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| ESRF | **Experiment title: Surface diffraction of Fe monolayers on W(110)** | **Experiment number**: SI-543 |
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| **Shifts:** | **Local contact(s)**: P. Staedman, S. Ferrer | *Received at ESRF:* |


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## Report:

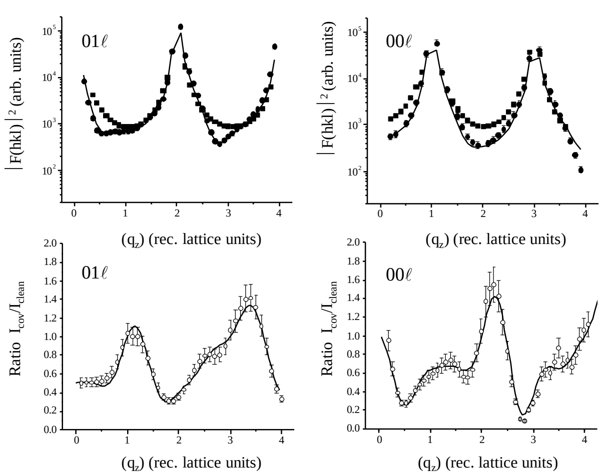


*Fig. 1: Measured (symbols) and calculated (lines) intensities (upper panels) and corresponding ratios (lower panels) for the clean and Fe covered W(110) surface. Fits are only shown for the Fe-covered sample and the ratios.*

We have investigated the geometric structure and the stress of the Fe/W(110) interface. In addition to the SXRD experiments on the clean W(110) surface and at low Fe coverages reported earlier [1,2] we have carried out experiments at 1.7 ML and 5 ML Fe-coverage [3]. After deposition of 1.7 ML Fe the intensity distribution along several crystal truncation rods was measured.

The upper panels of the figure 1 compare the (01ℓ) and the (00ℓ) CTRs' measured for the clean and the 1.7 ML sample. The lower panels show the corresponding ratios R between the covered and the clean sample (R= $I_{cov}/I_{cln}$). Solid lines are fits to the data. From the rapid intensity modulation along $q_z$, it is qualitatively directly evident that several pseudomorphically grown Fe ad-layers contribute to the scattered intensity. The structure model is shown in figure (2).

In total three pseudomorphic layers have to be taken into account to fit the x-ray intensities. The occupancies of 0.80(10), 0.60(10) and 0.20(10) for the first three Fe-layers indicate incomplete layer-by layer growth consistent with scanning tunneling microscopy data [4].

In general, the contractions of the normal interlayer distances are in fair agreement with previous experimental and theoretical work [5,6].

Pseudomorphic Fe growth on W(110) including a third Fe-layer were not considered so far, neither theoretically, nor experimentally. It is worth emphasizing, that the normal distance between the second and third Fe-layer is significantly less contracted than the deeper layers (5% versus 8 to 11%). This rapid "contraction-damping" can be attributed to the formation of small Fe islands that become more bulk-like with increasing thickness.

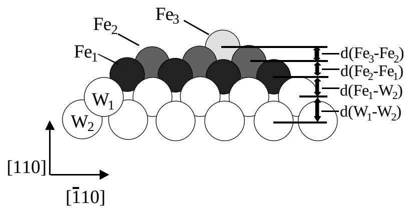


*Fig. 2: Schematic view of the Fe/W(110) interface as derived on the basis of the SXRD analysis. The relaxations are given with respect to the bcc W (2.23 Å) and the Fe (2.03 Å) interlayer distances.*

*d($W_1$-$W_2$) : - 1±1 % (W)*

*d($Fe_1$-$W_1$) : - 8±2 % (W)*

*d($Fe_2$-$Fe_1$): -11±3 % (Fe)*

*d($Fe_3$-$Fe_2$): - 5±2 % (Fe)*

In another experiment 5 ML Fe were deposited on W(110). Due to the large misfit between Fe and W, at coverages larger than about 2 ML a regular array of dislocations is formed which gives rise to a satellite pattern which has been observed by low energy electron diffraction (LEED) and STM [7,8].

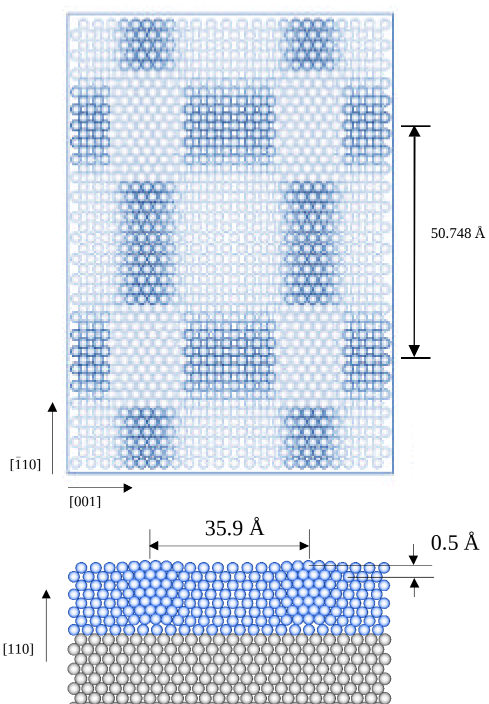


*Fig. 3:*
*Top (upper part) and side view (lower part) of the two-dimensional dislocation network for nominally 5 ML Fe/W(110). Draker regions correspond to protrusions.*

The intensity distribution along 16 satellite rods was measured. The data were fitted to a structure model assuming a sinusoidal modulation of the Fe-positions (figure 3.).

This structure model uses 8 layers, one pseudomorphic, a second layer with a fraction of 0.5ML pseudomorphic and non-pseudomorphic Fe-atoms, and 6 non-pseudomorphic layers. Interatomic distances were confined to be within 15% of the bulk Fe-Fe distances (2.48 Å). The lateral and normal modulation amplitude is in the range of 1.0 and 0.5Å, respectively. It is in the same range for all layers. The periodicity of the intensity oscillations along $q_z$ requires a model assuming 8 Fe-layers in contrast to the nominal thickness of 5 ML. This indicates the growth of Fe islands.

References:


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