EUROPEAN SYNCHROTRON RADIATION FACILITY

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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:** Probing the mesoscopic misfit in Co/Cu(001)	**Experiment number:** SI-1409
Beamline: ID03	**Date of experiment:** from: Dec.4 2006 to: Dec. 12, 2006	**Date of report:** February 20, 2007
Shifts: 21	**Local contact(s):** N. Jeutter	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

H. L. Meyerheim(*), O. Mironets(*), J. Kirschner (Max-Planck-Institut f. Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Germany)

Report:

It was the aim of the experiment to analyze the mesoscopic misfit of small Co-islands deposited on Cu(001) at T=150K. The experiments could be carried out successfully and the analysis of the data based on a static disorder approach and ab-inito molecular dynamics (MD) calculations provide first evidence for the theoretically predicted "mesoscopic misfit" concept.

As pointed out by Stepanyuk et al. [1], small Co islands consisting of several tens of atoms (diameter in the nanometer range) should exhibit a "mesoscopic" misfit, which means that the (average) inter-atomic bond length (2.50 Å in bulk Co) is reduced by several percent as shown in Figure (1).

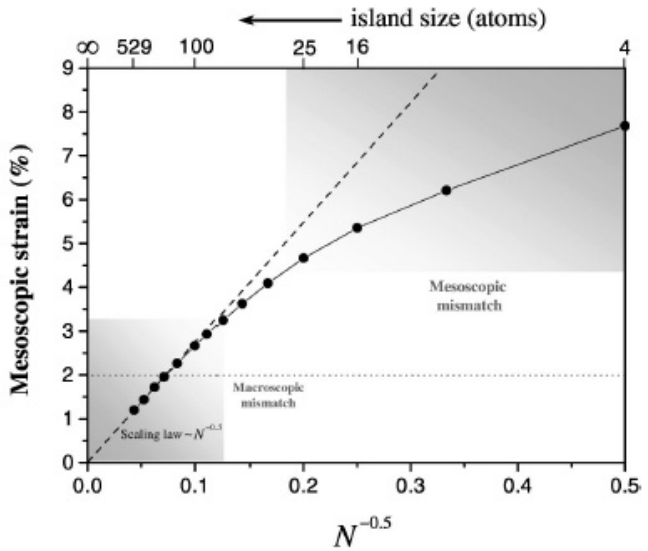

Fig.1: Calculated mesoscopic misfit vs. island size

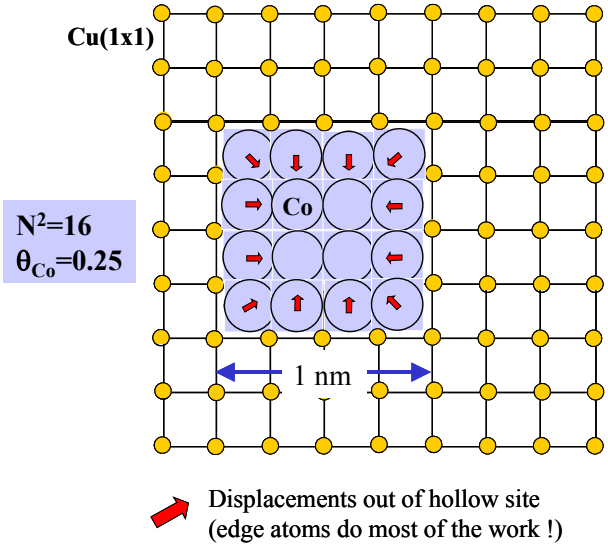

Fig.2: Schematic of a 4x4 Co-island on Cu(001).

The situation for a small island on Cu(001) is schematically represented in Figure (2). Ab initio MD calculations predict that the Co-atoms in the contracted island do not reside in hollow sites of the substrate but laterally shift towards the island center.

This situation can be described in a first approximation by a static disorder of the Co-atoms where the Cu-hollow site is the equilibrium adsorption position. To test this model we prepared small Co-islands and measured crystal runcation rods (CTR's) yielding information on the registry of the adsorbate atoms. As an example, Fig. (3) shows experimental (points) and calculated (lines) structure factor amplitudes for 0.3 ML Co/Cu(001) measured at T=150K. At this temperature island growth by diffusion and intermixing is inhibited. STM experiments indcated an island diameter of about 1 nm.

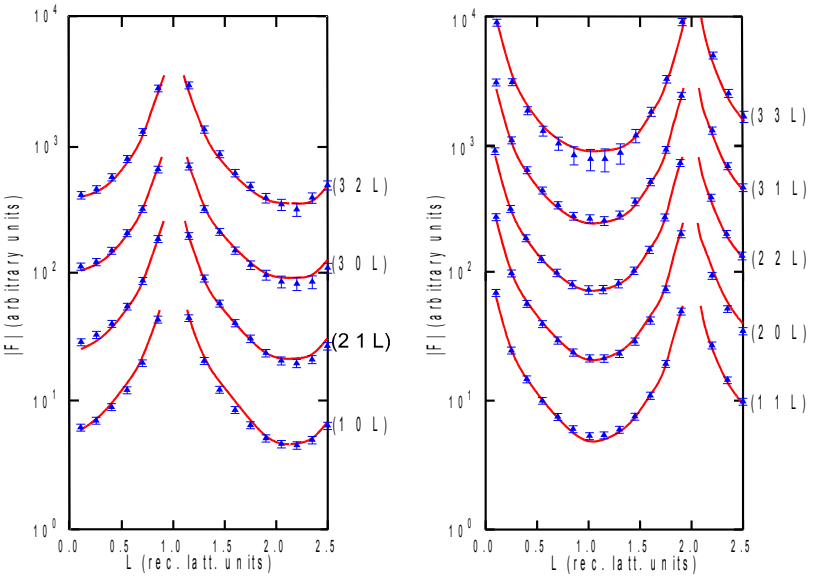

Fig.3: Measured (symbols) and calculated (lines) intensities along CTRs for 0.3ML Co/Cu(001)

In order to obtain meaningful results of the disorder analysis, highly accurate data need to be collected. The beamline ID03 with its improved optics supplying an approximately fivefold increased flux was ideally suited for this purpose.

Preliminary results are summarized in Figure 4. The filled circles represent the (static) Debye parameters ($B=8\pi^2\langle u^2\rangle$) derived from the fit of the CTR data for several Co-depositions.

In general, for the Co-atoms huge B's in the range between 1.7 and 3.2 Å^2 are obtained, the latter corresponding to $[\langle u^2\rangle]^{1/2} \approx 0.2$ Å

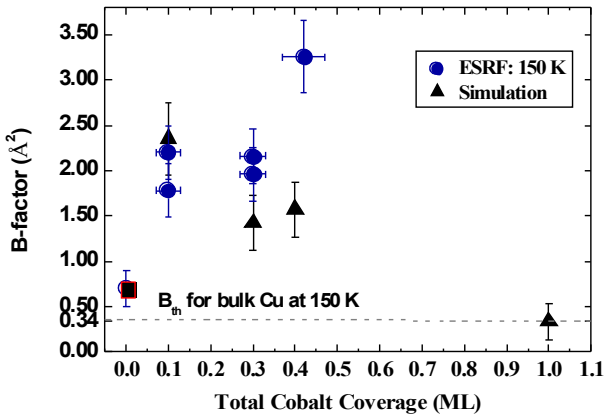

Fig.4: B-factor vs. Co-coverage

These values are in good agreement with simulated data based on 4x4-atom islands (triangles) and much larger than the contribution of the thermal disorder, which at T=150K equals to 0.34 Å^2 (dashed line). The validity of the analysis is also supported by the study of the uncovered Cu(001) sample (θ=0; solid square), where for the top Cu-layer a twofold enhanced (thermal) B-factor (≈ 0.7 Å^2) over the bulk value is derived.

In summary, the SXRD experiments have provided first experimental evidence for the mesoscopic misfit in small Co islands on Cu(001).

References: [1] V.S. Stepanyuk, D.I. Bazhanov, A.N. Batanov, W. Hergert, P.H. Dederichs, and J. Kirschner, PRB 62, 15398 (2000)