Kinetic Monte Carlo Simulation: an Accurate Bridge Between Ab-Initio Calculations and Standard Process Experimental Data

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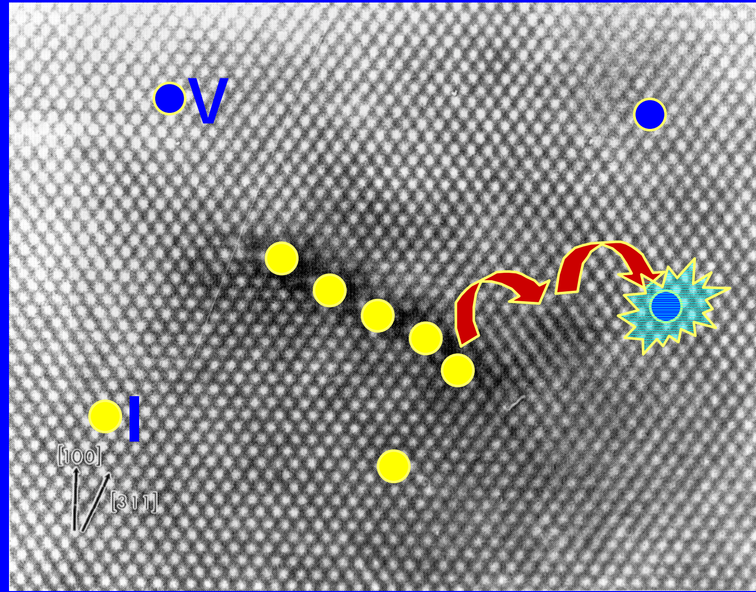
Outline

- Why Kinetic Monte Carlo?
- Ion Implantation damage simulation:
  - Simulation Scheme
  - Examples
- Polycrystalline thin film deposition:
  - Nucleation and Grain Boundaries
  - Examples
- Channeling Implants: Relevance of the Electron Density Distribution

The Kinetic Monte Carlo approach



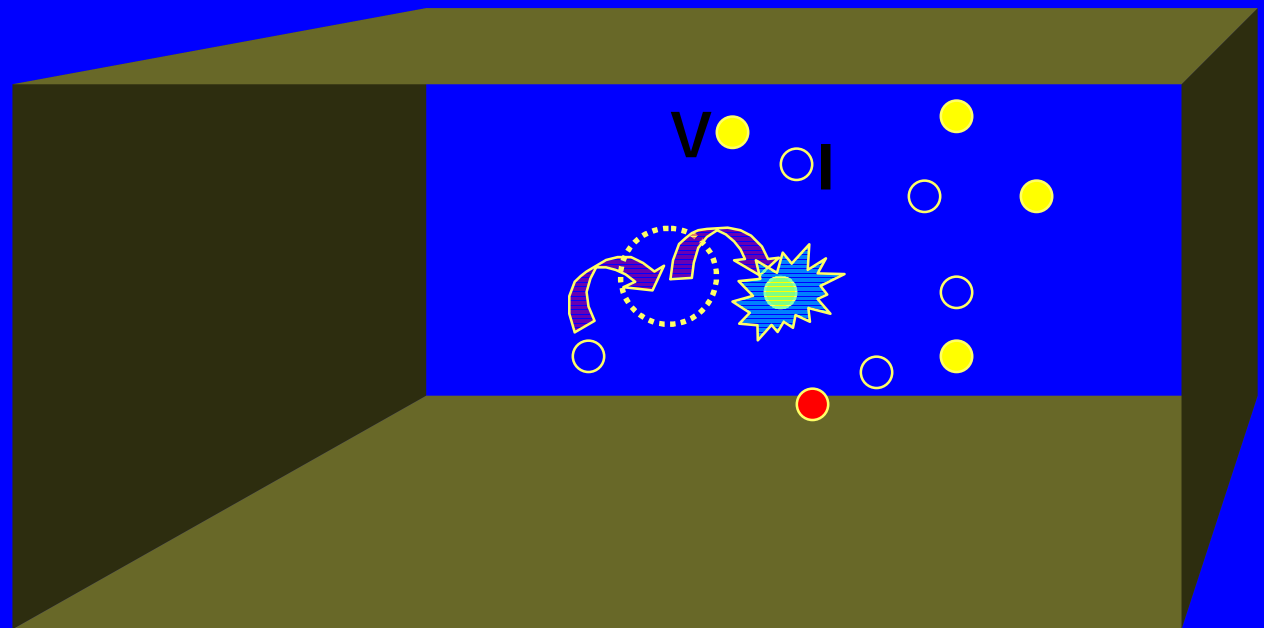
- Simulate only defects (Point & Extended)
- Use ab-initio or classical MD (off-line) to get the necessary parameters (migration energies, binding, …)
- Use BCA to generate each cascade (I,V coordinates)
- Anneal using kinetic Monte Carlo (kMC)

Atomistic Simulation
of
Diffusion and Clustering

SIMULATION SCHEME

SIMULATION BOX

FRONT SURFACE ↓



BACK SURFACE

LATERAL BOUNDARY CONDITIONS:

- **PERIODIC**
- **MIRROR**

DEFECT TYPES

1. POINT DEFECTS

- **SINGLE POINT DEFECTS: V, I, B, C, ...**
  - **POSSIBLE EVENT: JUMP**

$$Jrate = 6 * D_o * \exp(-Ea / kT) / L^2$$

- **PAIR POINT DEFECTS: IB, Bi, VO, ...**
  - **POSSIBLE EVENTS:**
    - **JUMP:**
    - **BREAK UP:** IB $\rightarrow$ I + B
    - **SWITCH:** IB $\rightarrow$ Bi

INTERACTION BETWEEN DEFECTS:

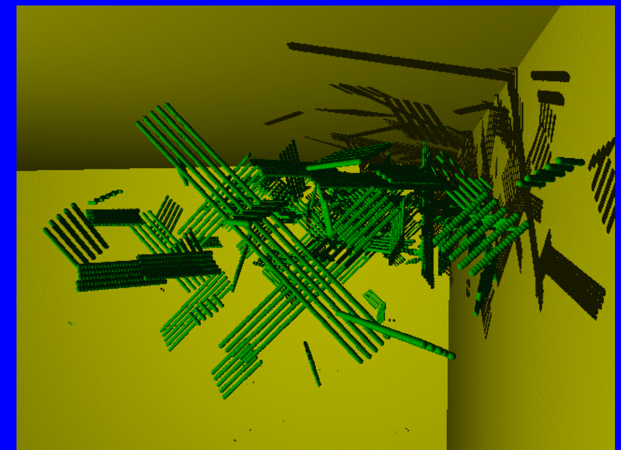
- **CAPTURE RADIUS = 3.84 Å**
- **WITH / WITHOUT AN INTERACTION BARRIER**

DEFECT TYPES

2. CLUSTERS

{311}'s

- **SHAPES:**
  - **IRREGULAR (blob): V, B, C, ...**
  - **SPECIFIC:**
    - **VOIDS**
    - **{311}'s**
    - **DISLOCATION LOOPS**
    - **STACKING FAULTS**



- **POSSIBLE EVENTS:**
  - **CAPTURE of a point defect**
  - **EMISSION of a point defect**

DEFECT TYPES
3. COMPLEXES

COMPOSITION:

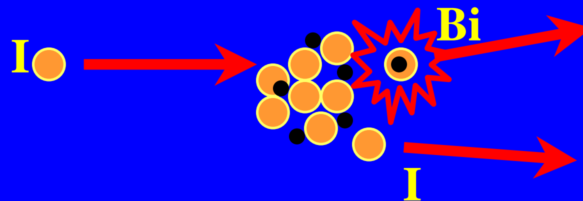
BINARY: I_nB_m, I_nC_m, V_nO_m, ...
TERNARY, ...

SHAPE:

IRREGULAR (small sizes)

POSSIBLE EVENTS:

CAPTURE or EMISSION of a point defect (SINGLE or PAIR)



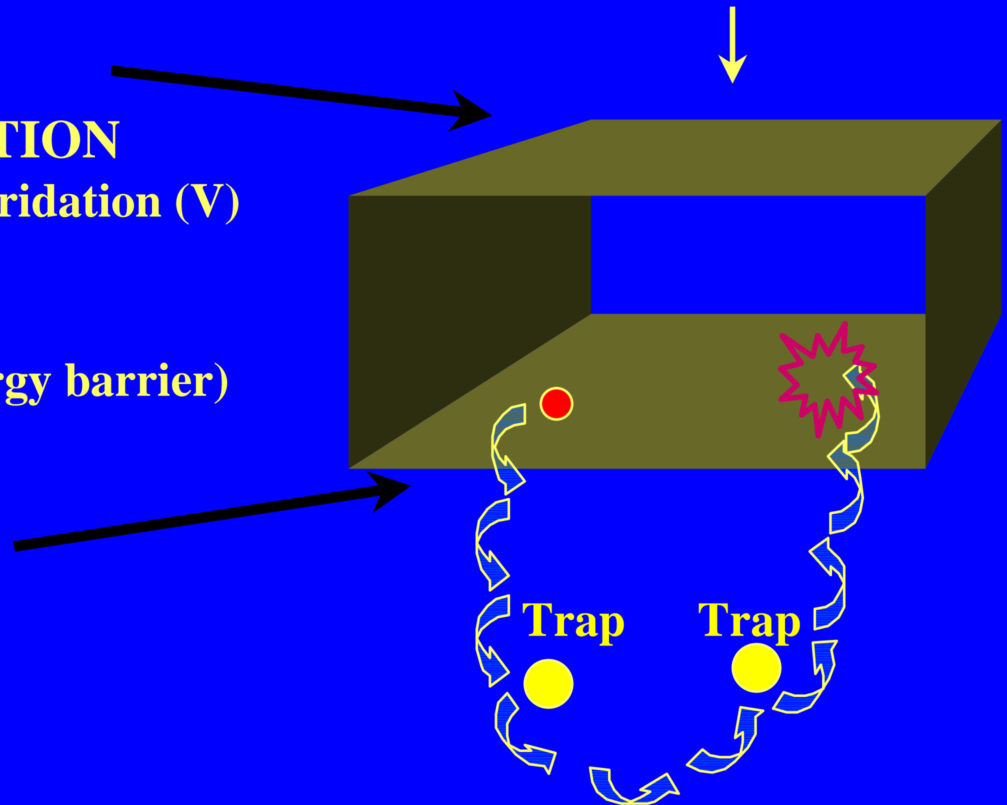
DEFECT TYPES
4. SURFACES

FREE SURFACE (Front):

- **THERMAL I-V GENERATION**
  - **Neutral, Oxidation (I),Nitridation (V)**
- **SINK for point defects:**
  - **from perfect SINK**
  - **to perfect MIRROR (energy barrier)**

BULK (Back surface):

- **DELAYING SURFACE:**
  - **Random walk**
  - **Bulk Traps**
  - **Re-emission from Traps**



SIMULATION SCHEDULER

EXAMPLE:

	n	J_{rate} (jumps/s)	Total Jumps/s
V	2	1000	2000
I	5	10	50

- **To simulate 1 second anneal we need to simulate 2050 Jumps $\Rightarrow \Delta t = 1/2050$ seconds per Jump**
- **We have to pick up V's and I's with a probability of 2000/2050 and 50/2050, respectively.**

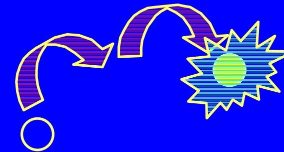
DIFFUSION SIMULATOR

CONTINUUM | **ATOMISTIC**

TO SIMULATE:

SOLVE:

$dI/dt = D\, d^2I/dx^2 - R_{Bulk}$



PROGRAM:

annihilate(I);
annihilate(V);

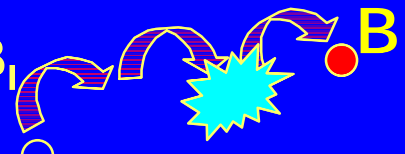
TO ADD NEW MECHANISM:

SOLVE:

$dI/dt = D\, d^2I/dx^2 - K_{IF} B_S I + K_{IR} B_I - R_{Bulk}$

$d B_I /dt = D\, dB_I^2/dx^2 + K_{BIF} B_s I - K_{BIR} B_I$

$d B_S /dt = - K$



PROGRAM:

annihilate(I);
annihilate(B_S);
create(B_I);

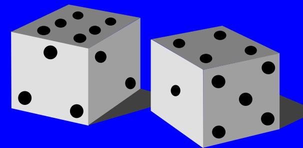
$\Rightarrow$ ALMOST NO ADDITIONAL COMPUTATION TIME

SIMULATION EXAMPLES

AT THE UNIVERSITY OF VALLADOLID WE HAVE IMPLEMENTED A FAST ATOMISTIC SIMULATOR :

DADOS

(**D**iffusion of **A**tomistic **D**efects, **O**bject-oriented **S**imulator)



PERFORMANCE: 1.4 seconds / Million events

(450 MHz Pentium II Xeon, Microsoft Visual C++ compiler)

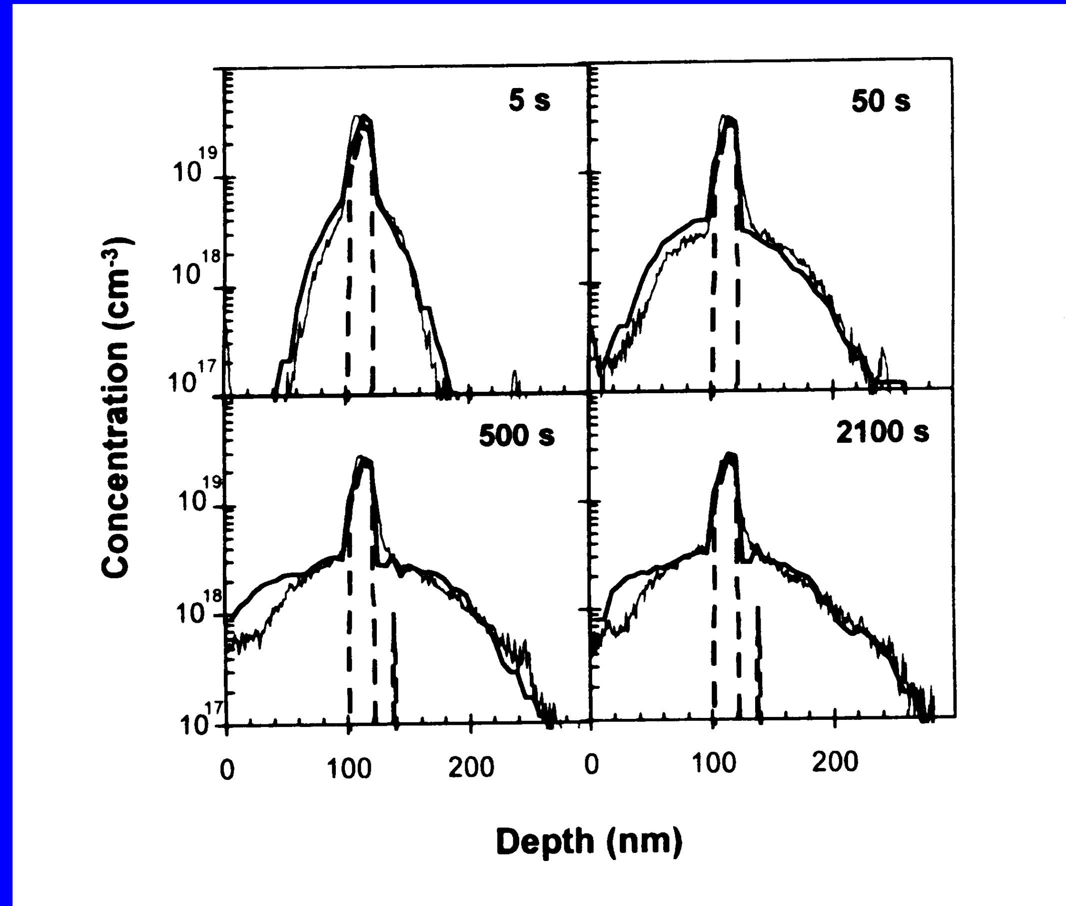
On average, simulates one event in the time it takes to calculate three Jump rates:

$$\text{Jrate} = 6 * D_o * \exp(-Ea / kT) / l^2$$

Anomalous Boron Diffusion in Silicon Processing

Anomalous Boron Diffusion in Silicon Processing:

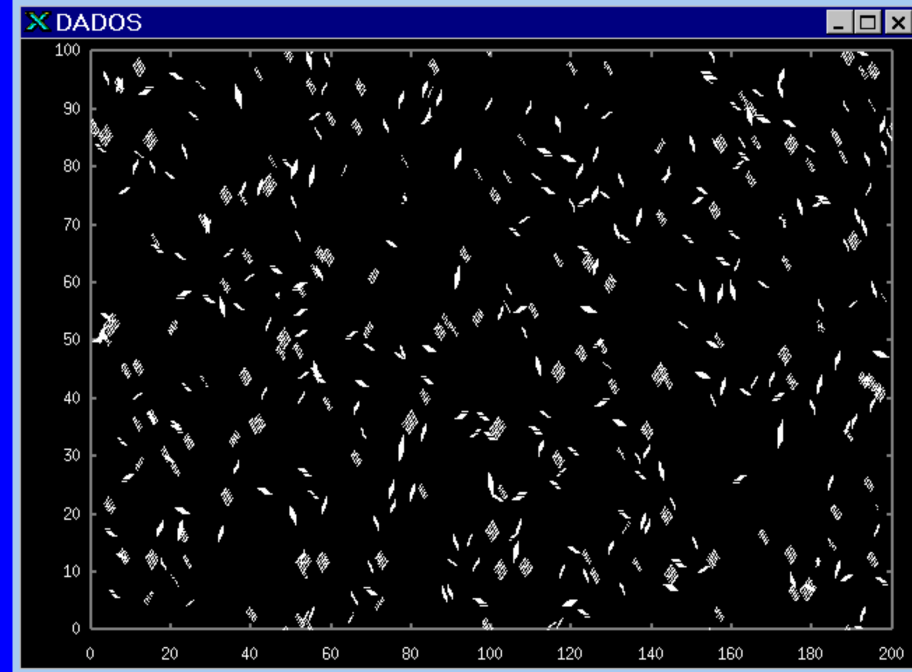
Experimental data (SIMS) and Kinetic Monte Carlo simulation



Appl. Phys. Lett. **70**, 2285 (1997)

Ion Implantation damage in Si: {311} self-interstitials Defects

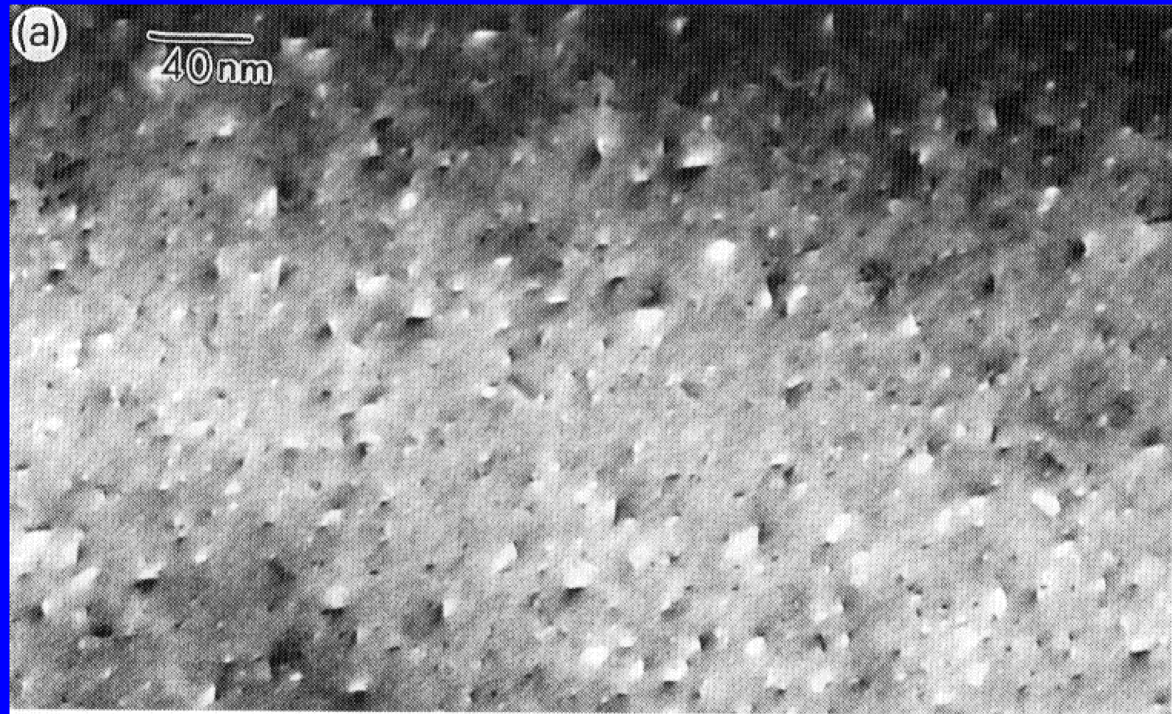
DADOS simulation



40 keV Si implant

after **5 seconds** at 800C

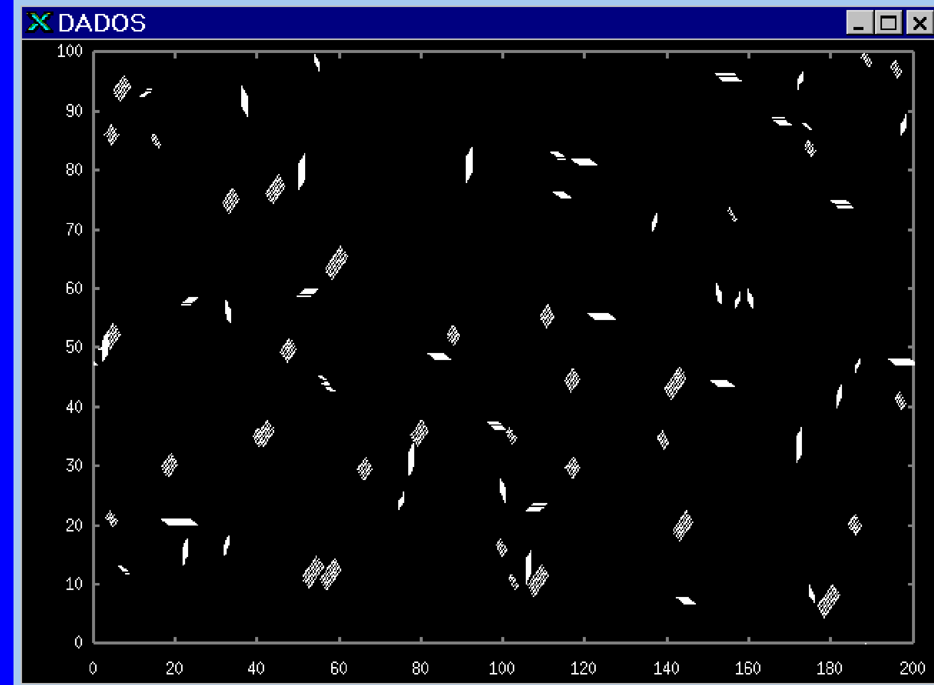
Experiment (TEM)



DADOS simulation

40 keV Si implant

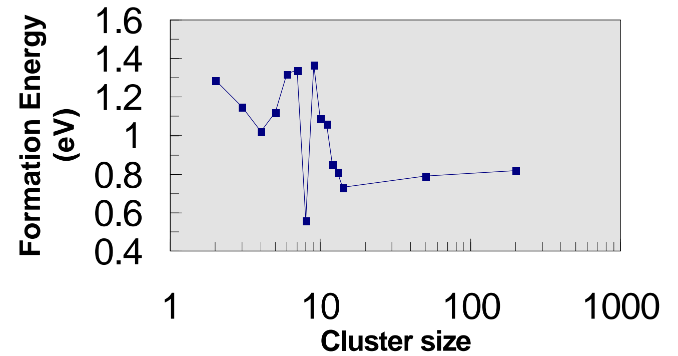
after **30 seconds** at 800C



Experiment (TEM)

Energetics of {311} Defects

Interstitial Supersaturation vs. Annealing Time



1.E+08
1.E+07
1.E+06
1.E+05
1.E+04
1.E+03
1.E+02

1.E+00 1.E+01 1.E+02 1.E+03 1.E+04 1.E+05 1.E+06

Experiment 600C
Experiment 700C
Experiment 800C
DADOS 600C
DADOS 700C
DADOS 800C

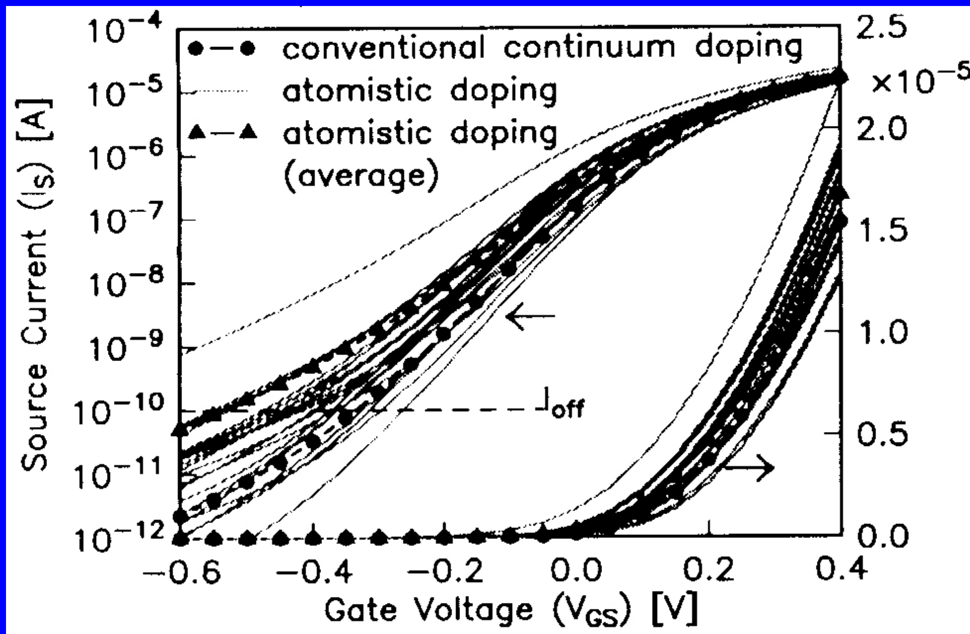
Cowern et al, Phys. Rev. Lett., in press

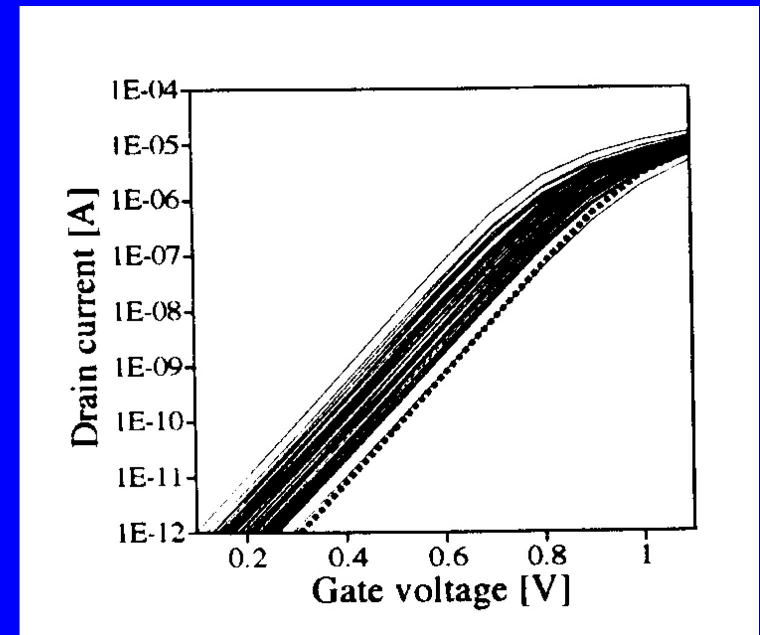
Dopant Fluctuations

Discreteness of Channel Dopants =>Average Shift of Threshold Voltage

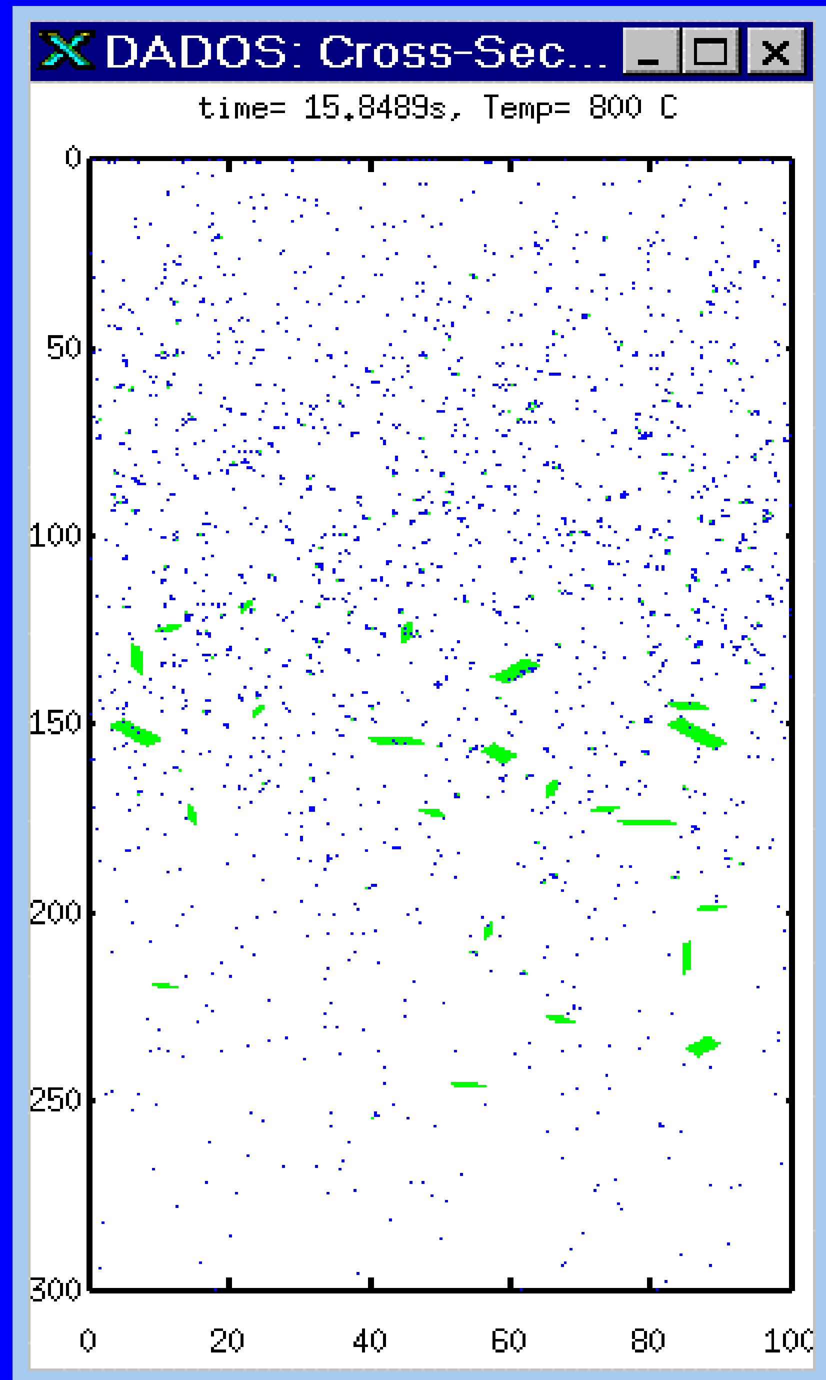
H.S Wong and Y. Taur, IEDM 93

A. Asenov, IEDM 98





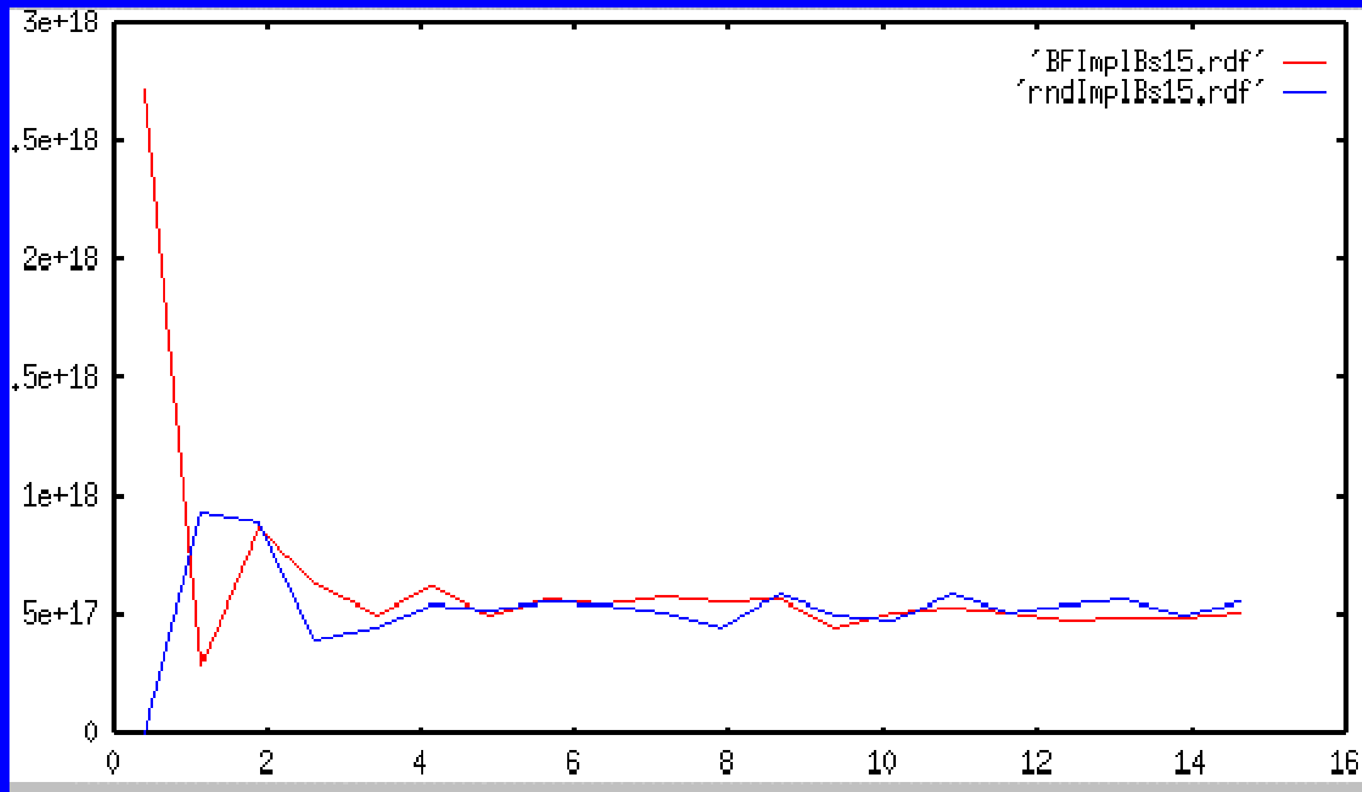
=> Do the local inhomogeneities due to clusters induce a spatial correlation in the dopant atoms?



Comparison between same dopant depth distributions generated:

- Randomly
- With the actual ion cascades

Radial Distribution Function



Blue: Random

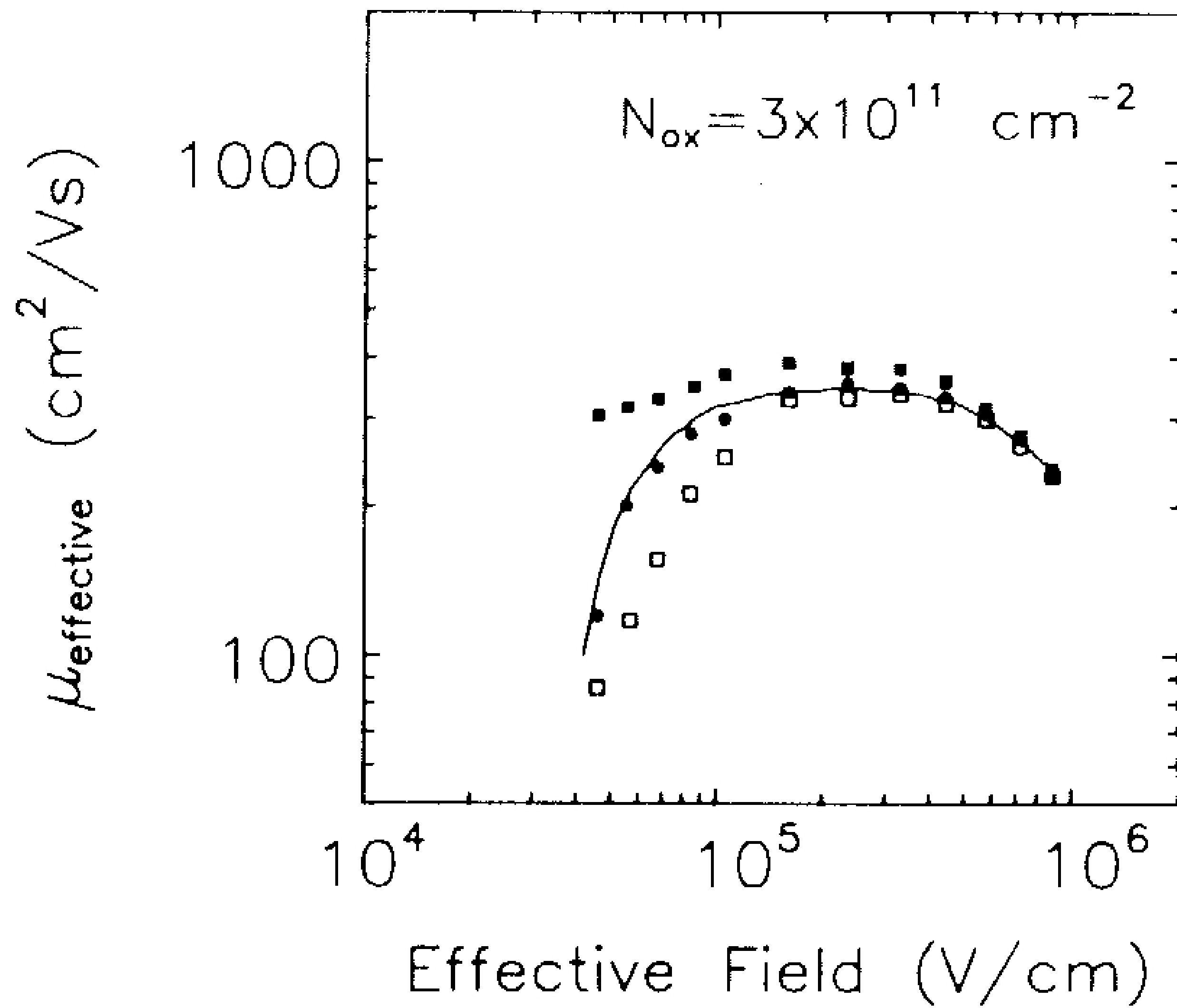
Red: Cascades

=> The diffusion process fully randomizes any local inhomogeneities due to clusters

However, diffusion of charged point defects could still give rise to space correlation (local fluctuations).

In fact, similar effects have been shown to occur in the oxide charge distribution in MOS structures => increase in the effective mobility.

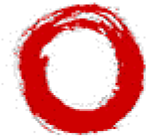
F. Gamiz et al., Semic. Sci. And Technol. 9, 1102-1107 (1994)

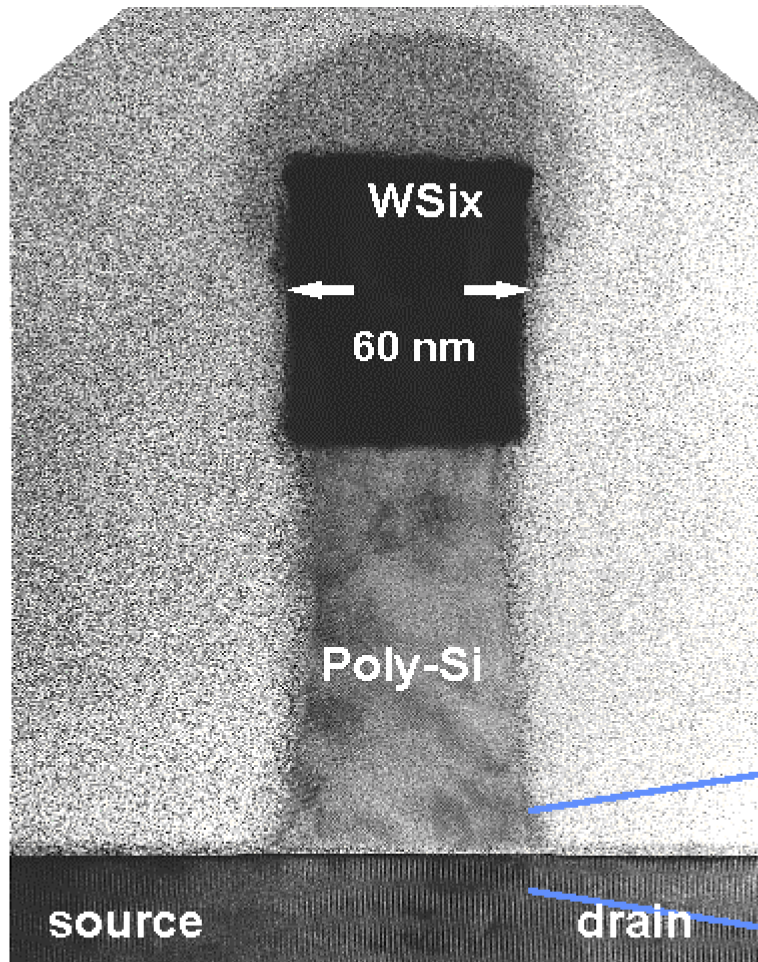


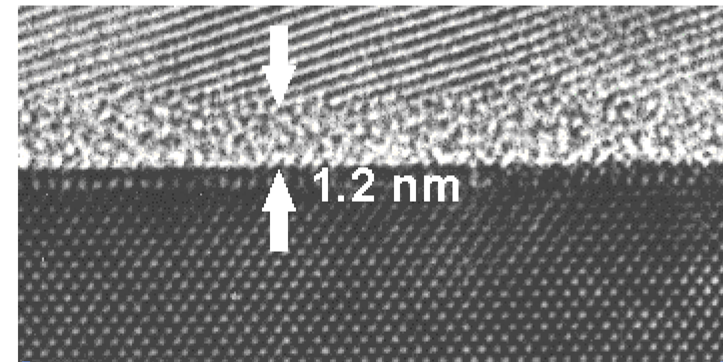
$N_{ox} = 3x10^{11}$ cm^{-2}
1000
100
$\mu_{effective}$ (cm^2/Vs)
10^4
10^5
10^6
Effective Field (V/cm)

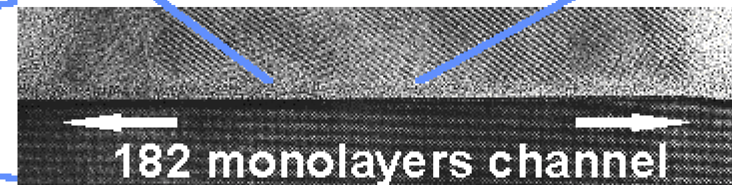
0.12 μm MOSFET

Towards sub-0.1 μm technology







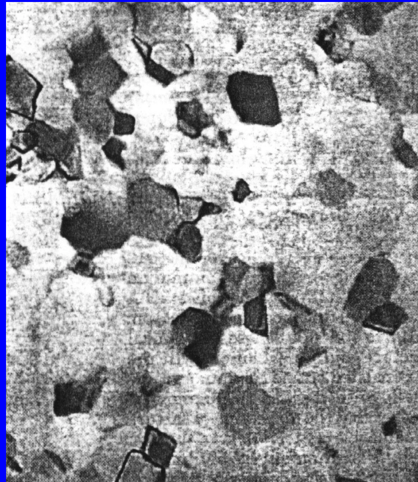


TEM micrograph: F. Baumann

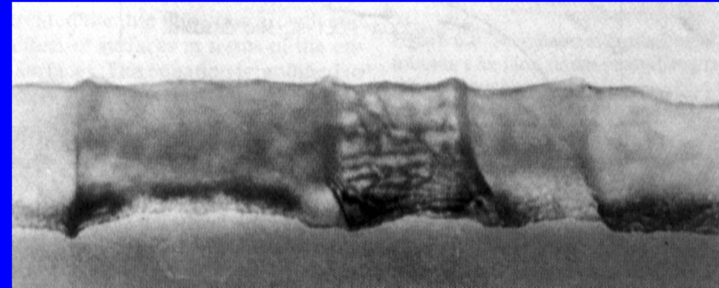
KINETIC <u>LATTICE</u> MONTE CARLO SIMULATION OF <u>POLYCRYSTALLINE</u> THIN-FILM DEPOSITION

INTRODUCTION

Aluminum: Polycrystalline structure



100 nm



0.5 μm

* Y-S Kang et al, J. Electron. Mater. 26, 805 (1997)
* S.P. Murarka, "Metallization", Butterworth-Heinemann, 1993

Microstructure of the deposited films during deposition and annealing:

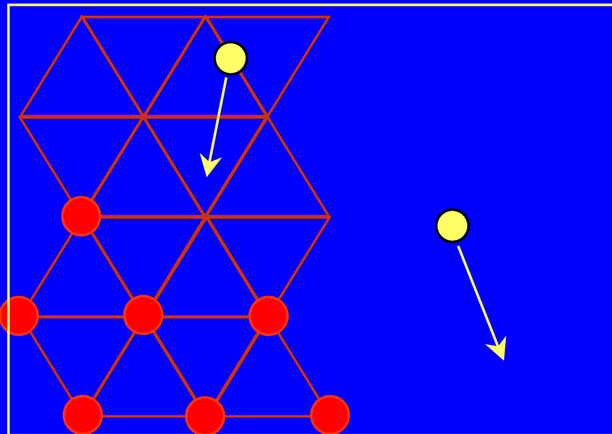
Grain sizes, surface texture

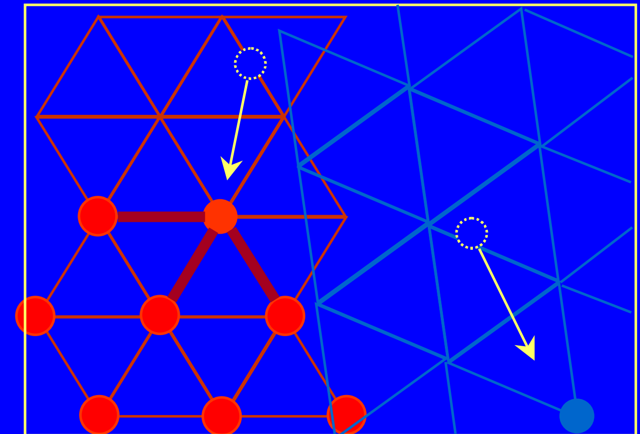
It depends on: temperature, deposition rate, substrate conditions

DEPOSITION

- Random initial position on the top of the simulation box
  Random velocity angles according to the desired angle distribution.

- Atom travels in a straight line until either:
  - It finds some neighbors:
    it finally get attached to the lower energy site
    in the neighborhood
  - It finds no neighbors: It starts a new orientation.





GRAIN BOUNDARIES

Jump to the Site which minimizes the energy:

Grain growth competition

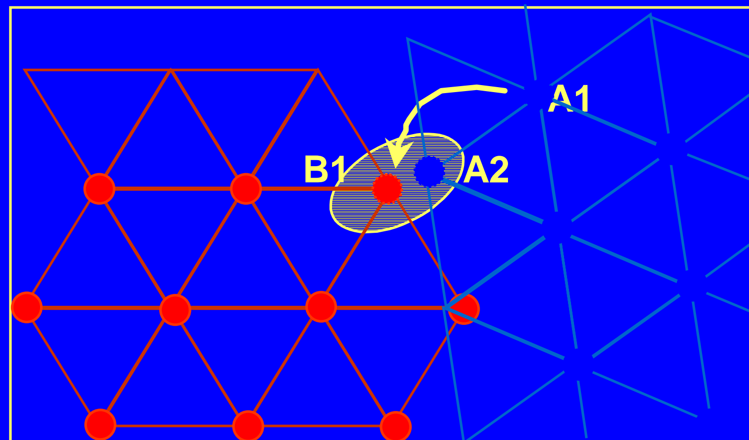
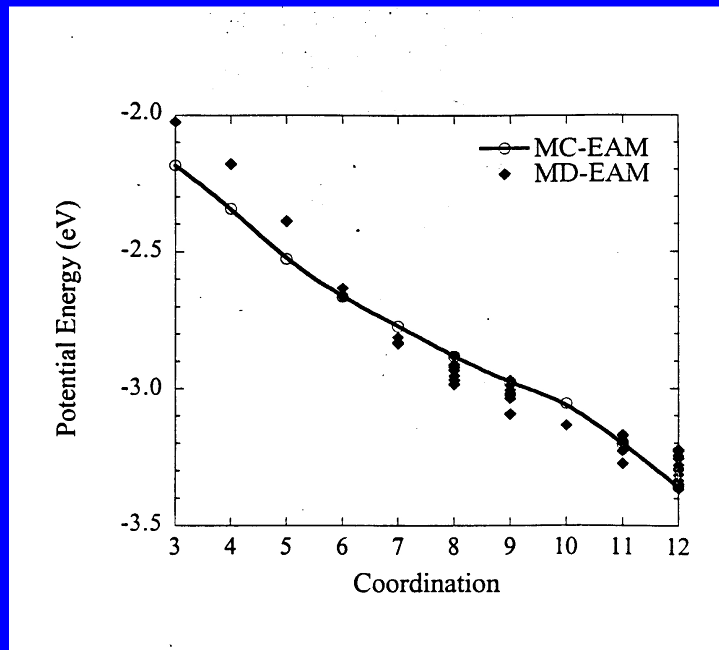


TABLE II. Prefactor (D_a^0) and migration energy (E_m) of each atom used in the MC model is given as a function of coordination (M_i) at the top; and self-diffusion coefficient (prefactor, D_s^0, and activation energy, Q) on three low index surfaces are given below. For comparison, results according to MD[a] and LDA[b] calculations are also listed. (The unit of the prefactor is cm^2/s, that of energy is eV.)

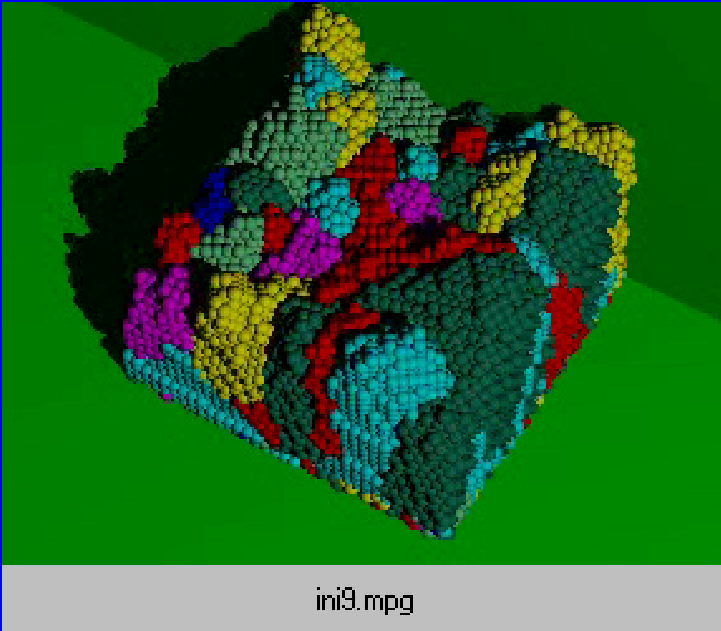
M_i	3	4	5	6	7	8	9	10	11
D_a^0	2.0×10^{-4}	4.0×10^{-1}	4.0×10^{-3}	1.0×10^{-2}	1.0×10^{-2}	1.0×10^{-2}	1.0×10^{-2}	1.0×10^{-2}	1.0×10^{-2}
E_m	0.10	0.33	0.33	0.60	0.60	0.60	0.60	0.60	0.60

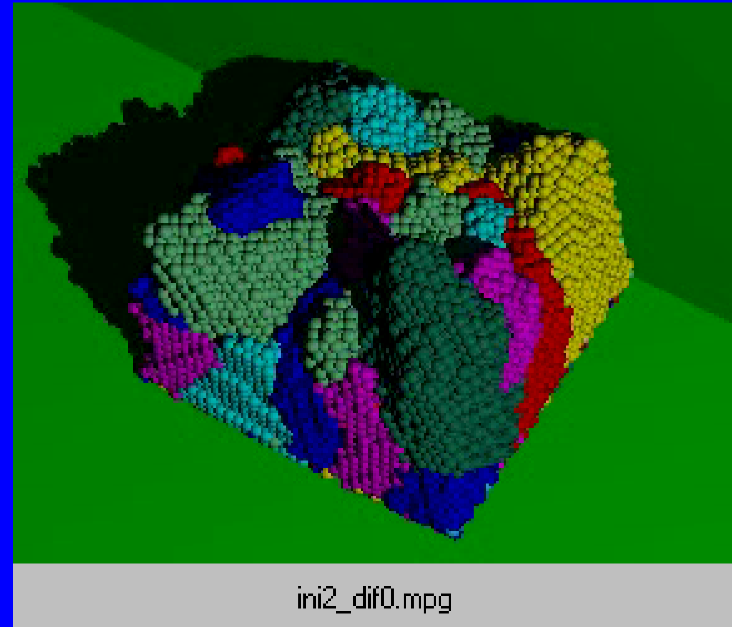
Diffusion \ Surface	(111)			(100)			(110)		
	MC	MD	LDA	MC	MD	LDA	MC	MD	LDA
D_s^0	2.0×10^{-4}	4.3×10^{-4}	2.0×10^{-4}	4.0×10^{-1}	4.0×10^{-4}	8.0×10^{-3}	4.0×10^{-3}	4.4×10^{-3}	1.0×10^{-2}
Q	1.04	1.02	1.09	0.97	0.68	0.73	0.56	0.56	0.57

[a]Reference 16.
[b]Reference 14.



SIMULATION RESULTS

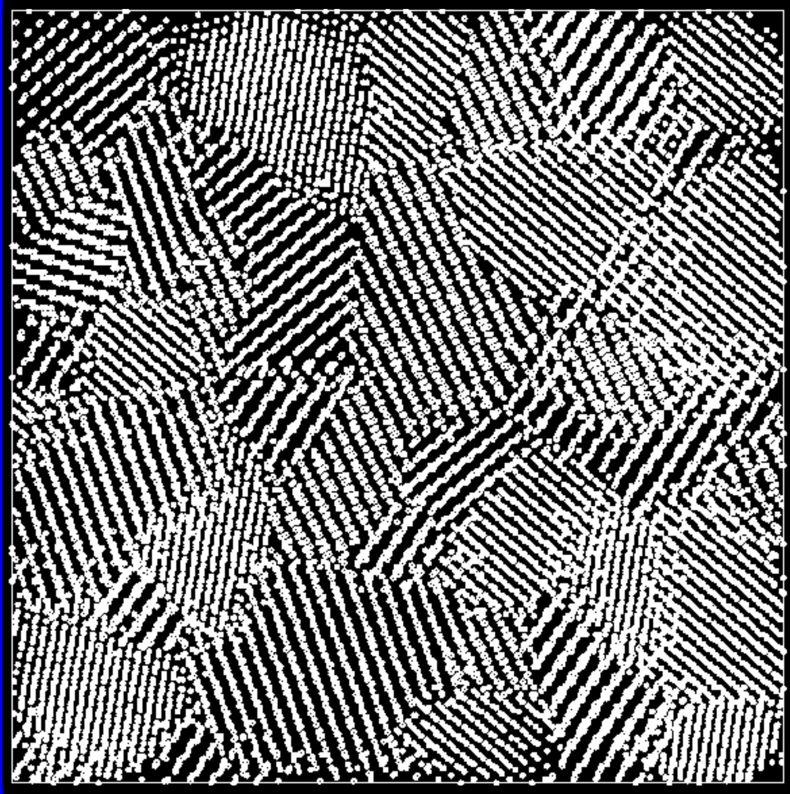




"Wetting substrate"
(Strong bonding)
=> smaller grains

"Non wetting substrate"
(Weak bonding)

Bonding to substrate:
effect on the grain size



“Wetting substrate”
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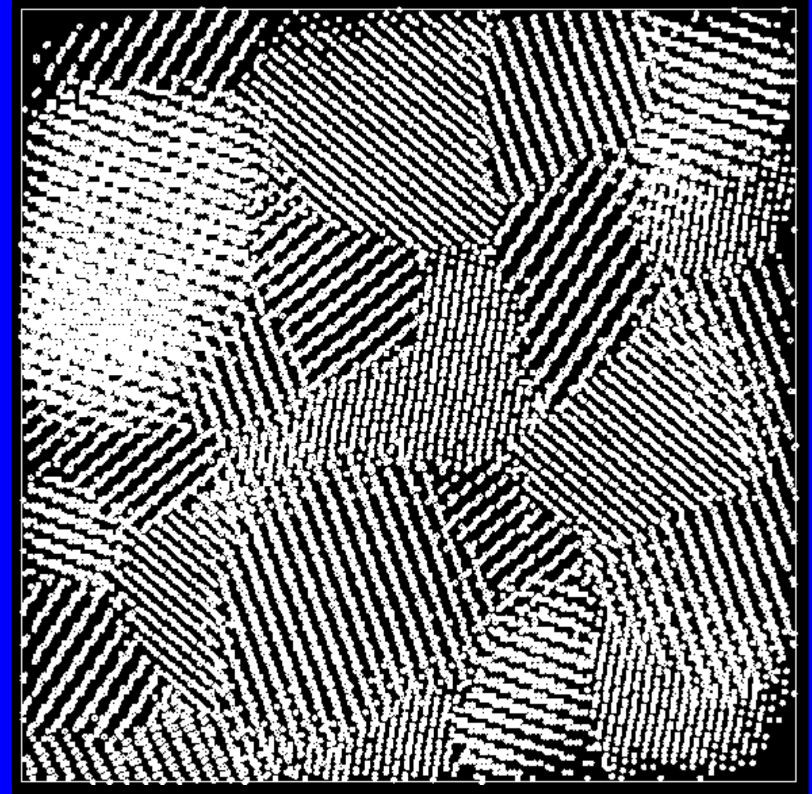


“Non wetting substrate”
(Weak bonding)

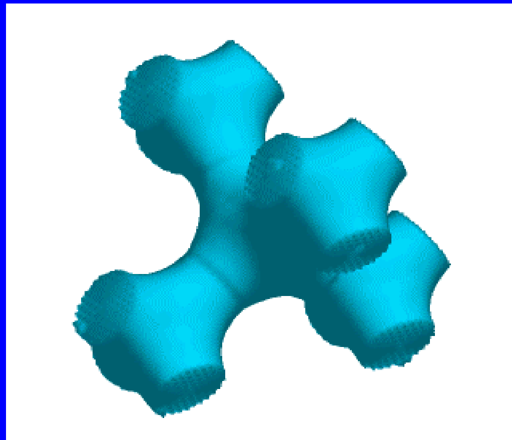
Channeling Implants:

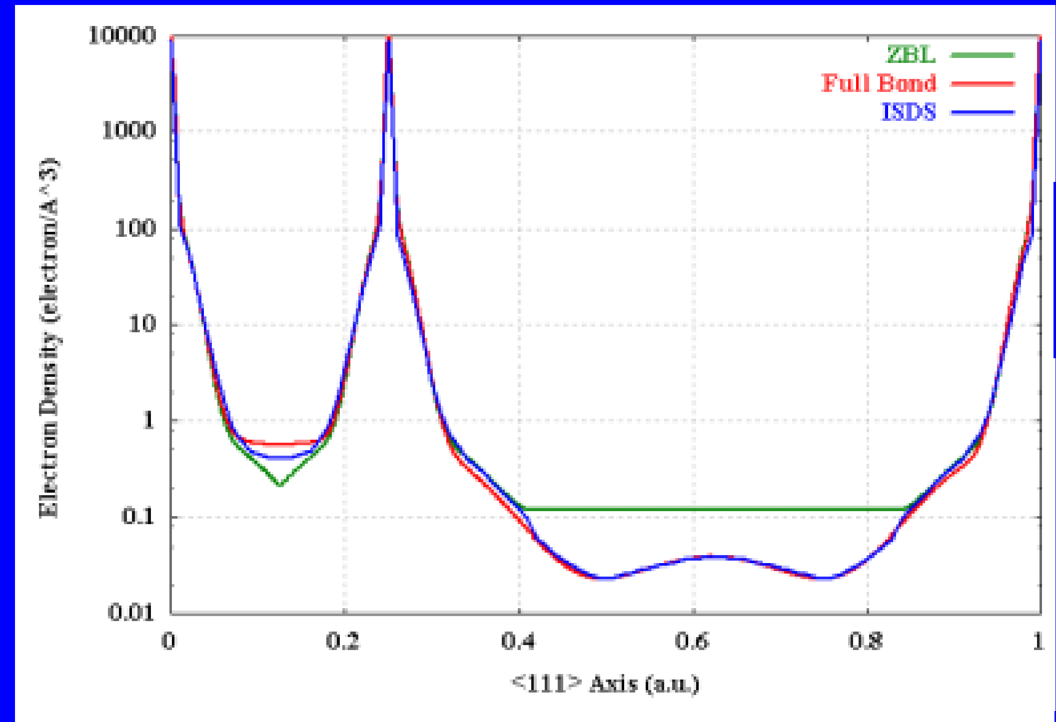
Relevance of the Electron Density Distribution

Channeling Implants:

Relevance of the Electron Density Distribution

- ZBL(Hartree-Fock)
- LDA
- LDA, radial

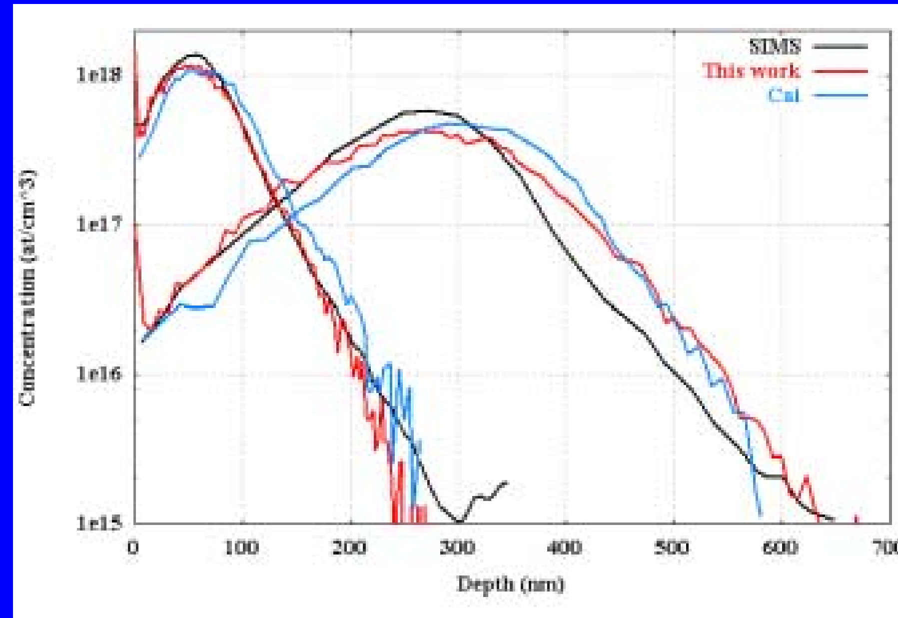


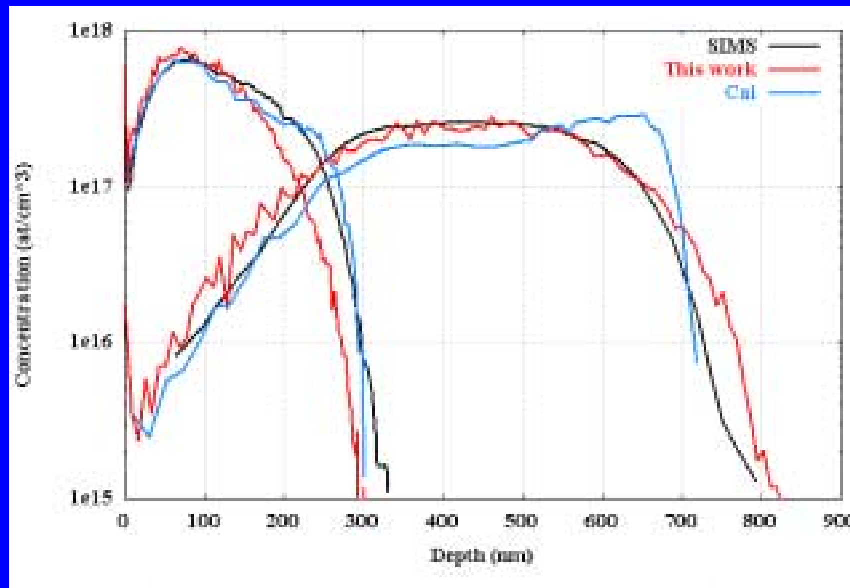


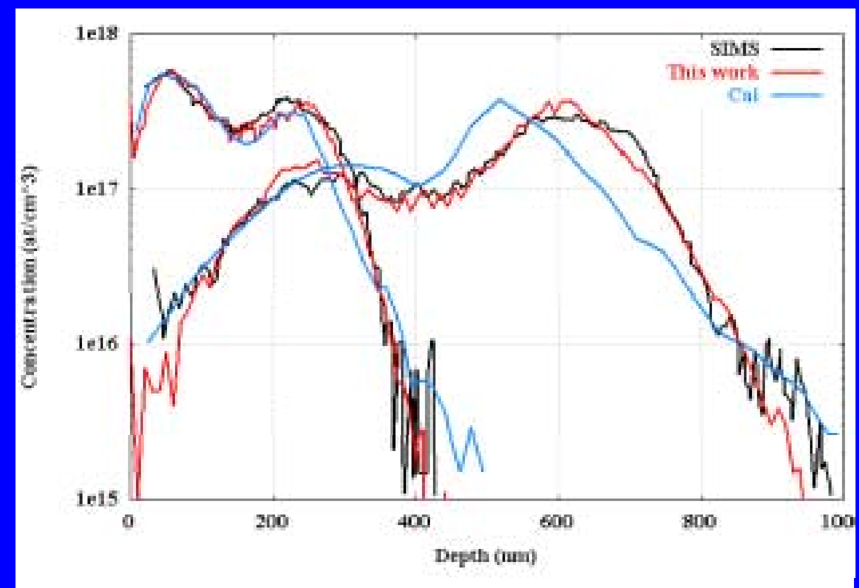
— SIMS

— This Work

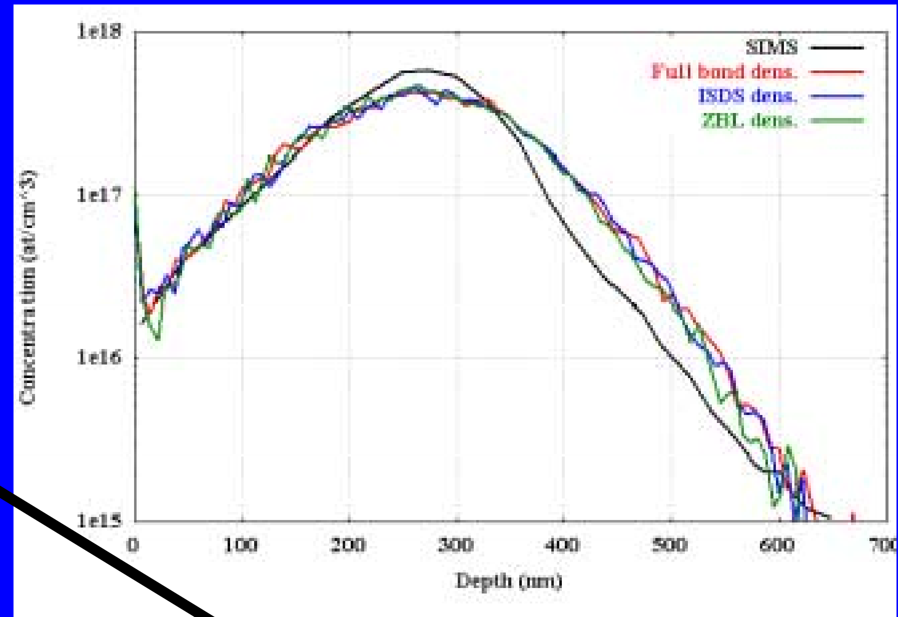
— Cai et al., Phys. Rev. B54, 17147 (1996)

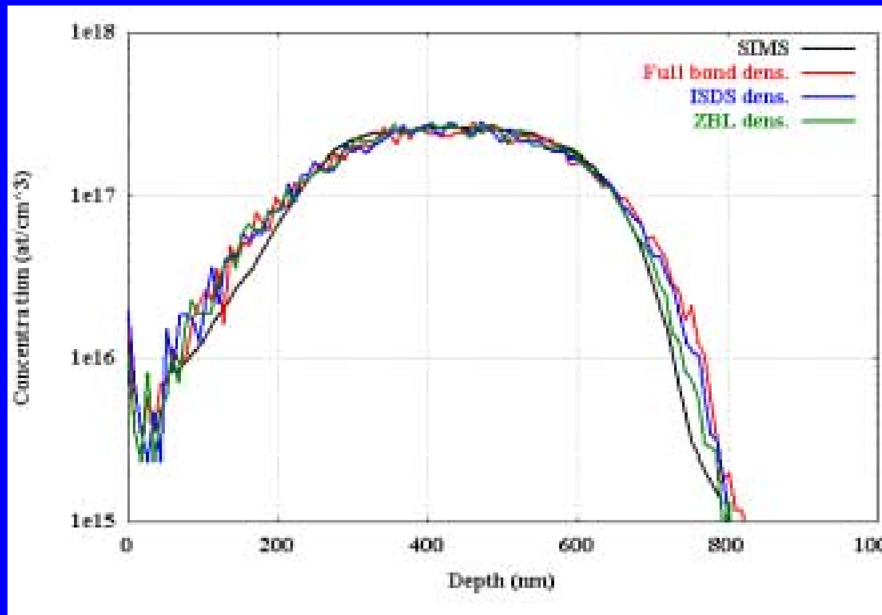


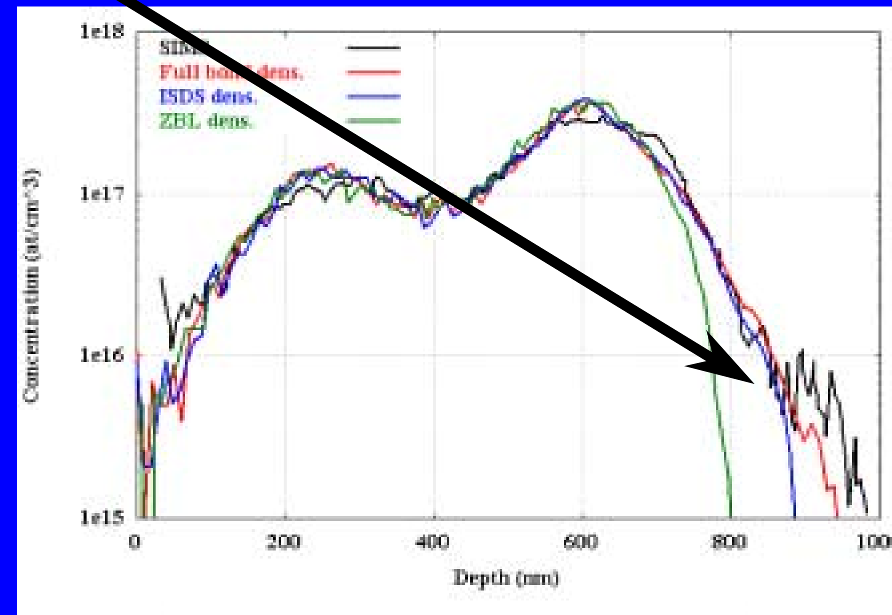




- SIMS
- LDA
- LDA, radial







Conclusions

- **Atomistic Process Simulators provide a bridge between ab initio calculations and standard process experimental data.**
- **Efficient and accurate 3D simulation.**
- **Straighforward implementation of new mechanisms.**
- **Microelectronics Device Processing: "Continuum physics models are no longer sufficient below 100 nm. Tools are needed for the physical and chemical processes at an atomic level"** (1997 USA National Technology Roadmap for Semiconductors)