ESRF	**Experiment title: Surface diffraction of Fe monolayers on W(110)**	**Experiment number**: SI-543
Beamline: ID3	**Date of experiment**: from: 21.Feb.00 to: 29.Feb.00	**Date of report**: Aug. 3, 2000
Shifts: 18	**Local contact(s)**: P. Steadman, S. Ferrer	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

D. Sander*, H. L. Meyerheim*, R.Popescu*, J. Kirschner,

MPI für Mikrostrukturphysik, Weinberg 2, D-06120 Halle

S. Ferrer*, P. Steadman*

ESRF, BP 220, F-38043 Grenoble, Cedex

Report:

We have investigated the geometric structure of the clean and Fe covered W(110) surface using surface x-ray diffraction (SXRD). This is of considerable interest given the large number of experimental and theoretical analyses concerning the magnetic, elastic and structural properties of this system [1-5].

In the first experiment the structure of the uncovered W(110) sample was investigated by means of analyzing the integer order crystal truncation rods (CTRs). We determine a first interlayer contraction relative to the bulk $\Delta d_{12}/d$ by –2.7 (5)% at 300 K and find a bulk like second interlayer spacing $\Delta d_{23}/d$ within an error of about 0.3 %. The data support previously reported results ($\Delta d_{12}/d$ =–3.1%) based on low energy electron diffraction (LEED) [6], but are somewhat smaller than predicted by theory (–4.1%) [7]. The results of this part of the experiment will be presented at the ECOSS conference [8] and have been submitted to Surface Science for publication [9].

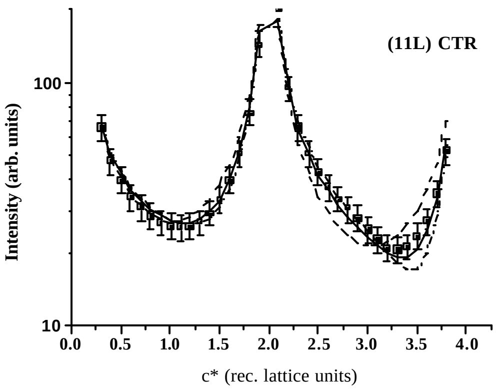

Figure 1: CTR data of the clean W(110) surface.

Figure 1 shows as a representative example the (11L) CTR. The measured structure factor amplitudes are plotted as solid squares, the fits to the data based on different contractions ($\Delta d_{12}/d$) are shown by the lines: $\Delta d_{12}/d$= 0.0% (long dashed)

$\Delta d_{12}/d$=-4.1% (short dashed)

$\Delta d_{12}/d$=-2.7 (5)% (solid) best fit

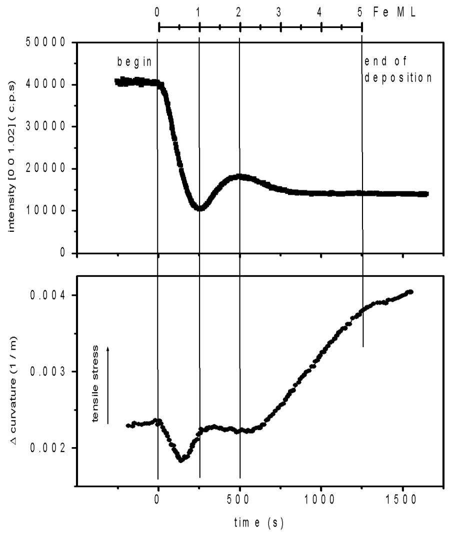

Figure 2: CTR intensity, upper panel, and simultaneously measured substrate curvature, lower panel, as a function of Fe

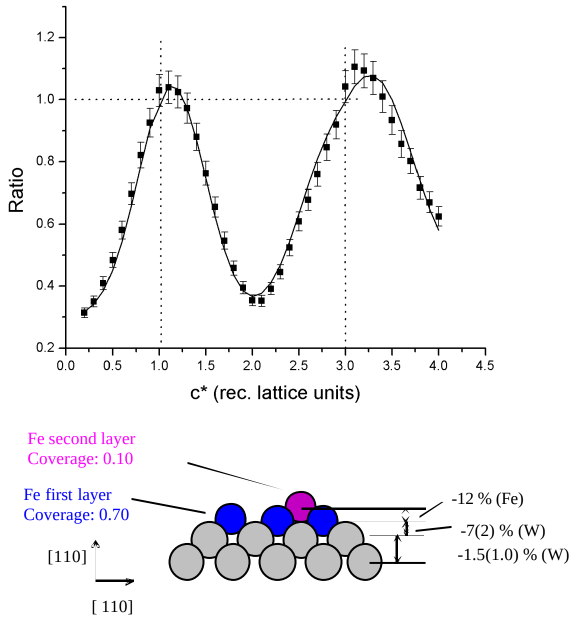

Figure 3: Upper panel: Ratio of the (01L) CTR intensities between the Fe covered and the clean sample, measured at the minimum of the CTR intensity of Fig.2. Lower panel: Structure model for an Fe coverage of 0.8.

In a second experiment the evolution of surface stress and the CTR intensity were monitored simultaneously as a function of the Fe-coverage. Our results are the first combined measurements of CTR intensities and substrate curvature [4, 5]. We shall exploit the results to investigate the correlation between film strain and film stress with submonolayer resolution. The upper part of Fig. 2 shows the (antiphase) 001 CTR-intensity in the coverage range between 1 and 5 monolayers (ML). It shows a damped oscillating intensity. The first minimum can be attributed to the completion of the first ML. The lower panel shows the curvature measurement that was taken simultaneously. The negative slope indicates Fe induced compressive stress below 0.6 ML. At higher coverage tensile stress sets in. The kink in the stress curve at 1.2 ML indicates the formation of misfit distortions [5]. The coverage of the kink closely coincides with the first SXRD intensity minimum.

SXRD measurements were carried out at this coverage of the minimum of the CTR intensity of Fig. 2. The ratios of the (01L) CTR intensities are shown in the upper panel of Fig. 3. The symbols represent the ratio between the measured intensities of the Fe-covered and of the clean W(110) surface. This procedure allows a data analysis that minimizes the influence of experimental correction factors. The data can be fitted by placing 0.7 ML Fe in pseudomorphic sites of the first layer and adding about 0.1 ML Fe in the second layer, as indicated in the model of the lower panel in Fig. 3. We find a downward relaxation of the first layer of Fe, e.g. towards the bulk of W, of -7(2)% with respect of the bulk W layer spacing and a downward relaxation of -12(4)% for the second Fe layer with respect to bulk Fe. The first W interlayer relaxation is considerably reduced from its value for the uncovered surface to -1.5%. The total coverage of 0.8 ML of this model is smaller than the coverage of 1.2 ML indicated by the position of the kink of the stress curve [5]. This discrepancy between SXRD derived structural models and the curvature measurement is tentatively ascribed to Fe atoms that are bonded in non-epitaxial sites, where they do not contribute to the coherent diffraction.

Measurements were also carried out at higher Fe coverage including the analysis of satellite reflections. The data analysis is presently in progress to model the relative satellite intensities for periodic distortions of the Fe bonding sites.

References:

[1] H. J. Elmers, J. Hausschild, H. Fritsche, G. Liu, and U. Gradmann, Phys. Rev. Lett. 75, 2031 (1995)

[2] J. Hausschild, U. Gradmann, and H. J. Elmers, Appl. Phys. Lett. 72, 3211 (1998)

[3] D. Sander, R. Skomski, C. Schmidthals, A. Enders, and J. Kirschner, Phys. Rev. Lett. 77, 2566 (1966)

[4] D. Sander, A. Enders, C. Schmidthals, D. Reuter, and J. Kirschner, Surf. Sci. 402-404, 351 (1998)

[5] D. Sander, Rep. Prog. Phys. 62, 809 (1999)

[6] M. Arnold, G. Hupfauer, P. Bayer, L. Hammer, K. Heinz, B. Kohler, and M. Scheffler, Surf. Sci. 382, 288 (1997)

[7] X. Qian, and W. Hübner, Phys. Rev. B 60, 16192 (1999)

[8] H.L. Meyerheim, D. Sander, R. Popescu, P. Steadman, S. Ferrer, J. Kirschner "Simultaneous determination of structure and surface stress in Fe / W(110)" poster Tu-P187, ECOSS-19, Sept. 5 – 8, 2000.

[9] H.L. Meyerheim, D. Sander, R. Popescu, P. Steadman, S. Ferrer, J. Kirschner "Interlayer relaxation of W(110) studied by surface x-ray diffraction", submitted to Surf. Sci., August 2000.