

# Report on experiment 32-03- 707: in-situ study of the SrTiO<sub>3</sub>/Si system

## Purpose of the experiment :

This experiment was aimed at :

-studying the early stages of the growth of STO/Si by means on surface diffraction, and obtain state of the art information on the structure of the x2 and x3 SrSi reconstructions used for Si surface passivation.

-understanding the formation of two phased during the early stages, and conclude on the possible ferroelectric behavior of these phases

## Methodology :

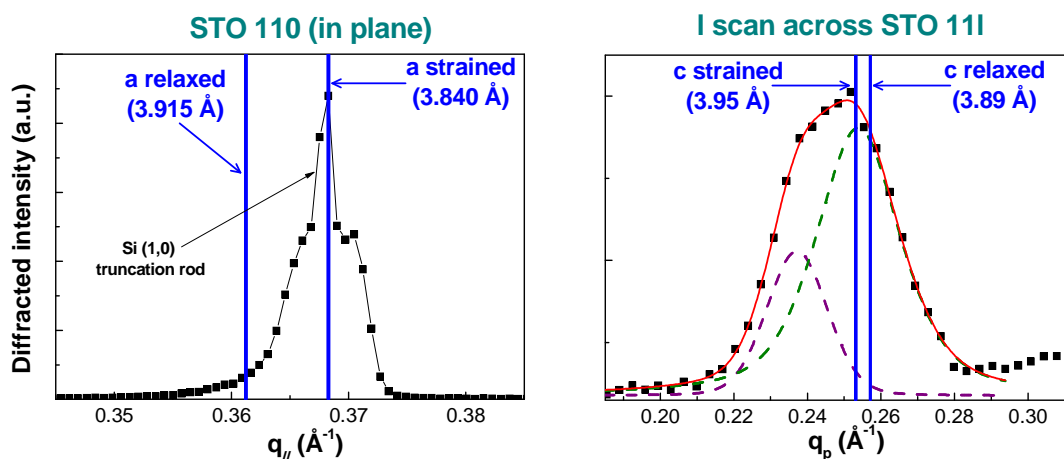
For studying the SrSi reconstructions, Sr was deposited on a bare and clean Si surface following the procedure commonly used prior STO growth. Diffraction signal from the SrSi reconstructions was recorded, and the results (truncation rod profiles) will be fitted and compared with ab-initio calculated surface models

In- and out-of plane diffraction was used to measure the lattice parameters of 3 and 7 monolayer thick STO/Si layers as well as their evolution during annealing under vacuum and under different oxygen partial pressures.

## Preliminary results :

The study of the SrSi reconstructions has just started, and is still under progress. Once truncation rod profiles will be extracted, they will be compared to existing and home-calculated atomistic surface models

The study of the two STO phases is still under progress. It has already shown that for 3 monolayer thick films, two STO phases are present and that they are boss strained on Si, thus contradicting the interpretation published by Schlom et al that one of the two STO phases is formed during plastic relaxation.



These experiments also clearly that one of the two STO phases is standard cubic STO, fully strained up to at least 3 ML, and that the other phase is also cubic, and formed due to deficient oxidation conditions. In the end, STO is not ferroelectric as shown by our temperature dependent lattice parameter measurements

Expected results :

These experiments should allow for concluding on :

- the detailed atomistic structure au the SrSi passivation layer deposited prior to STO growth
- the space group of the O-deficient STO phase (using diffraction extinction rules) and the origin of its formation