ESRF	**Experiment title:** Nonowires, surface alloy and magnetism. Mn thin films on Pt(110)-(1x2).	**Experiment number**: Si-1120
Beamline: BM 32	**Date of experiment**: from: 2-2-2005 to: 8-2-2005	**Date of report**: 6-10-2005
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Report:

Our aim in this experiment was to exploit the well known Pt(110)-(1*2) MR (missing row) reconstruction to grow monoatomic Mn wires by depositing about 0.5 ML in the grooves. Such a surface seems quite attractive for studying magnetic interactions.However, such an arrangement fits with none of the known Pt-Mn phases and, hence, is not expected to be thermodynamically stable.

The surface structure was studied by x-ray diffraction performed on BM32 (CRG-IF). The beam energy was 18 *keV* and the incidence angle 1°. Full data sets of structure factors – including equivalents – were collected along Crystal Truncation Rods (CTRs) and non integer rods. The data analysis was performed using the ana-rod package.

High purity Mn was evaporated in UHV (10^{-11} mbar range) by a Knudsen cell, at a rate of 1 ML/12min. A quartz balance was used for calibration. The rate was further refined by measuring the diffracted intensity in antiphase along a Pt(110) rod: a 1st maximum in intensity is obtained at layer completion.

Deposition of 0.5 ML at RT resulted in a (1*2) reconstruction, which was explained with Mn filling the grooves of the clean (1*2) MR surface. The model is shown in Fig. 1*a* and the best fit parameters in Tab. I. Mn is shifted outward - rippling of 0.20 Å ($d_{Mn\text{-}Pt}$). Buckling in the 3rd layer, pairing in the 2nd and 4th layers as well as interlayer relaxations were considered, as for clean Pt(110)-(1*2) [1.2]. The composition of the two surface sites (C_{11} and C_{12}) was optimized. We find ~20% of the other species in each site.

By annealing about 0.5 ML deposited at RT, we switched to a (2*1) symmetry structure. This thin surface alloy was interpreted as a precursor of the $L1_2$ phase (Fig. 1*b*). The best fit and the optimum parameter values are given in Fig. 2 and Tab. I, respectively. Pt and Mn alternate along each rod. This time the pairing is along [1-10]. The rippling is 0.16 Å. *b3*, *p2* and *p4* are smaller – the structure is more rigid along [1-10]. C_{11} and C_{12} point to some intermixing in the top layer. The Mn content in deeper layers is considered. ~30% Mn atoms in layer 3 (C_{31} site, under the surface Pt) are necessary to fit the data.

A better understanding was reached by studying also a thicker alloy, obtained by annealing about 3 ML Mn at 520°C. An alternating sequence of mixed and pure Pt planes is expected, both from bulk structure and surface effects. An oscillating profile was already reported in the literature by annealing Mn/Pt(111) [3], although it does not correspond to any identified bulk phase. In our case the structure is a Pt_3Mn-like film, 7 layers thick + a top layer + 3 interface layers. The "bulk" is a periodic sequence of a Pt rich layer (Cal_{11} =86%) alternating with a mixed layer (Cal_{21} =7%, Cal_{22} =75%). This $Pt_{0.62}Mn_{0.38}$ alloy has a $L1_2$ structure, which doubles the Pt(110) cell in the [110] and [1-10] directions. The interlayer spacing d_{al} is weakly contracted with respect to Pt_3Mn whereas the surface layers reproduce the surface structure of the thin annealed film.

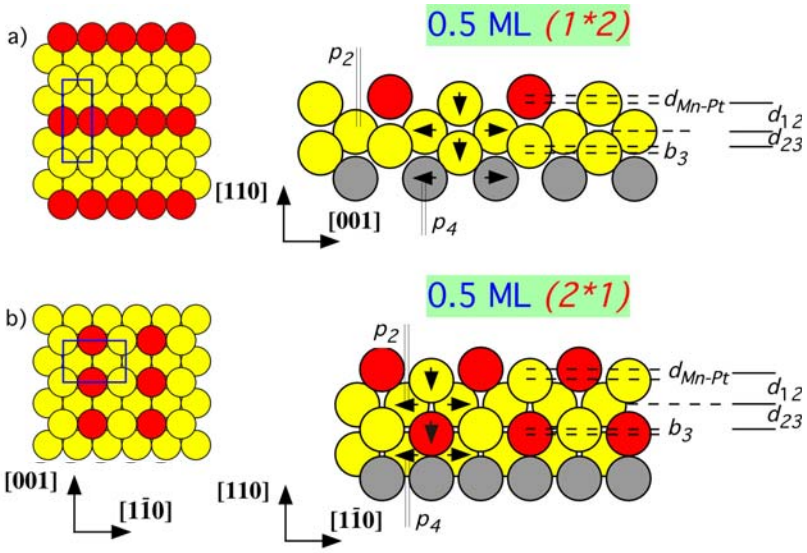

Fig.1: (1x2) (a) and (2x1) (b) surface models.

	0.5 ML (1*2)	**0.5 ML (2*1)**
d_{Mn-Pt} [Å]	0.20(2)	0.16(2)
b_3	0.120(6)	0.026(6)
p_2	0.04(1)	0.017(4)
p_4	0.025(5)	0.006(2)
d_{12}	1.160(6)	1.16(1)
d_{23}	1.445(6)	1.443(6)
C_{11} [%Pt]	80±5	80±4
C_{12}	20±5	5±13
C_{21}		96±4
C_{31}		70±4
χ^2	3.5	2.9

Tab. I: Best fit parameters.

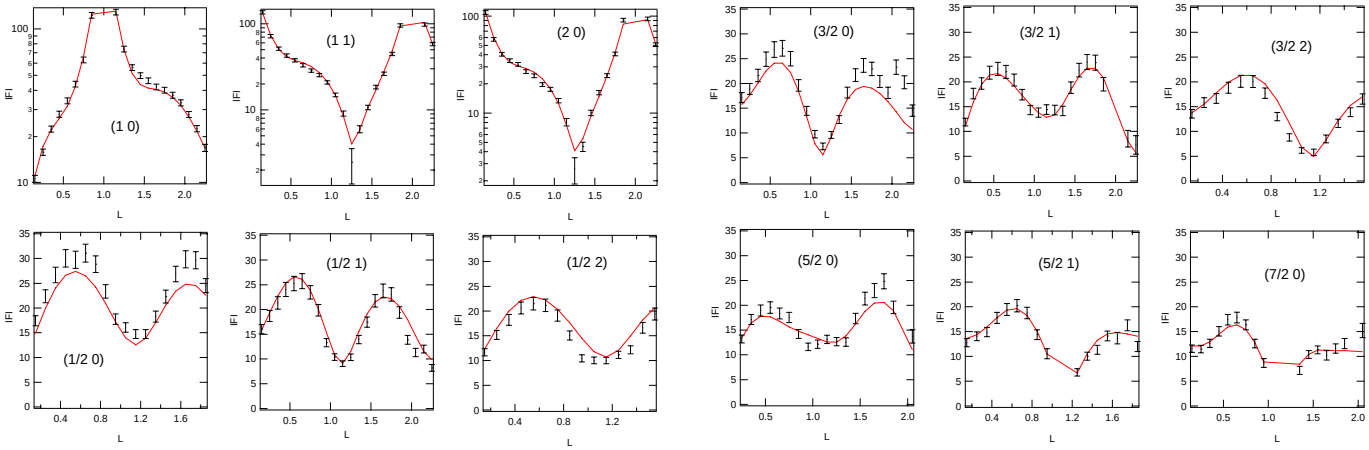

Fig. 2: Best fit of the (2x1) structure (~0.5 ML Mn/Pt(110) annealed at 380°C).

In conclusions, Mn/Pt(110) represents an original system where, by annealing, the surface layer structure switches from a (1*2) to a (2*1) surface alloy. In the (1*2), monoatomic Pt and Mn dense rows are parallel to the [1-10] direction. Conversely, in the (2*1), Pt and Mn sites alternate along each row, as in (110) mixed planes of $L1_2$ phase. In the former system, Mn atoms are nearest neighbors, while in the latter the interaction is mediated by Pt. In both cases a fraction of each site is occupied by the other species, resulting in long range order parameters S of ~ 0.6 and 0.75 respectively. In both arrangements, Mn is shifted outward by ~0.2 Å with respect to Pt, which seems at first looks surprising considering the Pt and Mn atomic radii. Indeed we find the same behavior as observed for several Mn based 2D surface alloys, and interpreted as the signature of surface magnetism. This looks promising for the magnetic properties of both surfaces.

The 3 ML film yields a $L1_2$ $Pt_{0.62}Mn_{0.38}$ alloy upon annealing. Taking into account the epitaxy relationship with the substrate, the interlayer d_{al} spacing gives a slightly expanded cell with respect to bulk Pt_3Mn.
Ab initio calculations provide a nice confirmation of the stability of the (2*1) arrangement and point to anti-ferro magnetic order

References

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