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ESRF

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.

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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	**Structure determination of thin chemically ordered antiferromagnetic films by SXRD: c(2x2) NiMn/Cu(001)**	**Experiment number**: SI-1588
Beamline: BM32	**Date of experiment**: from: 19.9.2007 to: 25.9.2007	**Date of report**: August 20, 2008
Shifts: 18	**Local contact(s)**: Dr. Maurizio DE SANTIS	*Received at ESRF:*

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Report:

We have proposed a surface x-ray diffraction (SXRD) study of the geometric structure of ultrathin $Ni_{50}Mn_{50}$ films deposited on Cu(001) at room temperature. Layers of 2, 4, 6 and 8 monolayers (ML) in thickness were prepared.
Complete datasets including superlattice (SL) and integer order crystal truncation rods were collected, however due to the limited beam intensity provided by the bending magnet, only the data of the thicker films (6 and 8 ML) allowed a meaningful analysis. Furthermore, even for these layers important details of the structural ordering escape from a clear-cut determination, which are very important for the interpretation of the magnetic properties of this system [1,2]. For this reason we are resubmitting a proposal to continue the experiment asking for beamtime at an undulator beamline. In the following we show the most important results on the basis of the 8 ML sample:

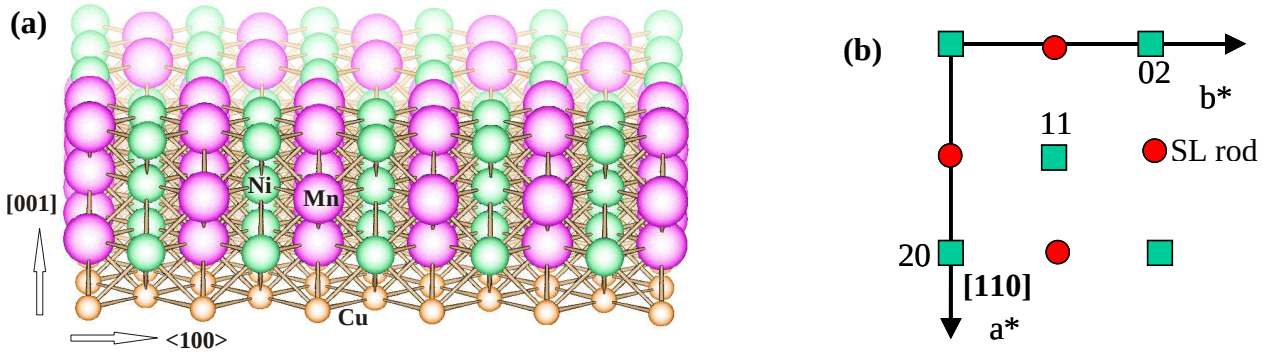

Fig.1: Schematic view of the $Ni_{50}Mn_{50}$/Cu(001) structure showing 3 chemically ordered layers (a) and the reciprocal lattice (b). Note, that there is a stacking fault in the topmost NiMn layer.

Fig. 1(a) and (b) show the basic structure model and the corresponding reciprocal lattice, respectively [1]. We chose the setting corresponding to the face-centered Cu(001) surface unit cell. In the model it is assumed that there are alternating sheets of Ni (small spheres) and Mn (large spheres) along the [100] direction, according to the CuAu- type structure of bulk MnNi. The chemical order leads to the apperance of extra diffraction spots (circles) at positions (H+K=2n+1, n integer) due to the lifting of the centering of the 2D unit cell. The intensity I at theses SL diffraction spots is proportional to the (squared) difference between the scattering amplitudes: $I \propto (f_{Mn}-f_{Ni})^2$. Chemical disorder leads to an intensity decrease of the SL reflections relative to the truncation rods resulting from the occupancy mixing of the lattice sites and the corresponding averaging of the f-values. Chemical disorder is characterized by local antisite defects and/or by stacking faults as shown in the topmost layer in Fig. 1a. Apart from a general expansion of the interlayer spacings by 1-2% relative to the Cu(001) bulk spacing, our SXRD data provide evidence for an unexpected layer-dependent chemical disorder as as shown in Fig. 2

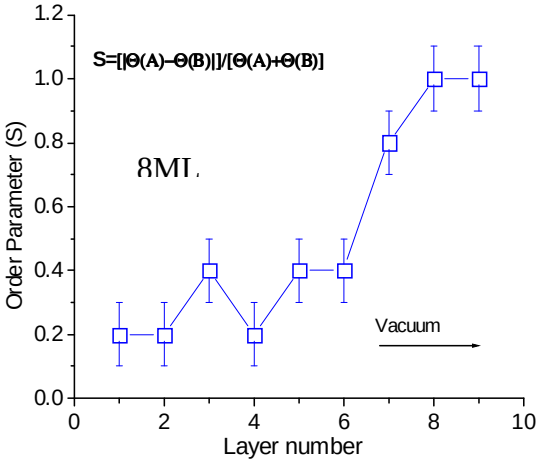

Fig.2: Order parameter (S) vs. NiMn layer number in the alloy for the 8 ML sample. (1)=bottom, (2)=topmost layer

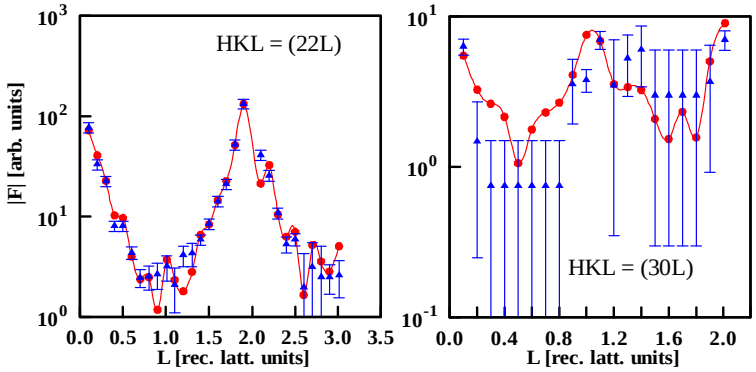

Fig.3: Structure factor amplitude along a high-q crystal truncation rod (left) and supperlattice rod (right) for 8 ML MnNi/Cu(001). Note the different scaling along the y-axis.

The order parameter (S) is plotted vs. the layer number. The values S=0 and S=1 indicate complete disorder and order, respectively. It can be seen that S increases from low values at the Cu/NiMn interface to S=1 at the topmost two (incomplete) layers. Although a similar trend is observed for the 6 ML sample also, models allowing for NiMn intermixing with Cu at the interface by simultaneously assuming a more ordered structure (S≈0.65) throughout the film lead to fits of similar quality (Ru≈0.10). The difficulty to distinguish between these models is due to the low accuracy of the high-q SL data as shown in Fig.3 on the right panel. The limited primary beam intensity does not allow the collection of SL intensities accurate enough to derive an unambiguous structure model. However, the precise determination of the Mn/Ni-order profile is a prerequisite for the understanding the striking magnetic properties of these alloy films. Examples are the appearance of antiferromagnetic order beyond 8 ML coverage and the observation of a non-collinear surface spin density [2].

References:

[1] C. Tieg, W. Kuch, S. G. Wang, and J. Kirschner, Phys. Rev. B **74**, 094420 (2006)

[2] C.L. Gao, A. Ernst, A. Winkelmann, J. Henk, W. Wulfhekel, P. Bruno, J. Kirschner, PRL **100**, 237203 (2008)