

# Kinetic Monte Carlo Technique in the MultiScale modeling of Micro/Nanotechnologies :

## Thermal silicon oxidation

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# Outline

- **Monte Carlo Basics**
- **Kinetic Monte Carlo**
- **KMC in MultiScale modelling**
- **How to build a KMC model**

- **Silicon oxidation**
- **Oxidation modelling and KMC approach**
- **What makes oxidation/KMC difficult**
- **Two examples:**
  - ✓ **Dry thermal oxidation growth –  $O_2/Si(100)$**
  - ✓ **Incorporation of oxygen atoms into Silicon surface under wet ambient –  $H_2O/Si(100)$**

- **Conclusions et perspectives**
  - ✓ **Towards CAD tools for the engineer – Monte Carlo / Continuum relationship**

# General nature of Monte Carlo Methods

## What is Monte Carlo ?

Simulation that uses random numbers to solve a given problem  
≡ Stochastic simulation procedure

This problem may be

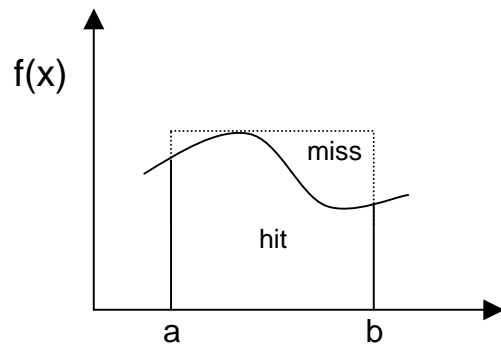
**probabilistic** => random numbers reproduce directly the physical process  
data analysis, statistics ...

**deterministic** => integral determination (high-dimensional integrals...)

# Monte Carlo: Brief history

Although the name of Monte Carlo is relatively recent (1949), roots are deep installed in the 19<sup>th</sup> century (statistical sampling)

- Method for estimating integrals



Sampling method

$$A = (b-a)/N \cdot \sum_{j=1}^N f(x_j)$$

Hit-and-miss method

$$A = A_{\text{ext.}} \cdot N_{\text{hit}} / (N_{\text{hit}} + N_{\text{miss}})$$

Importance sampling...

- Boost by the 2<sup>nd</sup> world war, named « Monte Carlo » for the first time (1949)

- ✓ 1947, neutron transport in the hydrogen bomb calculation

- ✓ 1949, first conference on the subject in Los Alamos

- ✓ 1953 Metropolis algorithm

- ✓ 1975 BKL algorithm

# Monte Carlo techniques used in physics

=> Monte Carlo terminology is extremely wide with overlaps

- Metropolis MC - algorithm that determines whether a process should happen or not
- Thermodynamics MC - thermodynamics quantities
- Lattice MC - MC through lattice based method
- Kinetic Monte Carlo > can be LKMC - time evolution of a system
- Quantum Monte Carlo - electronic structure calculation
- ...

# Monte Carlo techniques used in physics

## Recommendation

Always specify what kind of Monte Carlo method you use

+

Always describe how the method is implemented and/or  
where it is used in the simulation procedure

# Equilibrium Monte Carlo

**Metropolis = random walks probing phase space**

**Considering the transition from state**

$$\mathbf{a} = \{x_1, \dots, x_i, \dots, x_N\} \text{ to state } \mathbf{b} = \{x_1, \dots, x_i', \dots, x_N\}$$

**accompanied with a change  $\Delta E = E_b - E_a$  in energy**

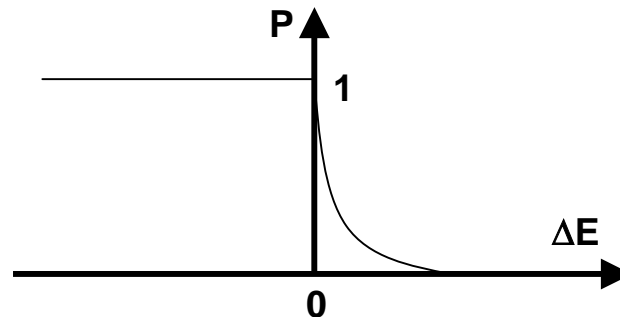
**If  $\Delta E \leq 0$ , the transition is accepted**

**If  $\Delta E > 0$ , a uniform random number  $z \in [0,1]$  is chosen,**

**if  $z < \exp(-\Delta E/k_B T)$  the transition is accepted**

**if  $z > \exp(-\Delta E/k_B T)$  the transition is rejected**

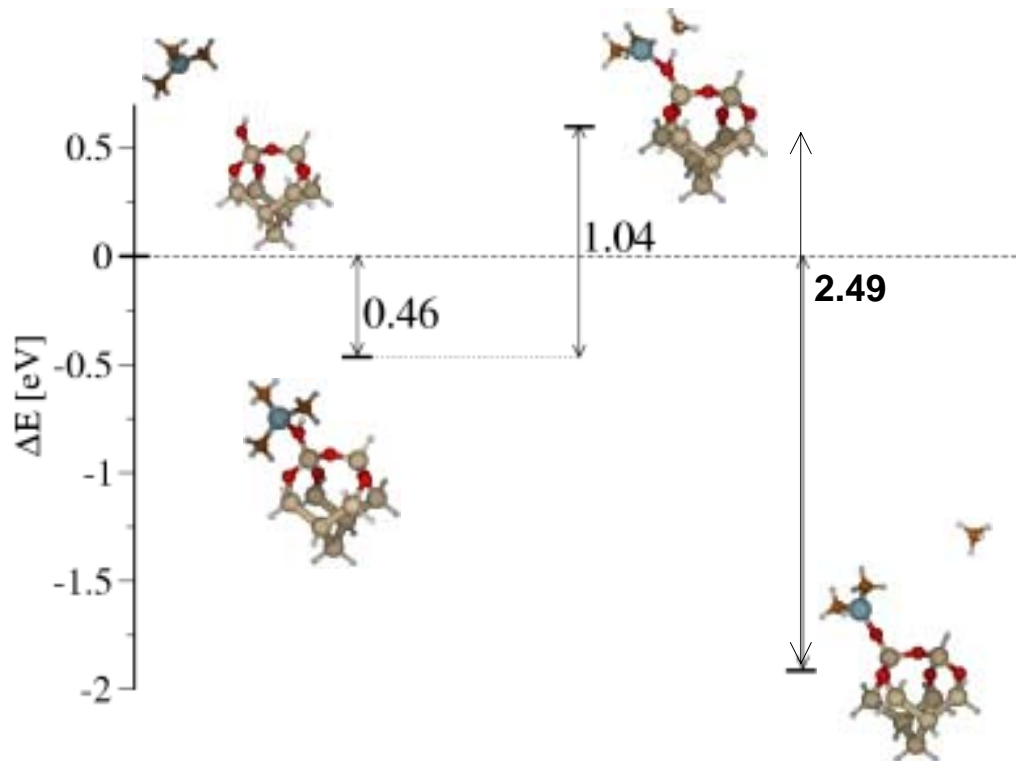
$$P(\mathbf{a} \rightarrow \mathbf{b}) = \min [1, \exp(-\Delta E/k_B T)]$$



# Kinetic Monte Carlo 1

Or how to reach the experimental time scale, the simulation of an actual experiment

Experiment = sequences of activated processes



E is not relevant, only  $\Delta E$  is

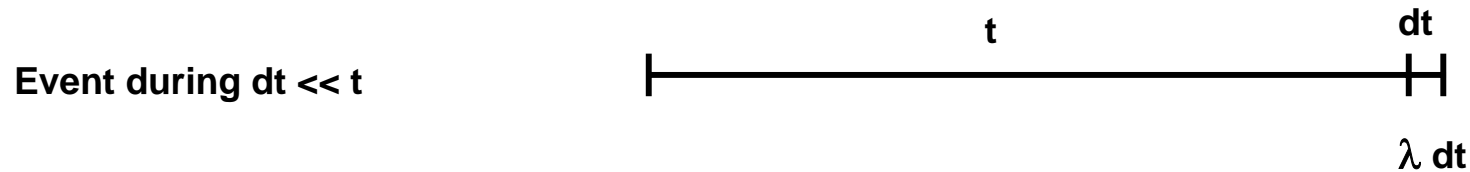
The Jump probability follows a Boltzmann distribution  
Therefore the event frequency = 1 to 100fs

# Kinetic Monte Carlo

The **hopping rate** at which an isolated is related to the activation barrier  $\Delta E$  by the **Arrhenius law**:  $\lambda = \nu \cdot \exp(-\Delta E/k_B T)$

$\nu$  is the attempt frequency

**Time dependence ? – Poisson process**



Probability of having an event between  $t$  and  $t+dt$ :  $P_c = \lambda \cdot dt \cdot \exp(-\lambda t)$

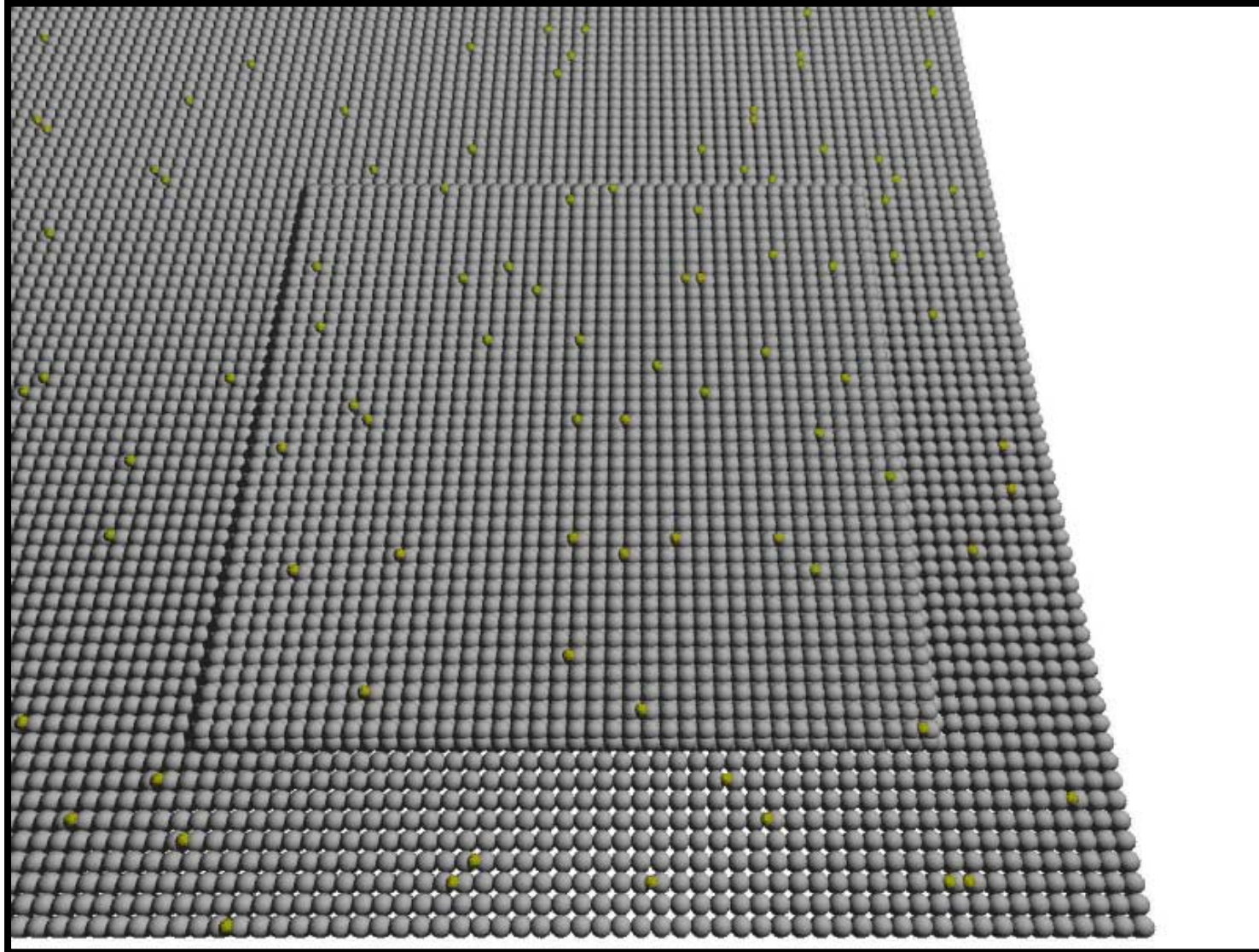
Mapping of the probability function through Monte Carlo sampling

$$\int_0^t \exp(-\lambda u) \cdot \lambda \cdot du = \int_0^z dz \quad \text{ou} \quad \int_z^1 dz$$

$$\Delta t = -(1/\lambda) \cdot \log(z) \quad \text{or} \quad \Delta t = -(1/\lambda) \cdot \log(1-z)$$

# Kinetic Monte Carlo:

## Formation of mismatch dislocation at the mesa step edges



GaSb on  
(001) GaAs  
 $\varepsilon=14\%$ ,  
 $T=700\text{K}$ ,  
 $J=2\text{ML/s}$ ,  
40x40 mesa.

# Kinetic Monte Carlo

## Advantages

- Relation to the experimental procedure
- No requirement of thermodynamic equilibrium in the algorithm
- Non preservation of the objects
- time follows mechanism changes...flexibility

## Disadvantages

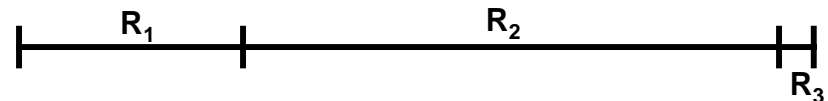
- Mechanisms and associated activation barriers have to be known in advance
- Much effort in an efficient coding of the mechanisms, data structures etc...forget transferability
- The Arrhenius law may not be fully adequate, for instance when kinetic energy is accumulated when crossing a barrier and can be used to cross other barriers  
= *transient mobility*

# Kinetic Monte Carlo

## Basic Bortz-Kalos-Liebowitz (BKL) algorithm

### *Sampling of the event*

1. Time  $t=0$
2. Establish a list of all possible transition states and calculate the cumulative function  $R_i = \sum_{j=1}^i \lambda_j$  for  $i=1, \dots, N$  total number of transitions
3. Get a uniform random number
4. Find the event by finding out the  $i$   $R_{i-1} < uR \leq R_i$
5. Occurrence of the event  $i$
6. Find all transitions and associated rates  $r$  that have changed
7. Get a uniform random number  $z = ]0,1]$
8. Update the time with  $t = t + \Delta t$  where  $\Delta t = -\log z / R$
9. Return to step 2



# Kinetic Monte Carlo

## Alternative algorithm

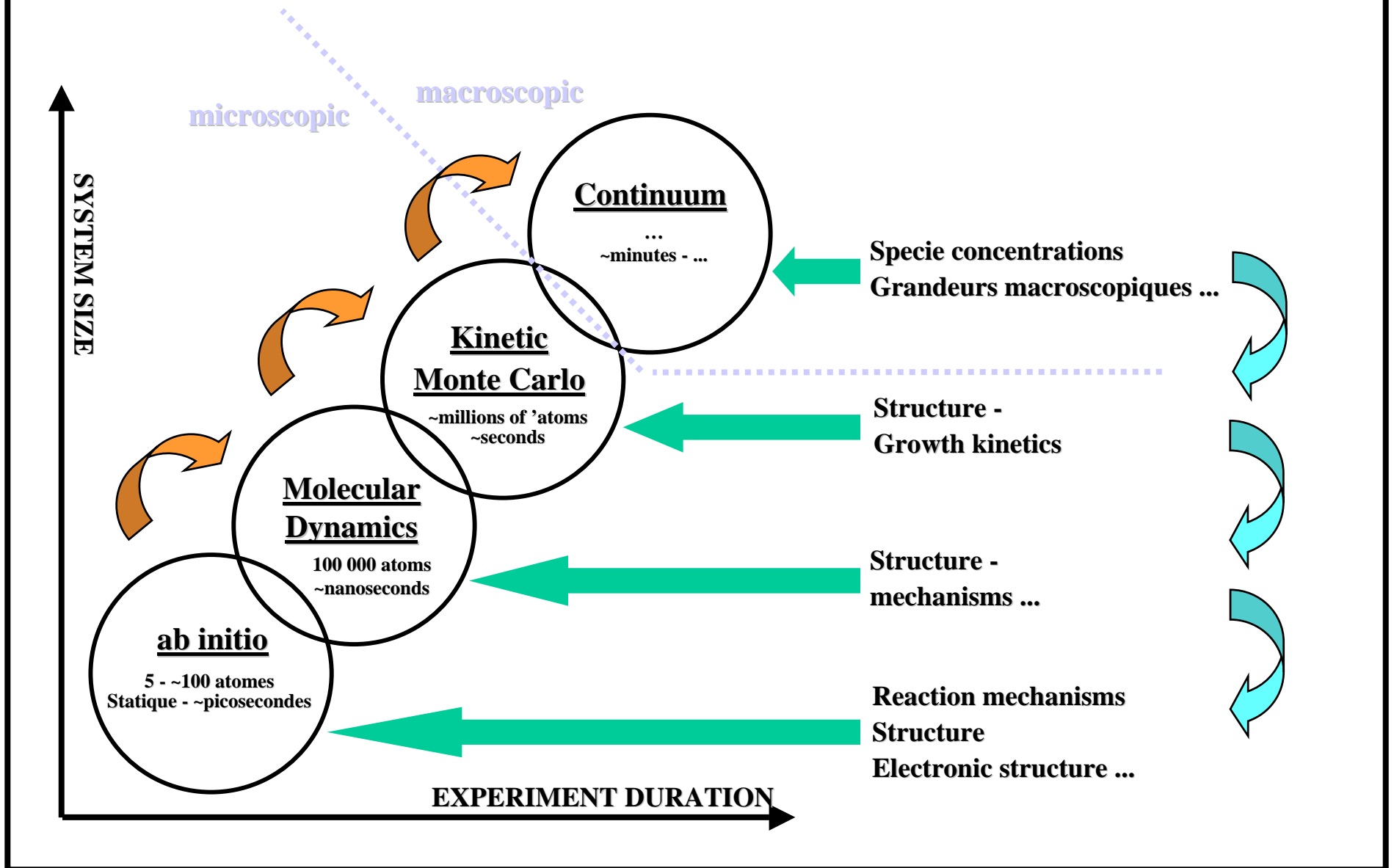
### *Sampling of time*

1. Time  $t=0$
2. Form a list of all possible transition states and calculate all possible rates
3. Schedule these transitions for all system sites
4. Choose the time minimum
5. Carry out the associated (site, event  $i$ )
6. Update the time with  $t = t + \Delta t$  where  $\Delta t = -\log(z) / \lambda_i$
7. Change the rate of all sites that have been modified due to event  $i$
8. Update the scheduler
9. Return to step 2

Main difference = this last algorithm authorizes a systematic change of the doublet (mechanism, activation barrier).

BKL => the event must be fully predefine

# Tools for materials design



# Kinetic Monte Carlo fields of application

- **Surface diffusion**
- **Molecular Beam Epitaxy growth (MBE)**
- **Chemical Vapor Deposition (CVD)**
- **Defects formation and diffusion, dislocation motion (...under irradiation)**
- **Oxidation (thermal growth, Atomic Layer Deposition techniques)**
- **...**

# Technical workplan

## What has to be built in concrete

### Lattice description

#### Periodic Boundary Conditions

(0,0)	(n,0)	(0,0)	(n,0)
(0,n)	(n,n)	(0,n)	(n,n)
(0,0)	(n,0)	(0,0)	(n,0)
(0,n)	(n,n)	(0,n)	(n,n)

### Writing of configuration

describe the chemical nature of each site of the grid

### Temporal dynamics

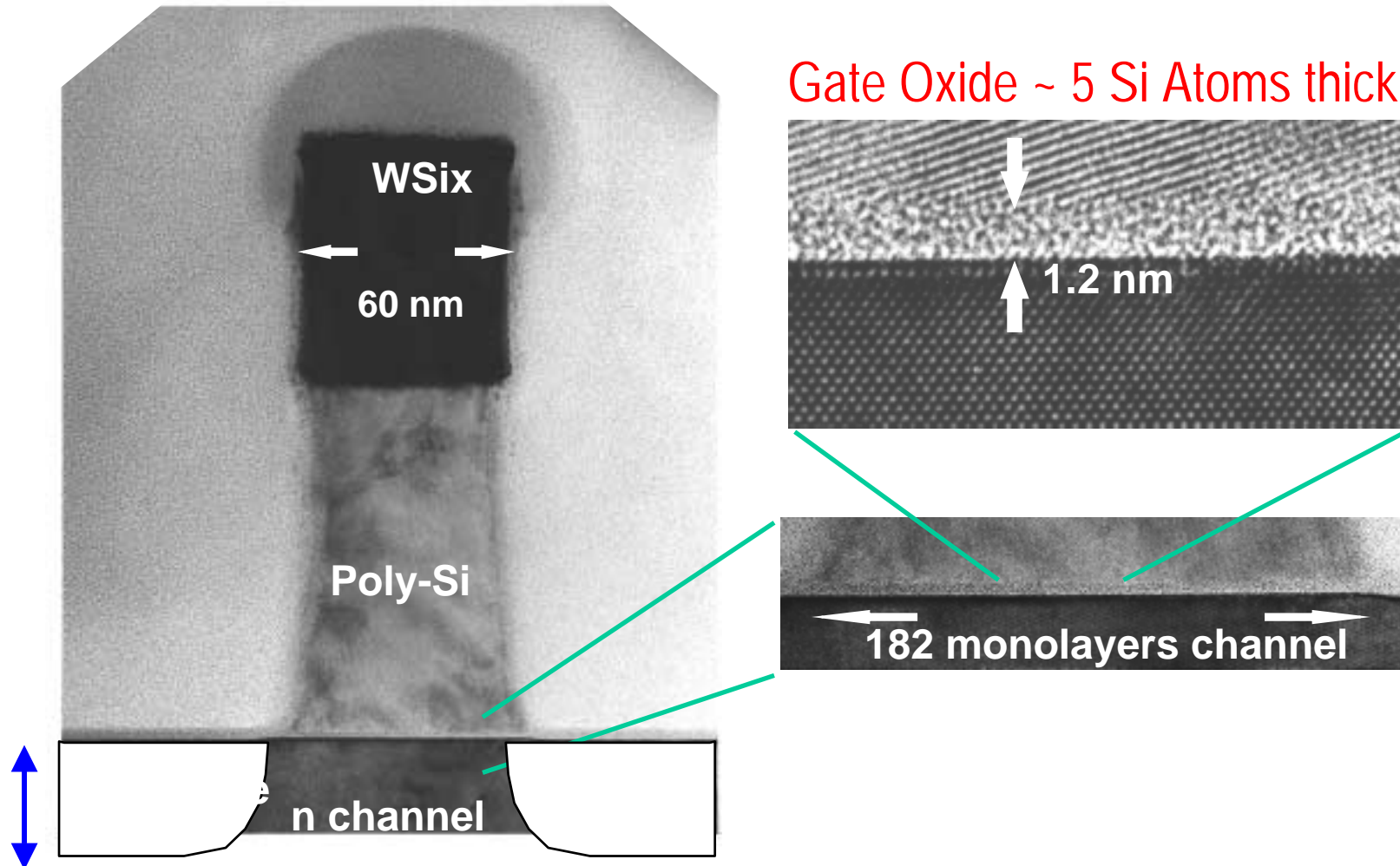
Function of the experimental procedure

### List of mechanisms

All pertinent mechanisms and associated activation energies, charge transfer, stress ....

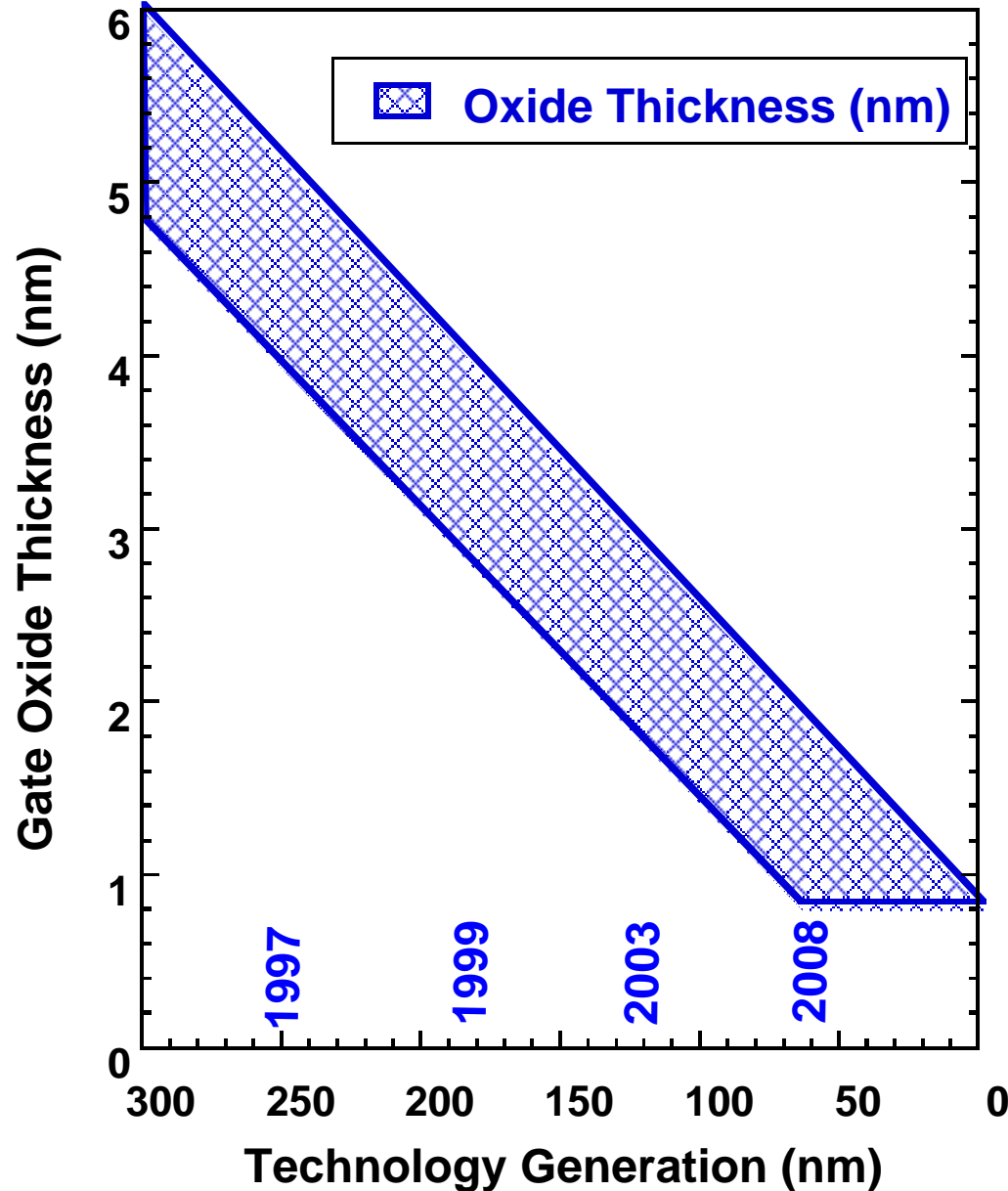
# Scaling limits to CMOS Technology

(For proper operation, all vertical and lateral dimensions scale simultaneously)



Shrinking the junction depth → increasing the carrier concentration

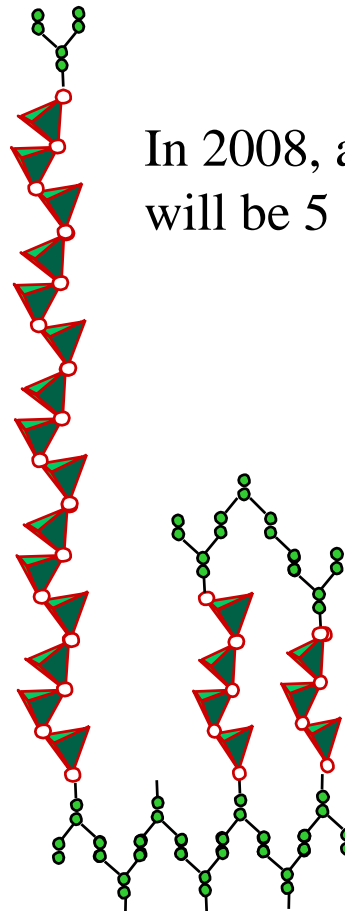
# Gate oxide: Roadmap



In 1997, a gate oxide was 20 silicon atoms thick.



In 2008, a gate oxide will be 5 silicon atoms thick.

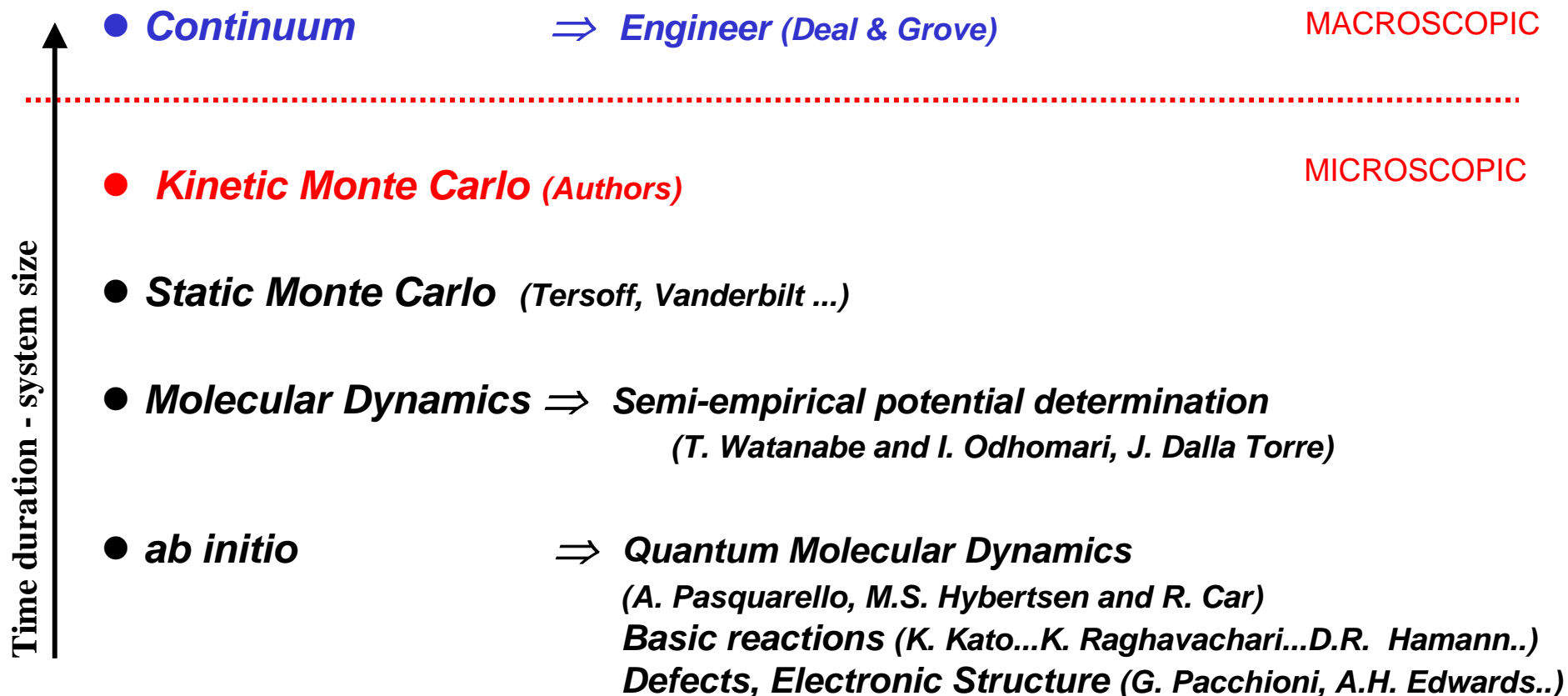


and at least 2 of those 5 atoms will be at the interfaces.

# Objectives

- **Development of a new generation of simulation tools for the nanometric scale technologies**
  - control and prediction of technological process at the atomic scale
  - Oxidation case = oxidation of the first silicon monolayers or growth – kinetics and structuring
- *Towards alternative High-k oxides (higher dielectric constant)*
  - $Al_2O_3$ ,  $ZrO_2$ ,  $HfO_2$ ...
  - *Formation of an interfacial silicon oxide: high-k/SiO<sub>2</sub>/Si*  
  
= what is the interface structure (experimental procedure dependent)

# State of the Art Methodology and tools



*Mixed methodologies: Static Monte Carlo then ab initio (D. Vanderbilt)*

## **Ex.I: Thermal oxidation growth $\text{SiO}_2/\text{Si}(100)$ via a Kinetic Monte Carlo technique**

How to build a KMC model in the frame of silicon thermal oxidation

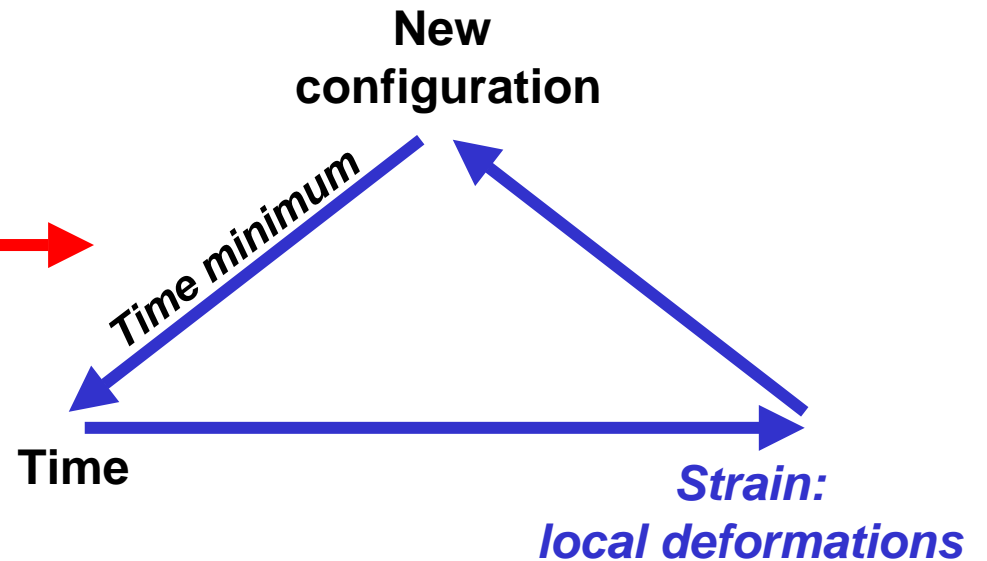
- **Monte Carlo Procedure – specific problems for the KMC model**
- **Crystallographic data**
- **Literature data**
- **Quantum calculation**
- **List of mechanisms for the KMC approach**
- **Results and discussion**

# Kinetic Monte Carlo

Time duration for each event  
 $t = (-1/\lambda) \cdot \ln(z)$   
 $\lambda = v \cdot \exp(-E/kT)$

events:

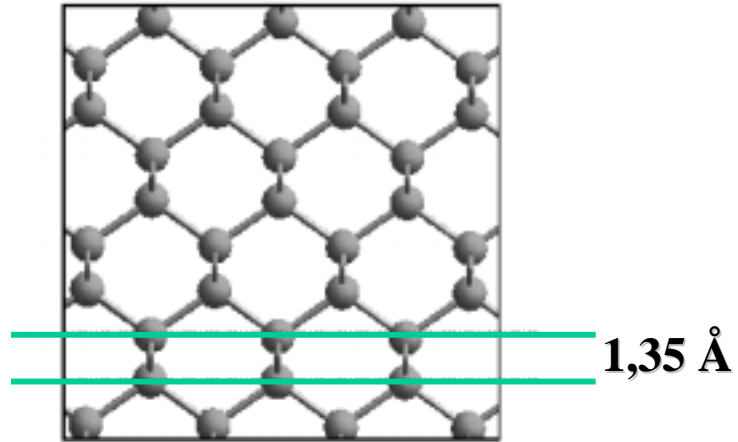
$E_1$   
 $E_2$   
.  
.  
.  
 $E_n$



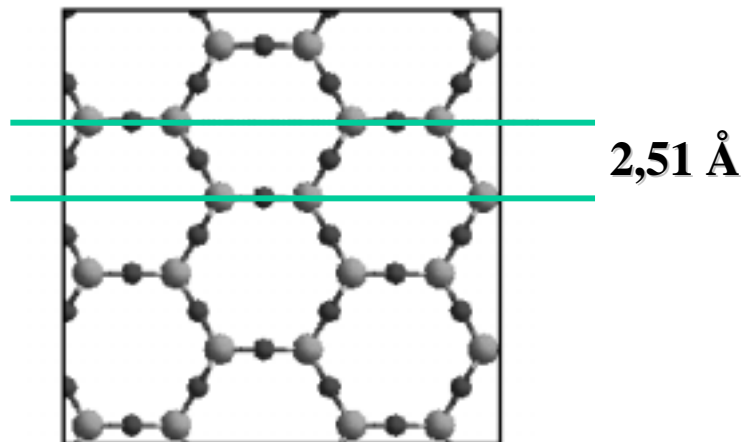
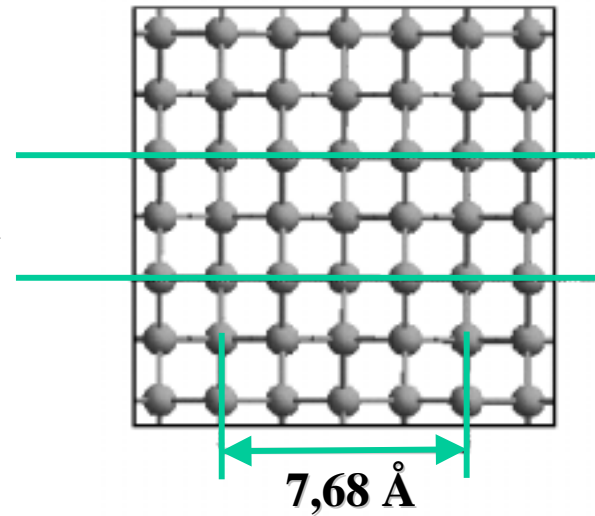
# What makes oxidation difficult

- **Knowledge of basic reaction mechanisms – complex chemical process**
  - Literature data
  - ab initio calculations
- **Lattice based model => network description of heterogeneous system hexagonal/cubic**
  - « Coincidence lattice site »

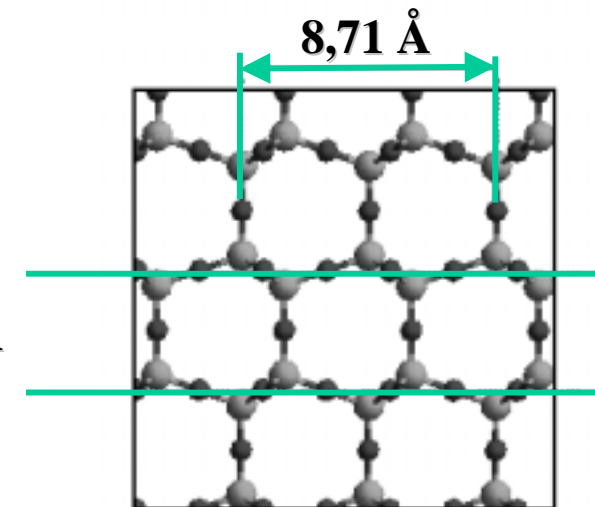
# Crystallographic considerations



3,84 Å



4,11 Å



**bi-axial compression => expansion ~11%  
along normal axis [100]**

# Elementary mechanisms through Literature considerations

- Oxidation = O<sub>2</sub> diffusion through SiO<sub>2</sub> towards the interface where it dissociates → B.E. Deal, AS. Grove, S. Rigo, D. Hamann, ...
- Amorphous/crystal duality → A. Ourmazd, J.C. Phillips, ...
- Viscosity of the formed layers → E.P. Eernisse, A. Fargeix et G. Ghibaudo, ...
- Reactive layer at the interface where chemical reactions occur → A.M. Stoneham, N. Mott, ...
- Molecular SiO presence → Y. Enta, H.Z. Massoud, ...
- Intrinsic Defects of the oxide → W.B. Fowler, A.H. Edwards, ....
- Elementary O<sub>2</sub> dissociation on Si(100) → Y.J. Chabal, G. Dujardin, ....

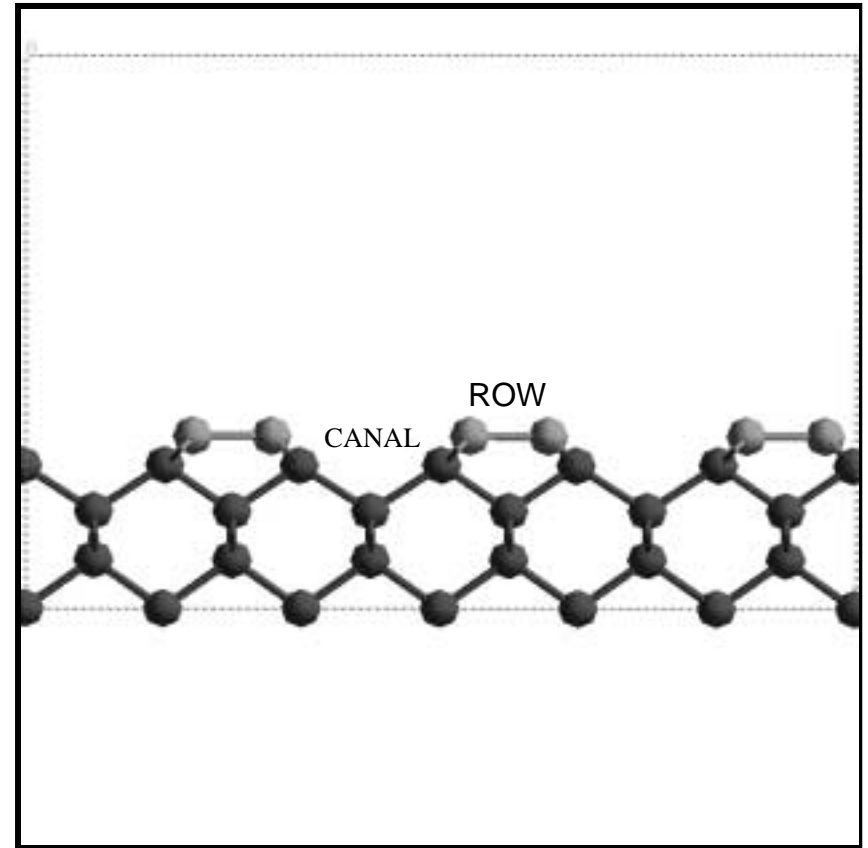
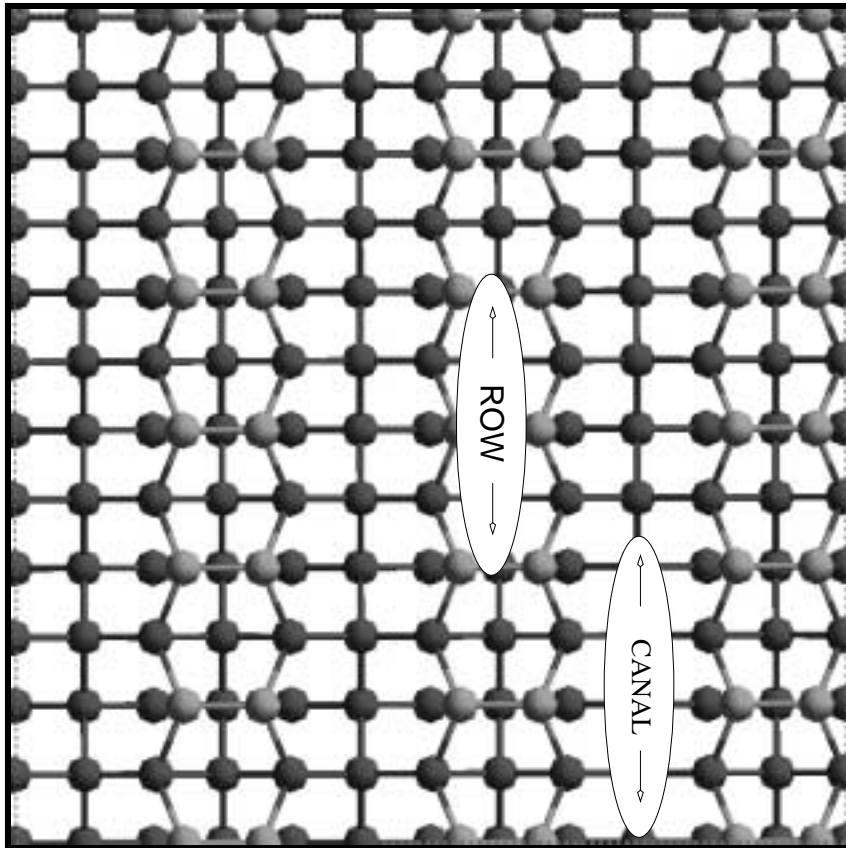
## Nature of the oxidation chemical reaction: first principle calculation

- **O/Si(100) interaction**
- **O/bulk silicon interaction**
- **O<sub>2</sub>/Si(100) interaction**
- **O<sub>2</sub>/bulk silicon interaction**
- *Same study with H<sub>2</sub>O*

*Castep, Vasp; DFT formalism, pseudopotentials,  
plane waves...*

# Si(100)x(2x1) surface morphology

## Influence of local minima

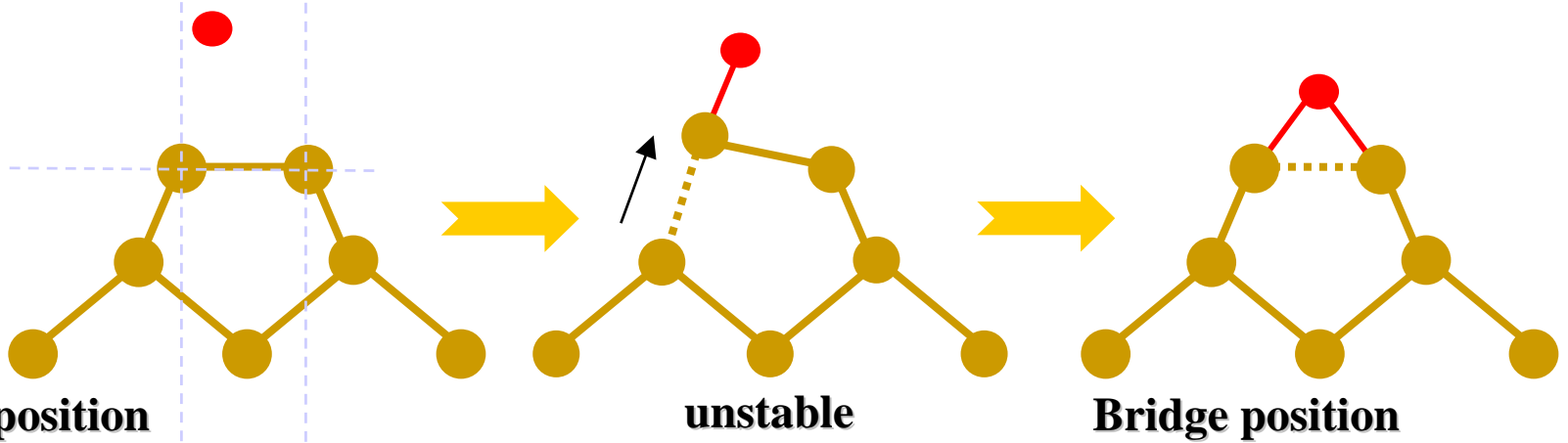


# O/Si(100) interaction O incorporation

[110]

1.

Initial position

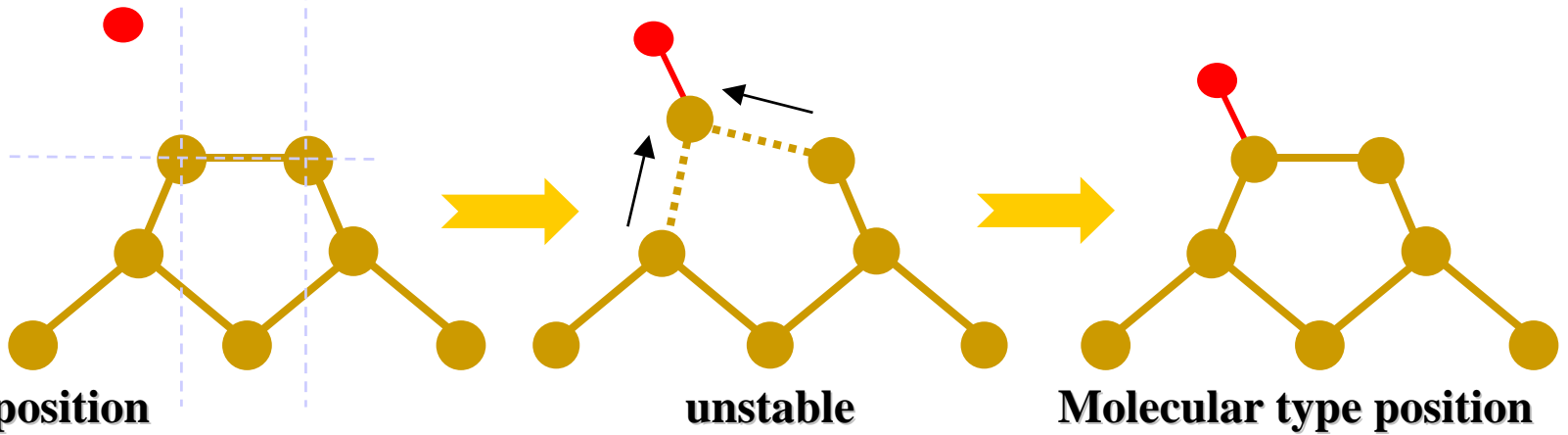


unstable

Bridge position

2.

Initial position

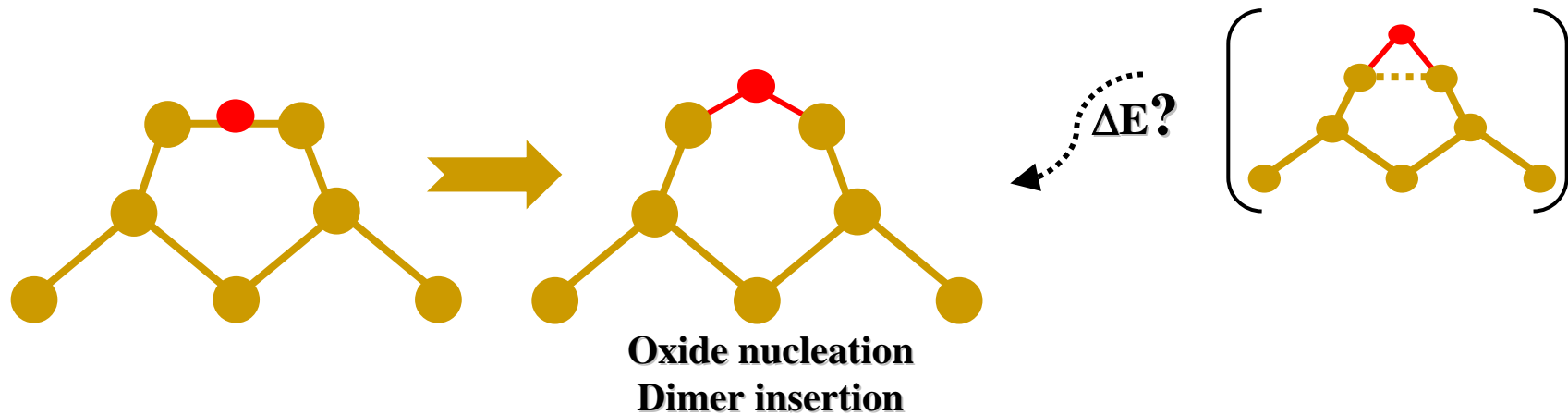


unstable

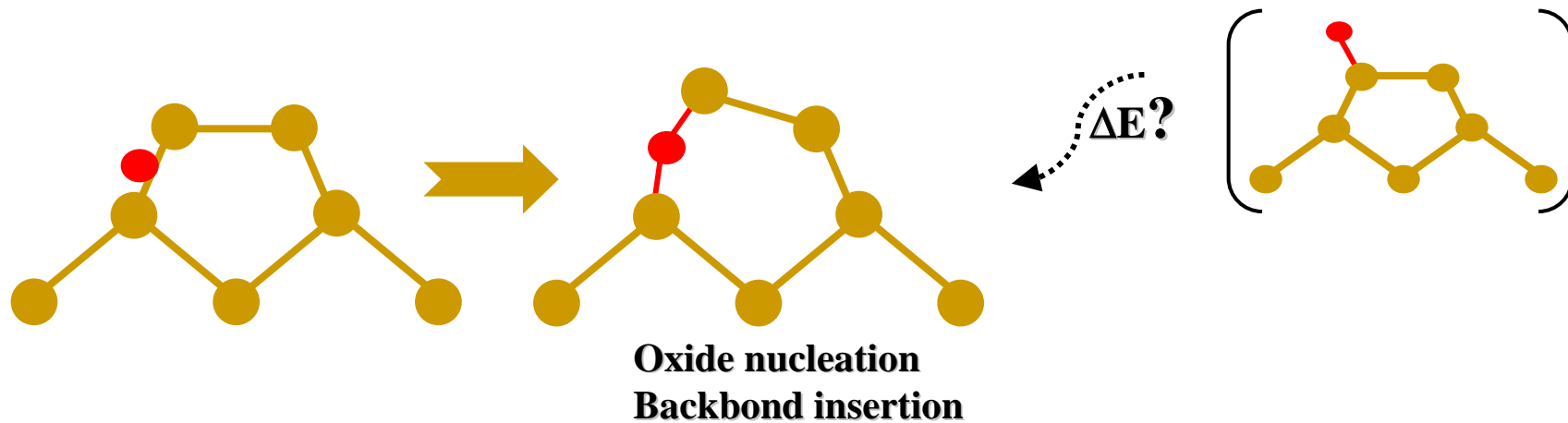
Molecular type position

# O/Si(100) interaction O incorporation

1.

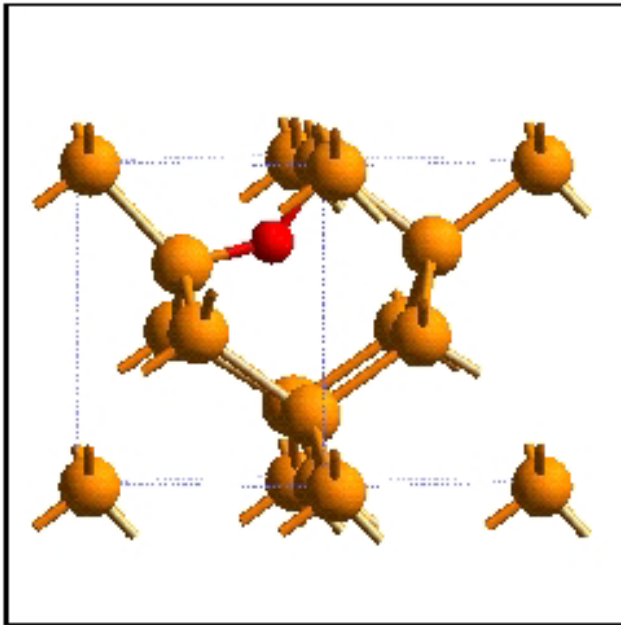


2.



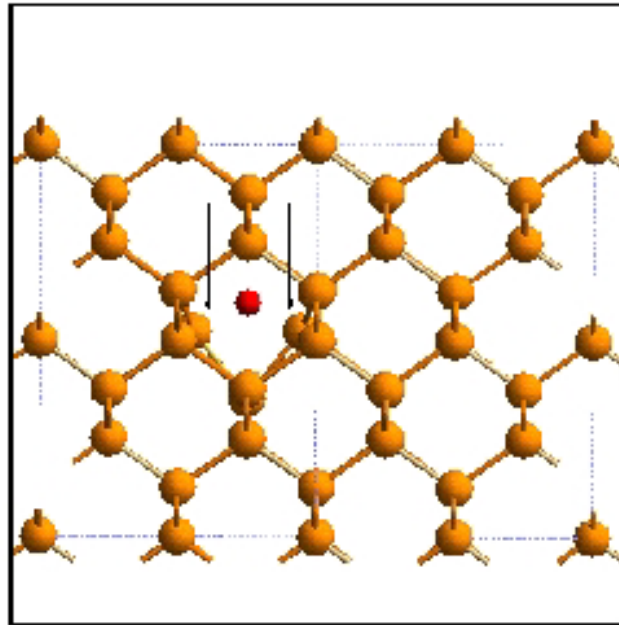
# Molecular oxygen in bulk Si

8 Si atoms unit cell



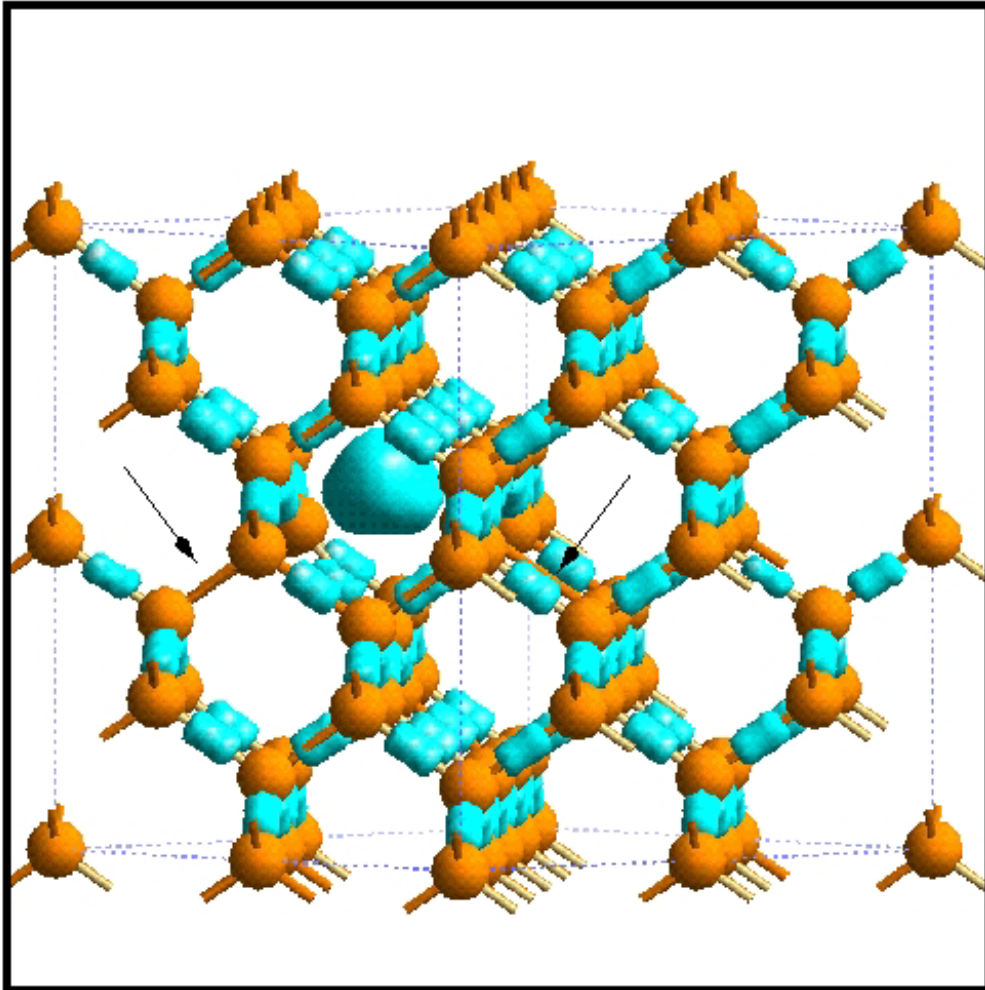
**directe silicium/oxyde transition  
= bond insertion (between Si first  
neighbours)**

64 Si atoms unit cell



**Elementary oxidation mechanisms  
= destructive aspects  
= bridging between 2<sup>nd</sup> neighbours**

**Charge isosurface =  $0.5 \text{ e}/a_0^3$**



**Charge transfer in the  
backbonds of the extracted Si  
atoms, due to oxygen presence**

# List of basics mechanisms considered for the Monte Carlo procedure

## Oxidation - step 1

**Non destructive**       $O_2 + Si_{\text{crist.}} \longrightarrow Brin^{-O} + 1/2 O_2$       =      **Strand formation**

**Destructive**       $O_2 + Si_{\text{crist.}} \longrightarrow Brin^{-O} + (SiO)$       =      **Strand formation**

**Adsorption of SiO = Si or O-terminated strand formation**

## Oxidation - step 2

**Junction of strands**       $Strand^{-Si} + Strand^{-O} \longrightarrow$       **perfect Si-O-Si sequences**

$Strand^{-Si} + Strand^{-Si} \longrightarrow$       **Oxygen vacancy**

$Strand^{-O} + Strand^{-O} \longrightarrow$       **Silicon vacancy**

## Diffusions

**Macroscopic diffusion of interstitial silicon**

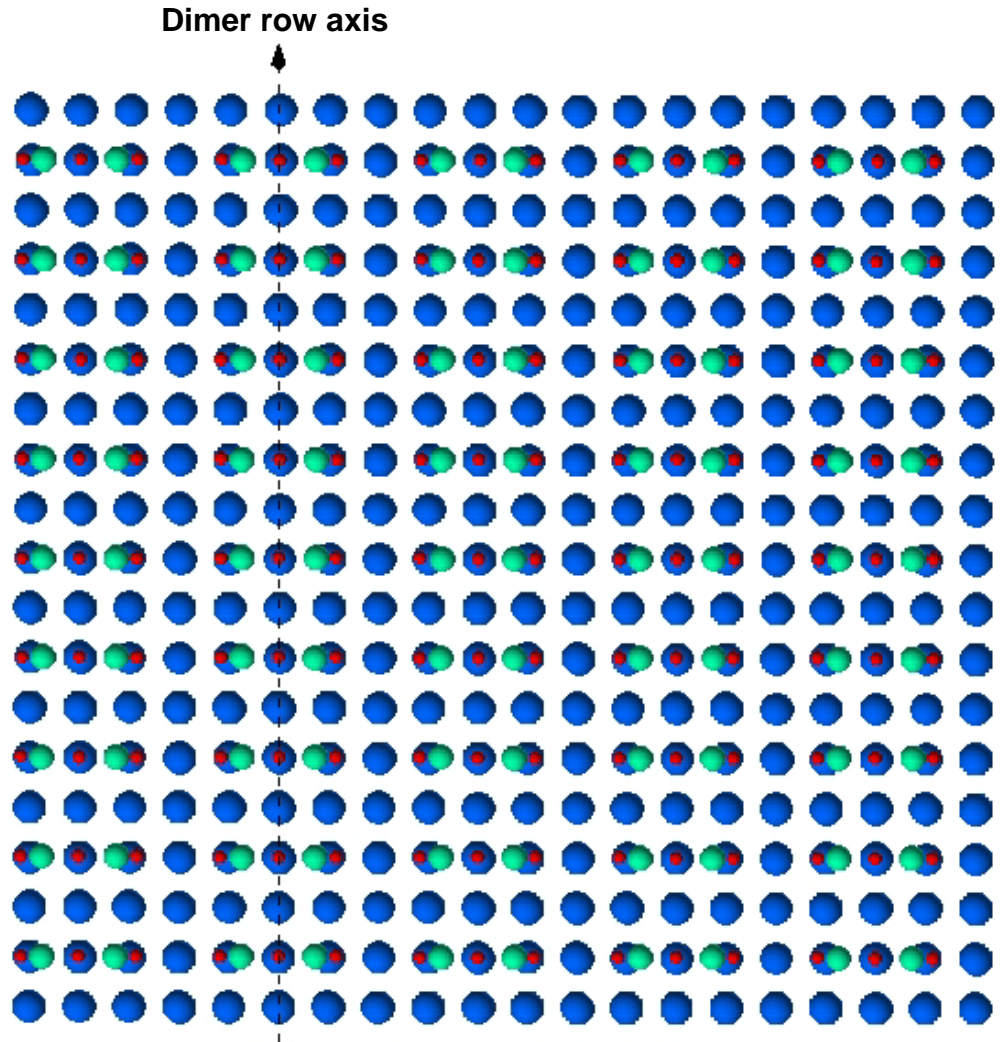
**Macroscopic diffusion of interstitial molecular oxygen**

**Microscopic diffusion of SiO interstitial**

# Non-destructive mechanism favoured

Pressure  $10^{-2}$  P.  
Temp. 1000 K  
Evnts 800  
Texp. 0.08 sec.

● surface order is conserved

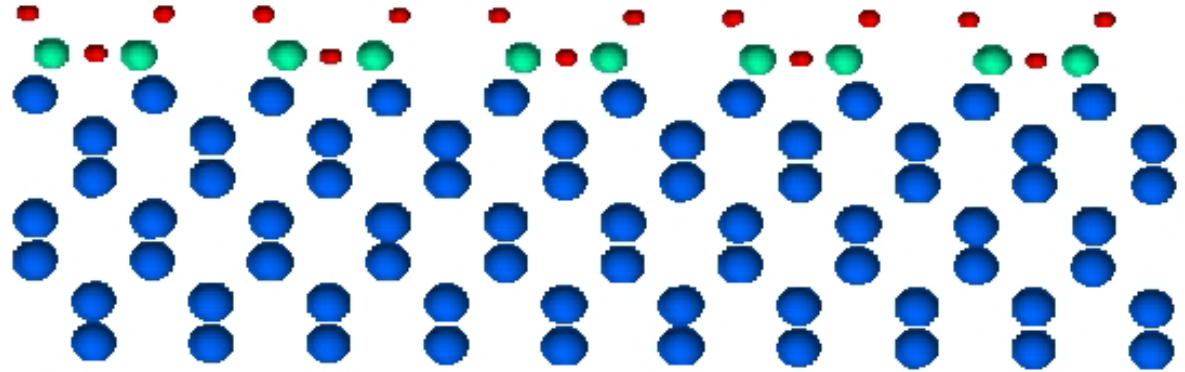


# Non-destructive mechanisms favoured

Pressure  $10^{-2}$  P.  
Temp. 1000 K  
Evnts 800  
Texp. 0.08 sec.

## Surface reconstruction

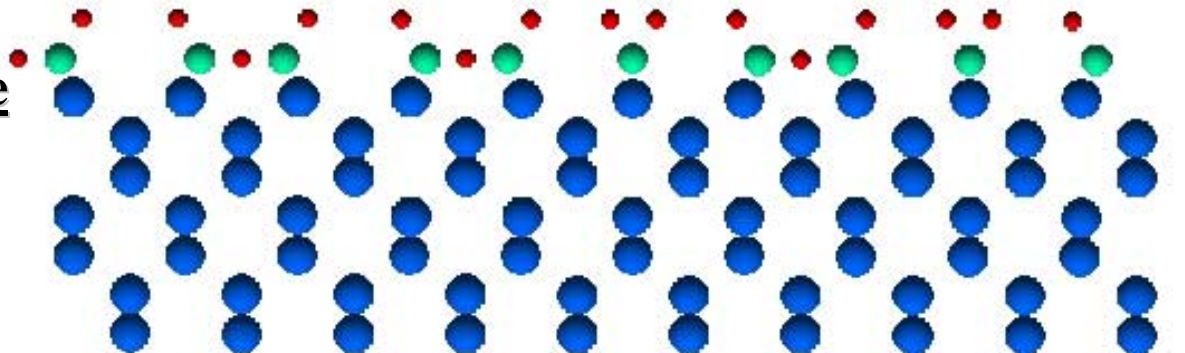
Nucleation of tridymite structure



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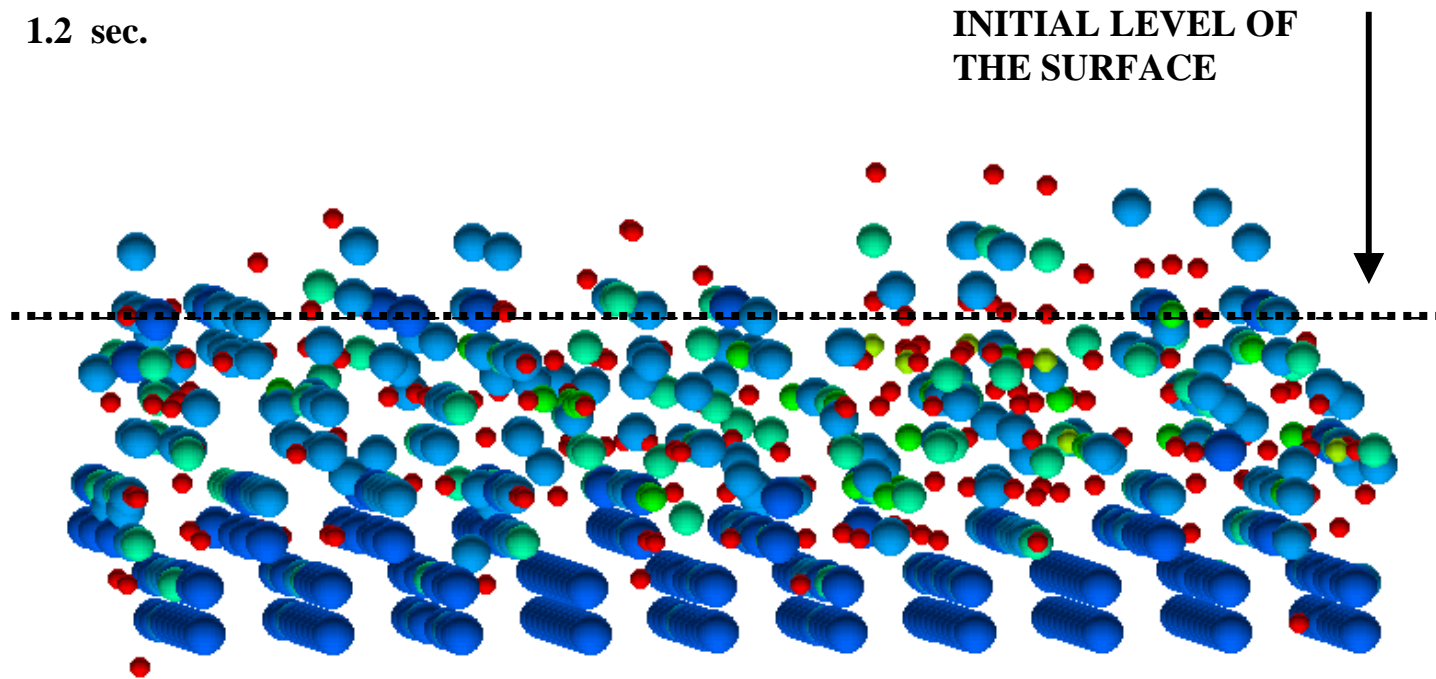
## Non reconstructed surface

Defect generation



# Destructive mechanism favoured No charge transfer

Pressure  $10^{-2}$  P.  
Temp. 1000 K  
Evnts 800  
Texp. 1.2 sec.



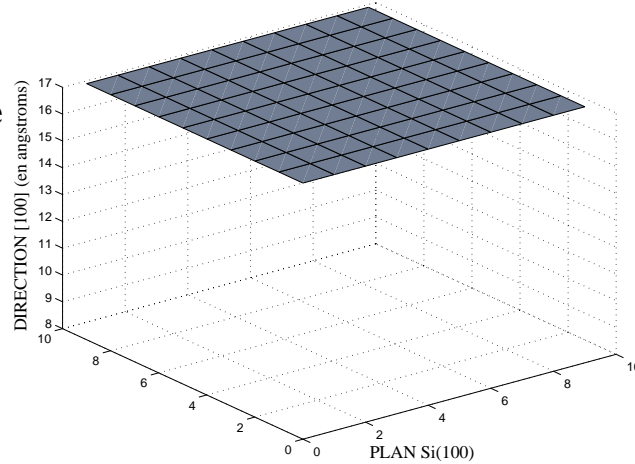


# Interface morphology

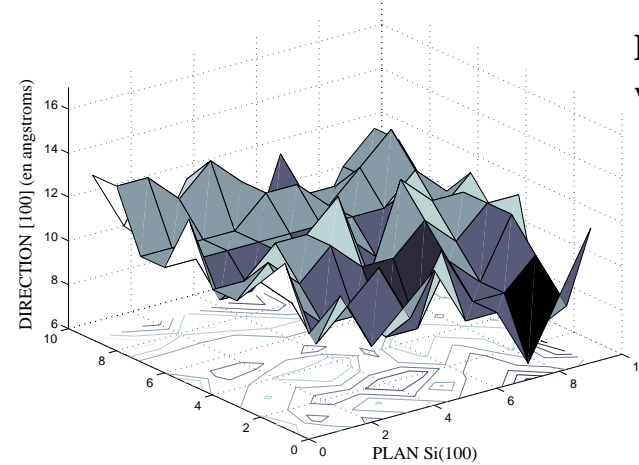
Pressure  $10^{-2}$  P.  
Temp. 1000 K  
Evnts 800

Charge transfer = CT

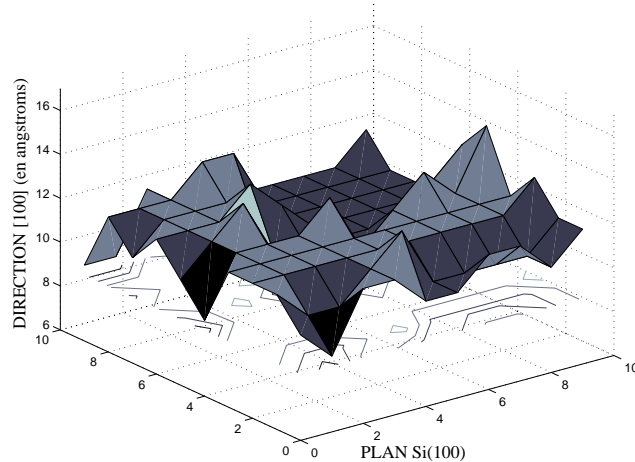
Non destructive



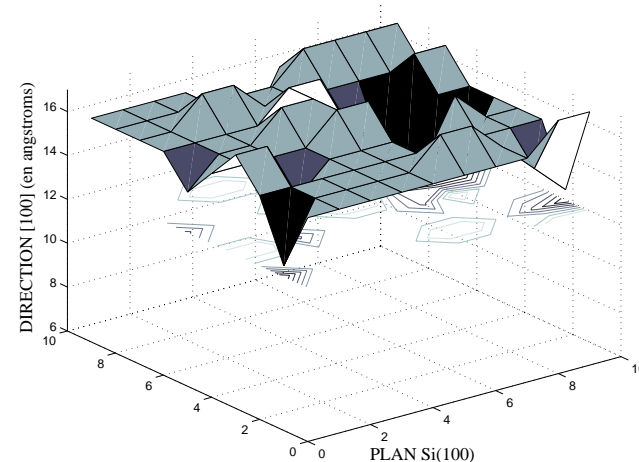
Destructive  
without TC



Destructive  
+ O-Si CT



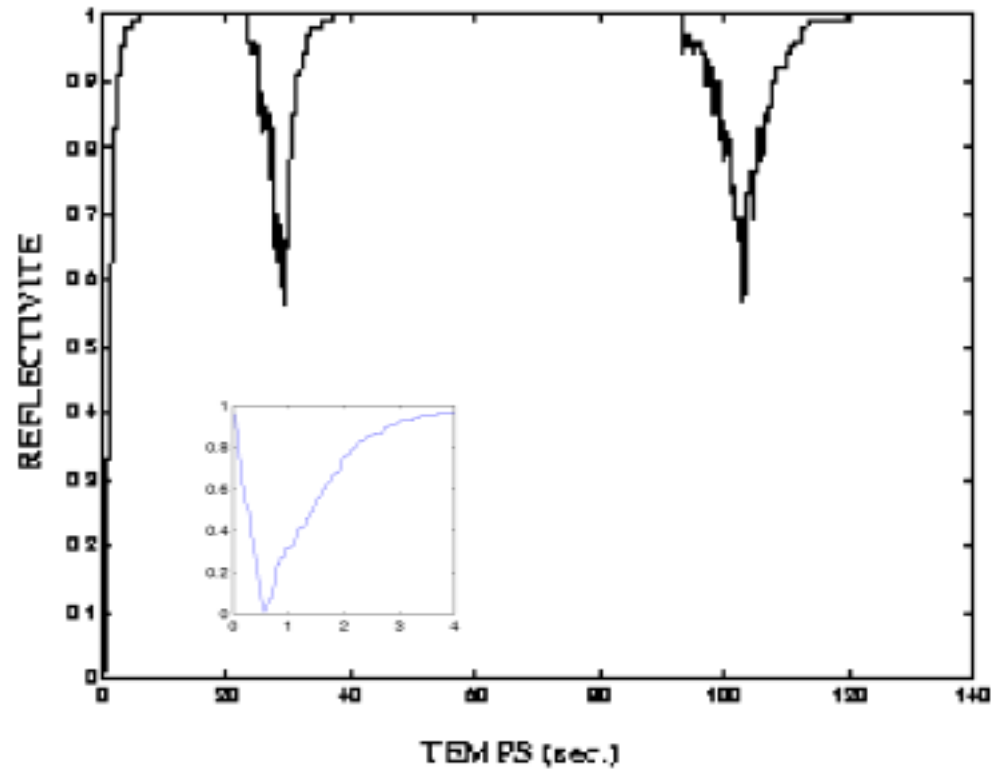
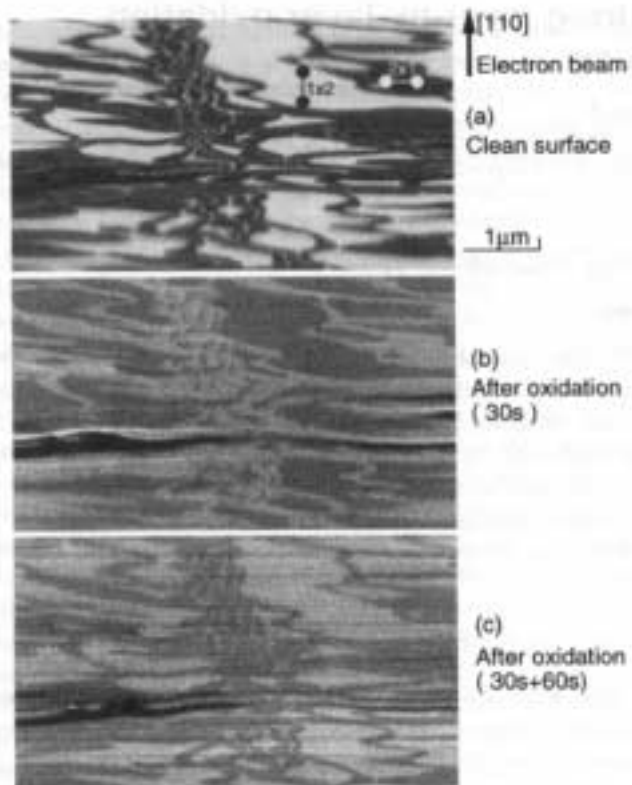
Destructive  
+ O-Si TC  
+ Si-Si TC



# Kinetic Validation

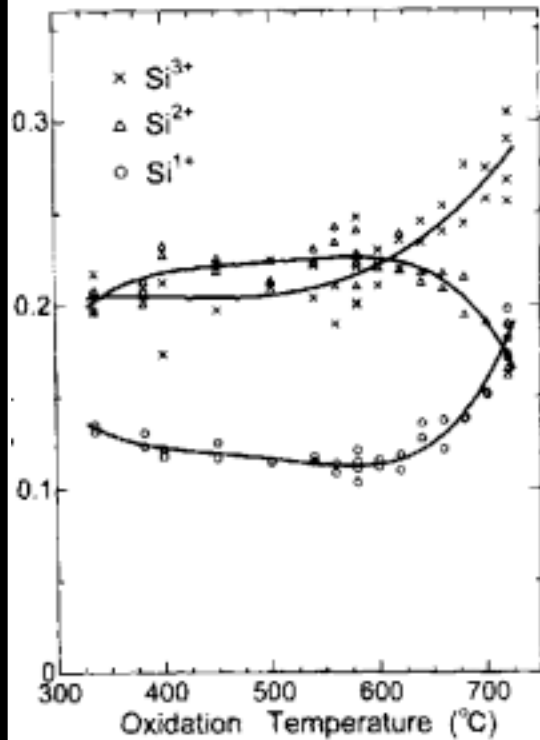
Oxidation reaction mechanism due to Deal and Grove data

Pressure  $10^{-2}$  P.  
Temp. 1000 K  
Evnts  $\sim 40\ 000$



Scanning RHEED  
Fujita et al. 1997

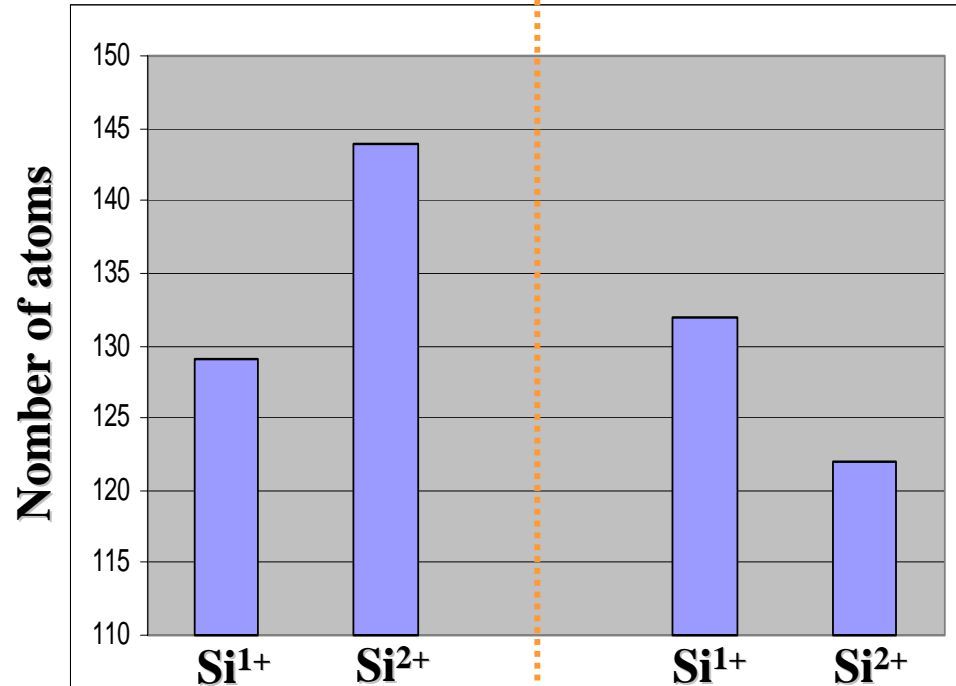
# Towards a XPS validation



**Inversion of Si<sup>1+</sup> and Si<sup>2+</sup> pics  
at 700 °C**

**Non destructive favoured**

**Equiprobability**



**Si<sup>1+</sup> et Si<sup>2+</sup> population inversion as a function of  
the balance between destructive and non destructive  
oxidation**

## Preliminar conclusion of this study

- Amorphosity of the layers
- Nanocrystallines portions of the interface
- Growth kinetics and layer by layer type of growth
- Transition zone or reactive layer at the interface (~2 to 3 Å at the interface)
- **Structural aspects = best knowledge of basic mechanisms of oxygen incorporation**
- **Additional mechanisms to treat annealing**

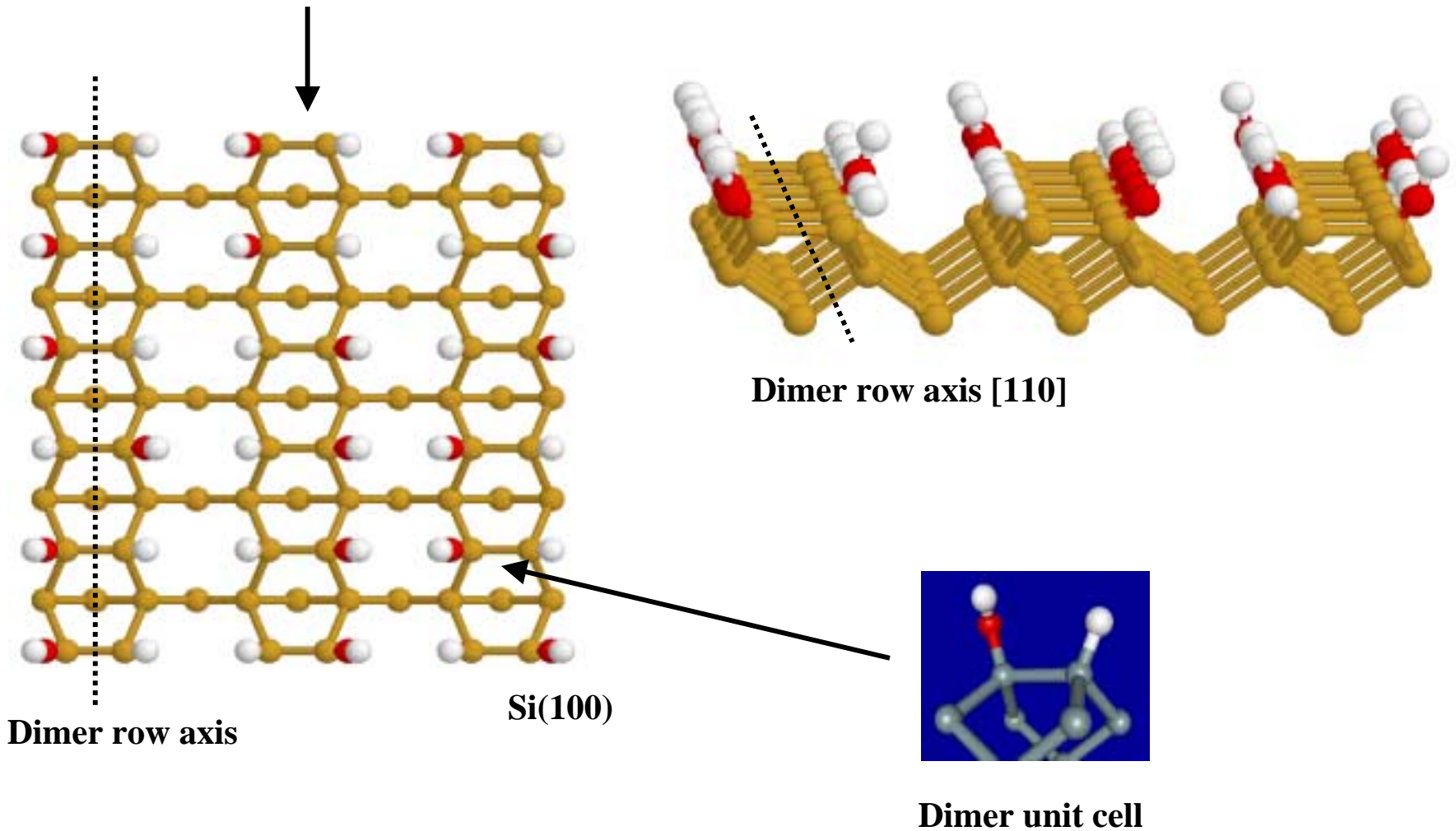
## **Ex.II: H<sub>2</sub>O/Si(100), oxygen incorporation reaction mechanisms and further migration**

- **Progress of advanced characterization techniques – new insights in the field of silicon oxidation**
- **How to organize the connection between Monte Carlo / Experimental Procedure / ab initio**
- **Results and discussion**

# Experiment

## Surface after initial water exposure

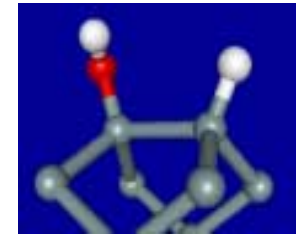
1. Initial configuration = H<sub>2</sub>O dissociated molecules (0.5 ML) / Si(100) 2x1



# Experiment Novel Features

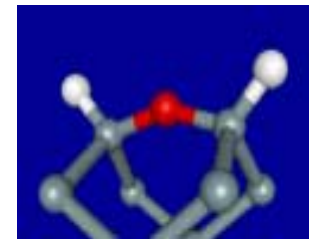
- ***Initial oxidation stage on water exposed Si(100)-(2x1) surfaces***

- ***initial H, OH distribution on each surface dimer***

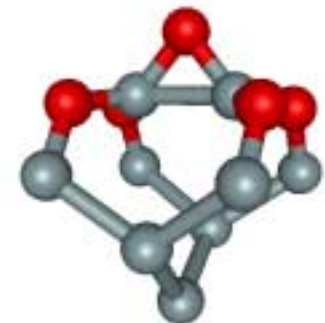


- ***a complex range of isolated surface configurations***

- ***conservation of the 2x1 (even if oxidized) structure***



- ***oxygen agglomeration from 1 O/dimer to epoxide (3 or 5 O/dimer) and associated kinetics***



# Framework

- Infrared spectroscopie

- *Vibrational modes*

- Quantum cluster calculations

- *Vibrational modes and associated atomic configurations*
- *Pathways and associated energies*

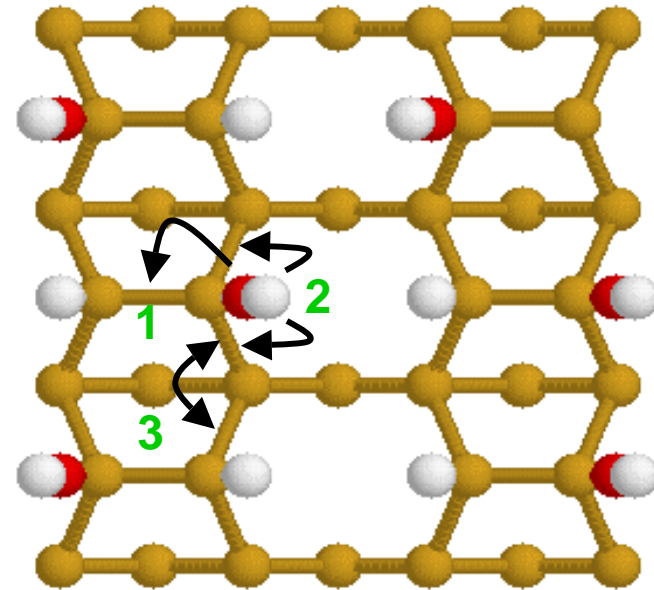
Final product of the oxidation

- Kinetic Monte Carlo Technique

- *Provides full kinetics of the species*
- *Evaluation of hypothetic mechanisms*

# List of proposed mechanisms in the Monte Carlo procedure before Hydrogen desorption

- 1 irreversible oxygen initial insertion from Si-O-H into Si-Si dimer bond
- 2 irreversible oxygen initial insertion from Si-O-H into Si-Si backbond
- 3 reversible oxygen backbond to backbond migration
- 4 Hydrogen desorption.
- 5 reversible oxygen insertion from Si-O into Si-Si dimer bond.
- 6 reversible oxygen insertion from Si-O into Si-Si backbond
- 7 reversible inter-dimer row oxygen migration

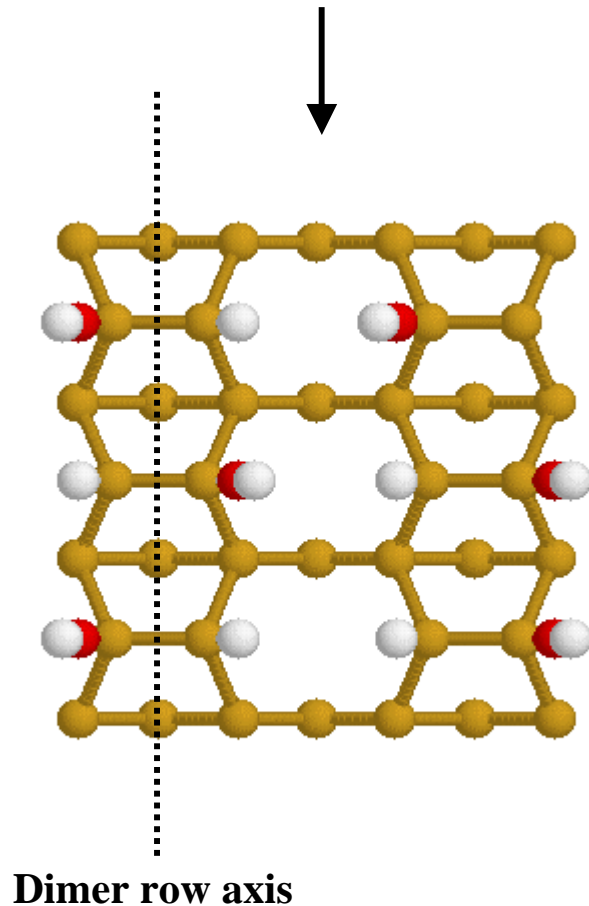


+ Charge Transfer

# Kinetic Monte Carlo Simulations

## Initial surface - First experimental procedure

1. Initial configuration = H<sub>2</sub>O dissociated molecules (0.5 ML) / Si(100) 2x1



2. Annealing : 2mn at 335 °C
3. Annealing : 2mn at 375 °C
4. Annealing : 2mn at 425 °C

### GUIDELINE

HSi-SiH  
HSi-O-SiH  
H(O)Si-O-SiH  
H(OO)Si-O-SiH

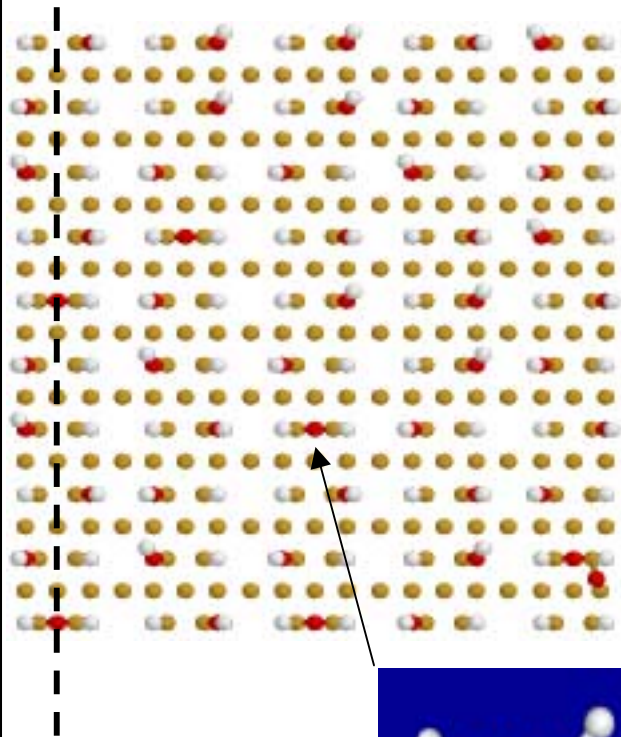
*No H(O)Si-O-Si(O)H*  
*No H(O) Si-SiH*  
*No H(OO)Si-SiH*

# First experiment - oxidation up to 700 K Si(100) top views

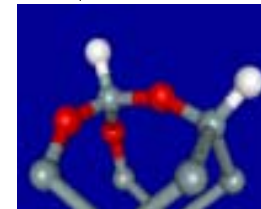
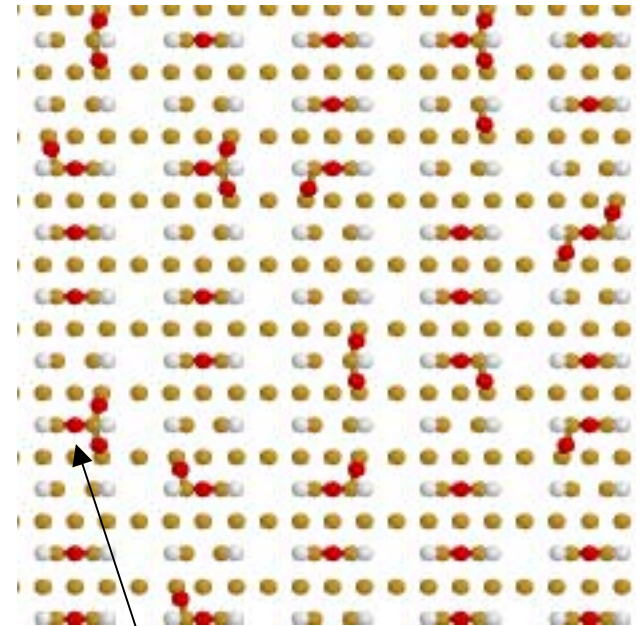
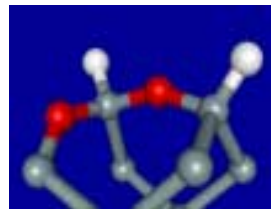
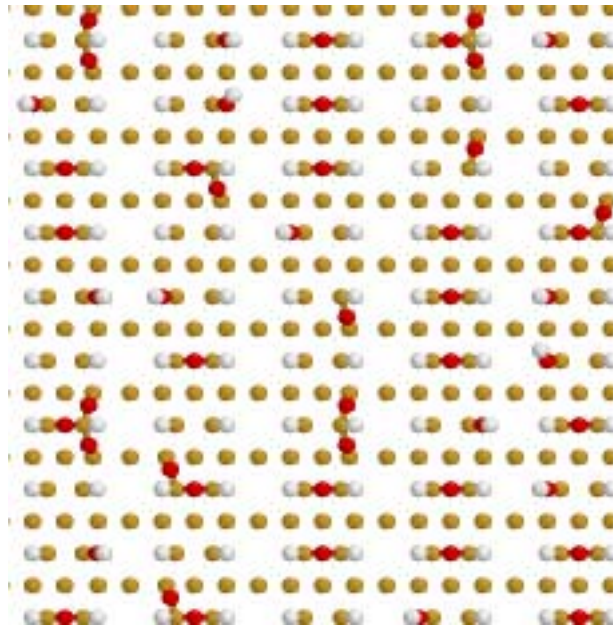
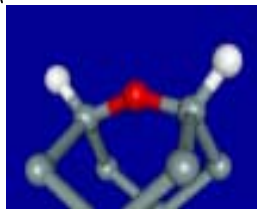
Annealing : 2mn at 608K

Annealing : 2mn at 648K

Annealing : 2mn at 698K

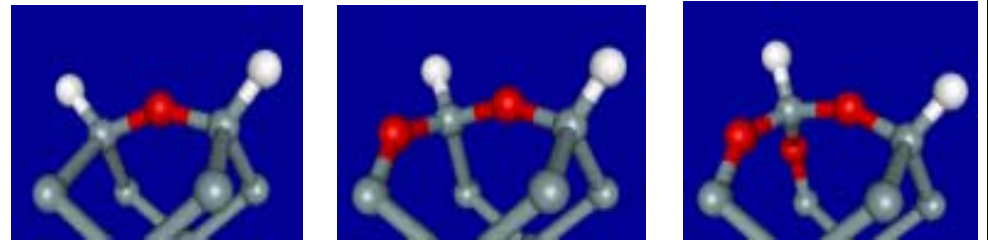
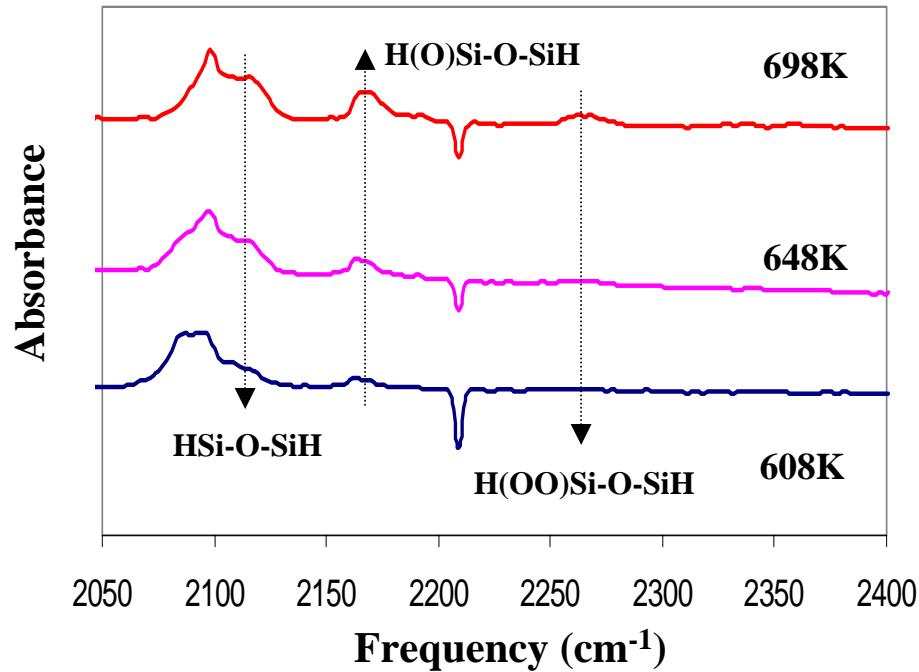


Dimer row axis



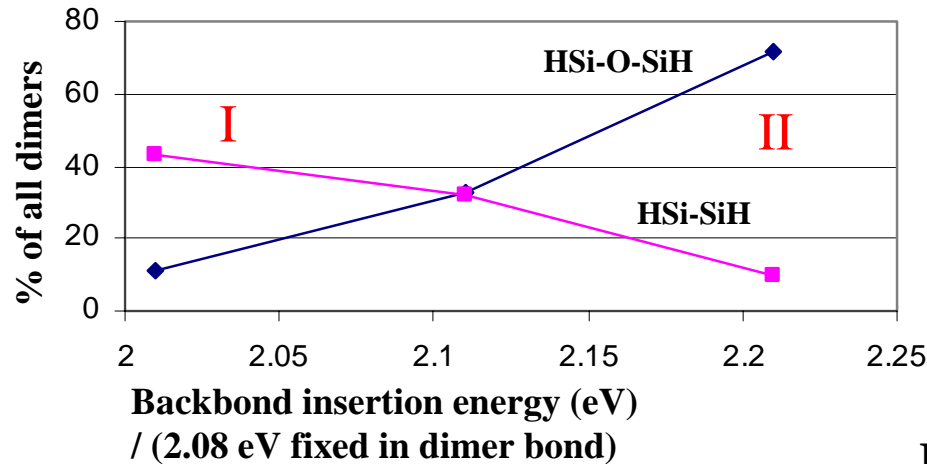
# First experiment - discussion

## Experiment



	Total OH (free)	one O	two O	three O	H-Si-Si-H
RT	100%	<1%	<1%	0%	0%
608K	66%	16%	9%	1%	8-16%
648K	33%	23%	17%	2%	25-40%
698K	1.5%	29%	24%	6%	>40%

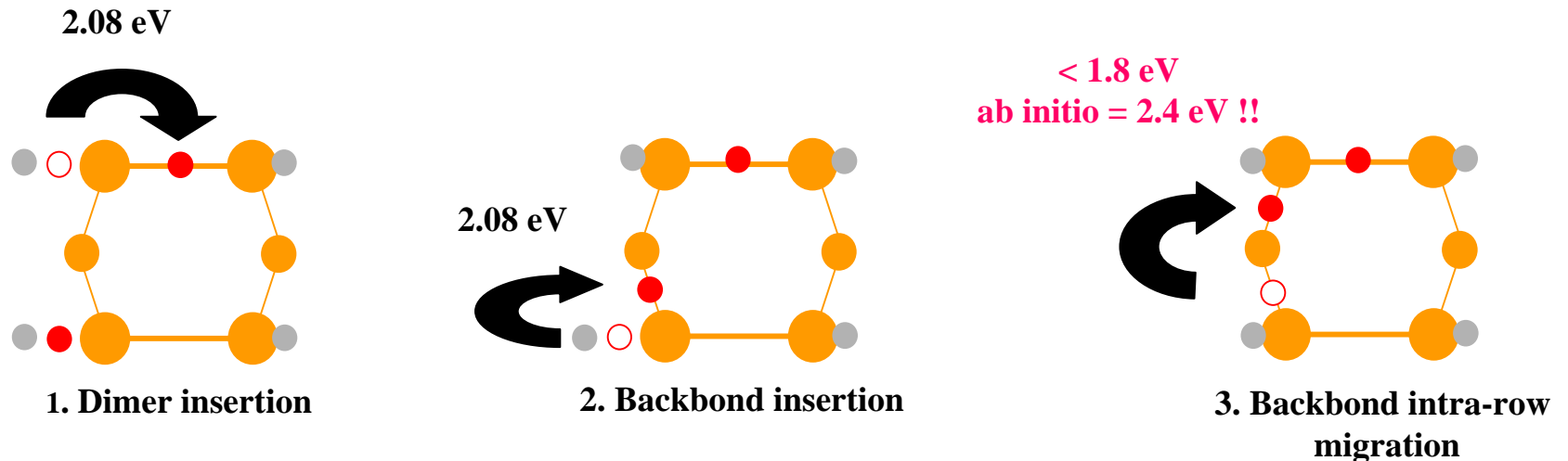
# Simulation - Energy calibration



I.  $H(O)Si-O-SiH > HSi-O-SiH$

II.  $H(OO)Si-O-SiH$  undetectable

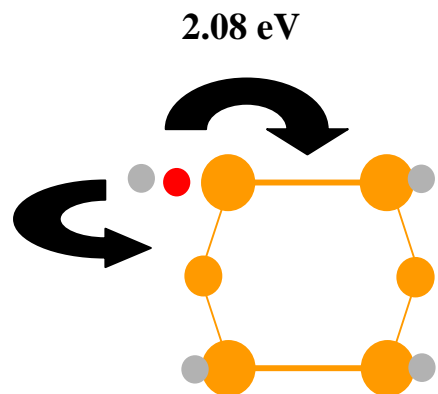
Preliminary agglomeration (up to 698 K)  
= three mechanisms



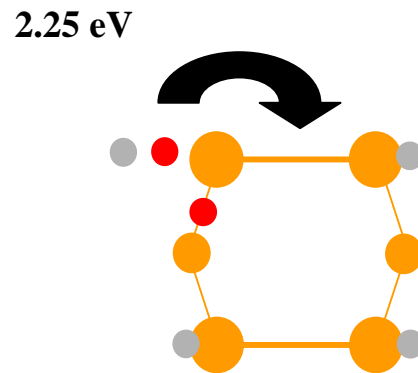
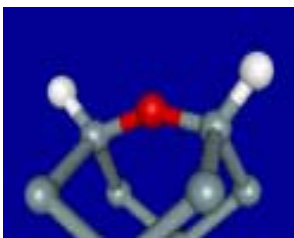
OH signal disappear after annealing two => retardation mechanism

2O signal lacking => charge transfer

# Simulation - O Incorporation

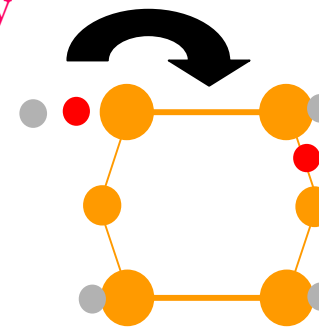


1. Dimer/backbond insertion

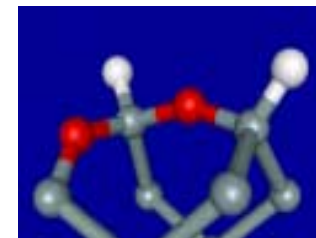


2. Retardation

< 1.9 eV

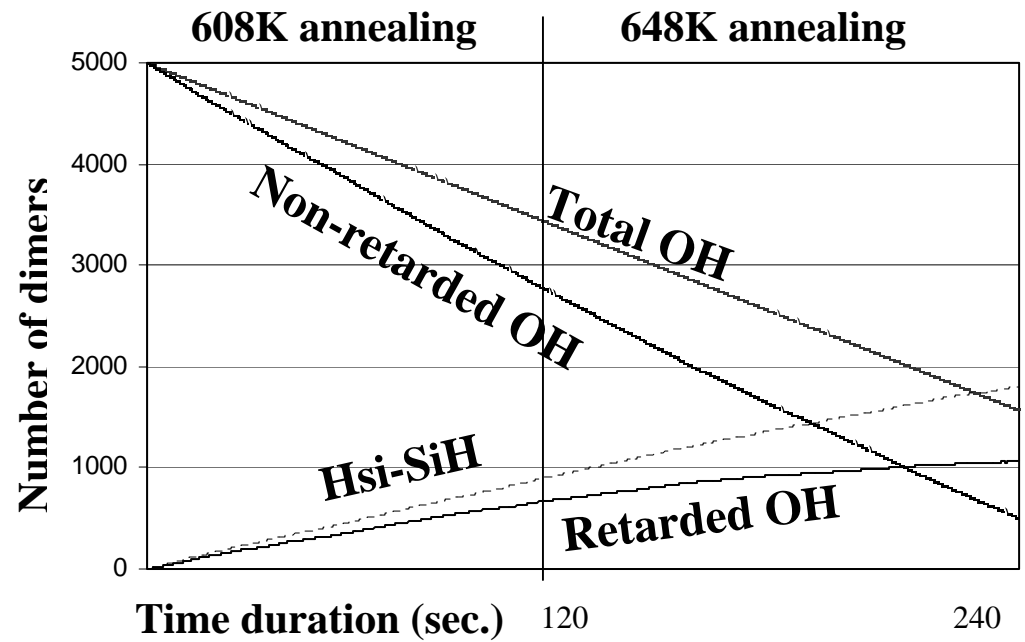
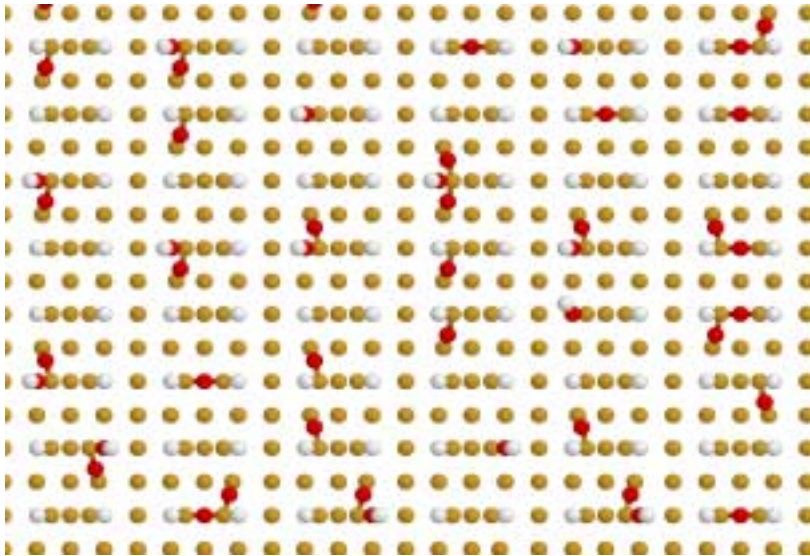


3. Charge transfer



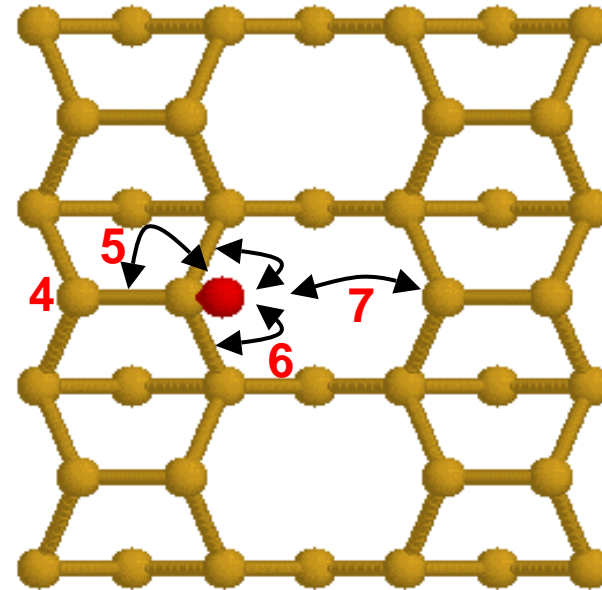
+ OH propension to be aligned after initial surface dosing with water

# Simulation - Energy calibration conclusions



# List of proposed mechanisms in the Monte Carlo procedure during Hydrogen desorption

- 1 irreversible oxygen initial insertion from Si-O-H into Si-Si dimer bond
- 2 irreversible oxygen initial insertion from Si-O-H into Si-Si backbond
- 3 reversible oxygen backbond to backbond migration
- 4 Hydrogen desorption.
- 5 reversible oxygen insertion from Si-O into Si-Si dimer bond.
- 6 reversible oxygen insertion from Si-O into Si-Si backbond
- 7 reversible inter-dimer row oxygen migration

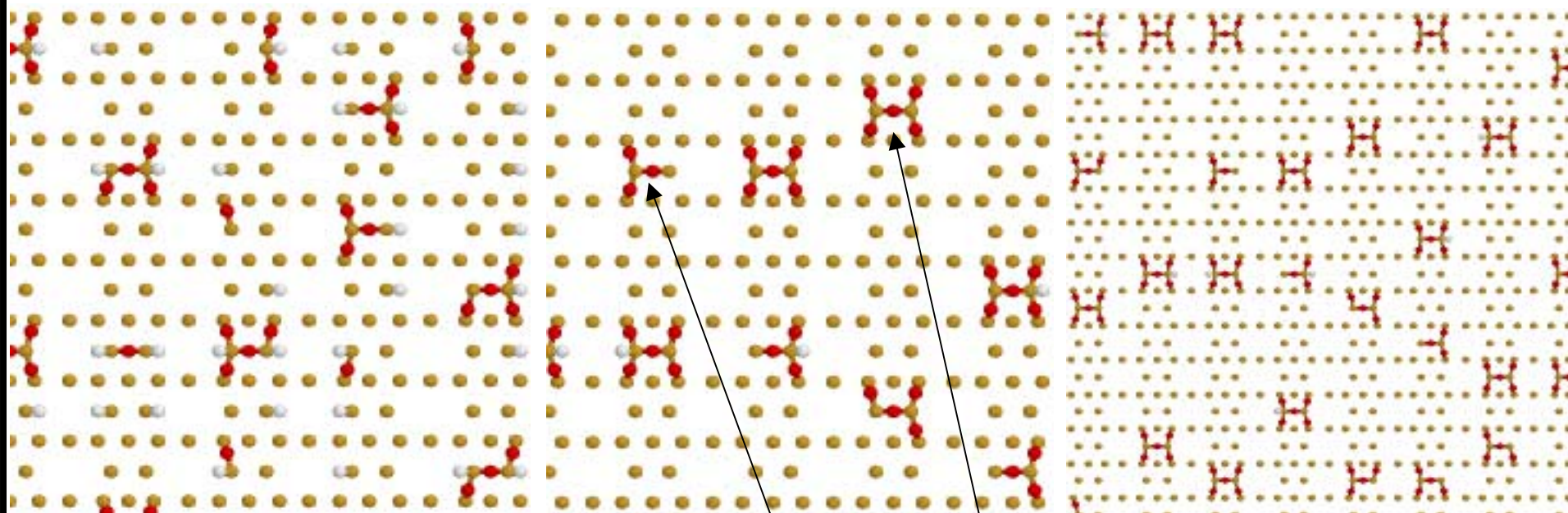


+ Strain, + Charge Transfer

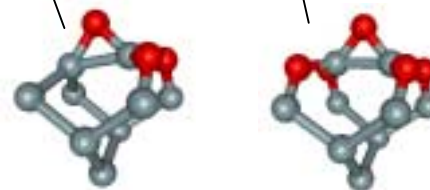
# Second experiment - oxidation up to 900 K Epoxide formation - Top view

Annealing : 2mn at 500 °C

Annealing : 2mn at 600 °C



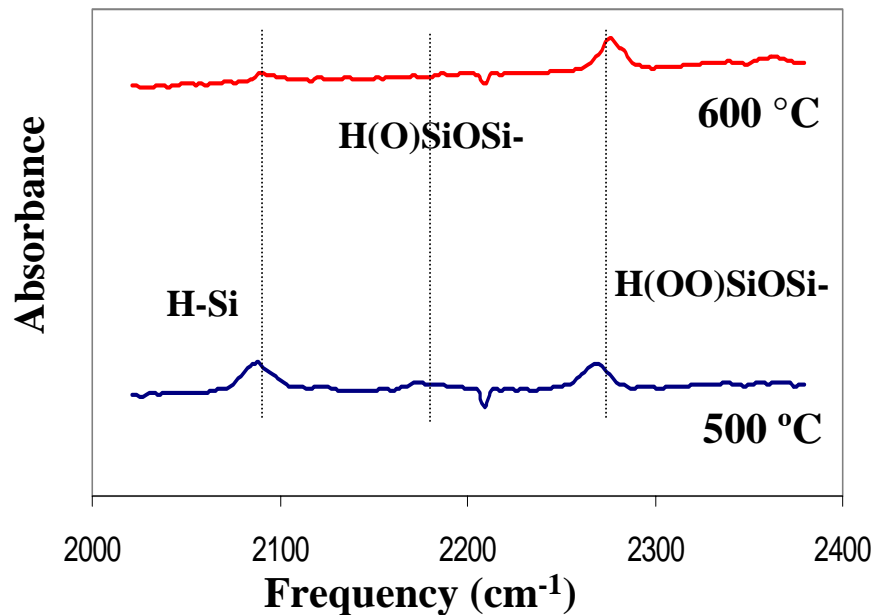
↓  
Isolated oxygen migrating  
doubly oxidized silicon nucleates epoxide



↓  
Isolated epoxide structure

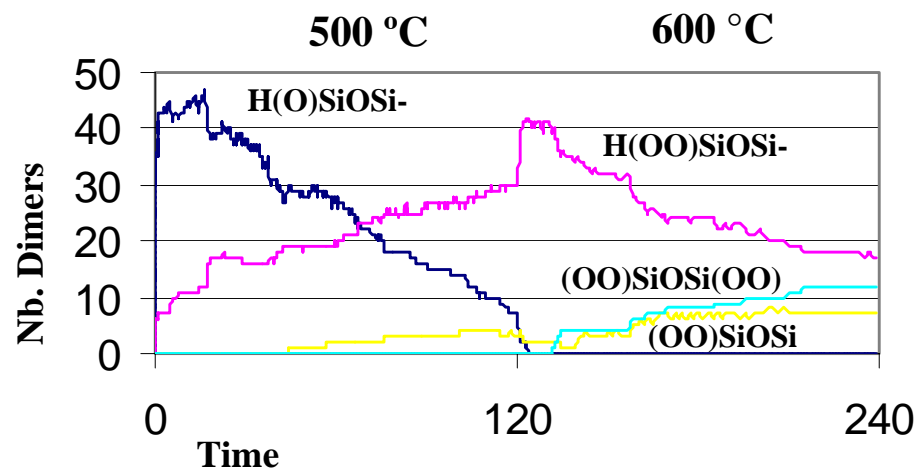
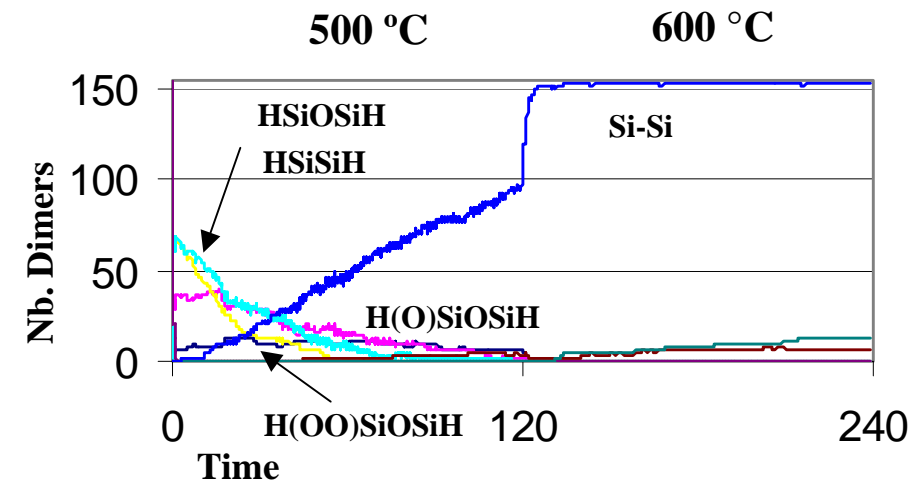
# Epoxide formation

## Experiment



Cross over between H(O)SiOSi- and H(OO)SiOSi-

## Simulation



# Conclusion

## ● *Kinetic Monte Carlo Tool associated with IR experiment and Quantum Cluster Calculations*

⇒ *Basic Mechanisms for initial wet oxidation*

= *Initial oxygen incorporation into the dimer bond  $\approx$  backbond = 2.08 eV  
dimer bond = 1.9 eV in the case of charge  
transfers  
retardation of oxygen incorporation*

= *effect of charge transfer for oxygen agglomeration even at the initial stage*

= *depassivation or dangling bond allow long range oxygen migration*  
*with up to 2 eV inter-dimer (in the same row) activation energies - desorption is a  
function of the local oxygen agglomeration (not linear: 2.42/2.45/2.49/2.81 eV)*

= *stability of doubly oxidized dimers has a role on the nucleation of final epoxide  
product at 900 K*

= *strain plays a role in the epoxide nucleation and repartition*

# Multi-Scale Perspective

- **Results can provide helpful informations for first principle validation and improvement of the KMC results, i.e. reaction pathways**

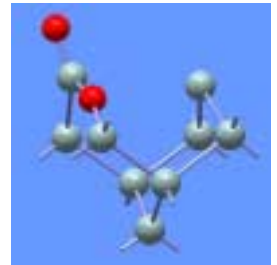
- **Progress in the Understanding of  $O_2$  Exposed  $Si(100)$  Surface**

  - ⇒ **novel experimental feature, G. Dujardin, Y.J. Chabal**

    - **initial insertion of the molecule in the backbonds of the same silicon atom**

    - **observed strands (according to the KMC  $Si=O$  stabilized by local strain)**

      - = **improvement of the corresponding mechanisms**



- **Towards Ultra Thin Film Growth**

  - ⇒ **introduction of strain, kinetics, layer by layer growth mode**

## **Key points of the oxidation process: towards CAD tools**

- **Charge transfer is a key issue**
- **Oxidation via water exposure driven by non destructive mechanism**
- **Oxidation via O<sub>2</sub> driven by destructive mechanism, the oxygen incorporation into silicon does not mean systematic insertion into Si-Si network bonds**
  - **Strand formalism**

**=> Next generation KMC model**

# Macroscopic formulation: chemical rate theory

$$\frac{dC_{si}(n)}{dt} = -K_{o2} * C_{si}(n) * I_{o2}(n) - K_{os} * C_{si}(n) * G_o - 4 * K_{o21} * C_{si}(n) * I_{o2}(n) - 4 * K_{os1} * G_o * C_{si}(n) - 4 * K_{31} * I_{o2}(n) * C_{si}(n)$$

$$\frac{dI_{o2}(n)}{dt} = D_{o2} * \Delta I_{o2}(n) - K_{o2} * C_{si}(n) * I_{o2}(n) - K_{o21} * C_{si}(n) * I_{o2}(n) - K_{31} * C_{si}(n) * I_{o2}(n) - K_{o1} * I_{o2}(n) * B_{si}(n) - K_{si_o} * I_{o2}(n) * G_i$$

$$\frac{dC_{sio}(n)}{dt} = D_{sio} * \Delta I_{sio}(n) - K_{o21} * C_{si}(n) * I_{o2}(n) - K_{os1} * G_o * C_o(n) - K_{si_o} * G_i * I_{o2}(n) + K_{osi} * G_i * G_o - K_{SIOX} * B_{si}(n) * I_{sio}(n) + K_{SIOX} * B_o(n) * I_{si}(n)$$

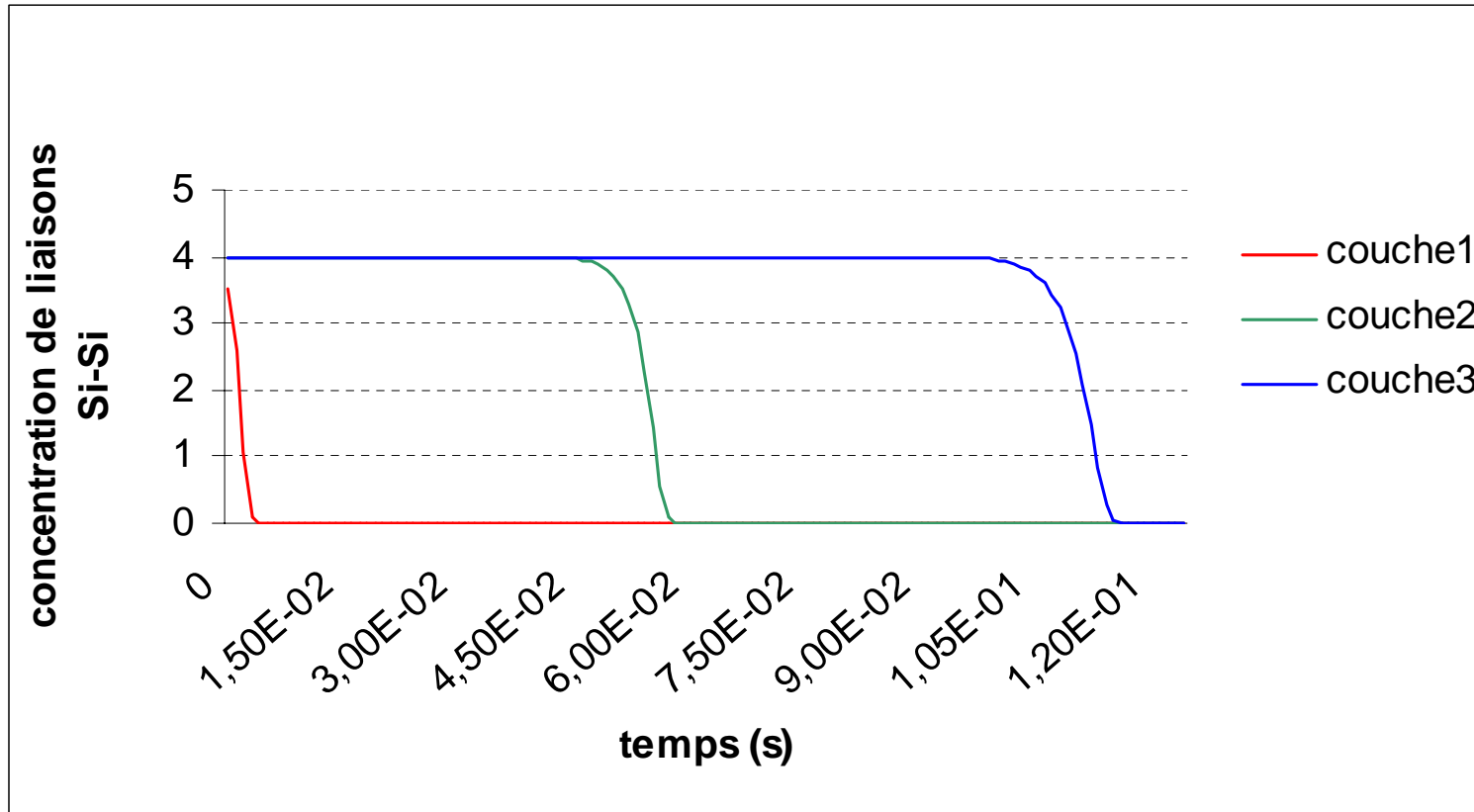
$$\frac{dB_o(n)}{dt} = K_{o1} * I_{o2}(n) * B_{si}(n) - K_{obs} * B_{si}(n) * G_o(n) - K_{si} * B_o(n) * G_i - K_L * B_o(n) * B_{si}(n) - K_p * B_o(n) * B_o(n)$$

$$\frac{dB_{si}(n)}{dt} = 4 * K_{o21} * C_{si}(n) * I_{o2}(n) + 4 * K_{os1} * C_{si}(n) * G_o + K_{si} * B_o(n) * G_i - K_{o1} * B_{si}(n) * I_{o2} - K_{obs} * B_{si}(n) * G_o - K_L * B_o(n) * B_{si}(n) - K_p * B_{si}(n) * B_{si}(n)$$

$$G_i = \frac{K_{31} * C_{si}(n) * I_{o2}(n)}{K_{si_o} * I_{o2}(n) + K_{si} * B_o(n) + K_{osi} * G_o + D}$$

$$G_o = \frac{(K_{o2} + K_{o21}) * C_o(n) * I_{o2}(n) + K_{si_o} * I_{o2}(n) * G_i}{(K_{o2} + K_{o21}) * C_o(n) + K_{31} * B_{si} + K_{osi} * G_i + D}$$

# Layer by layer oxidation



# Kinetics of species

## Time evolution of system species

