EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office using the **Electronic Report Submission Application:**

http://193.49.43.2:8080/smis/servlet/UserUtils?start

Reports supporting requests for additional beam time

Reports can now be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

	Experiment title: Reversible high temperature phase transition in $Pt_xRh_{1-x}(110)$ alloy surfaces	**Experiment number**: SI 577
Beamline: BM 32	**Date of experiment**: from: 19/06/2000 to: 26/06/2000	**Date of report**: 28/08/2000
Shifts: 18	**Local contact(s)**: **M. De Santis**	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

The sample originally planned ($Pt_{25}Rh_{75}(110)$) [1,2] revealed totally unfit to surface x-ray diffraction analysis (much too large mosaic spread); Fortunately, the crystal could be replaced at the last minute by another with very close composition and structure, $Pt_{50}Rh_{50}(110)$. By chance, all phenomena, expected on the former - phase transition with temperature in relation to segregation – do occur on $Pt_{50}Rh_{50}(110)$ too.

The experiments were performed from June 19 to June 26 2000 on the French -Interfaces line at ESRF. This system, $Pt_{50}Rh_{50}(110)$, was only partially known on a structural point of view at room temperature (RT) from LEED observations. The surface reconstructs, in the manner of (110) faces of Pt, Au and Ir , or of previously analysed bimetallic alloys ($Pt_{80}Fe_{20}$) with a (1x3) symmetry [3,4] : two dense rows, out of three in the top layer, and one in the second layer are missing. The surface is constituted of valleys the slopes of which are (111) micro-facets. This is at least what could be derived from the striking similarities in the I(V) spectra from PtRh and PtFe, the details of the structure requiring a thorough analysis of the data.

From LEIS (Low Energy Ion scattering) experiments performed on the other crystal ($Pt_{25}Rh_{75}(110)$) [1,2], we expect, on $Pt_{50}Rh_{50}(110)$, a modification of the composition of the outermost layers with increasing temperature, change related to the deconstruction of the surface which ends up with a (1x1) symmetry (?). However, as the composition is not the same – which means also slightly different interatomic distances –, an identical behaviour for both crystals was not obvious.

The low temperature structure was measured using integer and fractional order CTR. The quantitative analysis (in progress) should allow to extract the details of the atomic arrangement in the 3-4 surface layers. The high sensitivity of x-rays to lateral displacements

(i.e., parallel to the sample surface) should be an asset for deriving the pairing of the dense rows in layers 2 and 3. This work is being performed simultaneously with a quantitative LEED analysis : this latter method is more sensitive to concentrations and vertical shifts so that the combination of both techniques should give the whole picture.
The first results do confirm the missing row model. As for already known noble metals, this reconstruction is accompanied by an important contraction of interlayer distances and by buckling (0.1 à 0.Å) in several layers as well as pairing in at least two layers.
To this reconstruction is associated a strong Pt segregation in all dense rows exposed to vacuum and a marked depletion in the rows just underneath (Fig. 1).
Concerning the behaviour with increasing temperature, in the 0° à 950 °C range, we were able to show that *the (1x3) symmetry disappears* around 750 °C to yield *a (1x1) symmetry* which is quite typical of the volume phase. This is clearly obvious from the decrease – down to zero – of the intensity of the 1/3 order rods in the in plane scans (0k) and from the clear modifications of the intensity of integer rods. This symmetry change is totally correlated with LEIS measurements - realised early august – which reveal a striking reduction with increasing temperature of the Pt concentration in surface layers : this composition tends asymptotically

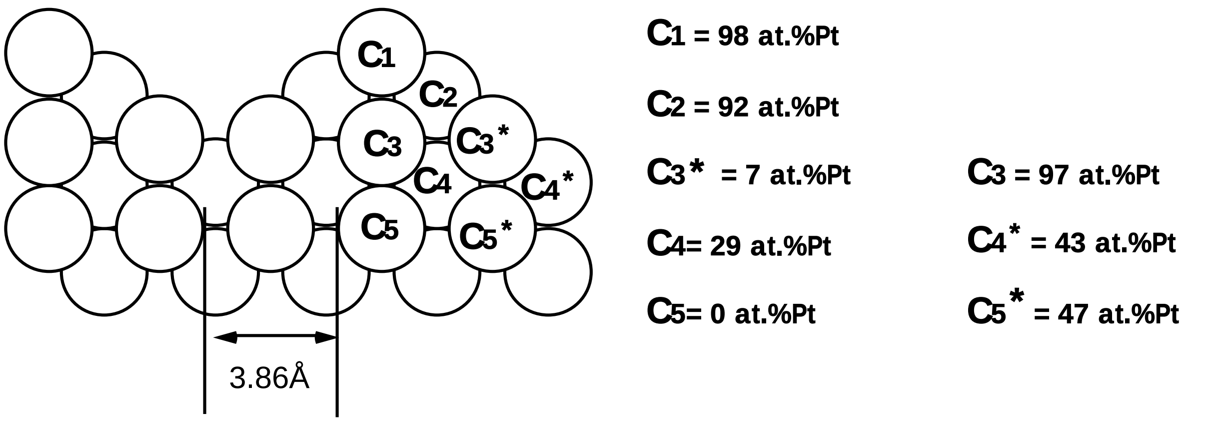

Fig. 1 : $Pt_{50}Rh_{50}$(110)-(1x3) . side view and concentration in the various surface dense rows

towards that of the deep bulk, 50-50%. Moreover, the total ion yield increases (for T increase from 0 to 850°C) is also characteristic of fully occupied surface layers (i.e. (1x1) symmetry). Surface segregation of Rh has the effect of a reduction of the elastic strains (Rh is ~2% smaller than Pt) which, likely, is at the origin of the observed deconstruction.

A detailed interpretation of the data is underway.

[1] E. Platzgummer, M. Sporn, R. Koller, Schmid M., P. Varga, Surf.Sci.423 (1999) 134
[2] E.L.D. Hebenstreit, W. Hebenstreit, M. Schmid, P. Varga, Surf.Sci. 441 (1999) 441-453
[3] R. Baudoing-Savois, Y. Gauthier, W. Moritz, Phys.Rev. B 44 (1991) 12977
[4] Y. Gauthier, Surf. Review Letters 3 (1996) 1663-1689