ESRF	**In situ GIXD study of the displacement field induced by steps on vicinal Si surfaces**	**Experiment number**: Si-1863
Beamline: ID3	**Date of experiment**: from: 8 April 2009 to: 14 April 2009	**Date of report**: 05/03/2010
Shifts: 21	**Local contact(s)**: Dr Roberto Felici (felici@esrf.fr)	*Received at ESRF:*

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High index Si surfaces are of strong interest both for fundamental and technological reasons. It has been shown that the surface morphology of vicinal Si surfaces can undergo huge transformations into ordered hill and valley structures with periods ranging from several nanometers [1] to microns [2]. Uniformly spaced step structures at surfaces could have applications for instance for the fabrication of 1D metallic nanowires or stripes. In particular Si(7 7 10) surfaces have attracted much attention due to the long range periodicity of the step network [3]. A complete understanding of this ordering necessitates having a better knowledge of the step-step elastic interactions. Indeed, due to the reduced coordination of the atoms at the step edges, elastic distortions propagate into the bulk and give rise to an overlap of the displacement fields between neighbouring steps. This overlap is the reason why steps interact elastically. Since the seminal work of Marchenko [4] it is known that this displacement field can be calculated by modelling the steps by a linear distribution of localised forces. Our goal in this experiment was to extract the force distribution at the step edges of several vicinal Si surfaces (with an emphasis on Si(7 7 10)) by Grazing Incidence X-ray Diffraction (GIXD) [5].

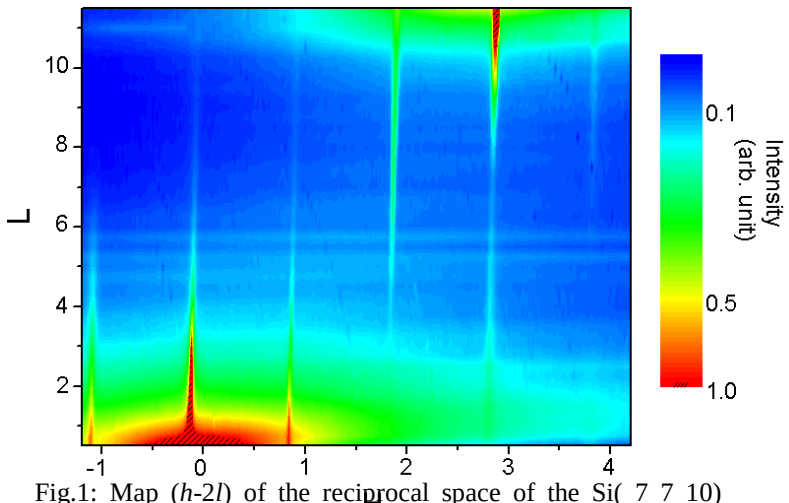

Fig.1: Map (*h*-2*l*) of the reciprocal space of the Si(7 7 10) surface. The elongated scattering rods are the signature of a well-ordered surface.

In this report we show that we have been able to measure accurately the elastic displacement field of the Si(7 7 10) surface. This surface exhibits a step bunching instability crossing the 1x1→7x7 surface phase transition temperature (860°C): monoatomic steps bunch together into a triple step organization with a high degree of order [3]. Fig.1 displays a map of the reciprocal space showing elongated Crystal Truncation Rods (CTR) revealing the long range order of steps.

The x-ray experiments were performed with 18 keV photons. We have measured quantitatively the intensity along the (1-2 *l*), (0-2 *l*), (-1-2 *l*), (2-2 *l*), (-6-1 *l*), (-7-1 *l*), (-8-1 *l*), (-9-1 *l*),(-10-1 *l*), (-6-3 *l*), (-7-3 *l*), (-8-3 *l*), (-11-1 *l*), (-6-5 *l*), (-7-5 *l*), (-8-5 *l*), (0-4 *l*) CTRs. Moreover we measured additional in-plane fractional high order spots to fit the complex Si(7 7 10) surface structure. The

integrated intensities were collected by rocking scans and corrected using the procedure reported in Ref. [6].

Using the proposed structure by Teys and coworkers [7], the surface structure and surface relaxations have been first systematically studied choosing different initial atomic positions. Then the elastic relaxations induced by step edges have been incorporated into the model. For the best fit we have a good agreement with the experiment. More importantly, the signature of elastic relaxations is clearly put in evidenced for instance at *l*=6 of (-1-6 *l*) CTR (see Fig. 2). As discussed in Ref. [8], the fast variation at such reciprocal lattice coordinate cannot be related to the relaxation of the sole surface atoms. It is related to elastic relaxations penetrating deep into the bulk. First results are encouraging but the amplitude, position and orientation of the dipole force moment at the step edges have still to be studied more quantitatively.

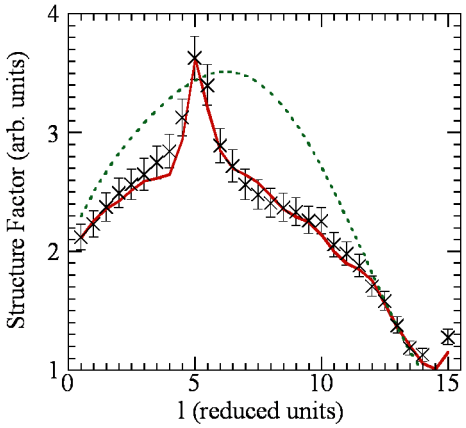

Fig. 2: Structure factor of (-1 -6 *l*) CTR (×) and best fit adding a line force dipole (—) and without force dipole (---).

In complement to these GIXD measurements, we studied by GISAXS the kinetics of the triple-step ordering at the 1x1→7x7 surface phase transition temperature. The long range order of the triple-step structure is reversible crossing 860°C (see Fig. 3). We have also been able to observe that different surface structures can be stabilized depending on the exact preparation conditions we used. In particular the triple-step structure (5.8 nm period) is stabilized by annealing the sample close to the 1x1→7x7 surface phase transition temperature whereas a high temperature flash and a fast cooling give rise to a shorter periodic structure (3.7 nm). The triple-step organization has been quantitatively characterized by GISAXS rocking the surface by steps of 0.2° over ±4° around the step edge orientation (see Fig. 4). These measurements will be compared with GISAXS simulations made with the IsGISAXS software [9] in order to extract the exact step organization inside the triple-step structure. These results will be compared with the model of the surface structure deduced from GIXD measurements. This work is in progress.

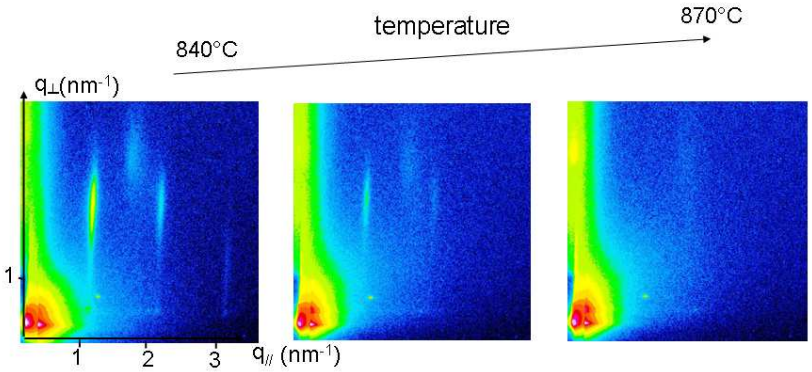

Fig. 3: Evolution of GISAXS patterns as function of temperature. Below 860°C intense scattering rods show a long range ordering of steps at the surface whereas at higher temperature, no organization is visible.

In conclusion this campaign of experiment has been successful even though we did not have time to study the other vicinal Si surfaces we planned, e.g. Si(1 1 11) and Si(105). Therefore a more complete set of data with different vicinal Si surfaces is still necessary to a have a detailed picture of the step interaction energetic at Si surfaces.

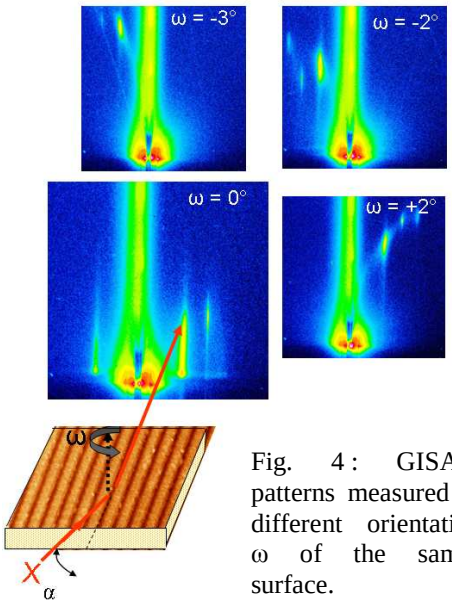

Fig. 4 : GISAXS patterns measured for different orientations ω of the sample surface.

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