NANOFACETING OF VICINAL Ni SURFACES INDUCED BY Ag DEPOSIT

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The deposit of small amounts of atoms on surfaces may induce the formation of well organised nanostructures, which can present a long range order. In the case of Ag adsorption on a vicinal Cu surface [1], the deposit induces a periodic faceting of the surface, with well defined facets; moreover, in this case, the Ag coverage can be used to tune the periodicity and the orientation of facets. The Ag/Ni couple was thought to be very similar to Ag/Cu: Ag and Ni are not miscible in the bulk, their cohesive energies and atomic sizes are very different, leading to Ag segregation at the Ni surface and to an abrupt chemical interface. However, the faceting behaviour of vicinal surfaces under Ag adsorption is found different, as observed on Scanning Tunnelling Microscope STM images and confirmed quantitatively by Grazing incidence X-ray Diffraction (GIXD), performed on the ID03 beamline at ESRF.

Ni (322) is a surface presenting a miscut of 11.42° with respect to (111) planes and is constituted by a regular succession of (111) terraces of 1.03 nm width separated by {100}-type monatomic steps. When Ag is deposited on this surface, in the monolayer range, and after a thermal annealing, a periodic faceting of the surface is observed, covering the whole surface only within a very restricted coverage range around 0.6 monolayer (ML). Fig 1a and b show this "ideal" faceted surface observed by STM and the corresponding X-ray reciprocal space map recorded at k=2 around two nickel Bragg peaks, on which the scattering rods diffused by the facets are well defined. Two orientations are observed for the facets: (111) and (211); the comparison with a parallel map going through the relaxed silver Bragg peaks (k=1.77), fig.1c, which shows only (211) facet induced diffuse rods arising from the Bragg nodes, enables to conclude that the surface is made of (111) bare Ni facets and (211) Ag covered facets. The narrow (111) oriented diffuse features in fig.1c do not stem from silver Bragg peaks and are presumably linked to planar defects in the nickel near surface region.

For different coverages and particularly for lower ones like 0.3 ML, a surface phase separation between faceted regions similar to the case previously described (same facets with similar local periodicity) and bare vicinal nickel as shown in the STM image and the two corresponding maps in fig.1d, e and f. The energetics of the system needs to be further investigated to understand the unicity of the surface faceting decomposition.

In addition, as already visible in the STM image, fig.1a, one of the facets shows a reconstruction and indeed accurate GIXD data could be collected on the reconstructed Ag covered (211) facets (fig.2a) corresponding to a (2 x n) surface cell ($8<n<9$). A starting model sketched in fig.2b involving 6 silver rows on top of two successive (111) terraces of the (211) Ni substrate with (n-1) Ag atoms for n Ni atoms along the $[01\bar{1}]$ direction has been used. When optimised by quenched molecular dynamics simulations involving about 60 bulk layers, this model renders satisfactorily the overall dynamics of the diffraction data but needs further

refinement to account for the whole in-plane and out-of plane measured structure factors. A mixture of different coverages of the individual terraces is presently investigated.

The knowledge of the system morphology and its surface structure are key parameters for its possible use as a nano-organized template for further growth of selected nano objects with magnetic or catalytic properties. This study shows how the coupling between GIXD, STM and atomistic simulations is fruitful as well as necessary to understand such phenomena.

References:

[1] A. Coati, J. Creuze, and Y. Garreau, Phys. Rev. **B 72** (2005) 115424
[2] Y. Garreau, A. Coati, A. Zobelli, J. Creuze, Phys. Rev. Lett. **91** (2003) 116101.

Figures:

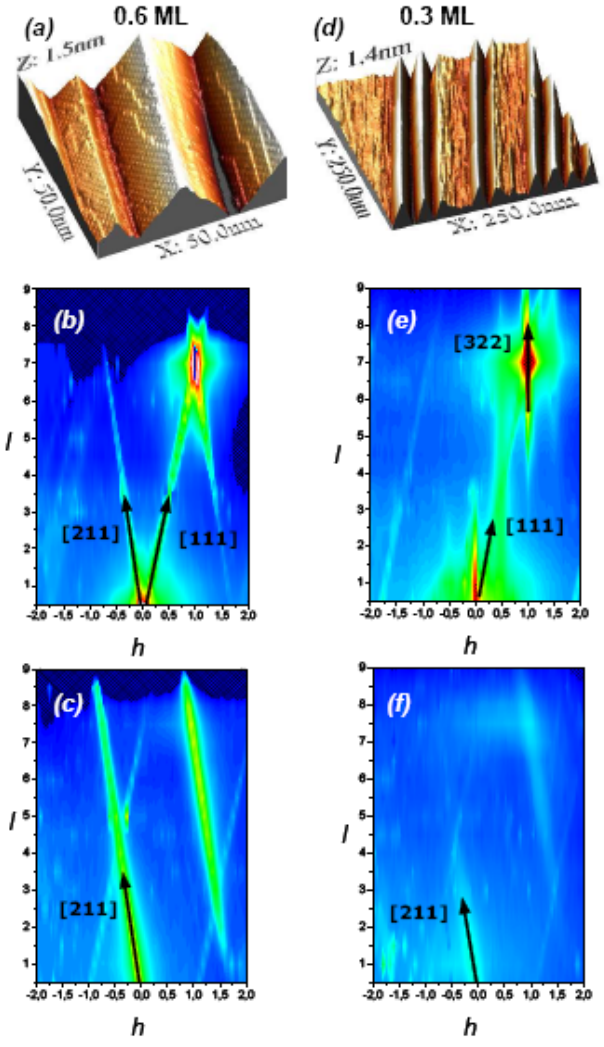

Fig. 1: Ni(322) surface after Ag deposit followed by annealing at 600 K. The Ag covered and bare Ni facets are clearly recognized: (a), (b) and (c) correspond to a 0.6 ML deposit, and (d), (e) and (f) to 0.3 ML. **(a)** 3D STM image (50x50) nm²; **(b)** *(h, l)* reciprocal space map at *k*=2; **(c)** *(h, l)* reciprocal space map at k=1.77; **(d)** 3D STM image (250x250) nm²; **(e)** *(h, l)* reciprocal space map at k=2; **(f)** *(h, l)* reciprocal space map at *k*=1.77.

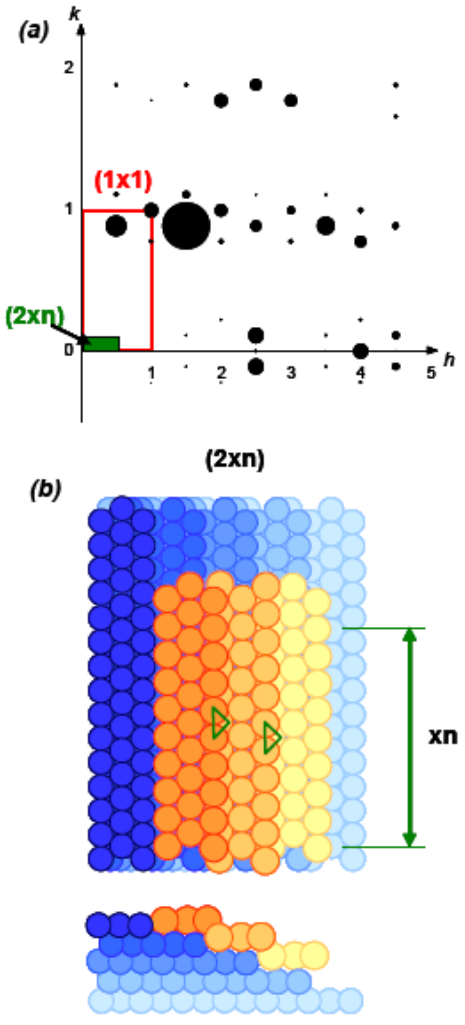

Fig. 2: Surface reconstruction induced by silver on the (211) facets. **(a)** GIXD in-plane data which shows the (2x*n*) surface periodicity; **(b)** model of the surface structure used for QMD simulations (Ag atoms in orange, Ni atoms in blue).