Reconstruction of the Mo(211) surface caused by the oxygen atoms

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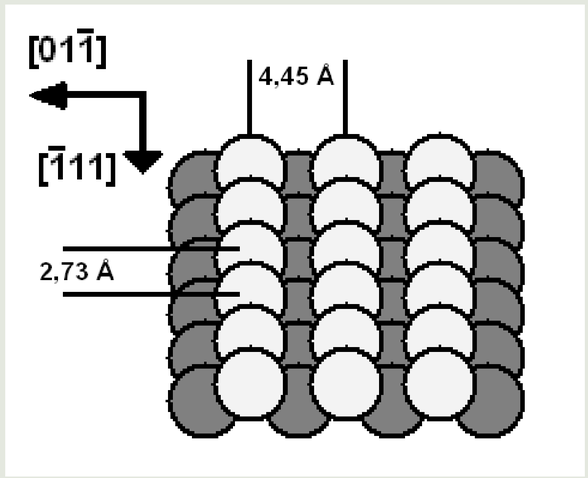
Abstract: *The Mo(211) surface was investigated by the scanning tunneling microscope (STM) and low energy electron diffraction (LEED) methods. Growth of Mo_2O layer and the surface structure reconstruction has been observed during an increasing of oxygen atoms concentration on the surface.*

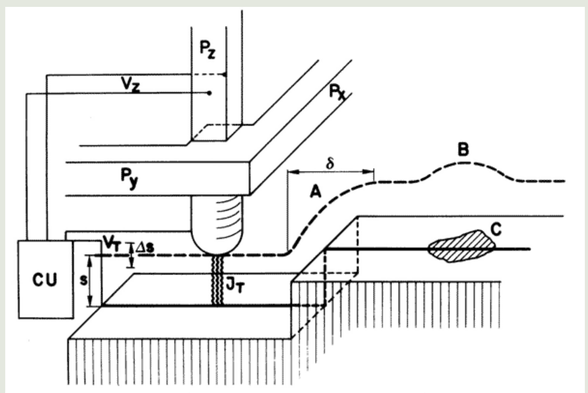
Introduction

Molybdenum is a metal crystallizing in a body-centered cubic (bcc) structure. Therefore Mo(211) surface is composed of close-packed rows along $[\bar{1}\,1\,1]$ direction with spacing of 2.73 Å between atoms in rows and 4.45 Å between rows, along $[0\,1\,\bar{1}]$ direction. This surface is used as a substratum in investigation of interaction between adsorbed atoms, especially rare earth and alkaline earth metals [1] and for the epitaxial growth of ultrathin oxide films [2] For the investigation it is necessary to get the clean surface. The main contamination of molybdenum is carbon which forms molybdenum carbide. Mo_2C can be removed from the surface by using the ion flood gun or by annealing the sample in oxygen atmosphere. In second case carbon reacts with oxygen and creates easily removable carbon oxide. Such a process was investigated by LEED and STM



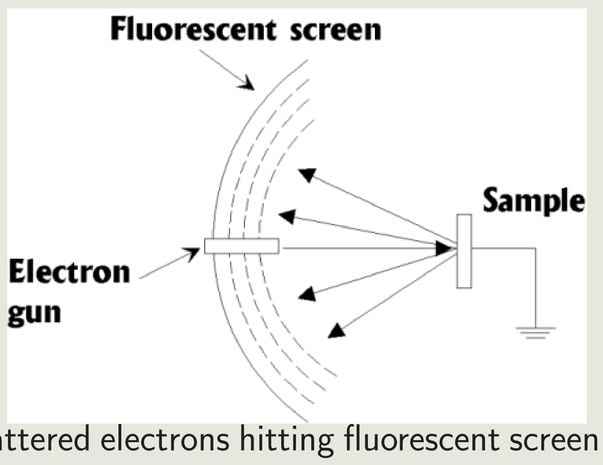
Techniques

Scanning tunnelling microscope (STM)[3] is an instrument based on quantum tunnelling, used for imagining surface topography and work function profiles at the atomic level. The basic scheme of STM is shown on picture (not to scale) from [3].



A sharp metal tip, controlled by piezoelectric drivers (Px, Py and Pz) is scanned over the sample close enough to the surface that electrons can tunnel between sample and tip .The control unit (CU) keeps a constant tunneling current by applying a proper voltage to Pz. At constant work function constant current yields constant tip height, so the surface profile can be obtained directly from CU voltage (broken line indicates z position of the tip). Changes in the work function (spot C with lower work function) result with changes of the tip height (B).

Low-energy electron diffraction (LEED) [4]is a technique used for obtaining image of the surface structure of crystalline materials. The idea of LEED is that the sample is bombarded by a beam of electrons with well specified energy from 20 eV to 250 eV. Such energies correspond to de Broglie wavelengths from 0.7 to 3 Å and give diffraction of the electrons beam on the sample surface. Scattered electrons hitting fluorescent screen give an image of reciprocal lattice of the surface structure. Scheme of LEED is shown on picture from [5]



Experiment

The experiments were carried out in UHV chamber equipped with LEED and STM. The base pressure was 4.5×10^{-10} Torr. Annealing process was carried out at 1200K with oxygen pressure 1.3×10^{-8} Torr. Dosing of oxygen was controlled by the time of annealing. The doses were 40, 10 and 90 langmuirs ($1L = 10^{-6}\,Torr \times s$). Then surface was flashed to 2000 K and studied by LEED and STM. Furthermore after getting the surface found as clean several steps were carried to check if obtained structures showed no more carbon contamination.

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Results

In the first two steps with doses 40 L and 10 L respectively observed structure was $p(5 \times 3)$ (Fig. 1) and was found as caused by carbon contamination. In further step (90 L) LEED showed $p(1 \times 1)$ structure (Fig. 2) what was interpreted as a clean surface.

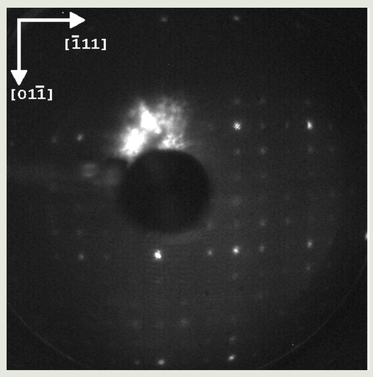

Fig. 1: collected at 212 eV

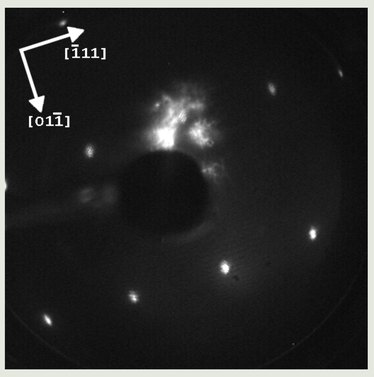

Fig. 2: collected at 90 eV

In the next steps oxygen adsorption was investigated. Structure of only annealed (without flashing) surface is strongly dependent on oxygen dose. For small doses (4 L and 6 L) no regular structures were observed (Fig. 3). For 12 L STM showed structure (Fig. 4) interpreted as the beginning of epitaxial Mo_2O growth and for 50 L shapes of observed terraces (Fig. 5) indicated, as interpreted by Schroeder et al. [6], presence of layer Mo_2O.

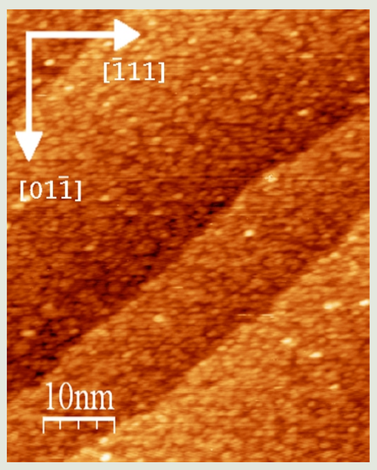

Fig. 3, U = 2 V
I = 0.2 nA

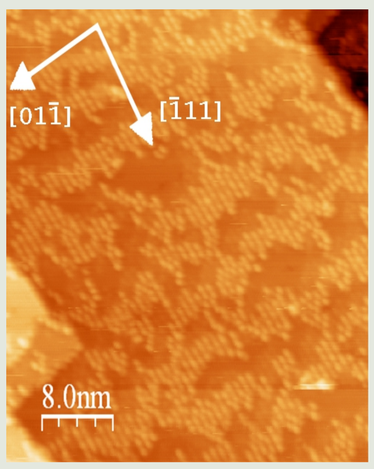

Fig. 4, U = 0.5 V
I = 0.5 nA

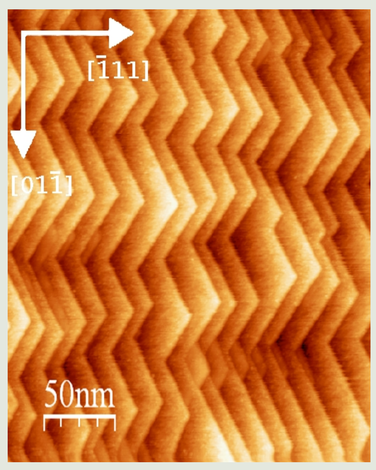

Fig. 5, U = 2 V
I = 0.2 nA

That was interesting that irrespectively to the oxygen dose the structures observed after flashing were both $p(1\times2)$ and $c(4\times2)$ (Fig. 6-7). Such $p(1\times2)$ structure was reported and interpreted as oxygen inducted reconstruction by Sierka et al. [7]. After longer flashing the only remaining structure was $p(1 \times 2)$ what indicates it is the most stable structure. To desorb all the oxygen higher flash (about 2300 K) was needed.

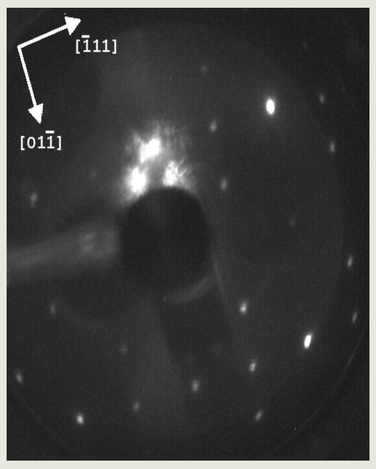

Fig. 6, collected at 83 eV

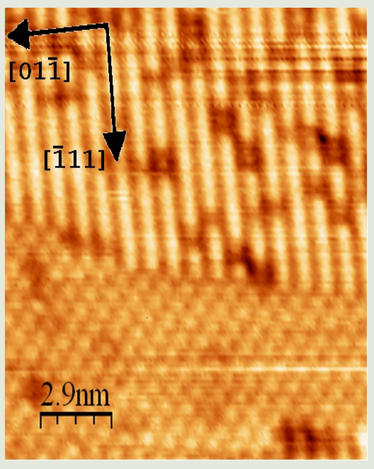

Fig. 7, U = 1 V,
I = 1.2 nA

References

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