

[o.m8.p7] Electron density topological analysis of silicon surfaces. The case of Si(100)(1x1):H and Si(100)(2x1):H. F. Cargnoni, C. Gatti, *Dipartimento di Chimica Fisica ed Elettrochimica, Università degli studi di Milano and Centro CNR per lo Studio delle Relazioni tra Struttura e Reattività Chimica, via Golgi 19, 20133 Milano (Italy).*

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Surfaces and interfaces of semiconductors play a fundamental role in many technologically important device applications. Passivation of silicon surfaces with H provides long-term protection against oxidation and adsorption of impurities.[1] The H-exposure of Ultra High Vacuum (100) cleaved Si leads to different structures of the H-covered surface as a function of H- exposure and of adsorption/annealing temperature.[1] The Si(100)(1x1):H and Si(100)(2x1):H structures have been extensively investigated [1]-[2], representing both the basic ideal models for the mono- or dihydride phases and the building blocks for the more complex (3x1) reconstruction.[1] In the monohydride (MH) phase, the symmetric Si-Si dimers of the nominally flat Si(100)(2x1) surface are preserved and the dangling bonds (DB) –one on each surface atom – are capped by H. Instead, in the dihydride (DH) phase, the dimer bonds are broken and the two DB on each surface atom are capped with H, leading to a (1x1) structure.

As in our previous investigation [3] on Si(111) clean and H-covered surfaces, we have studied the two basic H-terminated Si(100) phases using a slab model for the surfaces and fully-periodic first-principles calculations. The most relevant geometrical parameters were optimized and the electron density of each energy-optimized structure topologically analyzed according to the Quantum Theory of Atoms in Molecules [4]. The following points have been addressed:

- the diverse nature of H-H lateral interactions in the two phases, providing a rationale for the alternating rows of mono- and dihydrides observed in the (3x1) structure and for the lack of a pure DH phase;
- the nature of the dimer bond in the MH phase;
- how the bonds between surface Si and "bulk" Si atoms are affected by preserving (MH phase) or breaking (DH phase) the dimer bonds;
- which charge transfers take place in the top few atomic layers, in the two phases.

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[o.m8.p8] Surface Structure of SrTiO₃. S. Harkema, G.J. van Hummel, D.H.A. Blank, A.J.H.M. Rijnders, H. Rogalla, *Low Temperature Division, Dept. of Applied Physics and MESA⁺ Research Institute, University of Twente, POB 217, 7500AE Enschede, The Netherlands.*

Keywords: surface crystallography.

Strontium Titanate is an important substrate for layer by layer growth of oxidic materials like high T_c superconductors, ferroelectrics etc. An important issue in the growth studies is the termination of the substrate as well as that of the deposited layers.

The termination of the SrTiO₃ surface is normally a mixed one: part of the surface is terminated by TiO₂ planes, the other part is terminated by SrO planes. AFM scans reveal half unit cell steps in this case.

In our laboratory a method has been developed^[1] to prepare singly terminated SrTiO₃ surfaces with unit cell steps.

The structure of these (most likely Ti-terminated) surfaces has been studied by synchrotron X-ray scattering (ESRF beamline ID3)

A number of crystal truncation rods have been measured with good reproducibility. The measured data have been fitted with the ROD program^[2].

First results show an oxygen deficiency and small displacements of the heavy atoms in the topmost layers.

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