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.

ESRF	**Experiment title: Correlation of Structure and Magnetism in Ultrathin Fe-Layers on Cu(001)**	**Experiment number**: SI-658
Beamline: ID-03	**Date of experiment**: from: 28-June-01 to: 07-July-01	**Date of report**:
Shifts: 24	**Local contact(s)**: Odile Robach	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

1.) H. L. Meyerheim*, MPI f. Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

2.) R. Popescu*, as (1)

3.) D. Sander*, as (1)

4.) J. Kirschner, as (1)

5.) Odile Robach*, ESRF, BP220, F-38043 Grenoble, France

Report:

The aim of the experiments was to study the geometric structure of room temperature (RT) deposited ultra-thin Fe-films on Cu(001) using surface x-ray diffraction. While there is consensus that in the coverage range of up to 4 monolayers (ML) Fe orders ferromagnetic (FM), the magnetic structure in the coverage range between 4 and about 11 ML is controversial. Although many experimental and theoretical investigations have proposed that the magnetic structure of the (whole) film can be described by a type-I (collinear) antiferromagnetic (AF) ordering between successive layers or by an AF coupling between two FM coupled bilayers [1-3], a more recent study proposes a model of a spin-density wave (SDW) in resemblance to the SDW wave in fcc-Fe [4].

Further, theoretical studies have suggested that in general there should be a direct relationship between the interlayer distance (d_{ij}) between successive layers i and j. In this context, FM and AF coupling is correlated with an interlayer expansion and contraction, respectively [3,5]. In view of these studies we investigated in the experimental run the structure of 6 and 7 ML Fe deposited on Cu(001) at RT.

After Fe-deposition the experiments were carried out either at RT or after cooling to about 120K (in the following labeled by "LT"), which is below the Neel-Temperature (T_N~200 K) [6] of the AF underlayers.

In total, four different samples were prepared and investigated, namely three 6ML samples and one 7 ML sample. For all SXRD measurements a freshly prepared sample was used in order to minimize the influence of the surface contamination on the results. The accurate thickness calibration was carried out by monitoring the (010) anti-phase reflection oscillations as shown in figure (1) for the deposition of 6ML Fe. The first two layers grow in a double layer growth

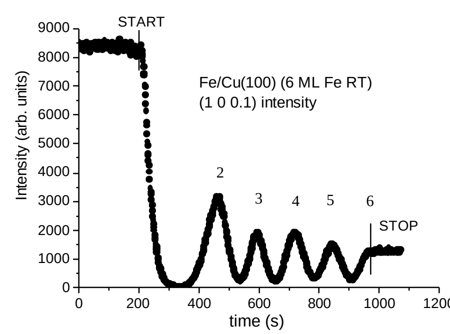


Fig.1: (010) reflection intensity versus Fe deposition time

mode, the following layers in layer-by-layer growth mode.

The figure (2) shows for the 6ML Fe/Cu(001) RT sample as symbols and lines the measured and calculated structure factor amplitudes, $|F_{hk\ell}|$ along four different crystal truncation rods, respectively. Highly accurate fits to the data were obtained as expressed by the unweighted residuum (R_u) in the order of 0.04.

For fitting the data the interlayer distances (d_{ij}) within the Fe-adlayers as well as the Debye parameters (B) describing the disorder were varied. The latter was very important for the low temperature data in order to take account of the lateral atomic displacements in the top layer as suggested by LEED [7]. The figure (3) shows the derived interlayer distances for all samples. The 6 ML samples (red, blue and black datapoints) are very similar, the d_{ij} are well reproducible within the error bars. While for the deeper Fe-layers, d_{ij} is in the range of 1.77 Å, which is characteristic for fcc-Fe, the top interlayer distance is expanded by about 5% to 1.87 Å. This is in agreement with the picture of the top two layers to be FM coupled. However we do not observe any variation of d_{ij} depending on either temperature or (theoretically) expected (Δd_{ij}= +,-,+,-,…) for a collinear bi-layer AF structure (↑↑↓↓↑↑) [2,3,5].

Further, for the 7ML (RT only) sample (green datapoints) the top interlayer distance does not exhibit a significant expansion relative to the fcc-value. The reason for this "unusual" behaviour is not clear at present. One could speculate that there might be a relation to the properties of the recently proposed SDW structure in this coverage regime [4]. In this model, the characteristic experimental feature was the significant minimum of the magnetization (MOKE measurements at 70 K) at 7ML, whereas at 6, 8 and 9ML larger moments are observed. This is because at 7ML the spins in the SDW nearly cancel each other, while this is not the case for the other coverages. In view of the present results, the high accuracy achieved in this study and the still unresolved details of the SDW model (e.g. still assuming the top two layers to be FM coupled) we apply for a continuation of the experiment to study samples of 8,9 ML Fe on Cu(001).

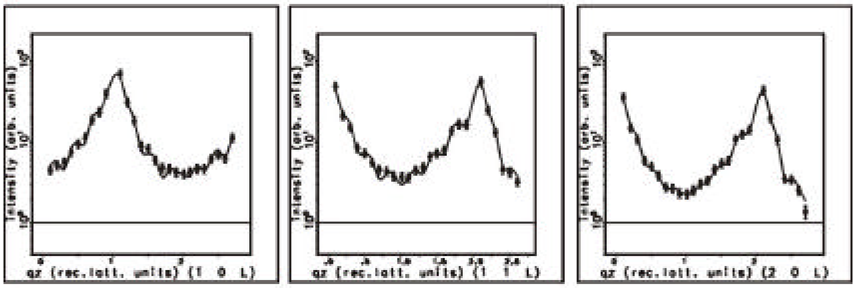
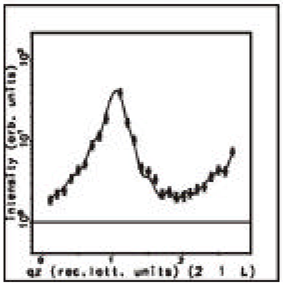
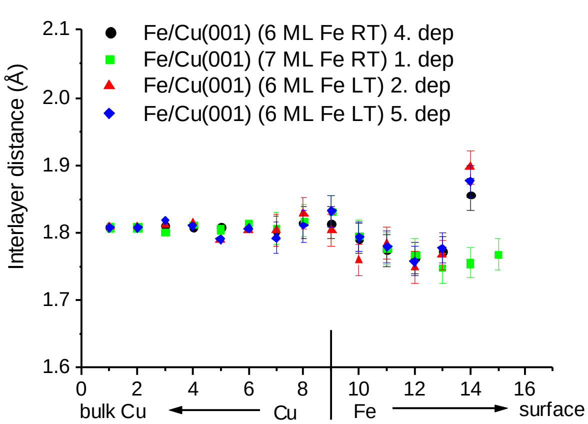



Fig. 2: Measured (symbols) and calculated (lines) structure factor amplitudes for 6ML Fe/Cu(001) at RT.



References:

[1] R.E. Camley, D. Li, PRL 84, 4709 (2000)
[2] E. G. Moroni, G. Kresse, and J. Hafner, J. Phys. Condens. Matter 11, L35 (1999)
[3] D. Spisak and J. Hafner, PRB 61, 16129 (2000)
[4] D. Qian, X.F. Lin, J. Barthel, M. Klaua, and J. Kirschner, PRL 87, 227204 (2001)
[5] X. Yin and K. Hermann, PRB 63, 115417 2001)
[6] D. Li et al., PRL 72, 3112 (1994)
[7] K. Heinz, S. Müller, and L. Hammer, J. Phys. Condens. Matter 11, 9437 (1999)