ESRF	**Experiment title: STRUCTURE OF THE GROUND STATE OF Sn/Ge(111)**	**Experiment number**: SI 2037
Beamline: ID03	**Date of experiment**: from: 16-06-2010 to: 22-06-2010	**Date of report**: 30-07-2012
Shifts: 18	**Local contact(s)**: R. Felici	*Received at ESRF:*

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Report:

We report an investigation on the structure of Sn on Ge(111) using surface x-ray diffraction at low temperature. The main goal of the proposal was to determine the structure of the ground state of Sn/Ge(111), in view of the observation with STM and electron spectroscopies of a phase transition below approx. 25 K, giving rise to a Mott insulating ground state with root3 structure. A well known (3x3) phase is seen in this interface below approx. 250 K. A Ge(111) sample of high quality was prepared in a straightforward manner. In turn, the preparation of a (3x3)-Sn/Ge(111) demanded a long time, as it was not possible to distinguish (3x3) superstructure reflections of sufficient quality. This was in part related to the fact that the (3x3) reflections present a very low intensity for low *l*-values. After tuning carefully the Sn coverage and inserting an analyzing crystal to remove background, good (3x3) reflections were observed and the main typical features of the (3x3) reconstruction, previously investigated by us at ID03, were identified.
Next, we took measurements as a function of temperature in the 100-10 K range. We monitored (3x3) and root3 specific reflections as a function of temperature, and indeed found that (3x3) reflections undergo a significant decrease of intensity below 60 K, followed by a total disappearance below approx. 40 K. Due to lack of time, we were not able to characterize

in detail the intermediate stages of the surface and had to concentrate our efforts in obtaining a sufficiently large data set at the lowest temperature achieved (in the range of 10 K at the sample), which corresponds to a root3 structure.

The main data set obtained includes 56 in-plane irreducible structure factor intensities and 172 out-of-plane irreducible structure factor intensities. In addition to this, 130 irreducible structure factors were measured for crystal truncation rods (CTR), providing a total number of 358 structure factors. The refinement of all the models includes horizontal and vertical displacements down to the fourth layer of the substrate and involves the use of a genetic algorithm implemented to be used along with ROD code. An example of the model fit is shown in Fig. 1 for the three independent CTRs. The model developed is based on the root3 conventional structure and agrees with its main features, but difficulties have been found to reach a satisfactory fitting of the in plane structure factors. We are currently using a Levenberg–Marquardt algorithm to refine the structure and test what could be the origin of the insufficient quality of the fitting of the in-plane data.

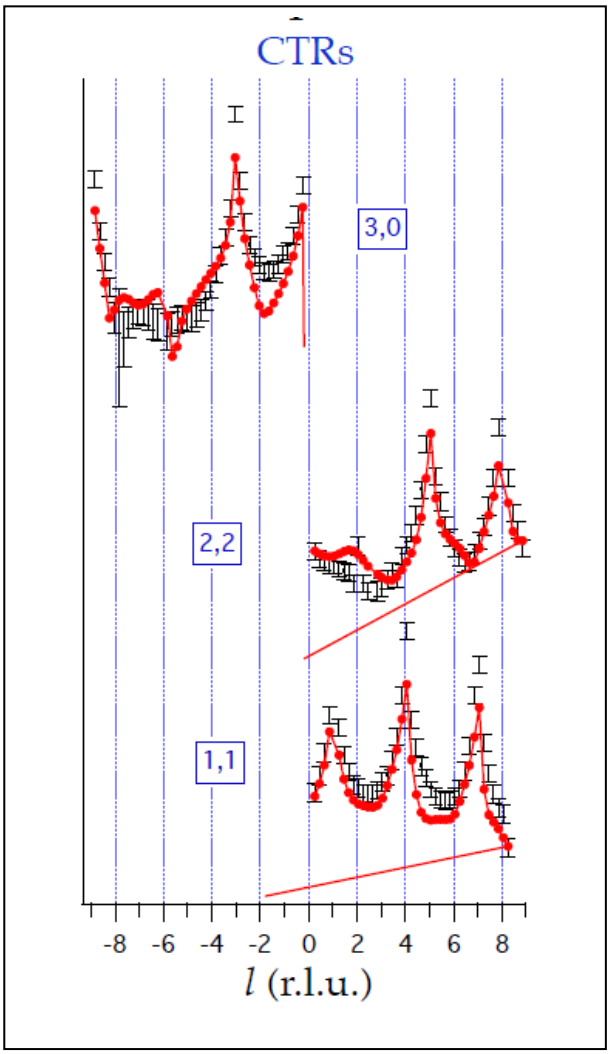

Fig.1 Example of the level of accuracy reached in the fit so far (only CTRs are shown), corresponding to a total chi2 of 2.3.