on mica. The experiment was carried out at elevated temperatures in the range of 300–500 K. A herringbone reconstruction was observed at a wide range of temperatures. However, at the highest temperatures studied a break down of the reconstruction long range order was noticed. Finally, the presence of a triangular-like reconstruction was reported. Changes in the reconstruction were explained in terms of the change in surface stress arising as a result of the tension at the gold–mica interface.

PACS : 62.40.+i; 68.37.Ef; 68.35.Bs; 68.35.Gy

Keywords: High temperature scanning tunneling microscopy; Gold; Surface stress; Reconstruction

1. Introduction

It is well known that surfaces of some metals reconstruct into an atomic arrangement different from the bulk one. It is very common behavior for all low index faces of FCC metals ((1 0 0), (1 1 0), and (1 1 1)) caused by surface stress arising from an abrupt crystal termination [1,2]. Reconstruction of (1 1 1) face was found only for Au [1,3,4] and in special conditions for Pt [4,5].

The surface reconstruction of Au(1 1 1) was studied intensively both theoretically [1,6–9] and experimentally among others using the scanning tunneling microscope (STM) [1,3,4,10–15]. Most of experiments were carried out below or at room temperature. High temperature investigations of a reconstruction on flat [16,17] and faceted Au(1 1 1) [18] were also carried out by the use of an X-ray scattering up to 1200 K. All those investigations described $23 \times \sqrt{3}$ reconstruction called a herringbone reconstruction where 23 surface atoms lie over 22 bulk atoms. This leads to 4.4% contraction of the surface layer which is composed of FCC and HCP regions separated by lines of higher corrugation (approximately 0.2 Å higher than an adjacent FCC region as measured by the use of STM) called discommensuration lines. Three rotational domains exist at the surface of Au(1 1 1) due to the threefold symmetry of gold which is energetically favorable to surface stress release. These domains are formed via a correlated $\pm 120^\circ$ bending of discommensuration lines which in consequence form the characteristic pattern of a herringbone reconstruction with supercell size estimated at 70×280 Å [12]. What is more, at approximately 860 K the first order transition of the herringbone reconstruction into discommensuration fluid phase was observed [16,17]. Transition temperature to the discommensuration fluid phase was estimated to be 150 K lower than in the case of faceted Au(1 1 1) [18] and took tens of hours to complete.

In recent years investigations of Au(1 1 1) surface have been the subject of constant interest. It was shown that a dipole surface layer was formed due to the reconstructed Au(1 1 1) surface [19] and that the reconstruction influenced the electronic surface of gold [20–22]. Deposition of organic molecules [23,24] and metals on the reconstructed Au(1 1 1) surface [10,25] was also investigated.

* Corresponding author. Tel.: +48 42 6355694; fax: +48 42 6790030.
E-mail address: pkowa@uni.lodz.pl (P. Kowalczyk).

0169-4332/$ – see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.apsusc.2006.10.037

It is believed that any disruption of an atomic arrangement could change type of the reconstruction [26]. For example, in the case of the surface with a big number of steps (vicinal surface) the presence of steps decreases the surface stress and in consequence the reconstruction could not form [27]. It was shown that deposition of oxygen [13,28–30] and sulfur [13] also influences surface morphology. Changes of Au(1 1 1) reconstruction were reported in electrochemical environment [14] and during Au electrodeposition [31]. It was shown that high electric field between STM tip and Au(1 1 1) surface could change the reconstruction [15]. Another way reported in the literature, which disrupted the atomic arrangement was applying a small mechanical distortion force to the gold film evaporated on mica which could change the herringbone reconstruction drastically [11].

In our experiment we made an effort to perform elevated temperature investigations of the reconstruction formed on a 300 nm thick Au(1 1 1) film evaporated on mica. We decided to use STM operating at high temperatures (HT-STM), mainly due to its resolution – STM is known to be capable of investigating surface of metals with the atomic resolution [4]. Our main goal was to investigate changes in the reconstruction due to elevated temperatures. It was shown earlier, that the herringbone reconstruction is stable at a wide range of temperatures particularly up to 500 K [10,16–18]. Our results (obtained on the Au film) contrary to the previous ones (collected on monocrystals) showed strong dependence of periodicity and size of the herringbone reconstruction on temperature. Therefore, our results are complement to the previous investigations of Au(1 1 1) herringbone reconstruction.

2. Experimental details

Commercially available 300 nm gold film evaporated on mica [32] was used in all experiments. The standard procedure of Au cleaning was used, namely, the Au(1 1 1) surface was prepared by repeated cycles of Ar^+ sputtering (Argon pressure of 2×10^{-5} mbar and voltage of 1 kV for 10 min) and annealing up to 800 K. Annealing temperature was increased in five stages – every 100 K and decreased rapidly in a single step. Typically three cycles of sputtering and annealing were enough to obtain a clean, reconstructed surface of Au(1 1 1).

HT-STM investigations were carried out in UHV with base pressure 8×10^{-10} mbar by the use of Omicron VT-AFM/STM system equipped with Auger spectrometer and a sputtering gun. The tips used in these experiments were prepared by mechanical cutting from 90%Pt–10%Ir ally wires. Investigations were carried out at four temperatures 296 K, 320 K, 430 K and 500 K. The same STM tip was used at all temperatures during the experiment.

In the first step the Au(1 1 1) sample was mounted on the STM head and investigated at room temperature. Afterwards, the tip was retracted up to 500 nm and the temperature was increased typically for 2–3 h up to the next temperature level and stabilized typically for 12 h otherwise, the parameters of stabilization will be given in the text. Next, the tip was approached to the surface and investigations at the desired temperature began. After finishing investigations at the desired temperature the tip was retracted ~500 nm backward and the temperature was increased as described earlier. This procedure was repeated to reach temperatures of 320 K, 430 K and finally 500 K.

3. Results and discussion

Fig. 1 shows a typical result obtained by the use of STM on the Au(1 1 1) surface at room temperature. Discommensuration lines forming the herringbone reconstruction are clearly visible over the whole scanned area. Two steps (denoted S1 and S2) and three terraces (denoted T1, T2 and T3) are seen in the image. The topographic data presented in the figure was filtered by the use of Laplace transform to obtain better contrast of the reconstruction on different terraces. The inset in the figure shows STM topographic image of the same area without filtering procedures applied. It is clearly seen, that far from the step edges discommensuration lines form a regular herringbone pattern with a supercell which size is estimated at 7.3 nm × 28.5 nm which corresponds to literature reports [12]. It has to be pointed out that a regular herringbone pattern indicates that the surface stress is uniformly spread over terraces. However, in the vicinity of the step edge the reconstruction changes slightly. In the case of S1 step it could be seen that discommensuration lines become less parallel. This effect is related to a change of the surface stress due to the presence of the step edge [10]. Discomensuration lines behave differently in the vicinity of S2 step edge. It is clearly seen, that lines do not cross the step directly but rather through distorted domains which are formed on the surface. In our opinion this kind of behavior is related to {1 1 1} microfacet formation of S1 edge and {1 0 0} microfacet of S2 one [10]. Unfortunately,

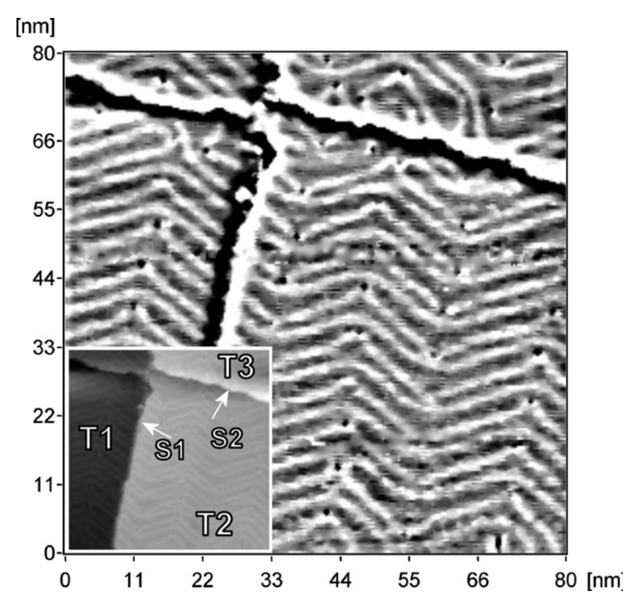

Fig. 1. A 80 nm × 80 nm STM topographic image of the reconstructed surface of gold at 294 K. The topographic data were filtered using Laplace transform to increase the contrast of the herringbone reconstruction on different terraces. The inset shows original topographic data. Three terraces were denoted T1, T2 and T3 and two-step edges were denoted S1 and S2.