EARLY STAGES OF GROWTH IN THE Ag/Ni(111) SYSTEM

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Metal on metal growth mechanism is a complex issue involving a large set of thermodynamic parameters. A good understanding of this process is of primary importance to interpret for instance the selective efficiency of bi-metal catalysts towards a given reaction [1]. The Ag/Ni couple, where both metals are immiscible in the bulk phase, has been the subject of a number of theoretical and experimental works.

The first stage of silver growth on Ni(111) up to 2 monolayer (ML) have been investigated by a combination of several experimental and theoretical tools. A detailed study by Scanning Tunnelling Microscopy (STM) [2] of the Ag growth process on Ni(111) as a function of coverage and annealing scheme has lead to the conclusion that Ag grows from the very beginning mainly as bilayer islands, without wetting layer (fig.1). Low energy electron diffraction (LEED) results have shown the occurrence of collinear or rotated registry of the silver plane on the Ni(111) surface depending on thermal treatment (fig.2). In order to determine the geometry of these tilted but still commensurate reconstructions, the adsorption energies have been calculated by quenched molecular dynamics (QMD) simulations for a large number of configurations [3]. Three of those tilted reconstructions, corresponding, respectively, to rotation angles equal to 1°, 2.2°, and 3.5°, have been found energetically more stable than the collinear one. These results support not only our data but also the tilted superstructures observed by various authors using LEED or STM.

In addition, soft X-ray photoelectron diffraction (XPD) in the forward scattering regime has been used to confirm the presence of bilayer Ag islands in the very early stages. Full photoelectron diffraction patterns collected on the clean substrate and on several deposits from about 1ML to 5ML thicknesses have shown twinning and asymmetric rotational effects of the order of magnitude mentioned above. Quantitative structural data have been extracted from hard X-ray reflectivity (XRR) and grazing incidence X-ray diffraction (GIXD) with the help of QMD simulations. These combined measurements have been performed on the ALOISA beamline at ELETTRA (Italy).

This study shows how the coupling between STM, synchrotron radiation techniques and atomistic simulations is fruitful as well as necessary to understand such phenomena.

References:

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[2] C. Chambon, A. Coati and Y. Garreau, Surf. Sci., **602** (2008) 2363
[3] C. Chambon, J. Creuze, A. Coati, M. Sauvage-Simkin and Y. Garreau, Phys. Rev. **B79** (2009) 125412

Figures:

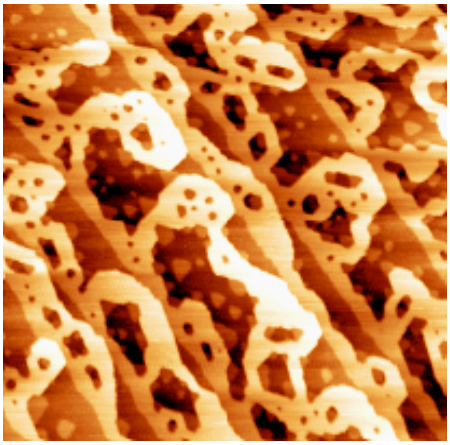

Figure 1 - STM image (250x250) nm² of Ni(111) surface after 1.2 ML of silver deposit and annealing at 525 K.

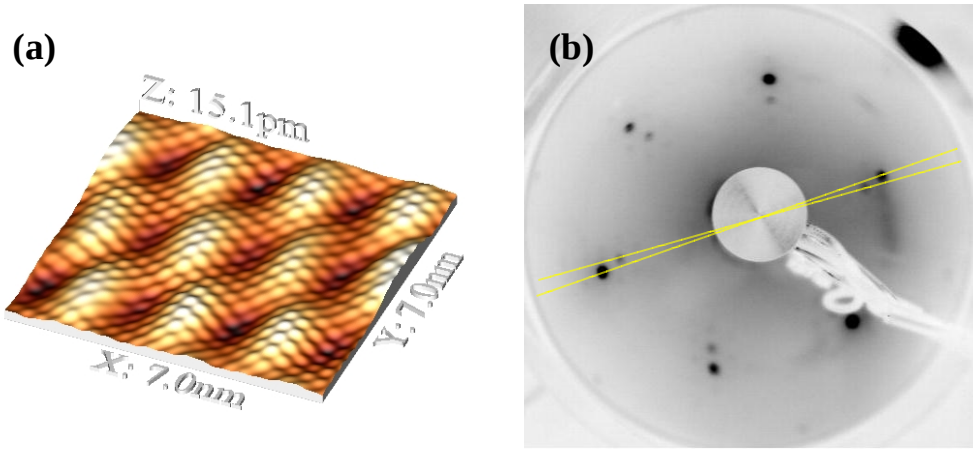

Figure 2 - (a) 3D atomic resolution STM image of "tilted" reconstruction moiré induced by silver layer on Ni(111) after annealing at 675 K – (b) corresponding LEED pattern.