(112) Oriented Growth of Au on the Periodically Corrugated (001) β-$MoTe_2$ Surface

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ABSTRACT – We have investigated the influence of the substrate topography on hetero-epitaxial nucleation and growth of Au by using STM and TEM. It is known that on atomically flat Transition Metal Dichalcogenide (TMD) surfaces Au grows isotropically with (111) [1$\bar{1}$0] Au || (001) [1$\bar{1}$0] TMD. Contrary, we show that the periodic troughs on the (001) β-$MoTe_2$ surface cause an anisotropic growth of Au nuclei with the orientation relationship (112) [1$\bar{1}$0] Au || (001) [1$\bar{1}$0] β-$MoTe_2$. It was found that by increasing the deposition temperature from 300K to 500K the long axis of the islands changed from [1$\bar{1}$0] to [0$\bar{2}$1] direction of Au.

[Keywords: Scanning Tunneling Microscopy; Transmission Electron Microscopy; Growth; Nucleation; Epitaxy; Gold; Molybdenum Ditelluride.]

Introduction

The growth of metals on Transition Metal Dichalcogenides (TMD) has been studied for many years but recently the research in this area is being paid attention not only due to their potential applications but also due to their usefulness as ideal model systems for the formation of metal-semiconductor junctions since the TMD surfaces are free from the surface states /1/. In general the crystals are composed of two dimensional sandwich-like X-M-X layers (X = chalcogen and M = metal) with strong covalent bonds inside and weak van der Waals interaction between the sandwiches. Most of the TMD crystals have hexagonal structures with atomically flat surfaces. They can be easily cleaved by an adhesive tape along (001) faces.

The fcc metals usually grow on these surfaces in the islanding (Volmer-Weber) mode with their (111) plane and <1$\bar{1}$0> directions parallel to the (001) plane and <100> directions of the substrate /2,5/. There have been several reports about anisotropic nucleation /3-5/ and different orientational relationship /4,5/ in case of Au grown on some TMD crystals with different surface structures /6-8/ e.g. WTe_2 and β-$MoTe_2$. The anisotropic nucleation on these surfaces is due to the existence of periodic troughs which influence the diffusion of the deposit. As a result the elongated Au islands with their long axis parallel to the troughs have been observed on WTe_2 and β-$MoTe_2$ at room temperature depositions.

The main objective of this work is to extend our previous work /5/ to elevated substrate temperature and to investigate its influence on nucleation behavior of Au.

Experimental

For STM investigations, we used a commercial Omicron UHV STM system with an operating pressure between 10^{-10} and 10^{-11} mbar. β-$MoTe_2$ crystals were grown by chemical vapor transport from 1170 to 1070 K with I_2 as the transport agent. The crystals were cleaved with an adhesive tape just before their introduction into the evaporation chamber connected to the STM chamber via a load-lock. The evaporation chamber was operated in UHV and was equipped with a rotational substrate shutter, a substrate heater and a quartz crystal thickness monitor. Gold of 99.999% purity was deposited onto the β-$MoTe_2$ crystals from a resistively heated Mo boat at 300 K and 500 K substrate temperatures.

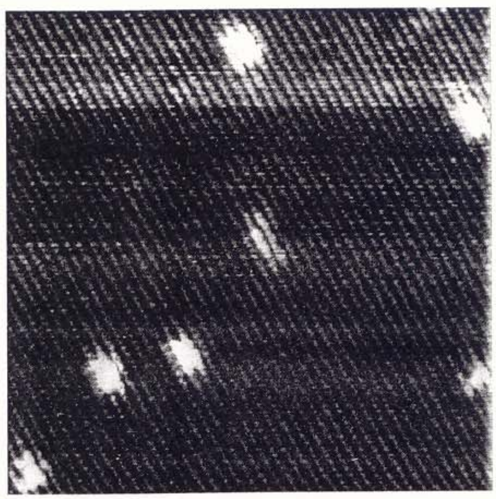

Fig. 1 – A 250 × 250 $Å^2$ STM image (I_t = 1.5 nA, U_t = 0.7 mV) of an early stage of Au nucleation (0.1 ML) on β-$MoTe_2$ (001) surface at room temperature. The troughs from the periodically corrugated surface are clearly visible. The Au clusters are 20 Å long, 6.5 Å wide and one monolayer high.

Deposition rates between 0.3 and 0.5 $Ås^{-1}$ were measured by the quartz crystal monitor while the specimen coverages were monitored by opening a shutter for corresponding times. Samples were transferred between the STM and the

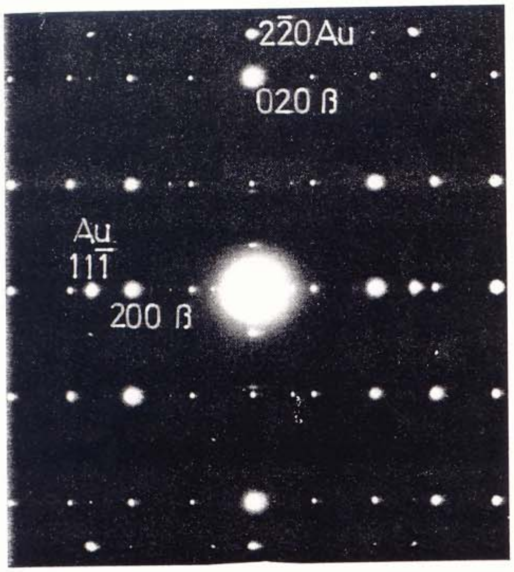

Fig. 2 – A transmission electron diffraction pattern of (112) oriented Au on β-$MoTe_2$.

preparation chamber without exposing them to atmosphere. The STM was operated in the constant current mode and electro-chemically etched tungsten tips were used throughout this work. The samples for transmission electron microscopy were prepared simultaneously in the same chamber and were examined with a Philips EM301 operated at 100 keV.

Results and Discussion

300K deposition temperature

During initial stages of growth gold forms clusters elongated along the rows of substrate Te atoms. The STM image of one mono-layer high Au clusters is shown in Figure 1. The occurrence of these anisotropic Au clusters is due to the preferential diffusion of Au along the surface troughs /3-5,9,10/. The nucleation of Au clusters starts by the formation of short close-packed chains of Au atoms in the troughs between the top-most rows of Te atoms.

With increasing coverage, the Au clusters continue to grow along the troughs and form long islands. At the later stages of growth however, new more isotropically shaped islands are formed which tend to agglomerate into larger finger-like aggregates preferentially aligned almost perpendicularly to the troughs /5/.

The orientation of the Au islands determined from transmission electron diffraction pattern (Fig. 2) is;

(112) [1$\bar{1}$0] Au || (001) [010] β-$MoTe_2$, and [$\bar{1}\bar{1}$1] Au || [100] β-$MoTe_2$.

The reason for this (112) orientational growth of Au is the topographical similarity between (112) Au and (001) β-$MoTe_2$ planes.

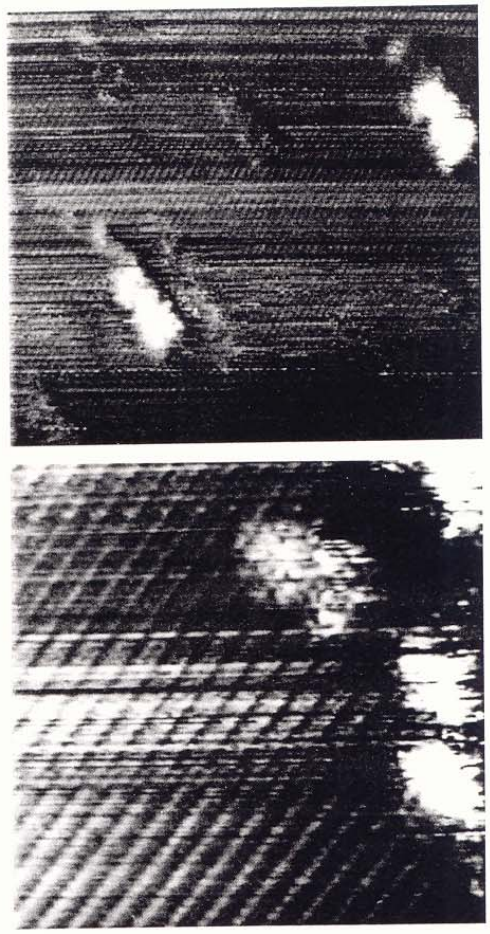

Fig. 3 – STM images (I_t = 30 nA, U_t = 0.2 V) of Au clusters on β-$MoTe_2$ grown at 500K. (a) 100 × 100 $Å^2$ image of atomic resolution of one monolayer high Au cluster (0.1 ML coverage) and (b) 500 × 500 $Å^2$ image of anisotropic Au clusters elongated parallel to the [0$\bar{2}$1] direction of Au (0.4 ML coverage).

500K deposition temperature

During the initial stages of growth at 500K substrate temperature, Au still formed anisotropic clusters on the (001) β-$MoTe_2$ surface as shown in STM images of Figure 3a and b. The long axis of these clusters are no longer parallel to the surface Te troughs as at room temperature but inclined for about 70°. Due to increased temperature the Au adatoms can overcome the existing trough barriers.

The substrate-deposit orientational relationship was determined by transmission electron diffraction from the thinnest measurable deposit and was found to be the same as at room temperature depositions i.e. (112) plane of Au was still parallel to the substrate.

The mentioned approximately 70° alignment of Au clusters toward the substrate troughs corresponds to the angle

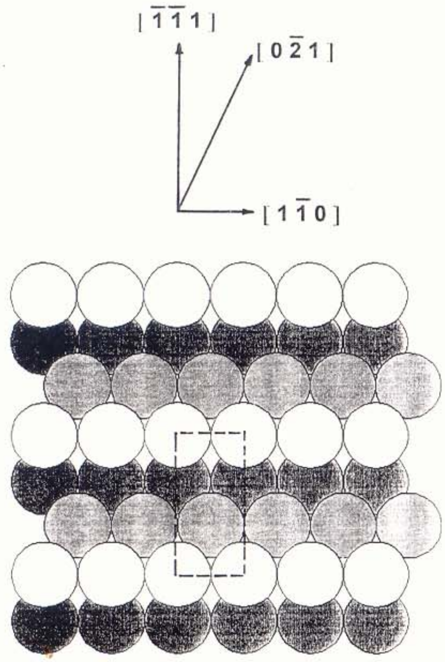

Fig. 4 - The schematic drawing of (112) Au plane. The surface unit cell is shown with dotted line. (White, grey and dark grey circles represent top, middle and bottom atoms).

between [$1\bar{1}0$] and [$0\bar{2}1$] directions of Au as schematically shown in Figure 4.

At the later stages of growth, more isotropic Au islands were formed and their size, height and density increased until coalescence.

Conclusions

The influence of substrate surface topography on the hetero-epitaxial nucleation and growth process in the Au/β-$MoTe_2$ system is clearly evident. The existence of periodic troughs on the (001) β-$MoTe_2$ surface causes Au to grow with its (112) plane instead of its common (111) growth on atomically flat TMD surfaces such as α-$MoTe_2$ /5/. A second consequence of the 1D diffusion along the substrate troughs is the elongation of Au clusters parallel to the troughs. The long axis of these clusters is the [$1\bar{1}0$] direction of Au.

At higher deposition temperature (500K), the diffusion of Au is not confined to the surface troughs which results in anisotropic clusters with their long axis parallel to the [$0\bar{2}1$] direction of Au.

Acknowledgements

This work was financially supported by the Ministry of Science and Technology of the Republic of Slovenia.

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