*CRG Committee Proposal Number : **32- 3- 65***

GROWTH AND STRUCTURE OF NEW PHASES OF PURE Pd ON THE Au(110) (1X2) SURFACE TO STUDY THE INTERACTION STRAIN-REACTIVITY OF Pd

LIGNE :	**BM32**	**SUV**

NUMBER OF RUNS USED : 24

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EXPERIMENTAL REPORT

We have carried out experiment to grow Pd on Au(110) with a substrate temperature below 300K. The clean Au(110) surface presents a (1X2) reconstruction due to a periodic missing row in the outermost layer. The lattice parameter misfit of Pd relatively to Au is + 5% and a Pd film on Au would suffer a substantial tensile strain.
The aim of this experiment was to obtain

- Ultra-thin Palladium film with dilated in-plane parameter for 3-4 ML deposits.
- In the submonolayer range (0.5ML), a filling of the missing row, to create Pd linear structures.

At room temperature, the growth is in a quasi layer by layer mode up to 3-4 ML, but due to Au segregation, the top layer is mainly filled by Au [experimental report 32-3-042 and ref 1]
We expected that at lower temperature it would be possible to freeze the Au segregation, while keeping a 2D growth mode.
The first stage was thus to explore the behavior of the Pd/Au(110) system by varying temperature below R.T.

Measurements were performed at 210, 240K and 270K in different ways:
During growth:

- we followed RHEED intensity oscillation of the (0 0) peak, to determine the growth rate, and of the (0 ½) to detect when the (1X2) reconstruction disappeared.
- we also recorded the X-ray diffraction intensity at (0 0 ½)

The main feature of deposit 0.5ML and 3ML thick at each temperature was then drawn by.

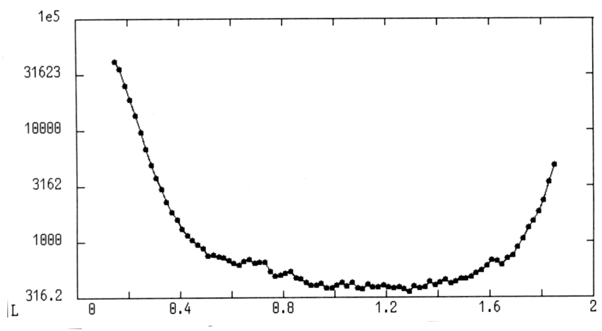
- Checking the Pd and Au concentration at surface by Auger spectroscopy.
- Linescan in the reciprocal space by X-ray diffraction, along the rods and parallel to the surface

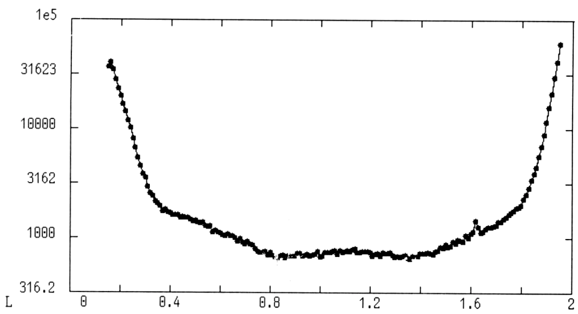
Afterwards, data for structural analysis were collected in some specific cases.
Most of the results are reported in ref. 2

During growth, except at the very beginning, the frequency of the (0 0) intensity of the RHEED pattern, was not very sensitive to the temperature, but the damping of the oscillations was more and more pronounced when decreasing the temperature. The frequency of the oscillations were used to calibrate the deposit. In the same time and whatever the temperature, the (0 ½) intensity essentially vanished for about 0.5 Pd ML, or slightly before.
Conversely the behavior of the (0 0 ½) intensity recorded by X-ray diffraction was strongly dependent on the temperature substrate. This apparently conflicting results for the (0 0) intensity for RHEED and X-ray, lye in the fact that for RHEED, the signal is essentially sensitive to the free surface roughness, while for X-ray diffraction it is due to interference between diffracted beam by the two interface: film/substrate and film surface/vacuum. This indicates thatthe process at interface strongly depends on the temperature.
The AES spectra recorded at the end of a 3ML deposit indicated that at 270K and below, the Au concentration is lower than at R.T.
We thus conclude that by decreasing the temperature we succeeded to limit the Au segregation

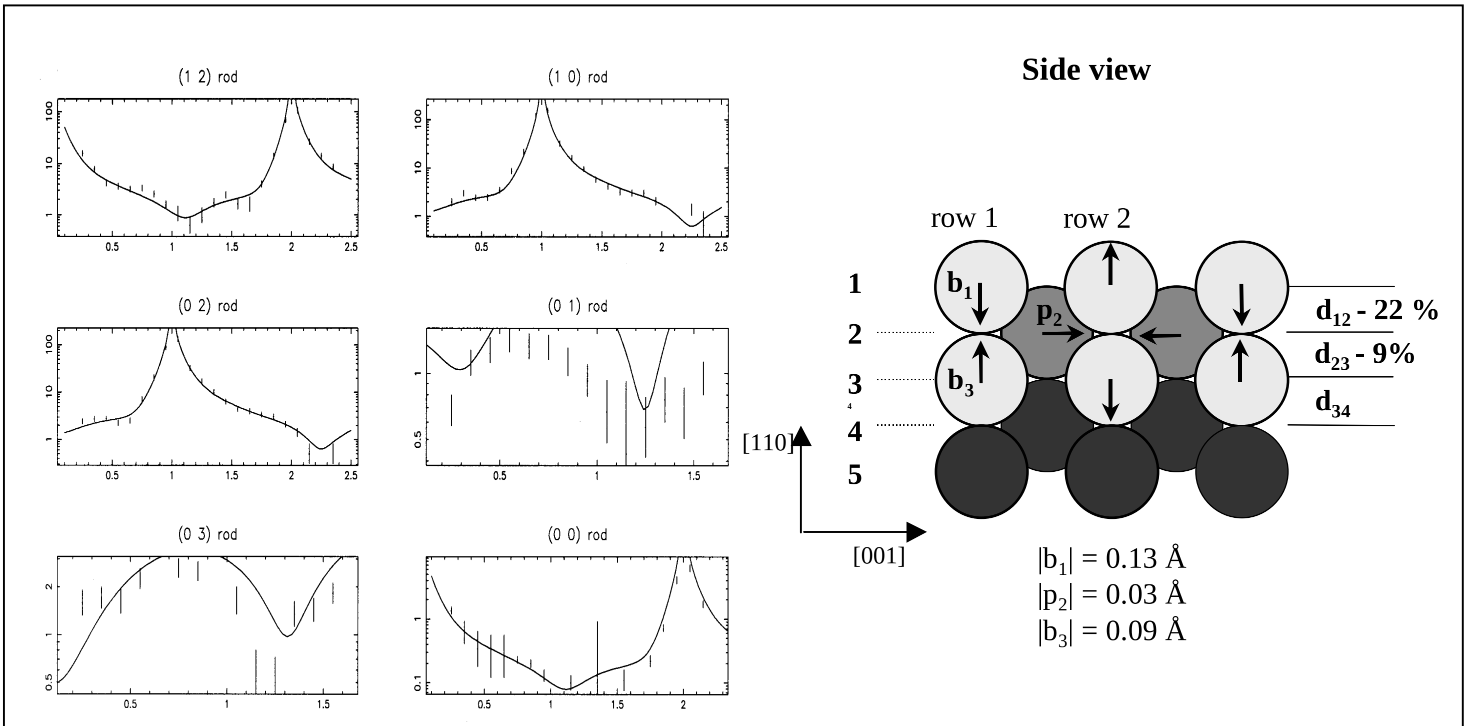
In the other way, by X-ray diffraction the linescan along (0 0) rod exhibited less and less well defined modulated intensity, consistently with the damping of the RHEED oscillations, this shows that roughness increases when decreasing temperature.

From all these experimental data, T=270K appears to be the better compromise, the figures below present the x-ray reflectivity for T= 240K at the left, and 270K on the right.





We recorded a set of x-ray data to solve the structure in two cases: 0,5ML and 3ML Pd deposited at 270K. We first analyzed the data for the 0,5ML. Results are illustrated on the figure below.



The interplane spacing is strongly contracted relatively to the pure Au one, and small atomic displacements, pairing and the buckling, are present contributing to the (1x2) reconstruction still observable by x-ray diffraction**. At this temperature, Pd stays mainly in the outermost layer**.
This is very different from the R. T. case where an interface alloy was formed buried under 2 Au (very incomplete) atomic planes [1].
However the real composition remains to be determined since the classical analysis of x-ray diffraction only fits an effective atomic scattering factor: we are not able to unambiguously affect at each site a partial occupation of Au or Pd. Especially we cannot conclude to a disordered PdAu atomic plane at surface or to a trend to an ordered atomic arrangement with one Pd row and one Au row.

[1] - "*Strained Pd films, by epitaxial growth on Au(110), to control catalytic properties*" P. Dolle, R. Baudoing-Savois, M. De Santis, M.C. Saint-Lager, M. Abel, J. C. Bertolini, P. Delichère, to be published in Surf. Sci.
[2] - "*Etude structurale par diffraction X de surface de dépôts du Palladium sur l'Or(110°, réalisés à une température inférieure à 300K*" rapport de stage de DEA de Aude Bailly, Université Joseph Fourrier, Grenoble.