# Current Capabilities
and
# Future Prospects
of
# Atomistic Process Simulation


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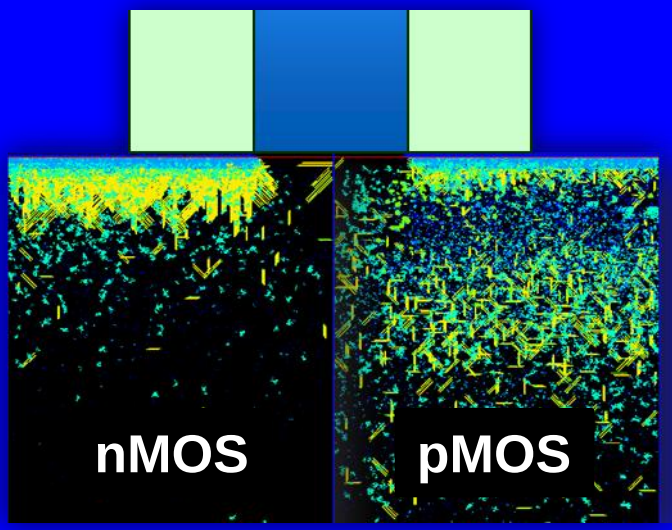
# Recent collaborators

- ***Univ. of Valladolid:***
  - Pedro Castrillo
  - Ruth Pinacho
  - Jose E. Rubio
- ***Synopsys:***
  - Ignacio Martin-Bragado
- ***Chartered:***
  - Caroline Mok
- ***NXP:***
  - Julien Singer

# Outline

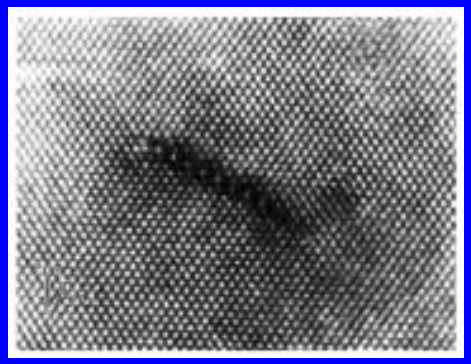
- The atomistic Kinetic Monte Carlo (KMC) scheme
- Atomistic KMC: Current capabilities
- Recent developments
- Prospects of Atomistic Process Simulation
- Conclusions

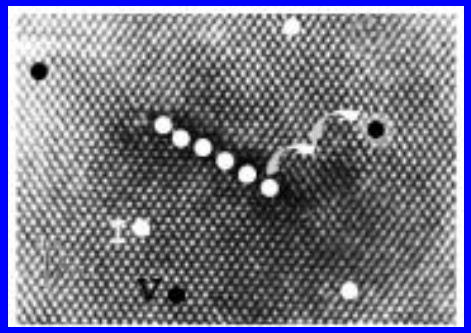
# Why Atomistic?

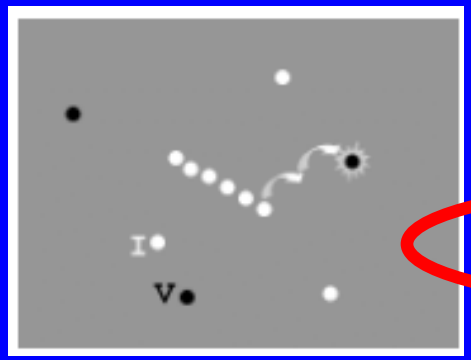



- Complex processing conditions: Many different, simultaneous, non-negligible mechanisms
- Detailed: Direct input from ab-initio parameters, facilitates model calibration
- Predictive: physically-based simulations
- Like fabrication, KMC simulates individual devices (accounts for Variability)
- … and is now feasible (small devices)

# The Atomistic KMC Approach






**Lattice** atoms are just vibrating

But only **defect** atoms move (diffusion hops)

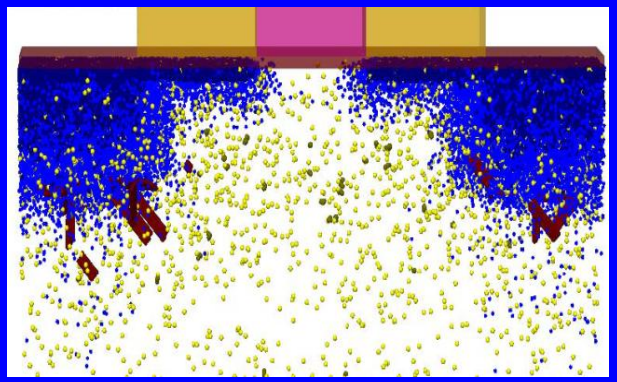
So, KMC follows defect atoms **only**

**Δt: ps … hours**

**Molecular Dynamics:**

**Δt ≈ 1E-15s**

**KMC output**



# Atomistic KMC capabilities

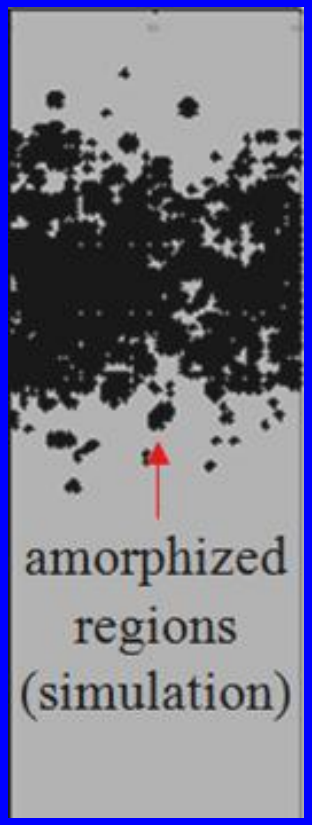
# Damage model: highly adaptive

- Accumulates I's & V's as agglomerates.
- These agglomerates behave both as Amorphous Pockets and Clusters, and have size-dependent activation energies.
- Amorphization: When local damage concentration reaches a threshold value.

# Implant damage - Amorphization

## Realistic

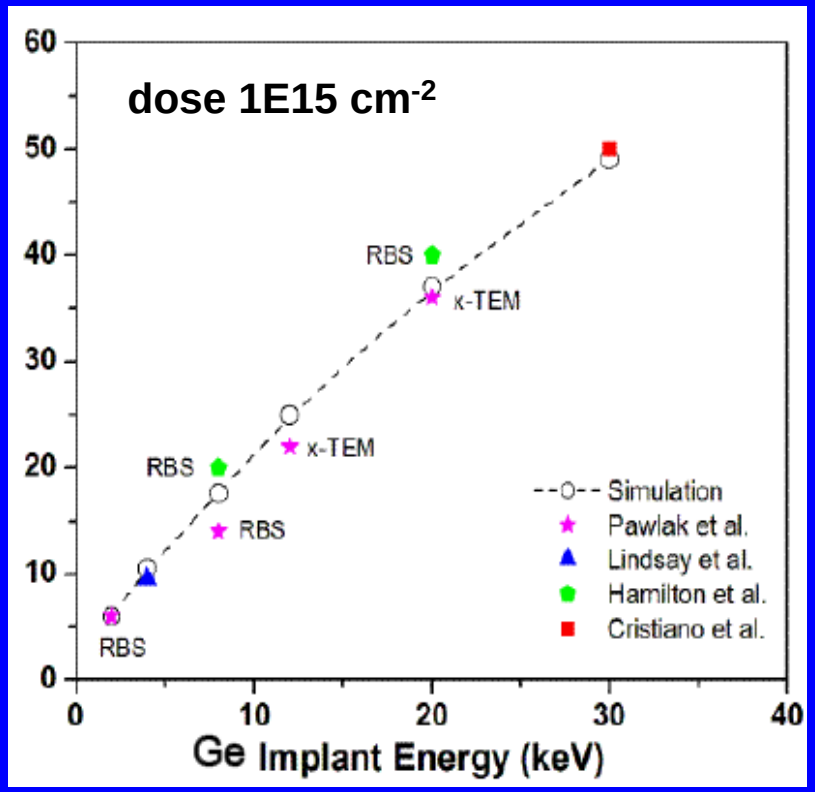
Simulation




Experiment


## Accurate

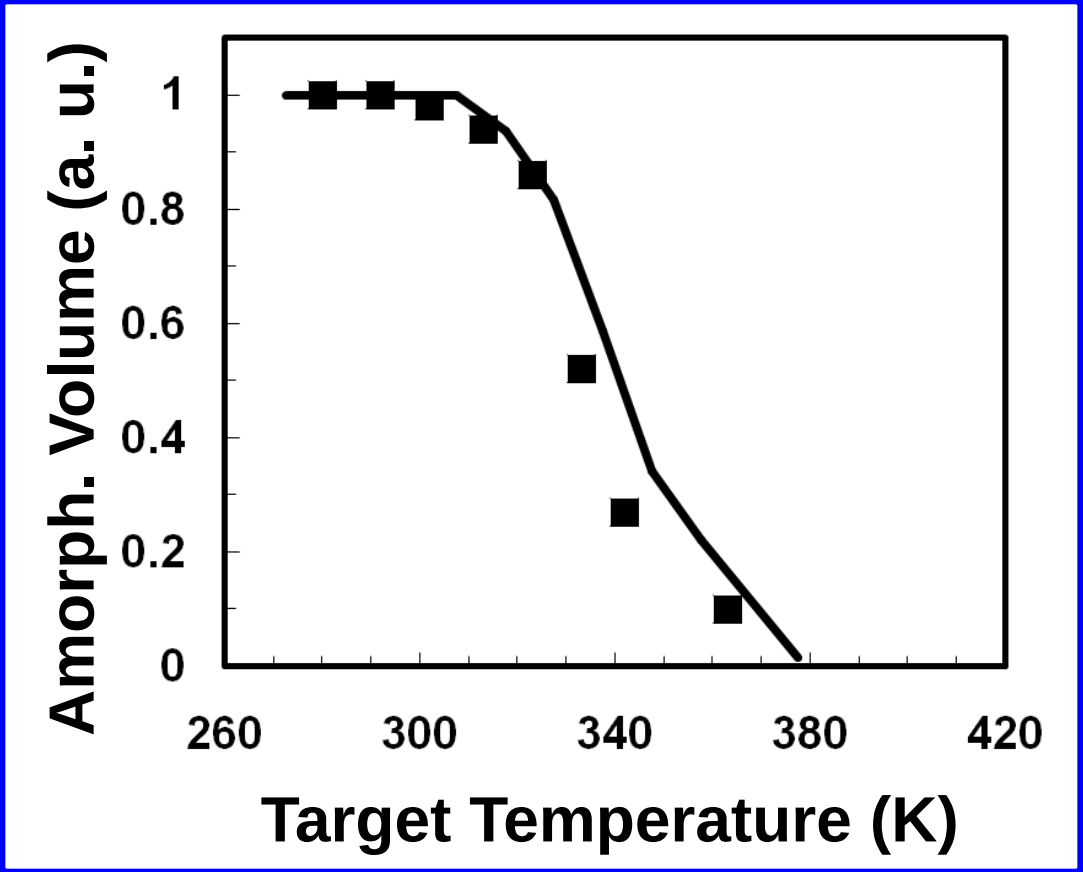
Amorph. Depth
vs. Implant energy



# Amorphization vs Target Temperature

**Accurate**

**Si, $1 \cdot 10^{15}$ cm$^2$**
**$3.57 \cdot 10^{12}$ cm$^2$/s**



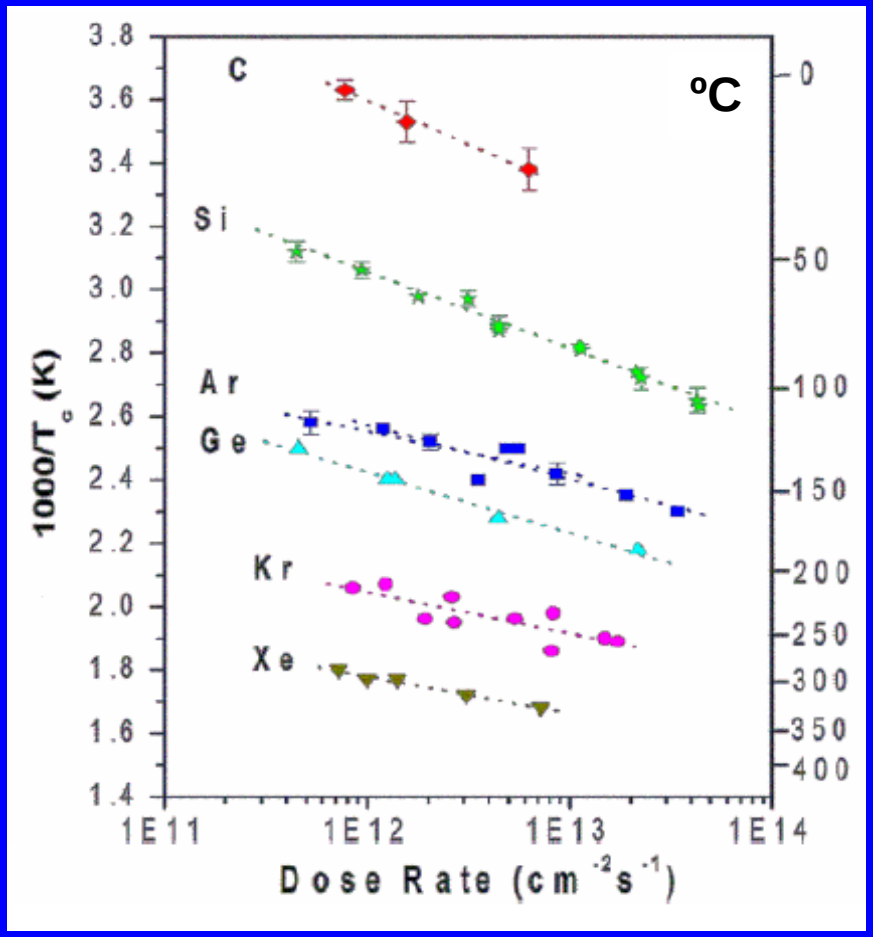

Symbols: Experim. (RBS)
Lines: Simulat.

# Amorphization: Dose rate & Temp.

**Accurate**

**Amorphization Temperature**
**vs.**
**Dose Rate**

(Dose = 1E15 $cm^{-2}$)

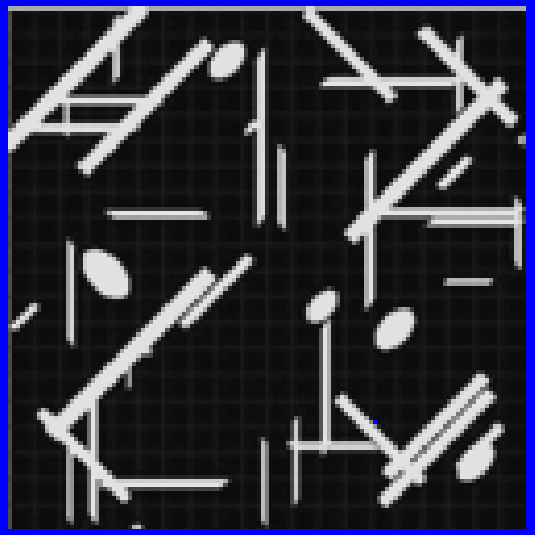



Symbols: Experim.
Lines: Simulat.

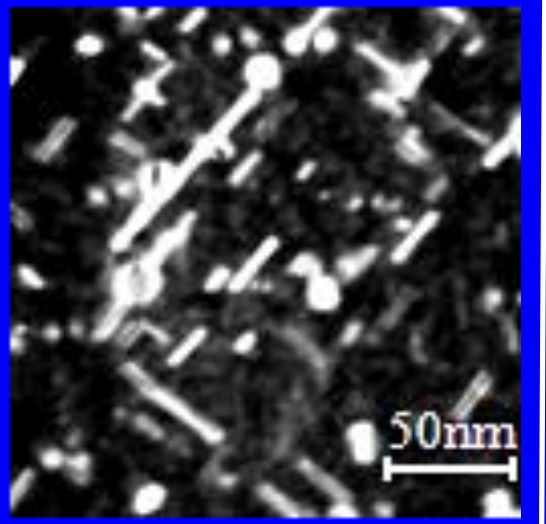
# Damage anneal: Extended defects

## Realistic

Simulation

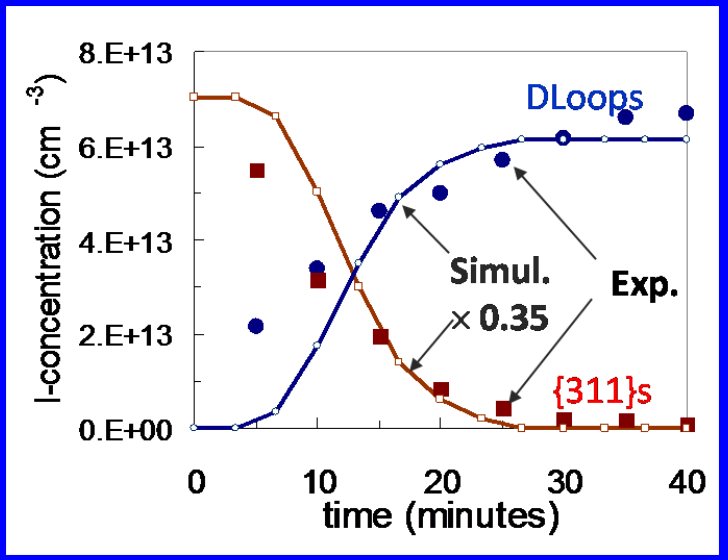


Experiment




## Accurate

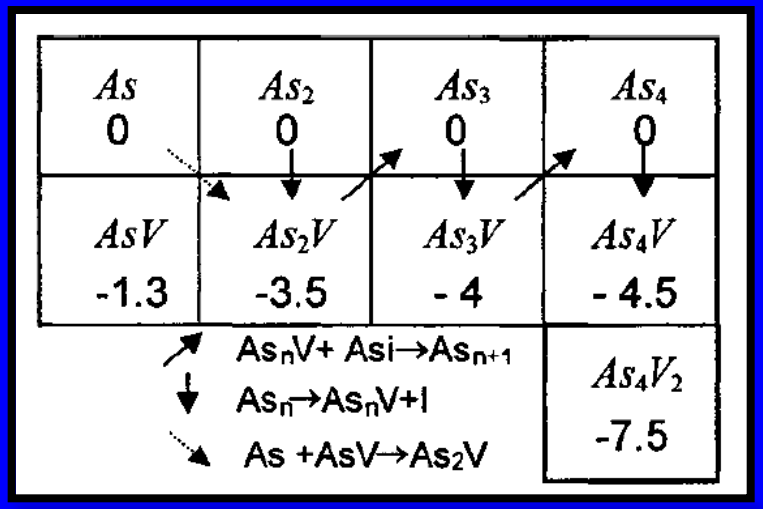
311's & DLoops vs. annealing time

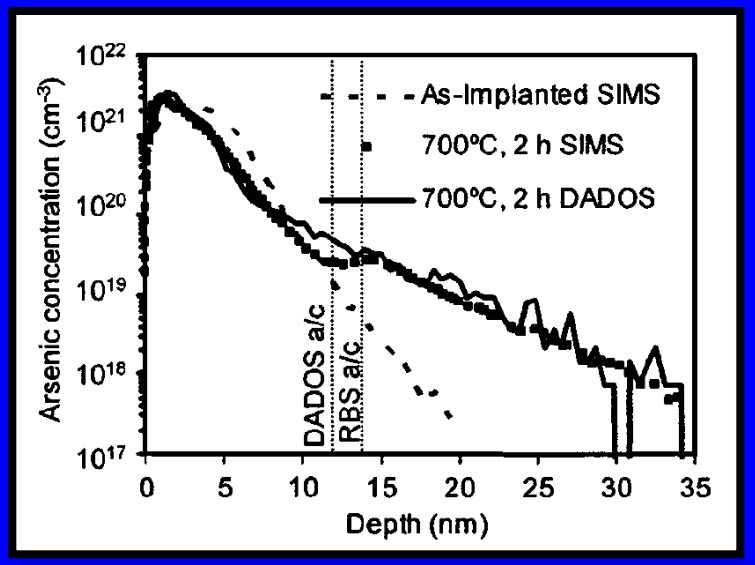



It's important to predict 311→DLoop transition because thermal budget can change considerably

# Dopant clusters: Activation / deactivation

**as many cluster compositions as needed**



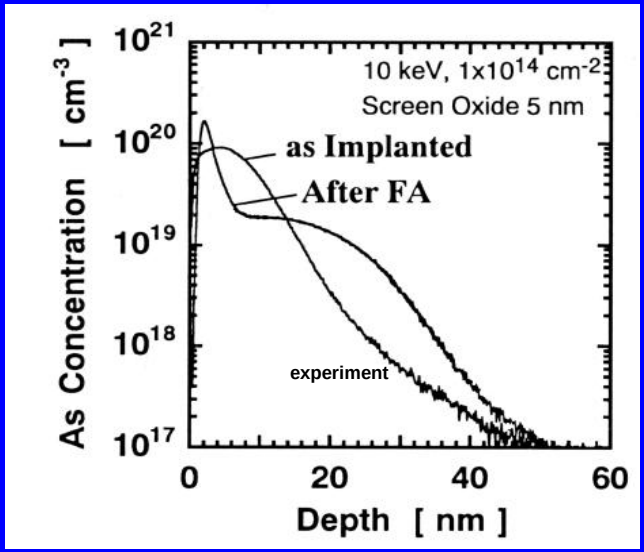



# Interfaces: trapping and segregation

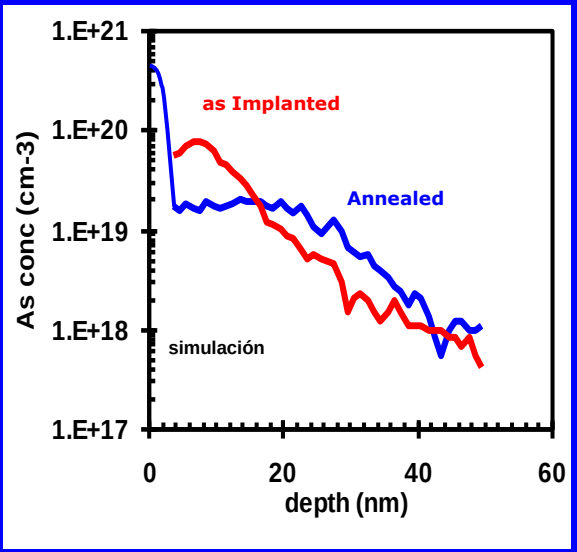
**Dose loss** cannot be neglected for small volume devices

- **Multiple species (B, As…)** simultaneously
- Combined Interface **saturation** level

Experiment



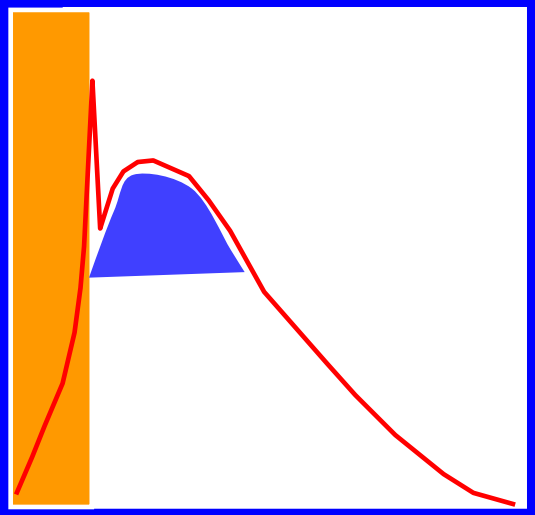

Simulation




- Also reproduces Energy, Dose and Time dependencies

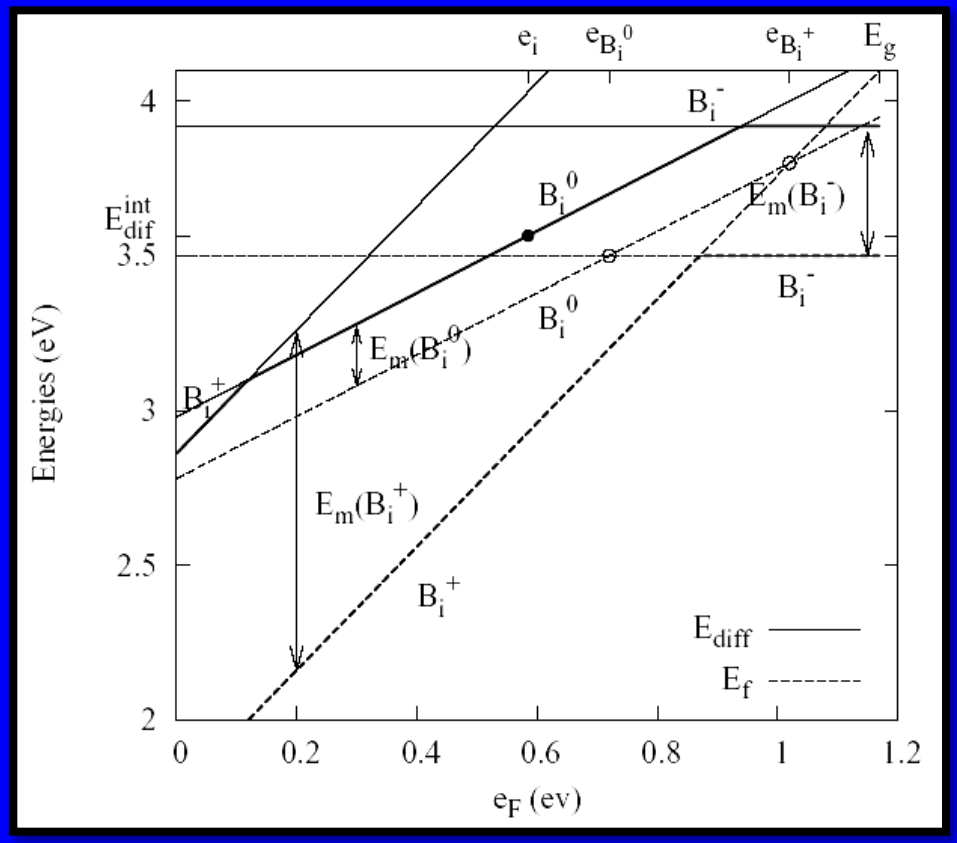
# Recrystallization, impurity sweep

1. Recryst. front moves with thermally activated velocity
2. Controlled trapping/deposition of impurities (snow plow)
3. Above solubility: Deposits minimum-energy impurity clusters



# Charge levels

- Each state implemented as a separate particle:
- Example: $B_i^0$, $B_i^+$, $B_i^-$



# Field effects

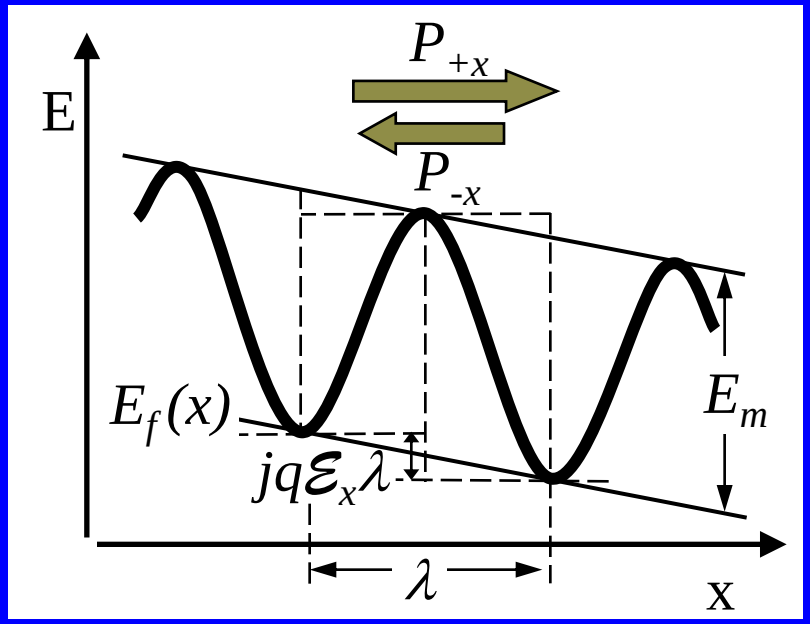
**Fields due to:**

- **Electric Charge**
- **Ge composition**
- **Stress (anisotropic)**

**Formation-energy gradient: different jump probabilities**

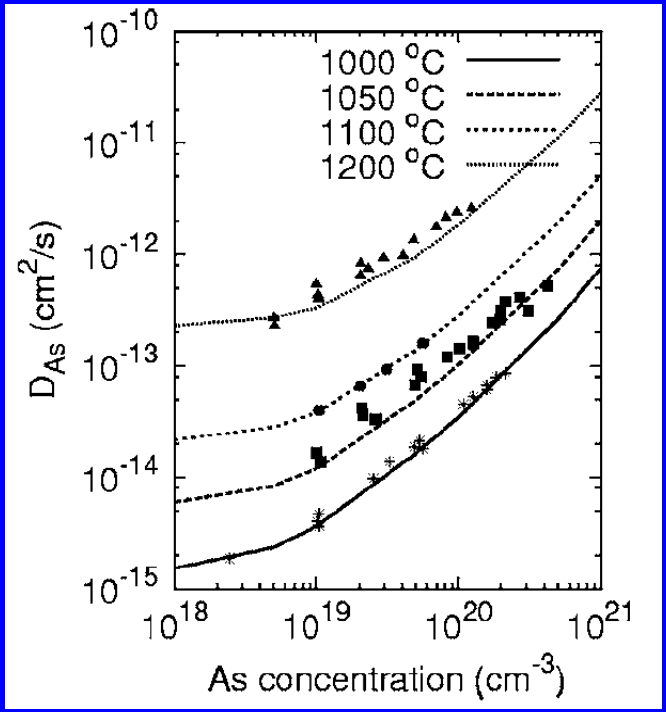
**Example: Electric field**

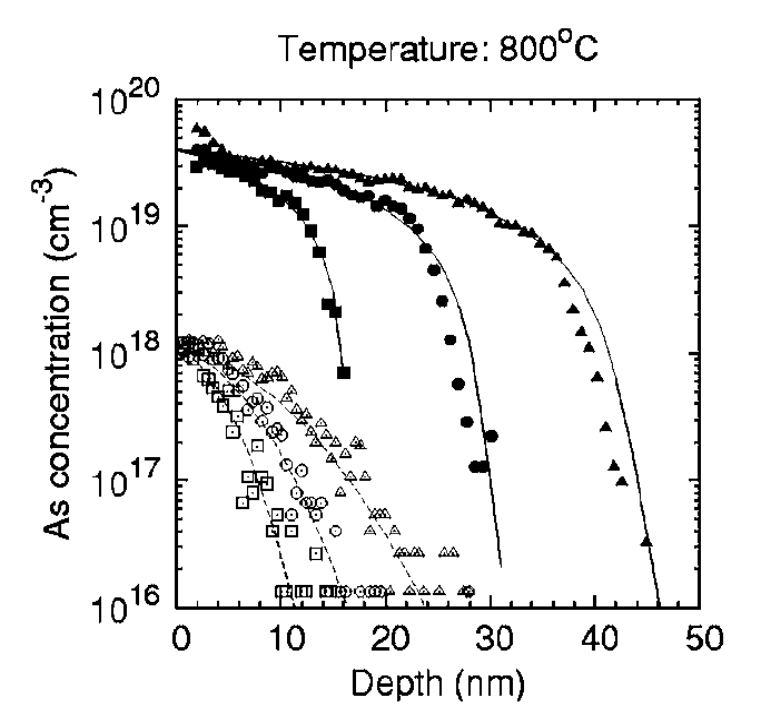
$$\frac{P_{+x}}{P_{-x}} = \exp\left(\frac{jq\mathcal{E}_x\lambda}{k_BT}\right)$$



# Fermi level effects

**Excellent agreement with experimental diffusion data, under intrinsic and extrinsic conditions**



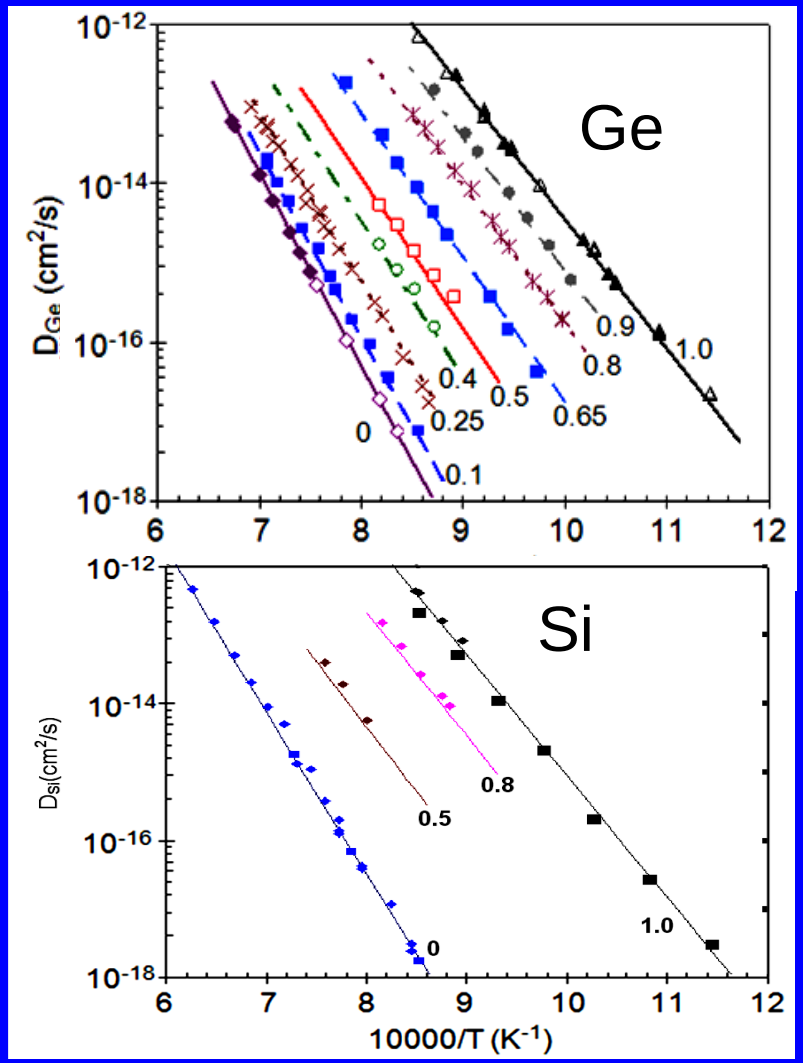
# Recent progress

# Si-Ge interdiffusion: Atomistic implementation

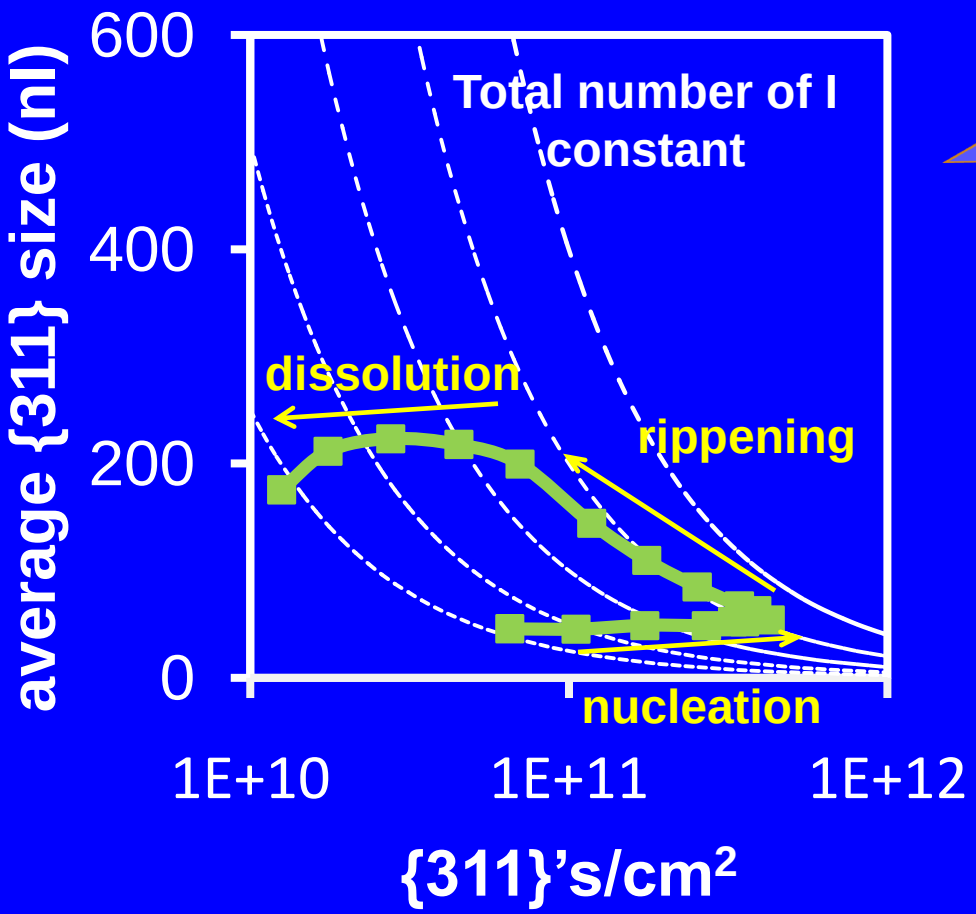
- Different probability for an I or V to move a Si or a Ge atom
- Thus, I or V supersaturation effects are automatically accounted for
- Dopants: $D_B \propto DC_I$, $D_{Sb} \propto DC_V$

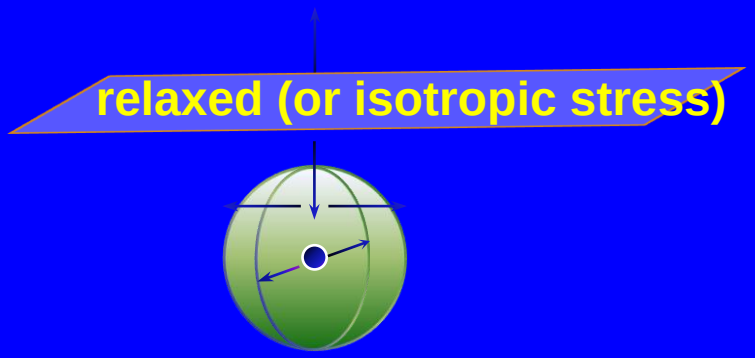
# Si-Ge interdiffusion: Atomistic implementation

- Excellent agreement with experimental self-diffusivities for all Ge compositions
- Provides a means for calibration of I, V parameters in SiGe

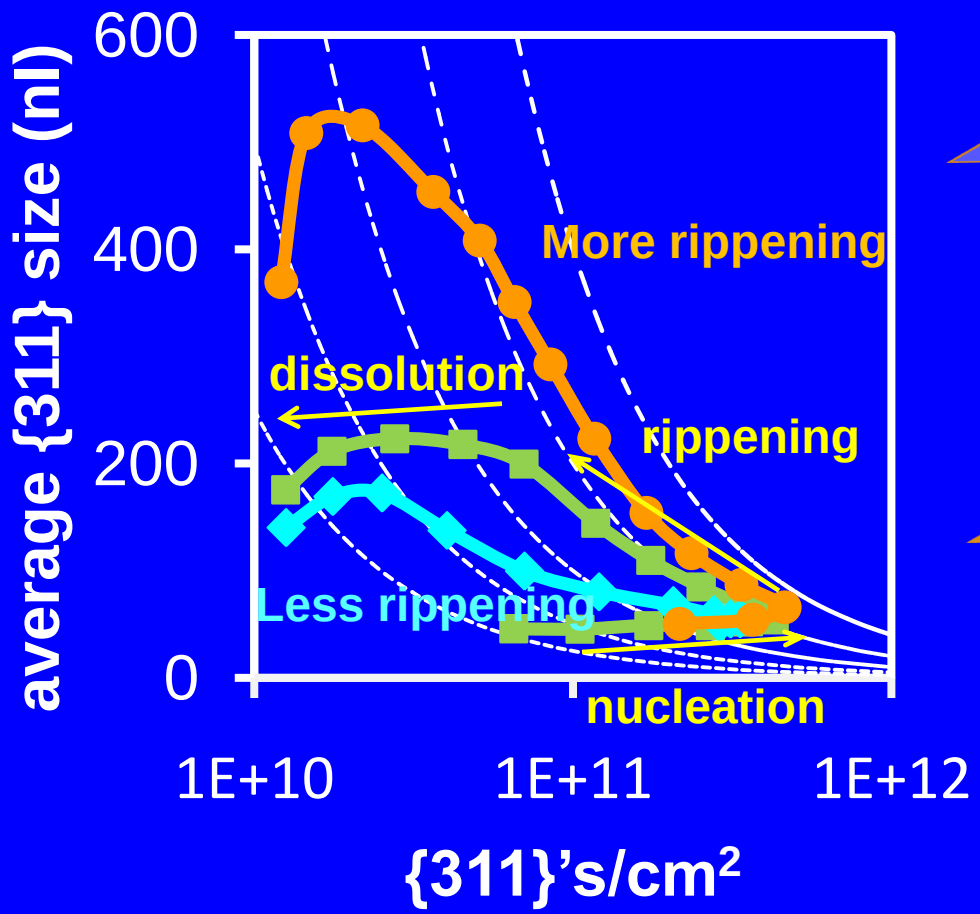


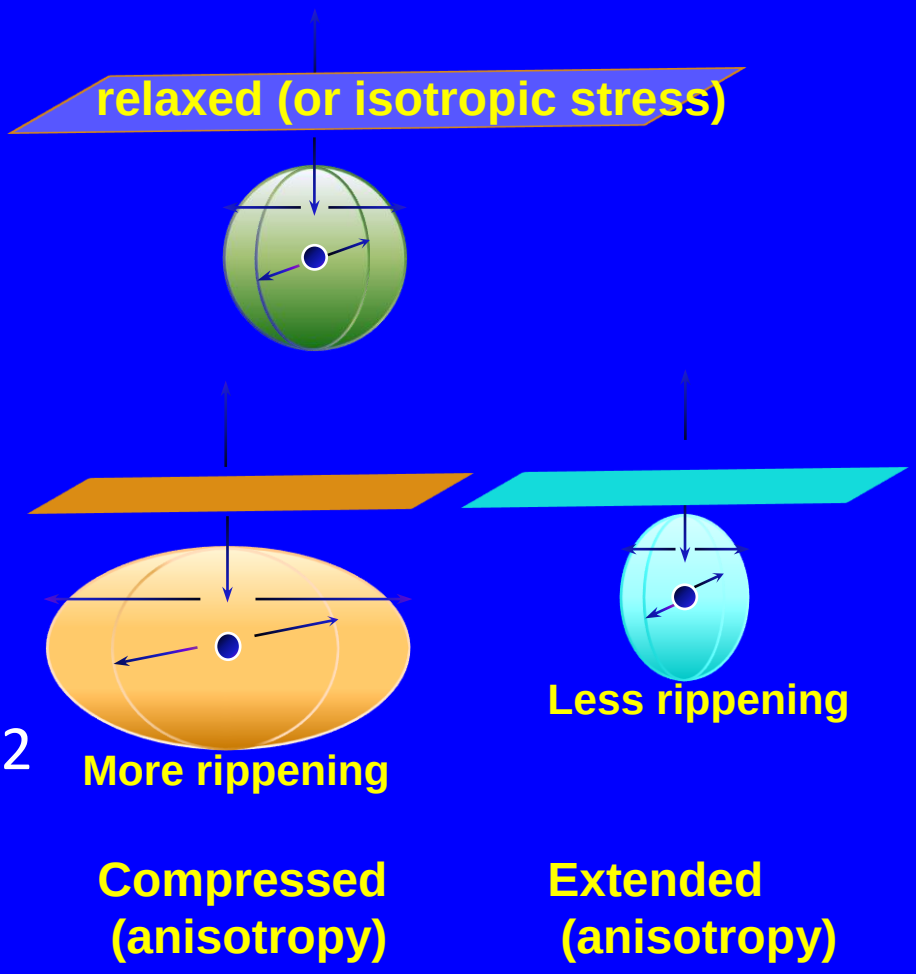
# Effect of anisotropy on {311} ripening



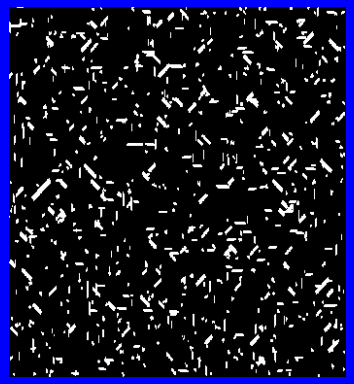



# Effect of anisotropy on {311} ripening

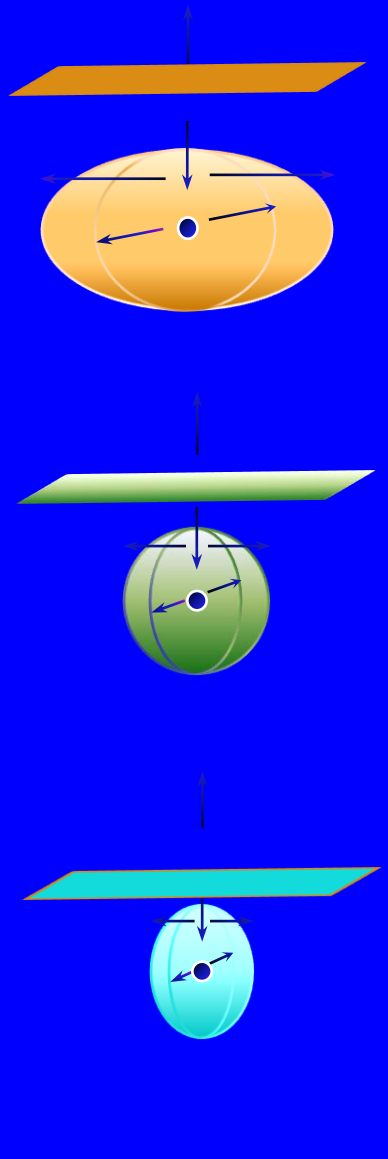


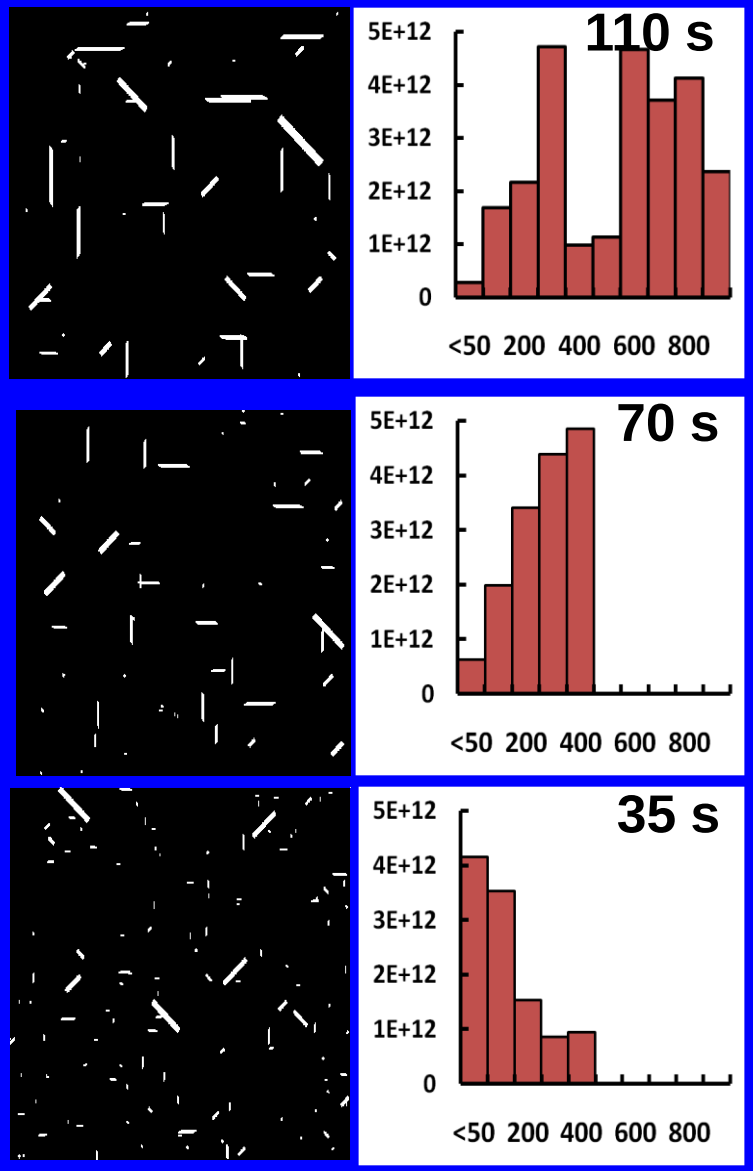
# Test for strain-induced I-diffusion anisotropy



Remarkable effect on {311} ripening: **suggests a test for strain-induced I-diffusion anisotropy**



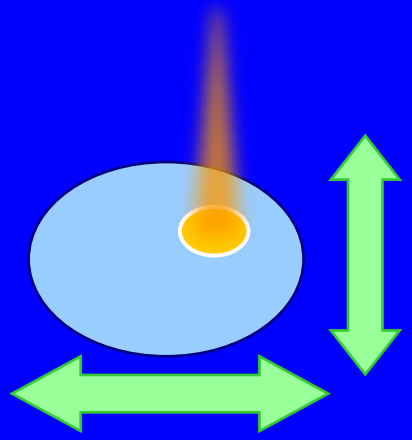
Dissol. time const.



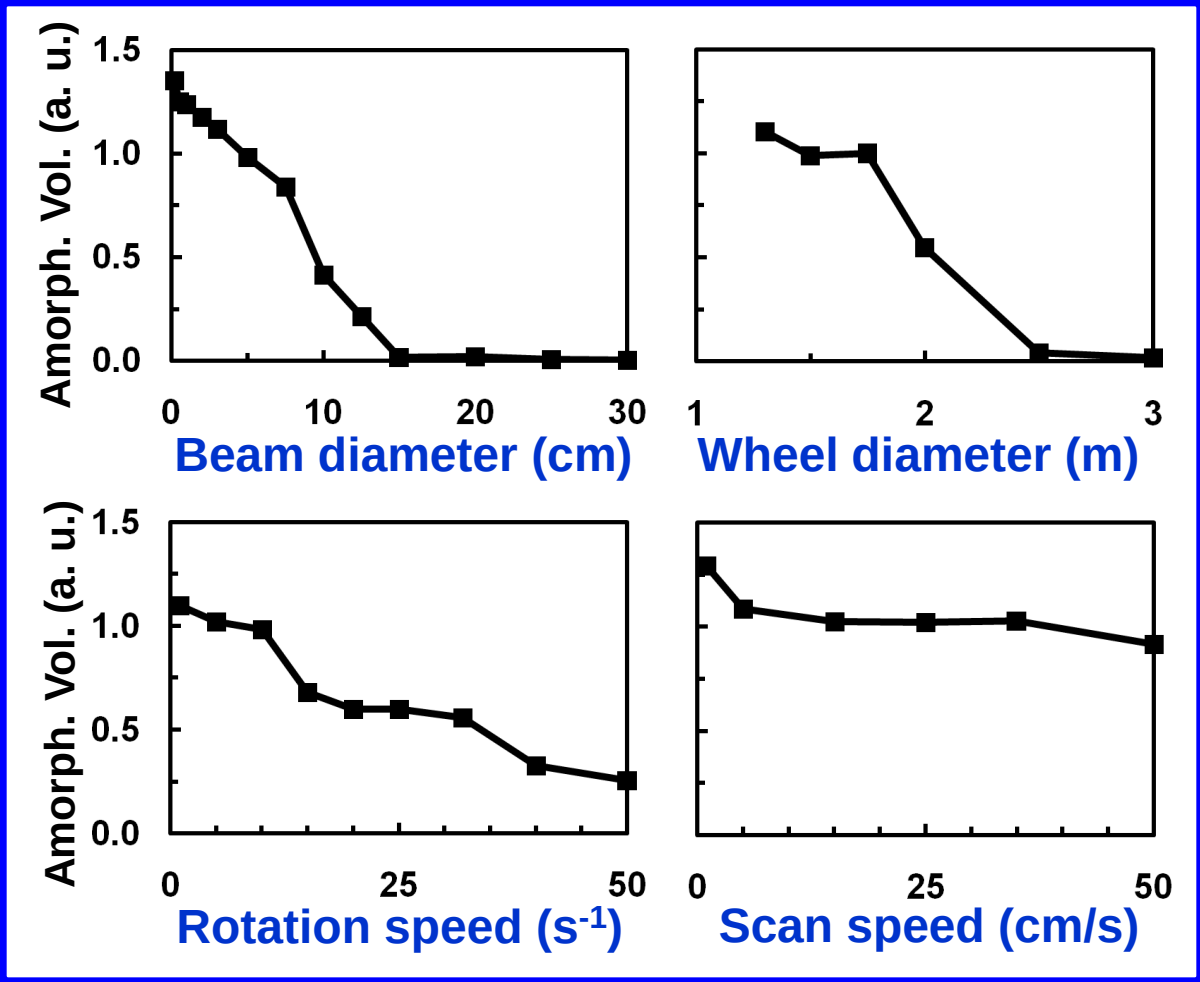
# Implanters: Batch

30 KeV, $1\times10^{14}$ $Ge^{+}/cm^{2}$, 90°C

Batch – spot beam



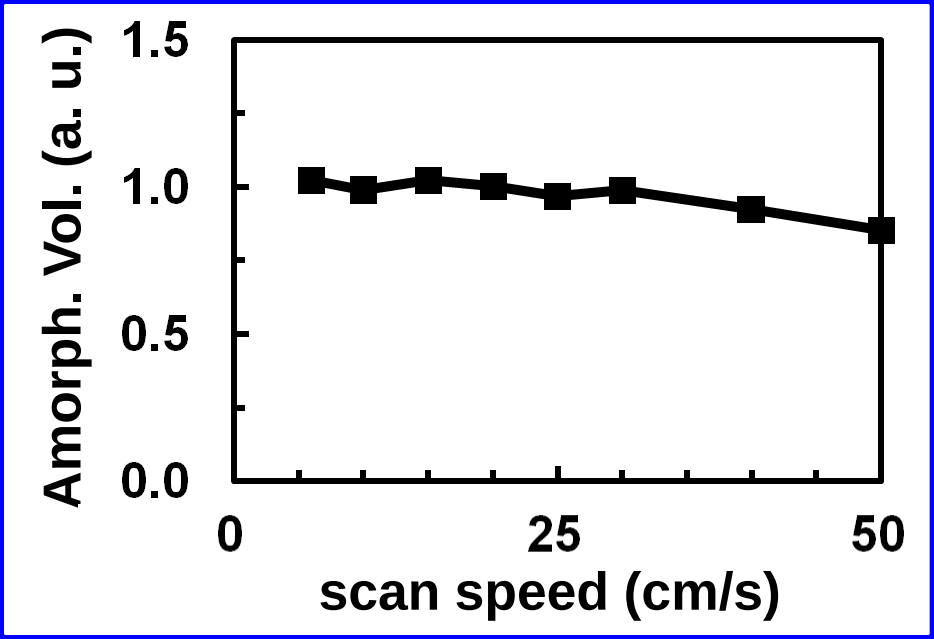
Amorphized volume vs. several parameters



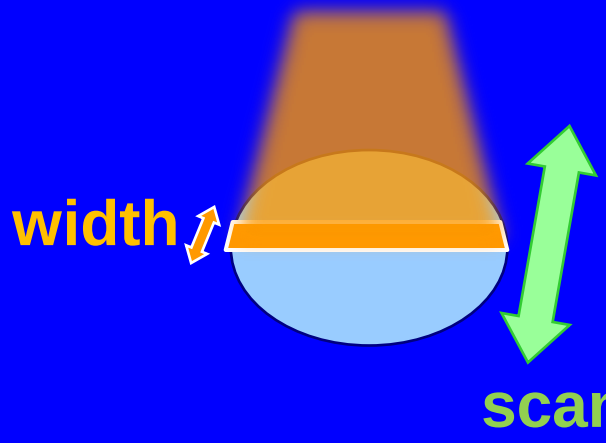

Atomistic KMC enables quantitative analysis of amorphization vs. different Implanter parameters

# Implanters: Single-wafer

## Amorphized volume vs. scan speed




## ribbon beam

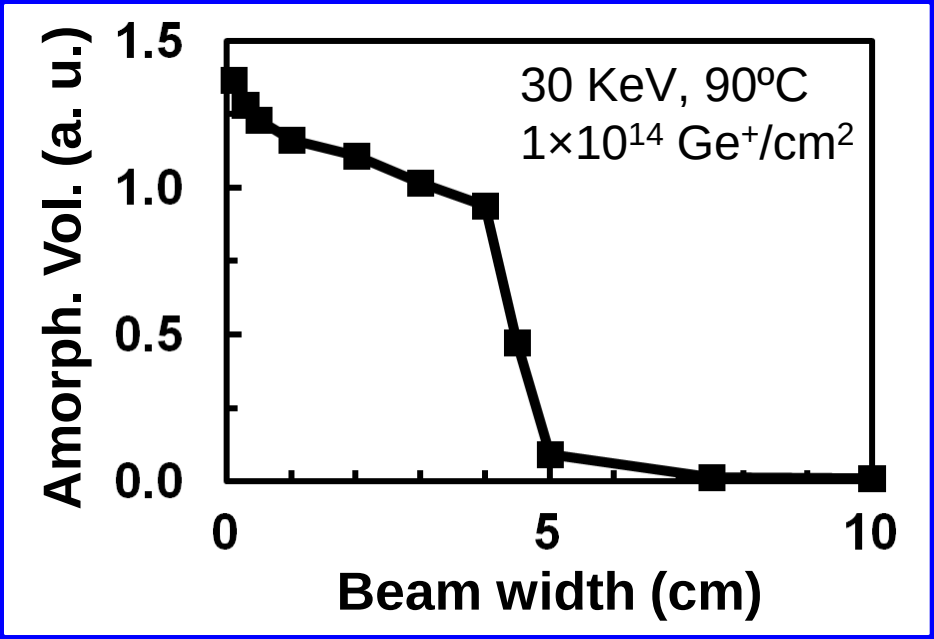



Wafer diameter = 300 mm
Beam current = 5 mA
Scan speed = 20 cm/s

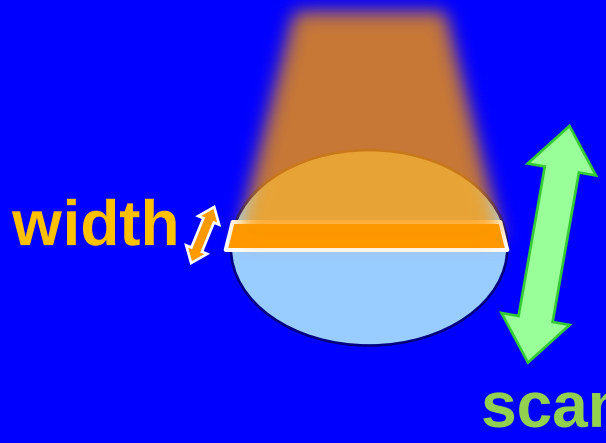
Almost insensitive to scan speed

# Implanters: Single-wafer

## Amorphized volume vs. beam width




## ribbon beam

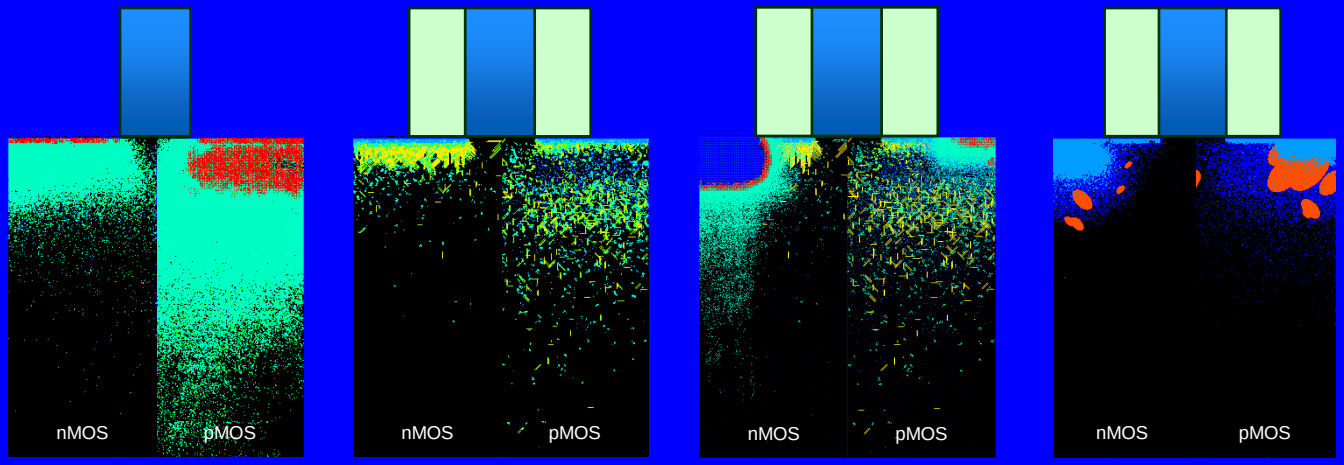



Wafer diameter = 300 mm
Beam current = 5 mA
Scan speed = 20 cm/s

**Effect of de-focused beam:**

**Abrupt change beyond a given beam width at critical amorphizing dose**

# Device fabrication

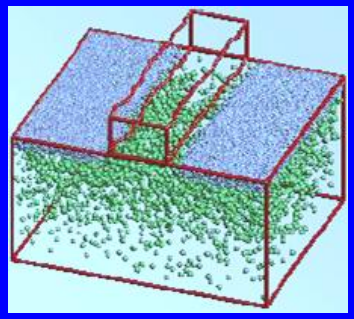


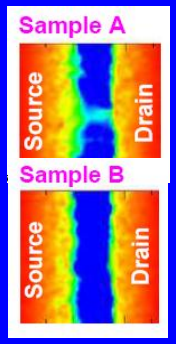

**All mechanisms are always active simultaneously:**

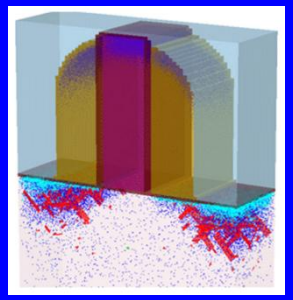
***No need for simplifying assumptions***

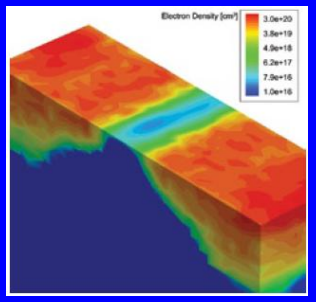
# Other results: KMC-Device

1. A. Asenov - DADOS
2. M. Hane (NEC) - Own KMC implementation
3. Chartered - DADOS
4. Synopsys - KMC/DADOS







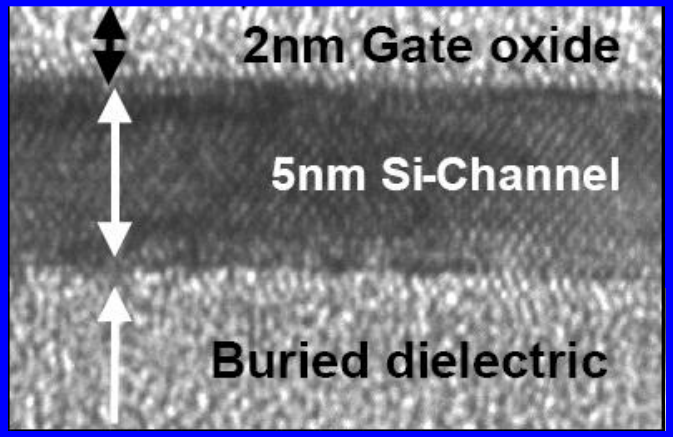
# Future Prospects of Atomistic Process Simulation

# Alternative Technologies

***Nothing beats MOSFETs overall for Boolean logic operations at comparable risk levels* (ITRS Analysis)**

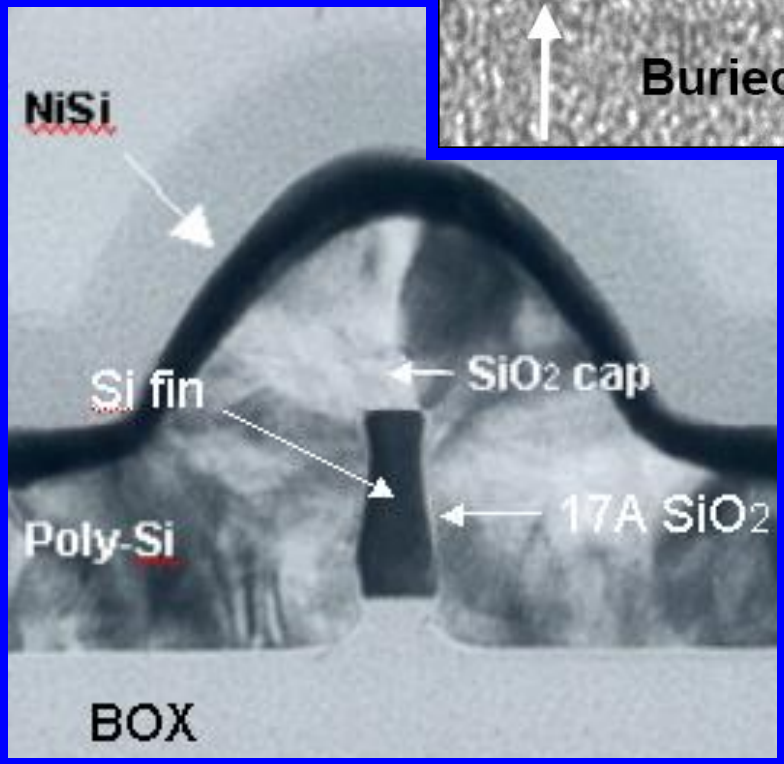
- **MOSFETs (Planar, FDSOI, FinFET, MultiGate…) likely to continue for the coming years:**
  - **Ion Implant: less relevant**
  - **Growth, Etch, Deposition: dominant role of *interfaces***

# Simulation Requirements for Upcoming Devices

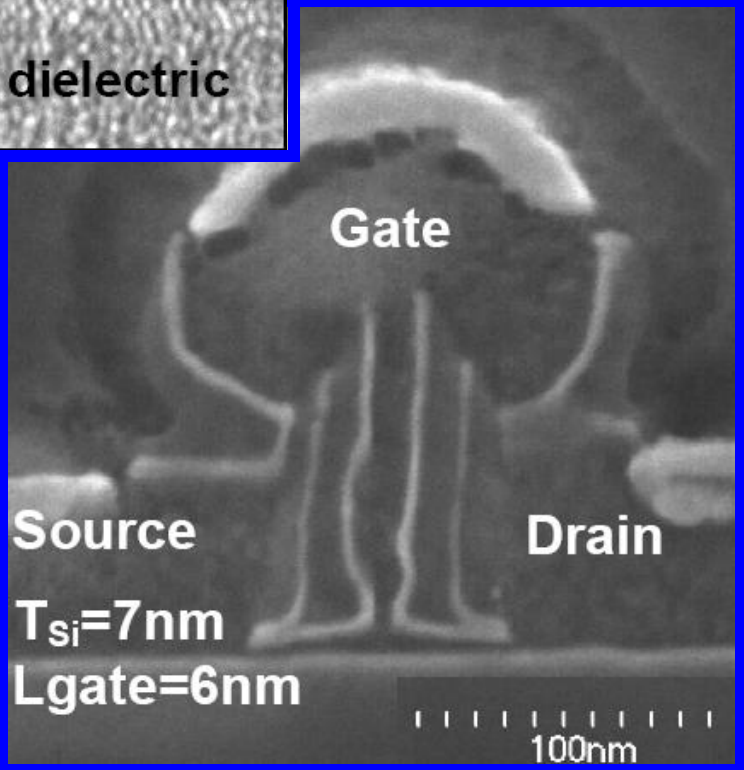



"Silicon On Nothing" *(Monfray et al)*

10 nm FinFET *(Yu et al)*

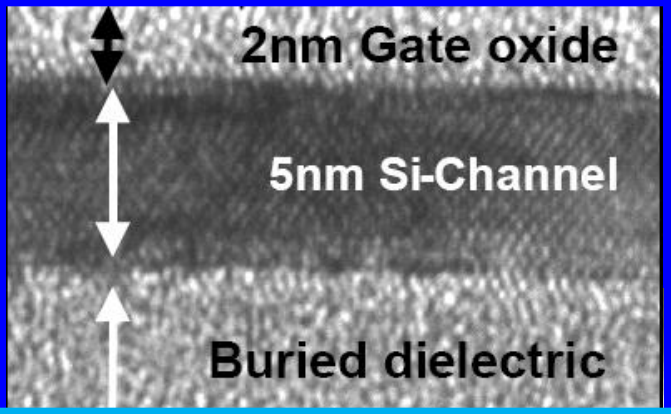



6 nm FinFET *(Doris et al)*



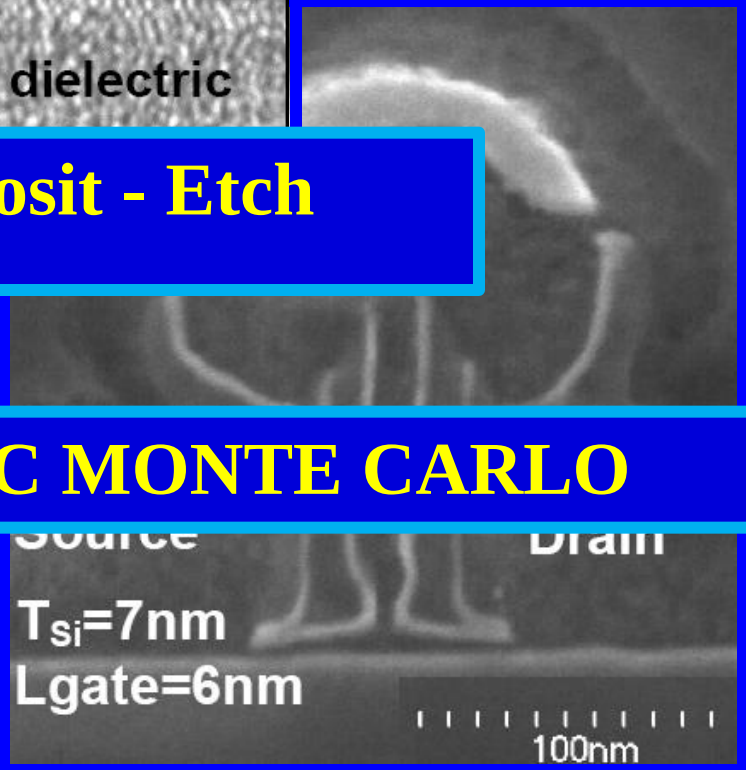
# Simulation Requirements for Upcoming Devices

**Different Materials and Interfaces**




**Atomic-scale resolution**

**Grow - Deposit - Etch**

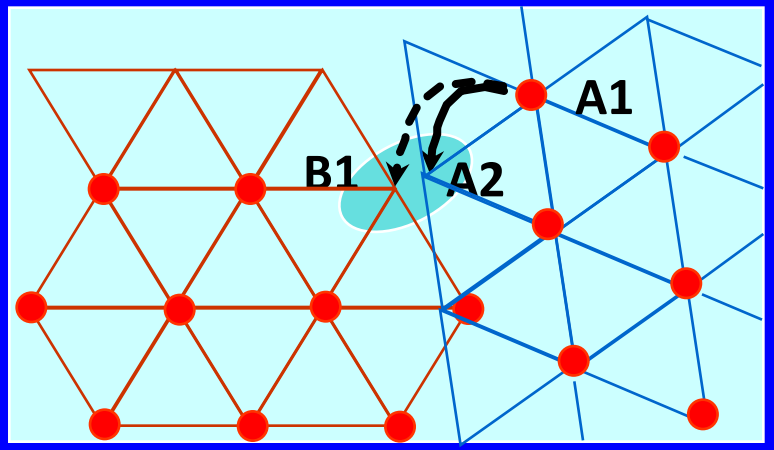

**⇒ LATTICE KINETIC MONTE CARLO**

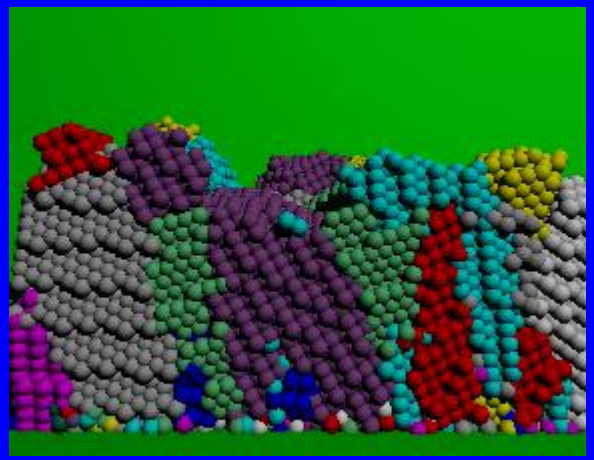
# Lattice KMC: Grain boundaries

If the destination site of a jump is at a grain boundary (A2):

1. Check the energy of sites belonging to other grain orientations (B) around destination site.

2. If energy(B1) < energy(A2) then the final site is B1.



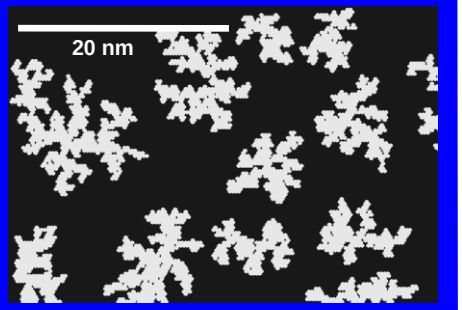



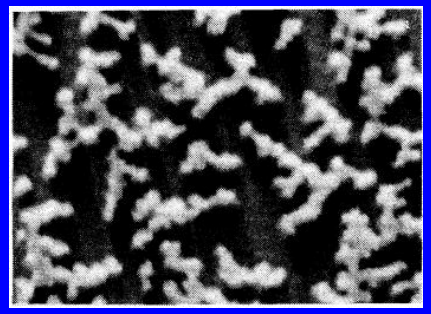
# Lattice KMC

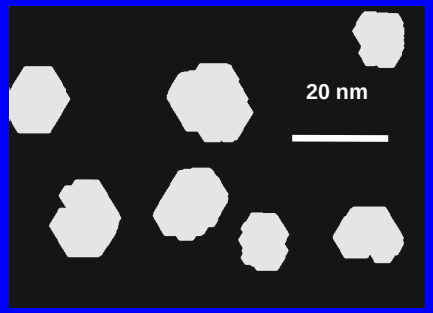
Can predict different morphologies depending on processing conditions

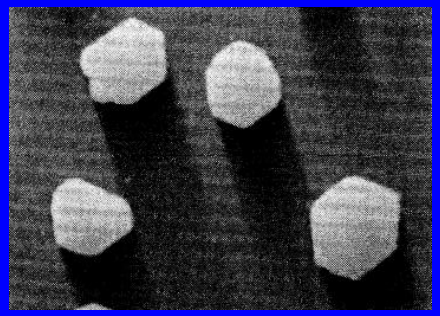
SIMULATION

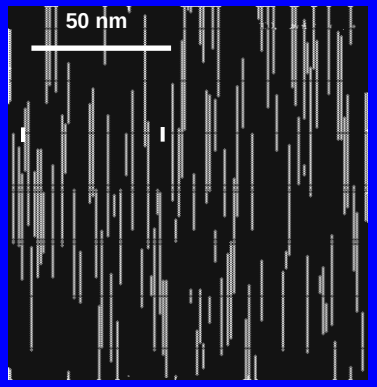
EXPERIMENT

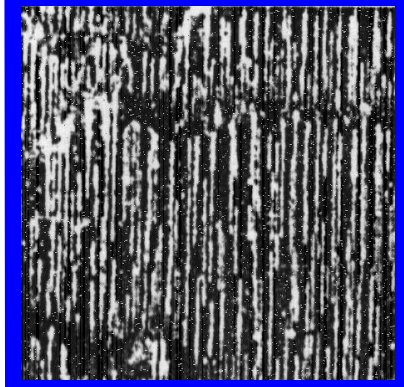






Al

Pt & Cu

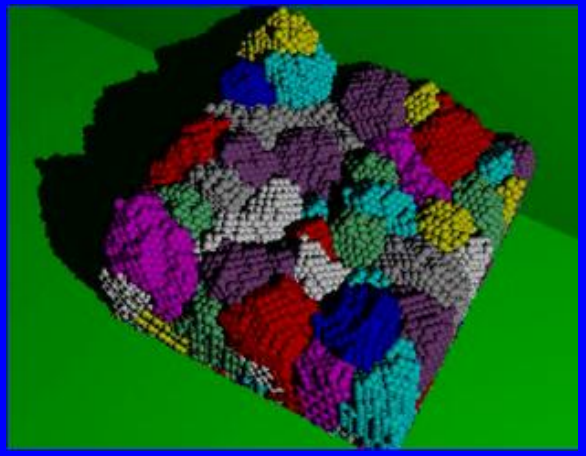
# Lattice KMC

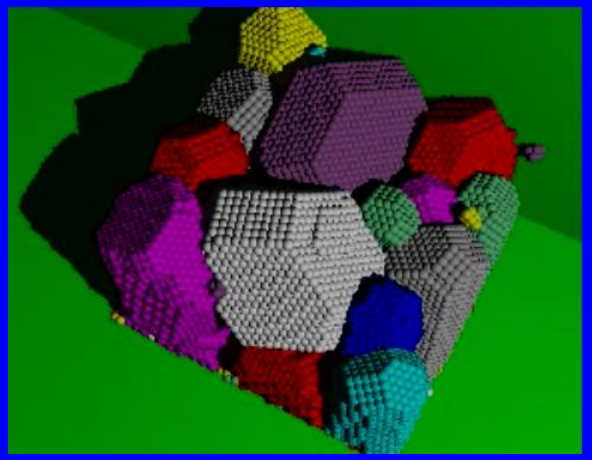
Grains: a) Growth-Shrinkage

b) Faceting

c) Diffusion along grain boundaries

**Aluminum, deposited @ 80 ºC, 0.25 µm/min:**





**as Deposited → → → → → → 2s anneal @ 300 ºC**

**Amorphous materials need to be incorporated**

# In summary…

- Atomistic KMC can handle many mechanisms ***simultaneously***.
- Basic ***microscopic mechanisms*** and ***ab-initio parameters*** can be directly plugged in.
- KMC is a ***predictive*** process simulation technique.
- The goal is to attain a simulator that, although not particularly accurate for any given simulation ***never gives a totally wrong result***, even for previously unexplored conditions.
- ***Lattice KMC*** looks like a promising process simulation technique for upcoming device generations.