EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

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.

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:** Solvent Dependence of the NaCl {111} surface structure	**Experiment number**: SI720
Beamline: ID03	**Date of experiment**: from: 13.09.2001 to: 20.09.2001	**Date of report**: 22.03.2002
Shifts: 21	**Local contact(s)**: Dr. Christopher Walker	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Drs. J. Arsic*, Drs. M. F Reedijk*, Drs. D. Kaminski* and Prof. Dr. E. Vlieg*

Report:

The crystallographic structure determines the shape and properties of crystals. Current theories that predict the growth shape of a crystal are based on the bulk crystallographic structure [1]. These theories ignore the role of deviations from the bulk structure at the growth interface. From the surface science point of view this assumption appears to be somewhat crude, but it is a good starting point that has been proven to be quite successful. By using the present generation of synchrotron radiation sources, surface X-ray diffraction is now starting to provide quantitative information about surface termination, relaxation and the role that impurities play.

Here, we rapport the surface structure of the NaCl(100). Sodium chloride crystallizes quite easily and is one of the most produced alkali halides. In these ionic crystals with their delicate balance between electrostatic forces and Van der Waals interactions, small changes in the surface structure may significantly influence the interaction potential. Thus, the detailed knowledge of the surface structure is needed.

NaCl crystals were mounted in a growth chamber [2] and data were collected for two different environmental conditions: air and 85% humidity. Data collection was quite difficult because the x-rays were found to generate significant amount of bulk defects in NaCl, so-called F and H-centers [3].

The surface structure is not directly affected, but the bulk defects give a rise to huge background signal, making it difficult to measure the surface signal (figure 1.)

We, nevertheless, were able to measure in total 167 non-equivalent reflections in air, consisting of the (20) and (11) rod and specular reflectivity data, with an agreement factor of 16% when averaged over all measurement conditions. Figure 2 shows the measured structure factor amplitudes of the (20) rod. For the 85% humidity conditions we collected in total 110 nonequivalent reflections with agreement factor of 15% consisting of the same rods.

Our data show that the surface layer of NaCl (100) is terminated with a top layer containing alternating Na^+ and Cl^- ions for the both experimental conditions, as expected. A good description of the data, however, is only obtained when small out-of-plane ion relaxations in the top layer are allowed and when a simple model for surface roughness on an atomic scale is included. In air, according to our analysis, Na^+ is relaxed outward 0.10Å (towards to bulk) and Cl^- is relaxed 0.04 Å inward (figure 2). For the measurements in the 85% humid environment relaxations are somewhat bigger. These analyses are still in progress.

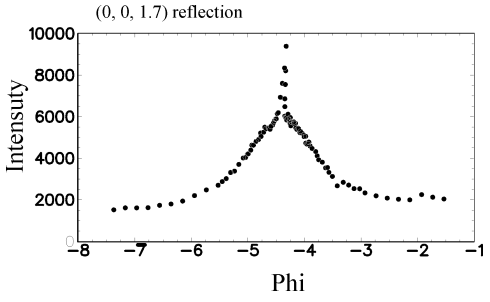

Fig. 1 (0,0,1.7) surface reflection with a broad background due to a bulk defects.

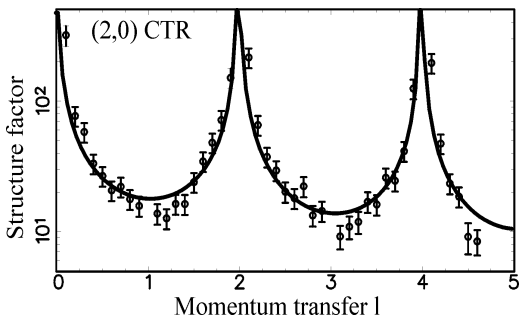

Fig. 2. (2, 0) rod of NaCl(100)measured in the air. Data are represented with circles. Line represents model calculations for alternating Na^+ and Cl^- in the surface layer with the relaxations included.

References:

1 P.Hartman and W. G. Perdok, Acta Cryst. 8, 49 (1955).

2 S. A. de Vries, P. Goedtkindt, S. L. Bennett, et al., Phys. Rev. Letters 80, 2229 (1998).

3 R. Bennewitz, S. Schar, V. Barwich, et al., Surface Science Letters 474, L197 (2001).