Task B-1

Investigation of Oxidation of H_x-Si Using Scanning Tunneling Microscopy and Infrared Spectroscopy

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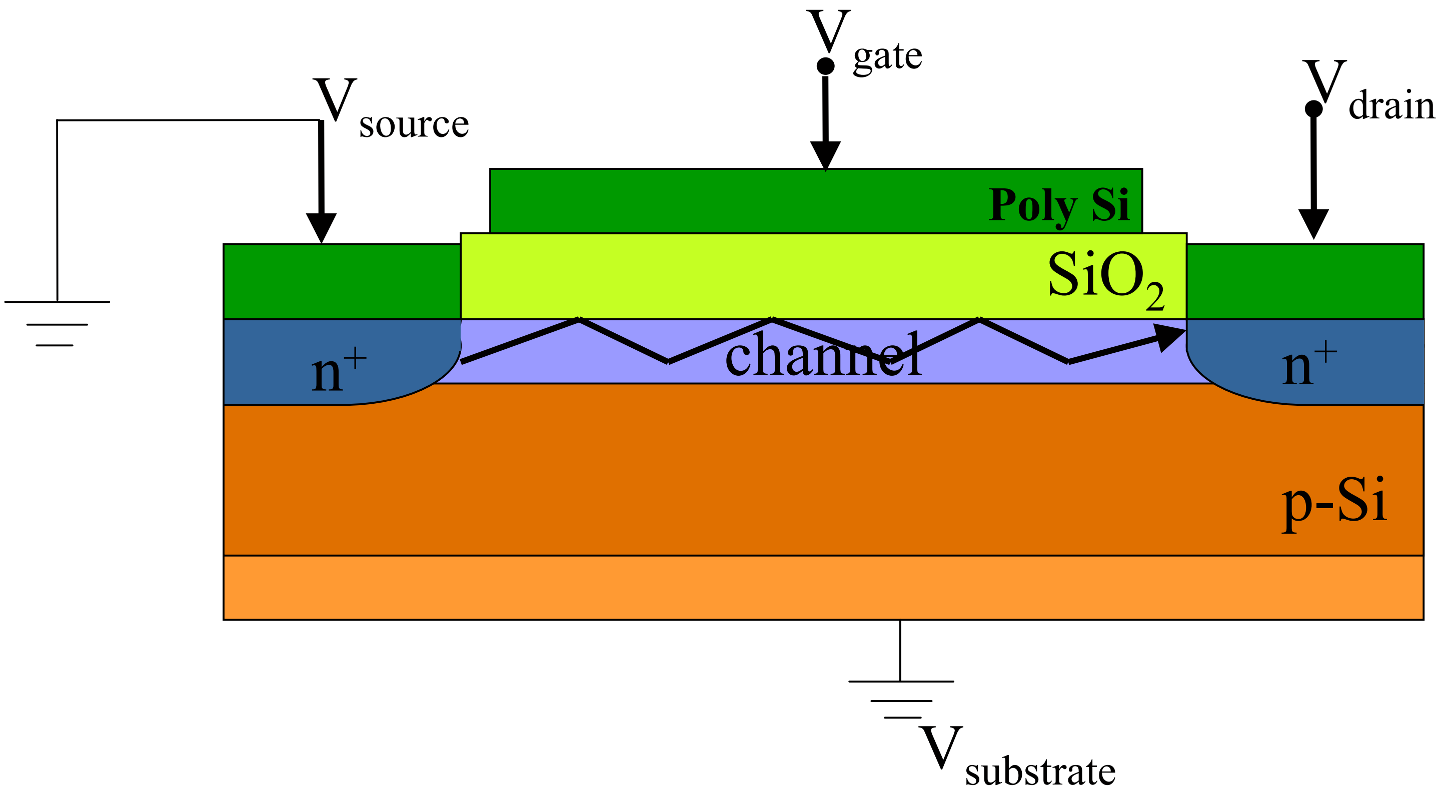
Stanford University, 01/07/00

Motivation

- **Use of H-terminated Si as a precursor surface for growing high quality ultra thin gate oxide**



Motivation: Current Understanding of Oxidation of H-Si

- **Known**: H_x-Si is stable in the presence of O_2 in the gas phase
- **Conditions that promote oxidation**:
  - water
  - UV light (350nm)
  - highly doped n^+ substrate
- **Not well understood**: Kinetics of these oxidation processes

Understanding these processes may be crucial for growing tomorrow's high quality ultra thin gate oxides (>20Å).

Key Questions in Oxidation

- **For a given set of conditions:**
  - **Where** does the **oxide** initially nucleate?
  - **What** is the **rate** of oxidation?
  - **What** is the **mechanism** of oxidation?

Silicon Surface

Complication:

H_x-Si(100)

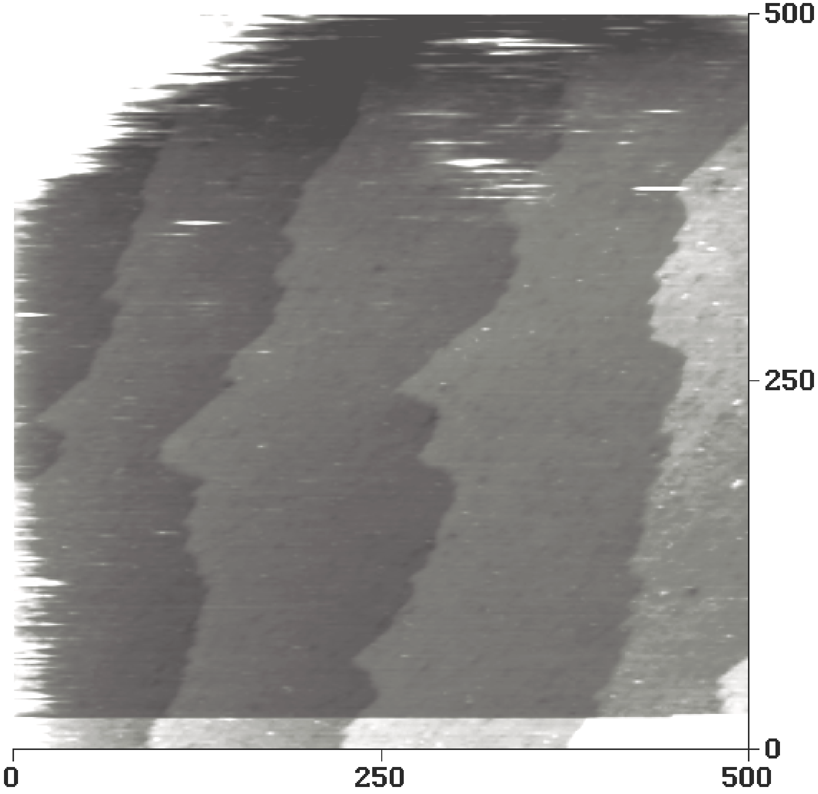
- Surface of current technological relevance is rough

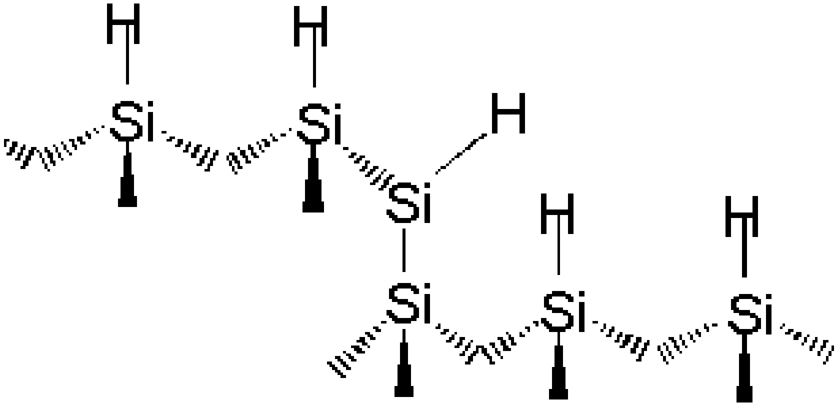
Simplification:

Model Surfaces

- H-Si(111)(1X1) is predominantly perpendicular monohydride.
- H-Si(100)(2X1) is predominantly tilted monohydride.

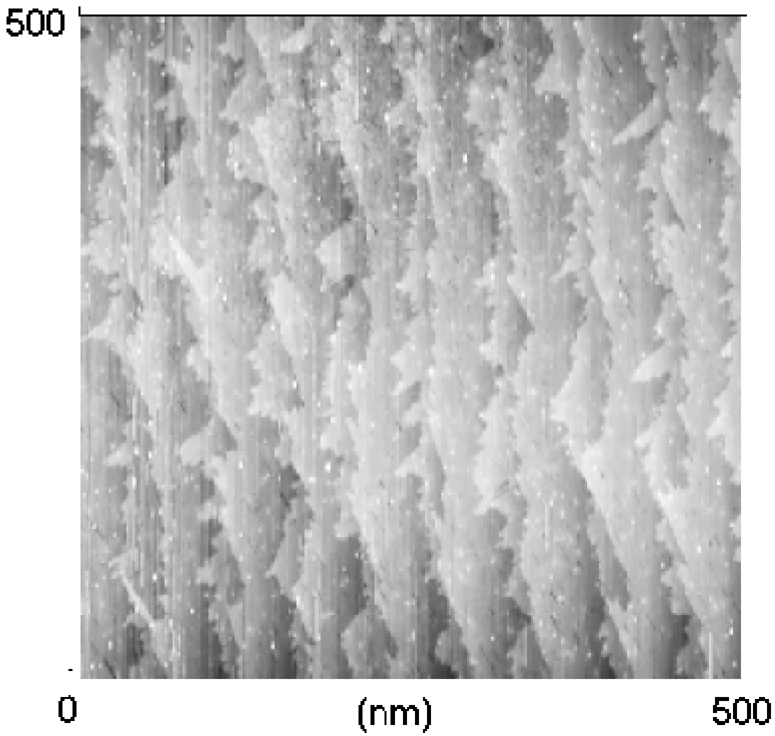
Model Surface: H-Si(111)(1X1)

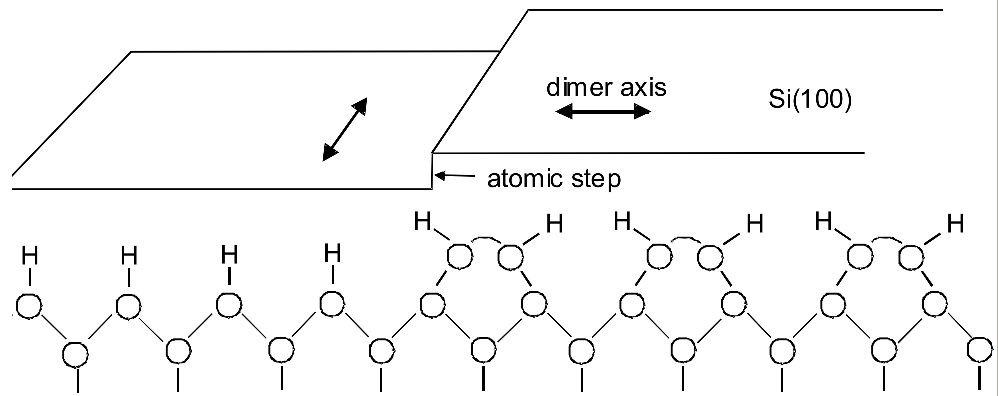




K.Morse, Stanford University, 1999.

Model Surface: H-Si(100)(2X1)



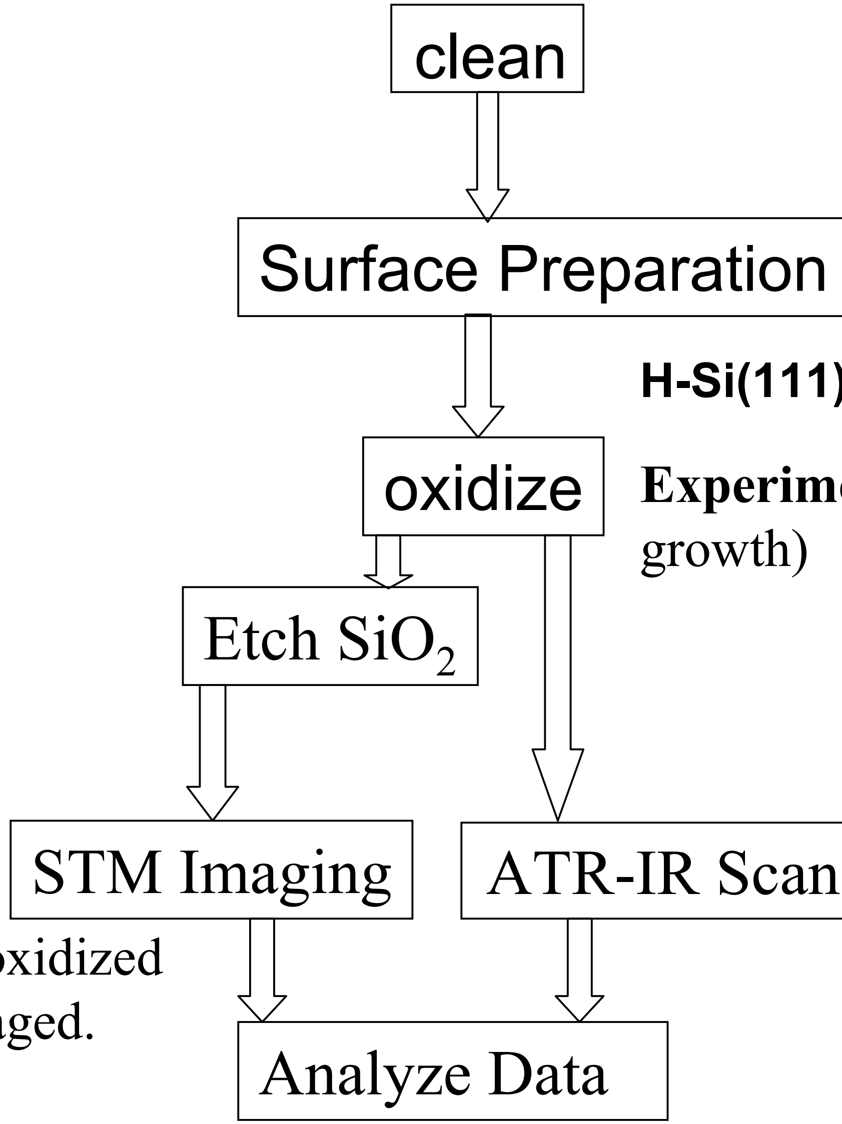


Luo, H., *Thesis*, Stanford University, 1998.

Previous Accomplishments in Research of Oxidation

- T. Yasaka and coworkers observed a dependence of **aqueous oxidation** rate on **dopant type** and on **dopant concentration**.
  (T. Yasaka, et. al, *IEICE Trans. Electron*, Vol. E75-C, No.7, July 1992.)
- C. Wade observed the relationship between [$\mathbf{O_2}$] and density of pits formed on H-Si(111) in **aqueous** fluoride **solutions** using STM.
- H. Luo observed the dependence of etching time of H-Si(111) on [$\mathbf{O_2}$] in **aqueous** fluoride **solution** using ATR-IR. No dependence observed for H_x-Si(100).
- M. Linford observed the relationship between **gas phase oxidation** of H-Si(111) and exposure to a critical wavelength of **UV light** using ATR-IR.
- B. Stefanov, Y.Chabal and coworkers observed intermediate structures in the **$\mathbf{H_2O}$ induced oxidation** of Si(100)(2X1).
  (B.B. Stefanov, et. al, *Physics Review Letters*, Vol. 81, No.18, 3908-3911, 1998)

Procedure for Analyzing H-Si



H-Si(111)(1X1) or **H-Si(100)(2X1)**

Experiment (sub-monolayer oxide growth)

Negative of oxidized surface is imaged.

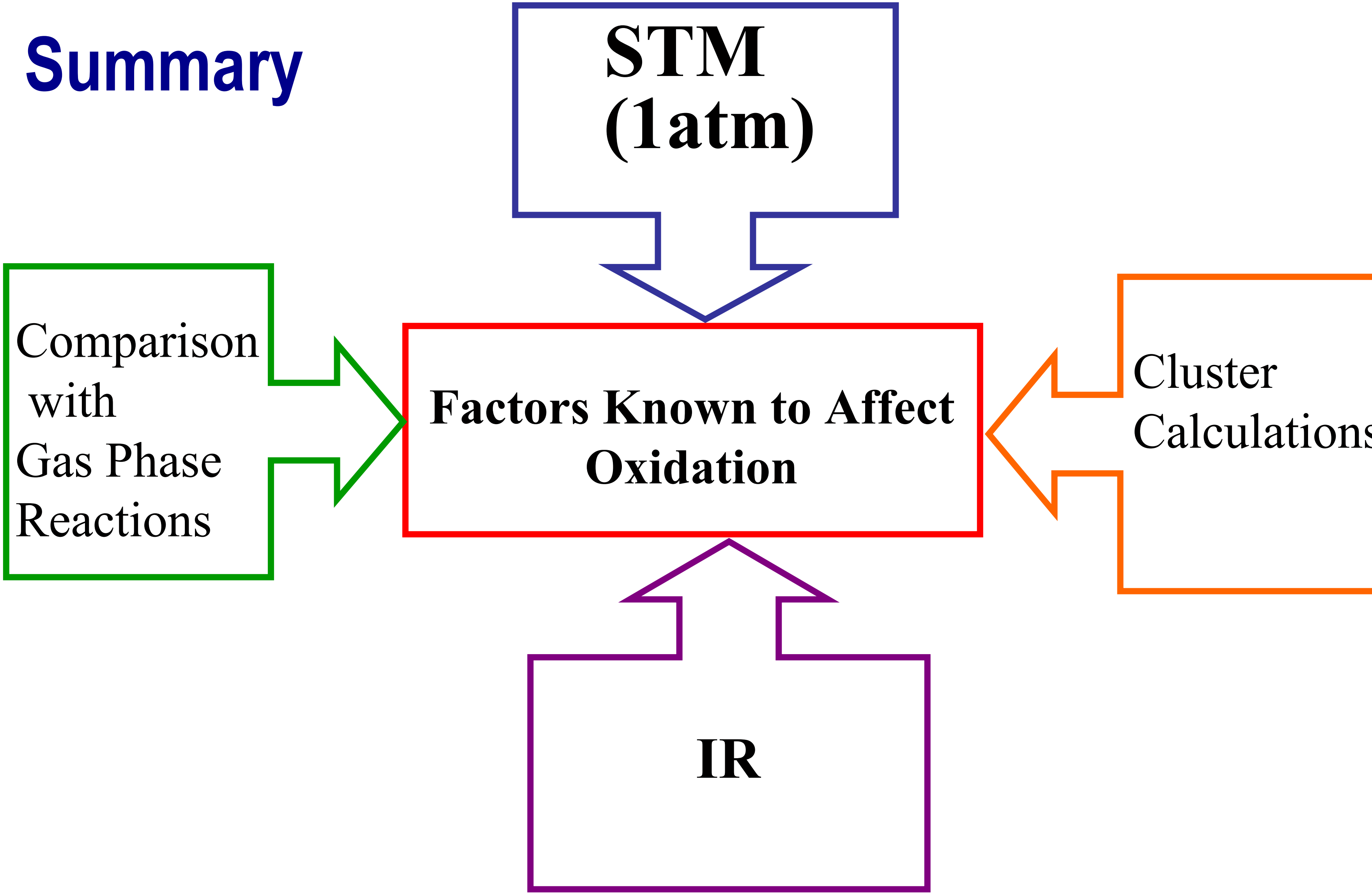
Short Term Research Plan: Investigate Factor known to Affect Oxidation

- **Observe changes in morphology and structure of model surface H-Si(111)(1X1) and H-Si(100)(2X1) using STM and ATR-IR for each of the following:**
  - **dopant type**
  - **dopant concentration**
  - **humidity**
  - **UV light (350nm)**

Long Term Research Plan

- Investigate Oxygen insertion mechanism for H-Si(111)(1X1) in O_2
  - **C. Chatgilialoglu proposed mechanism**
- After investigating factors affecting oxidation, propose possible mechanisms to explain the oxidation behavior.

Summary


STM
(1atm)
Comparison
with
Gas Phase
Reactions
Factors Known to Affect
Oxidation
Cluster
Calculations
IR