Atomistic Front-End Process Modeling

A Powerful Tool for
Deep-Submicron Device Fabrication

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Thanks to:

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C. S. Rafferty (Bell Labs.)

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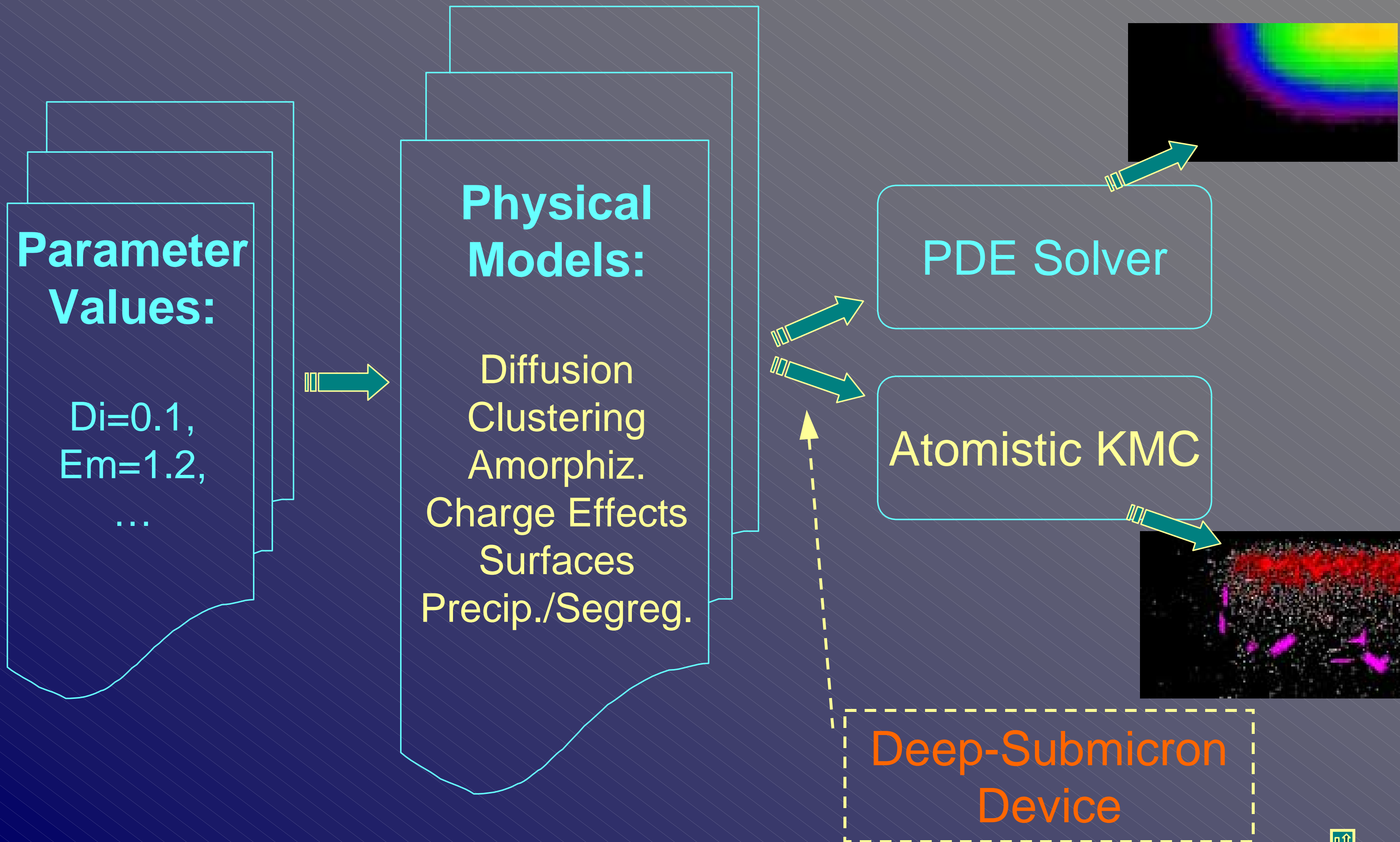
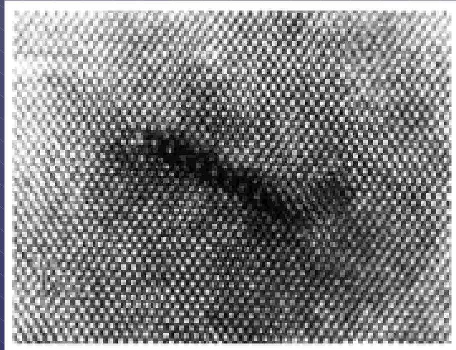
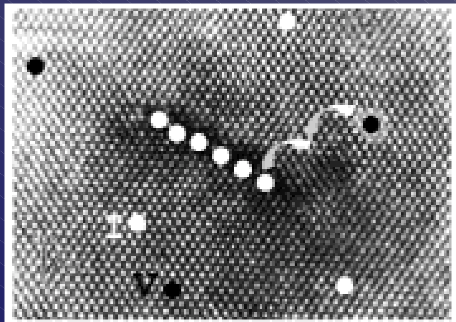
Front-End Process Modeling



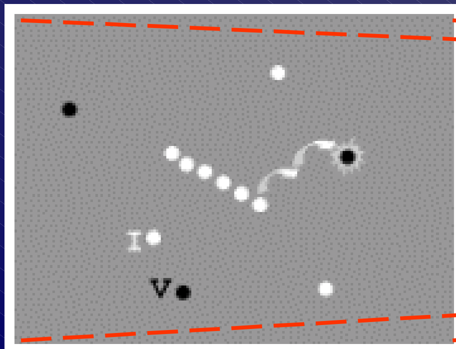
The Atomistic KMC Approach



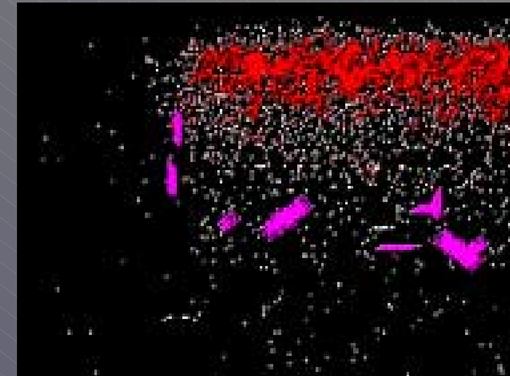
Lattice Atoms are just vibrating



Defect Atoms can move by diffusion hops

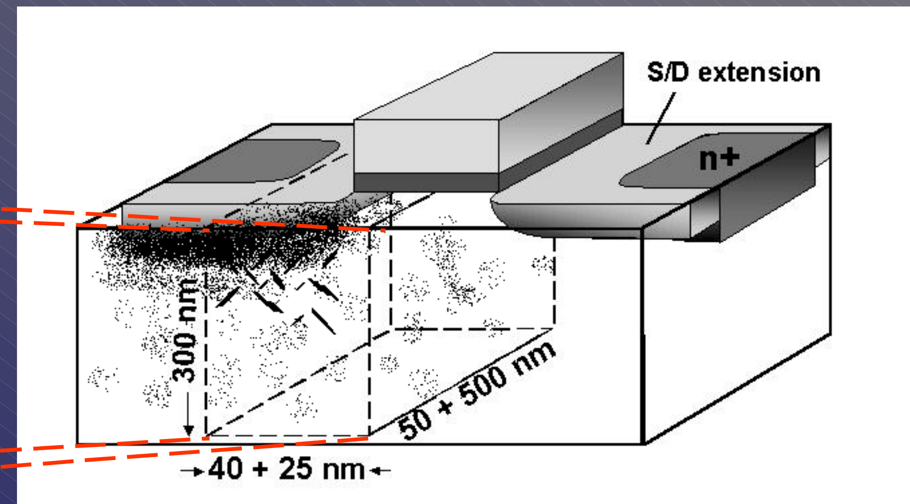


KMC simulates Defect Atoms only



Output

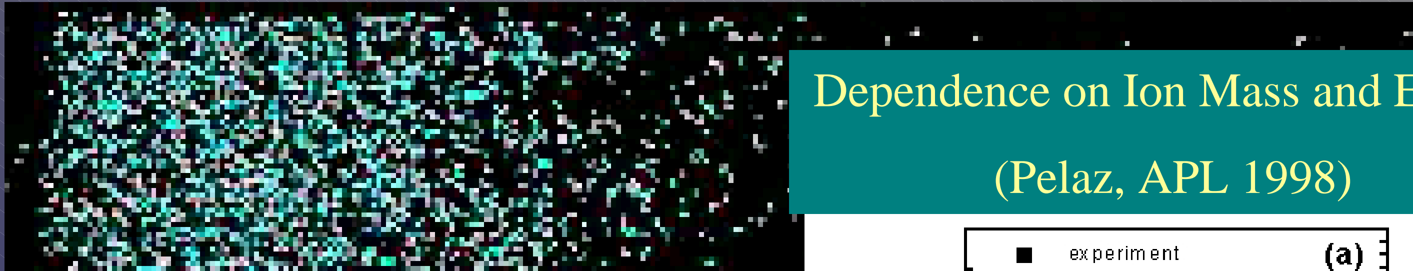
KMC Simulator



Ion Implantation: The "+1" model

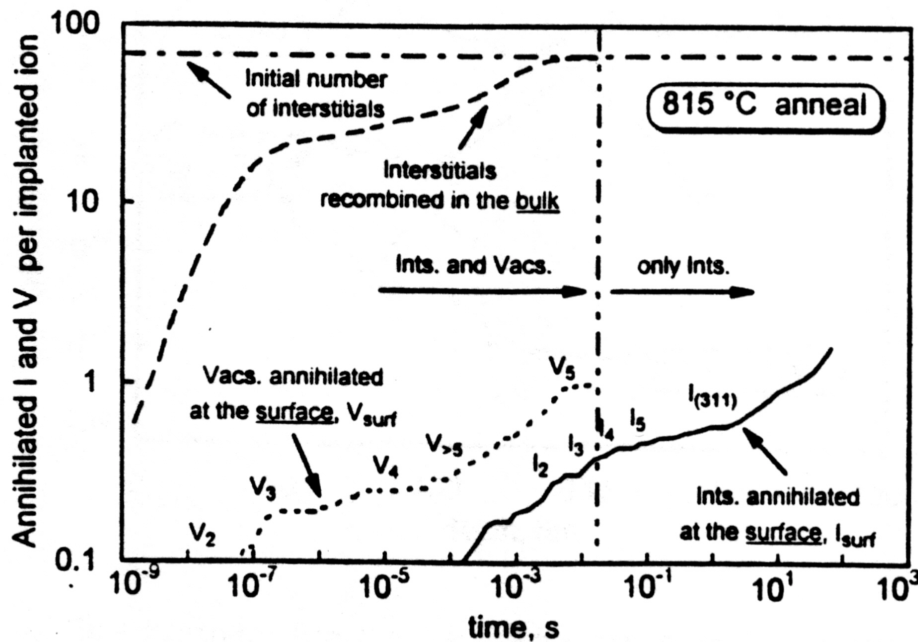
"One excess Interstitial per Implanted Ion" (M. Giles, 1991)

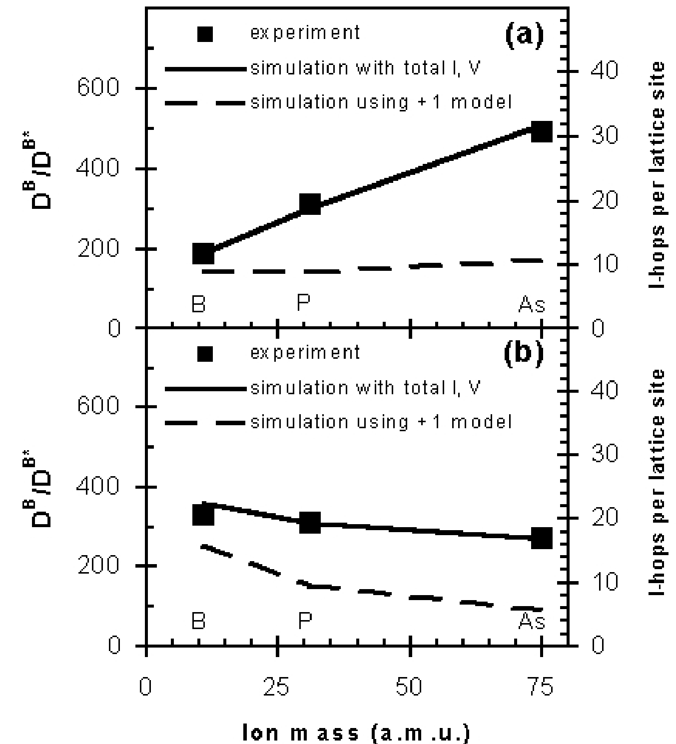
Atomistic KMC made **quantitative** calculations feasible (I):



Dependence on Ion Mass and Energy

(Pelaz, APL 1998)





"+1.4" (Jaraiz, APL 1996) In agreement with Eaglesham's measurements

Ion Implantation: The "+1" model

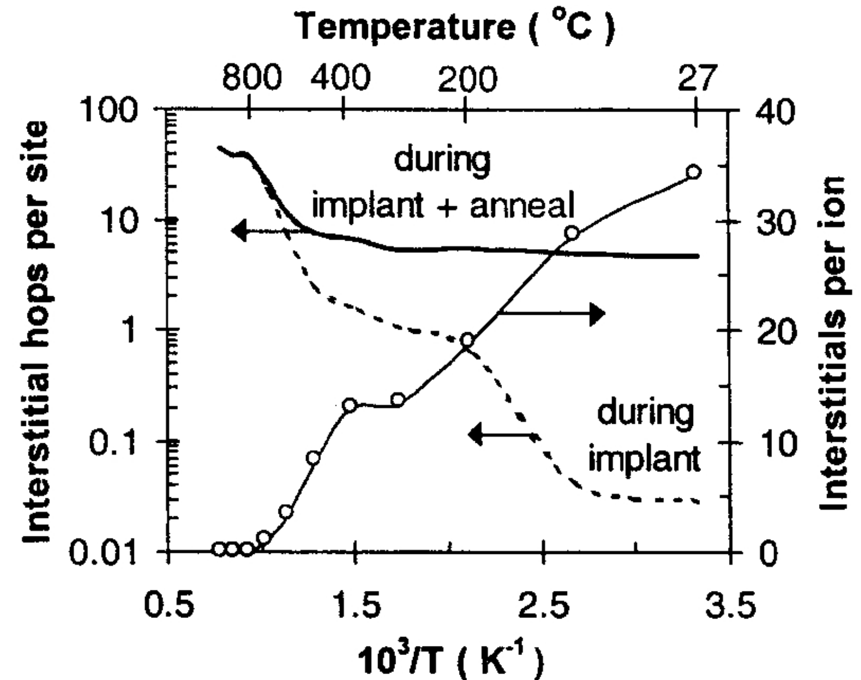
Atomistic KMC made **quantitative** calculations feasible (II):

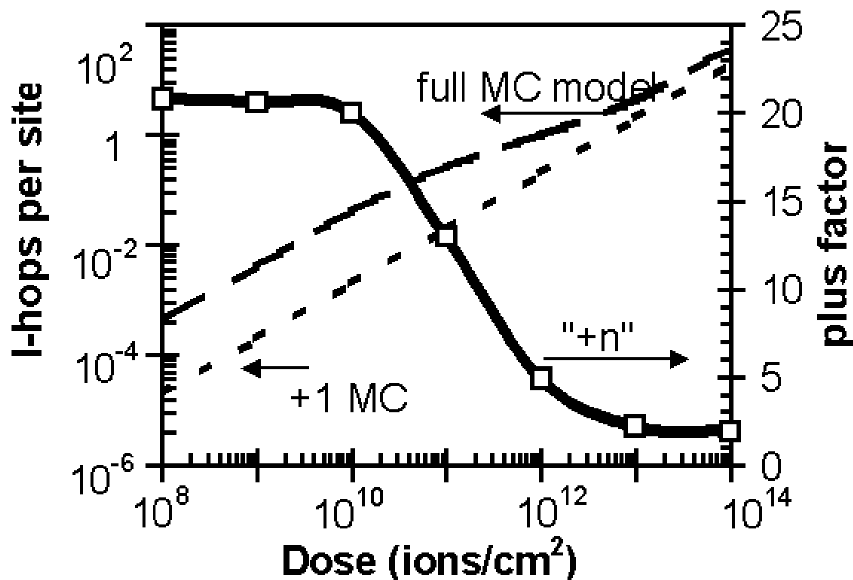
KMC Simulations (Pelaz, APL 1999)

Dependence on:

- Dose
- Temperature / Dose-Rate

Total diffusivity almost constant for T<500C, in agreement with Jones et al.





Sub-linear increase for intermediate doses, as observed by Packan et al.

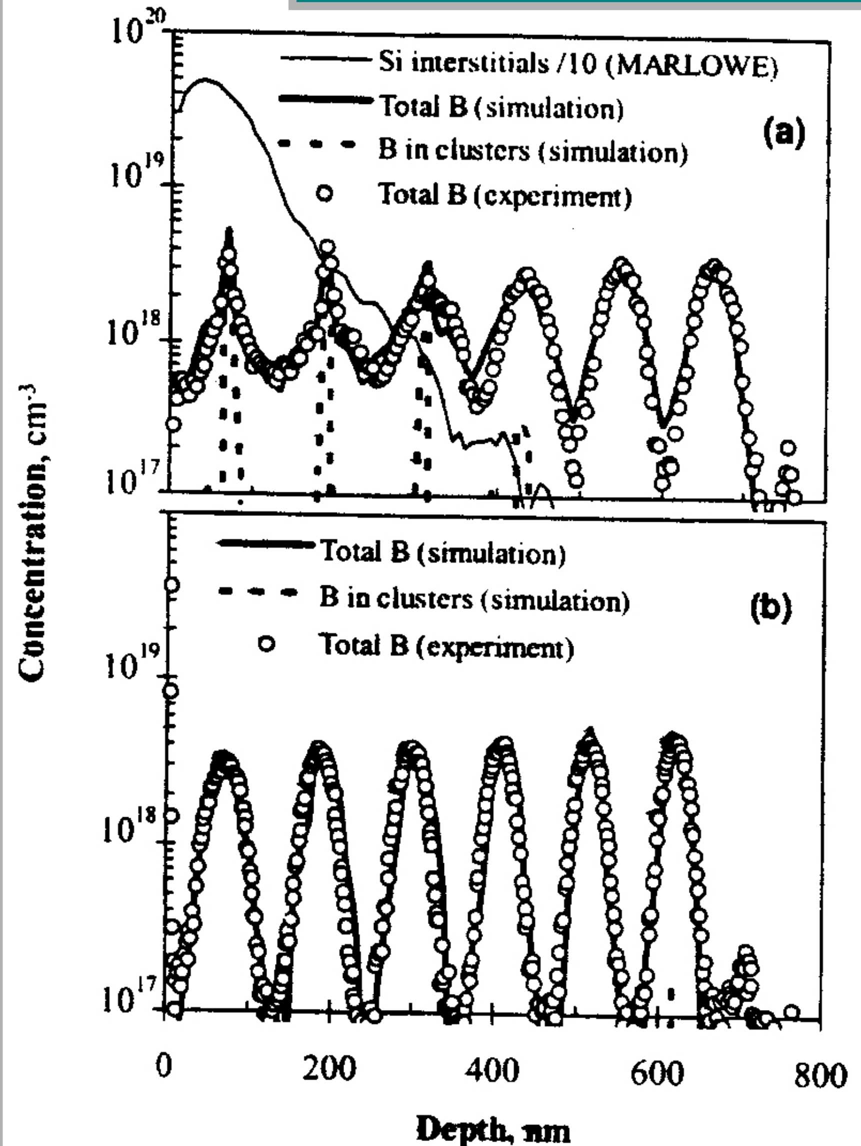
Impurity Atoms: Boron (I)

KMC Simulations (Pelaz, APL 1999):

- Kick-out mechanism
- I_nB_m complexes

Accurate annealed profiles:

- Diffused B (substitutional)
- Immobile B (I_nB_m complexes)

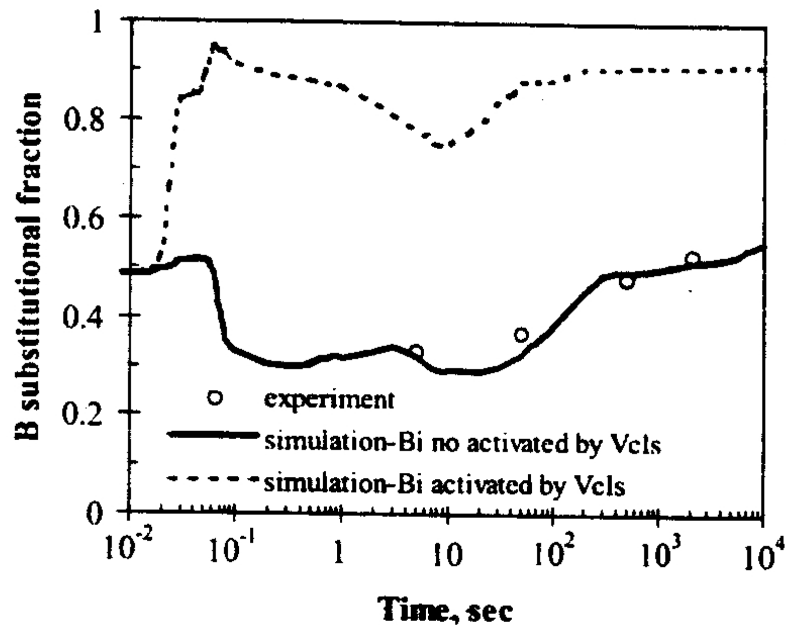


Impurity Atoms: Boron (II)

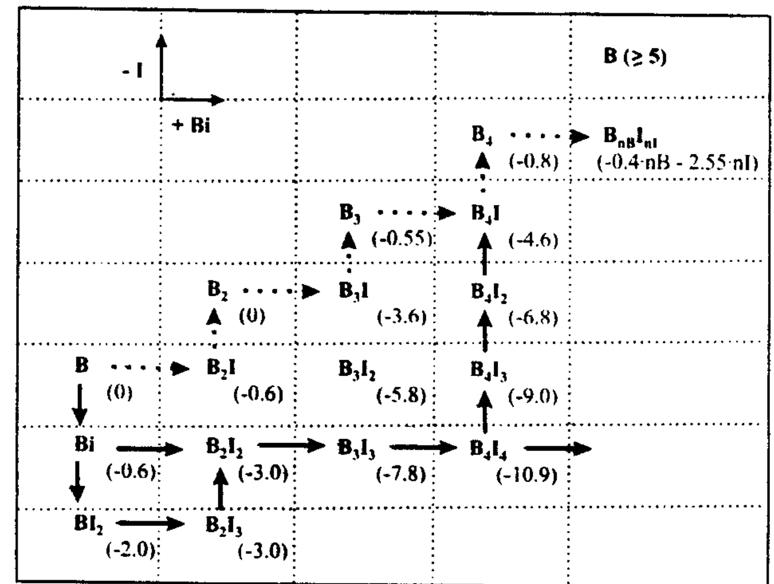
KMC Simulations (Pelaz, APL 1999):

- Accurate prediction of **electrically active** B

Electrically active B



I_nB_m Pathway

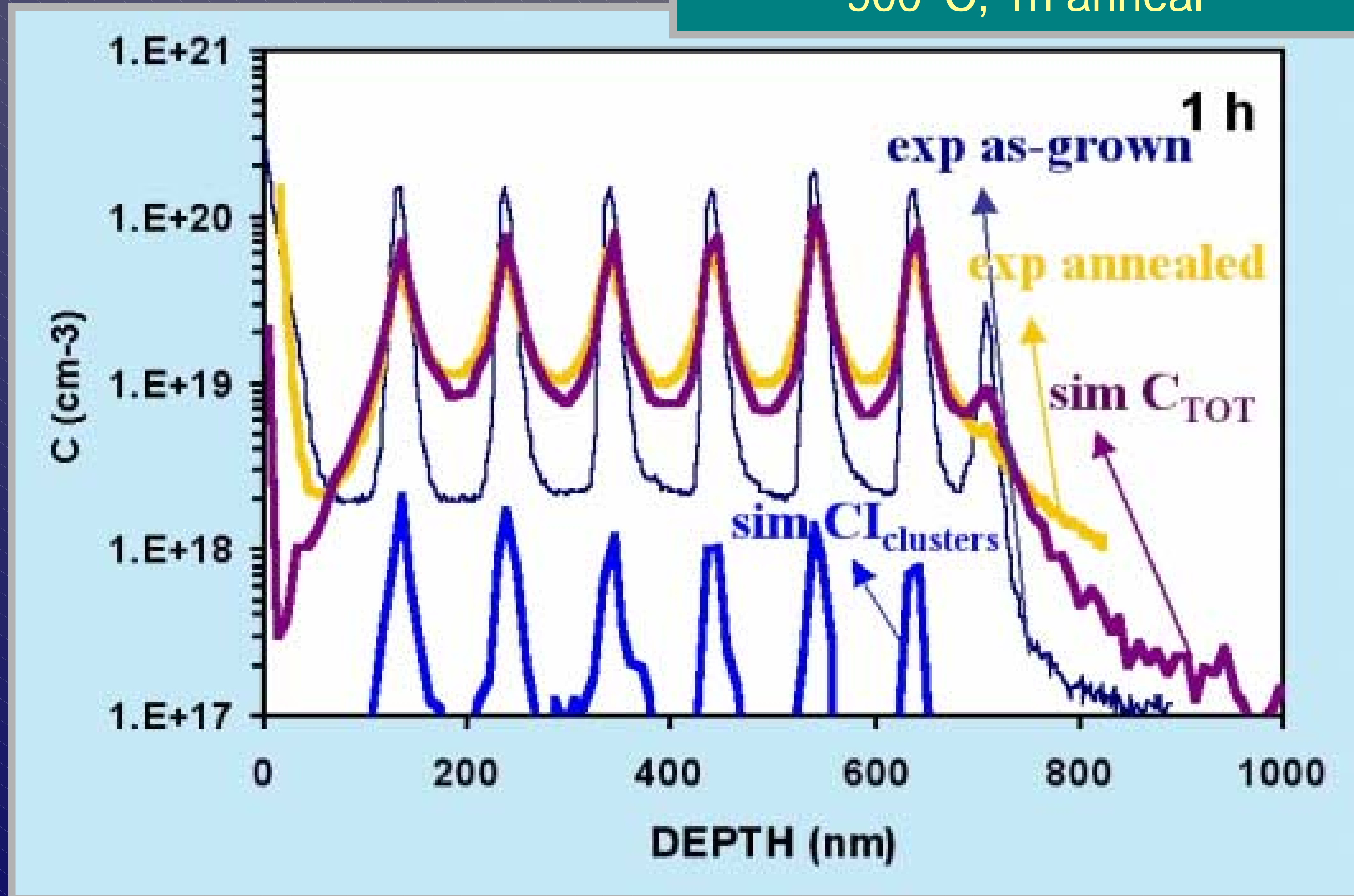


Impurity Atoms: Carbon (I)

KMC Simulations (Pinacho, MRS 2001):

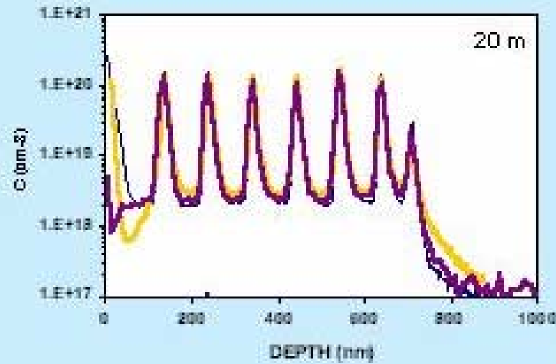
- Kick-Out Mechanism
- I_nC_m Complexes
- Frank-Turnbull Mech.

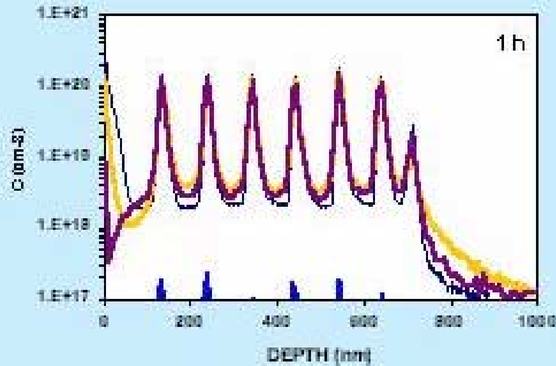
900 'C, 1h anneal

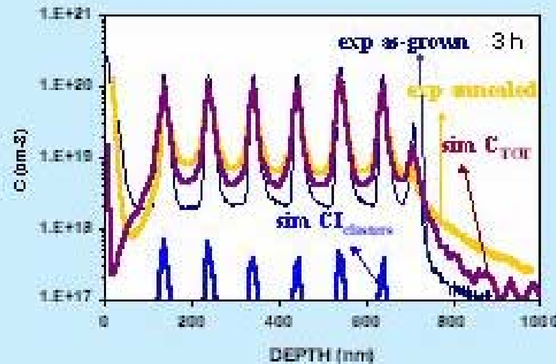


Impurity Atoms: Carbon (II)

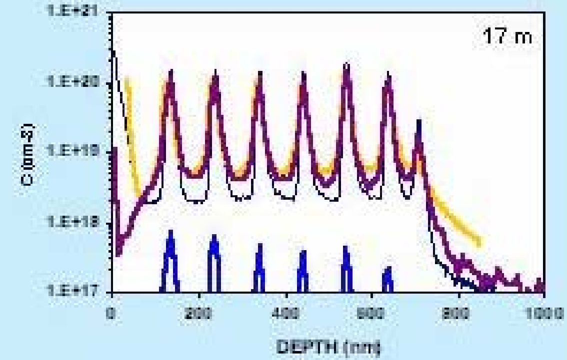
850°C ANNEALING

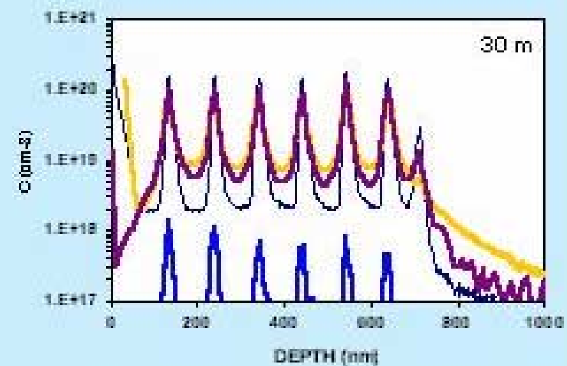


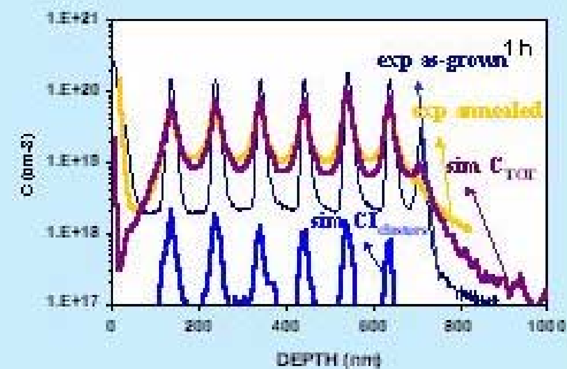




900°C ANNEALING







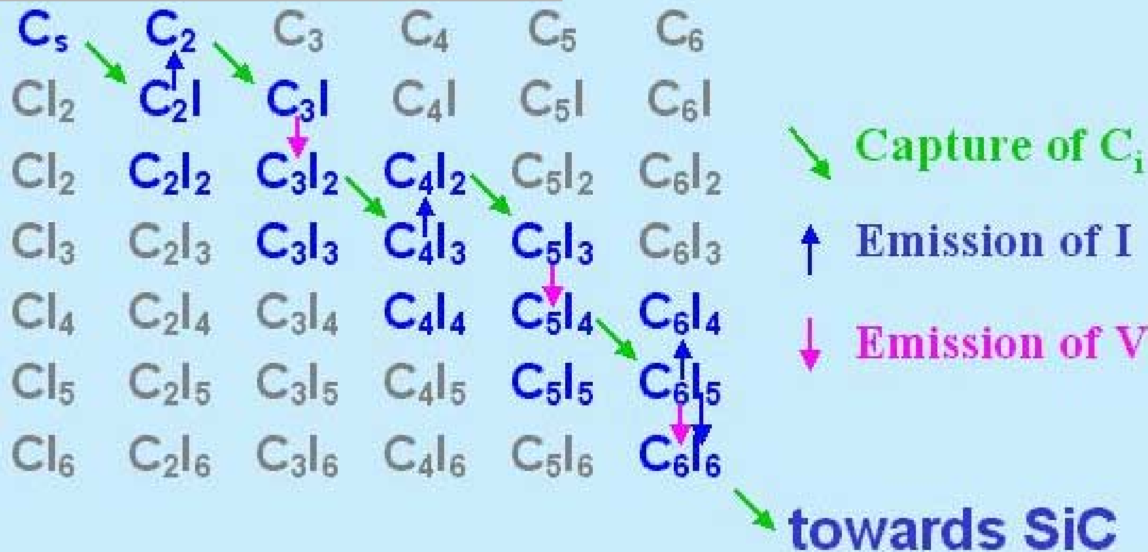
Impurity Atoms: Carbon (III)

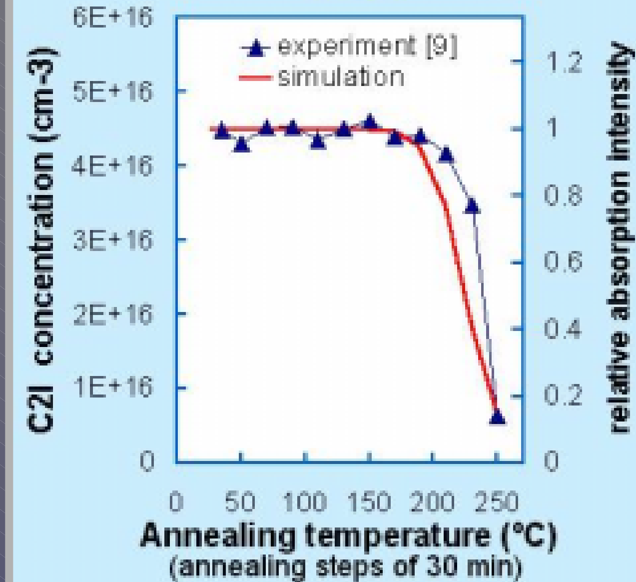
In agreement with experimentally observed C_2I complexes

Carbon is normally above its solubility

Clustering/Precipitation

I_nC_m Pathway





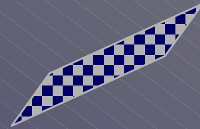
Extended Defects: Interstitials

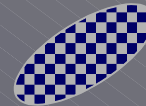
Small clusters

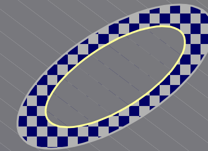
{311} defects

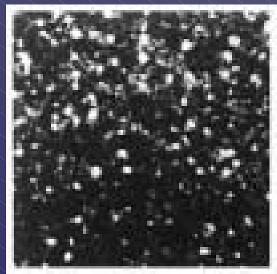
Faulted loops

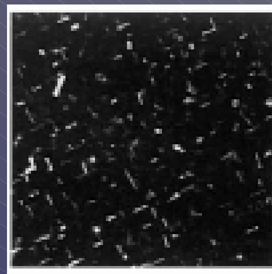
Perfect loops

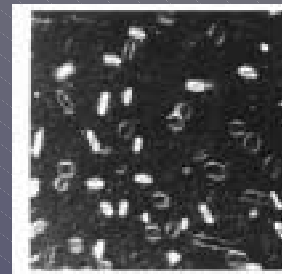


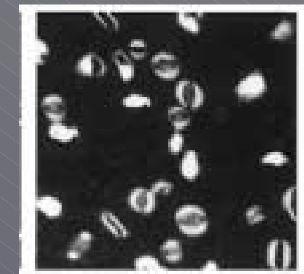




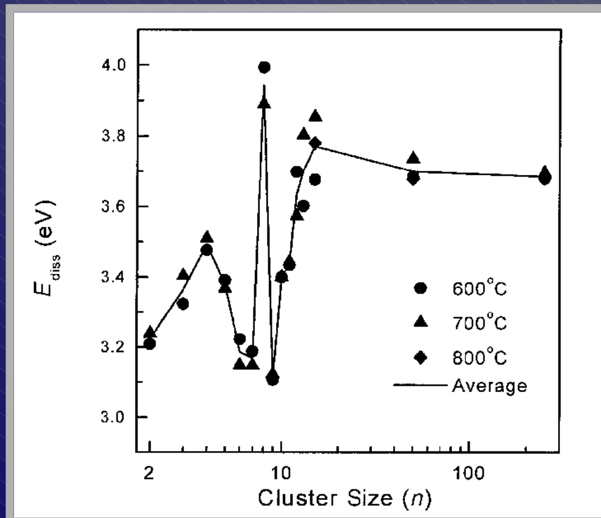




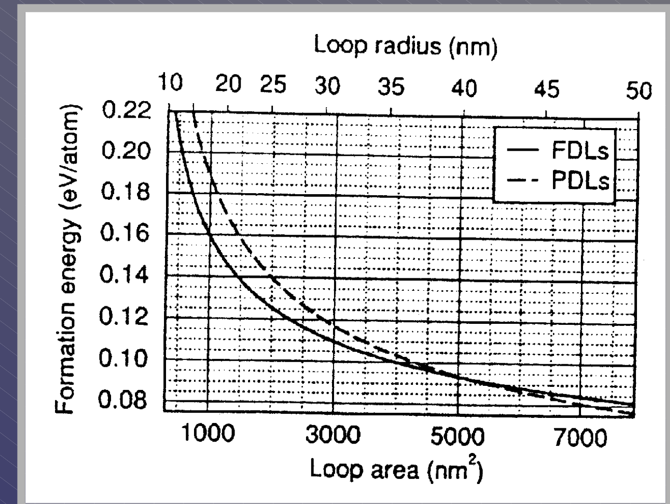




TEM images from Claverie et al.



Cowern et al.

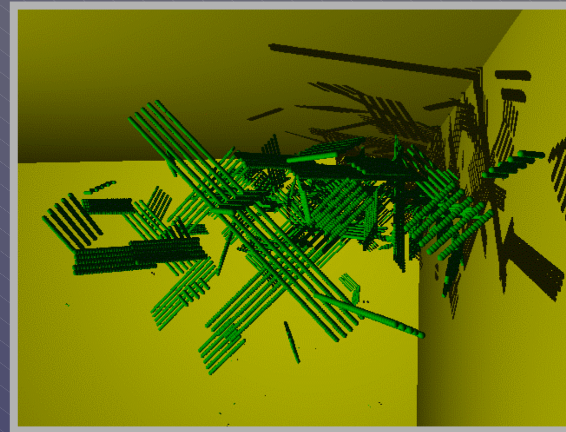


Cristiano et al.

Extended Defects: Interstitial {311}

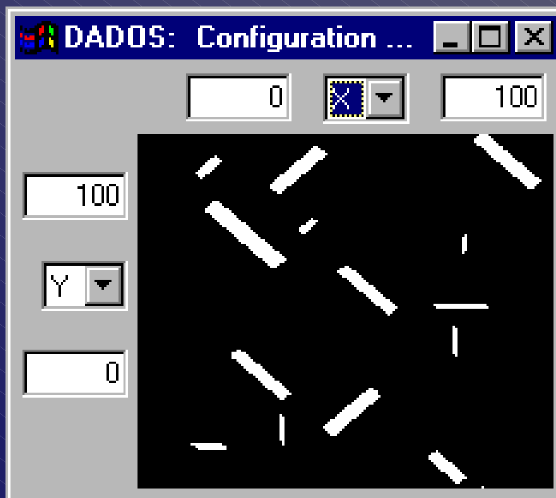
Simulated in DADOS with their actual crystallographic parameters

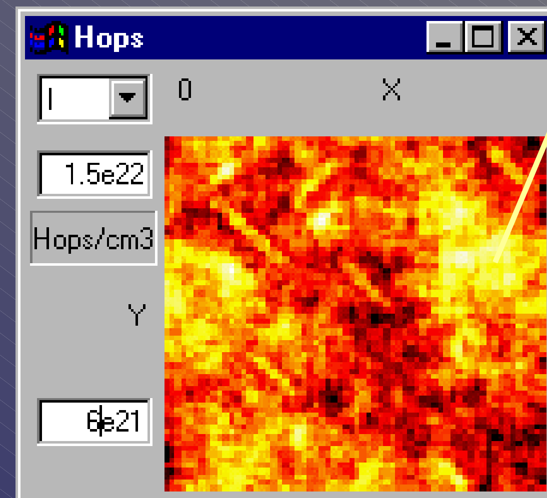
3D View



High B diffusivity

2D Projection





{311} defects → Interst. Supersat. (Hops)

311-defects dissolution

- Full damage simulation: No “+N” assumption
- Defect cross-section automatically given by defect geometry

interstitials in defects (cm-2)

1.E+15
1.E+14
1.E+13
1.E+12
1.E+11

1 10 100 1000 10000 100000

Anneal time (s)

Experimental:
815ºC
738ºC
705ºC
670ºC

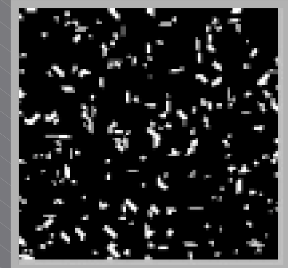
Lines: simulation

Experimental data from Eaglesham et al.

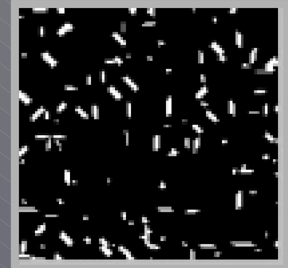
Simulation

738ºC

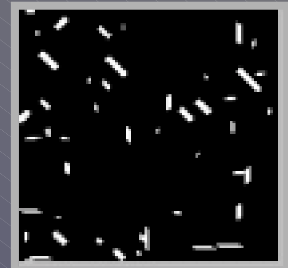
200 s



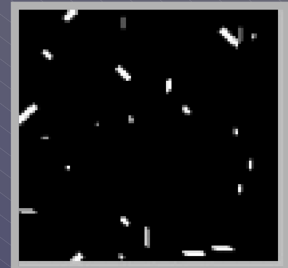
600 s



1200 s

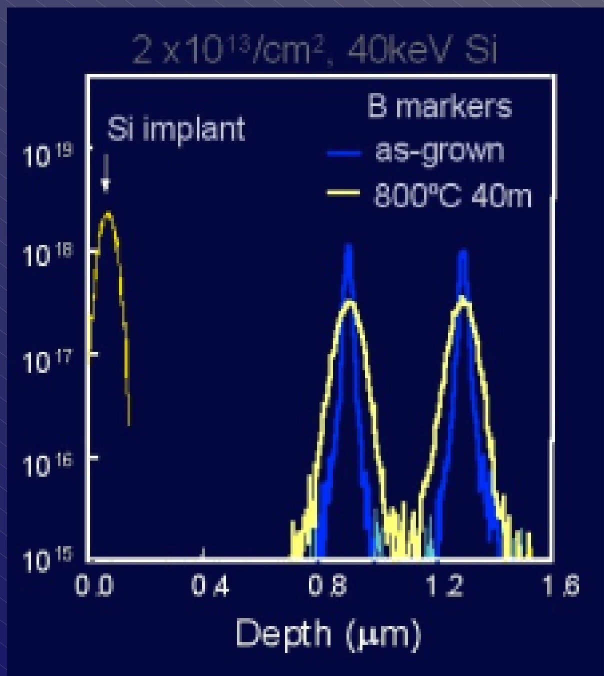


1800 s



Interstitial supersaturation

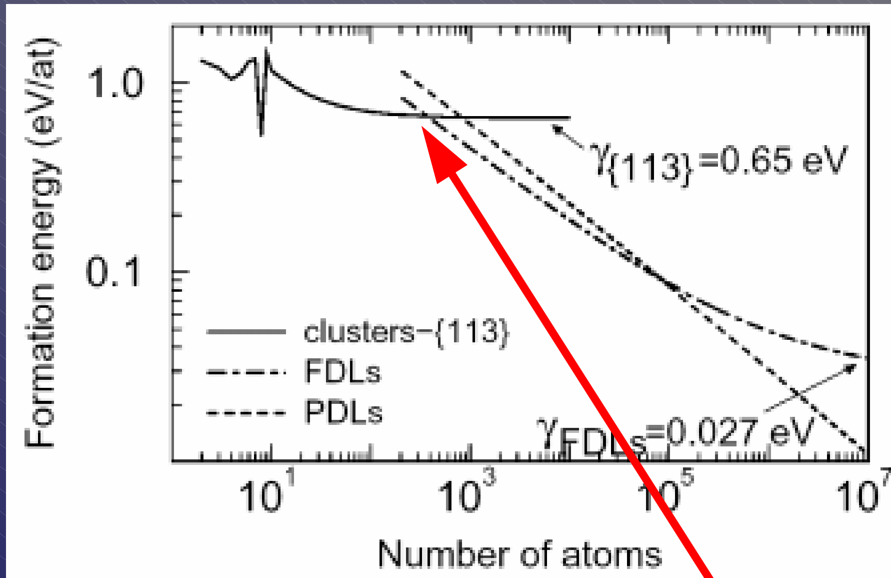
Determines dopant diffusivity



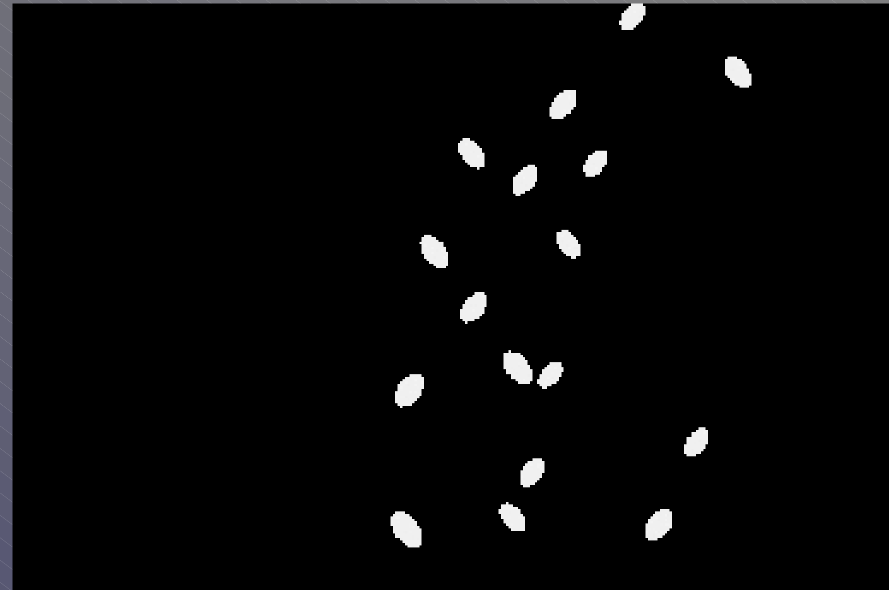
1.E+08
1.E+07
1.E+06
1.E+05
1.E+04
1.E+03
1.E+02
Interstitial supersaturation
Experimental
600°C
700°C
800°C
Lines: Simulation
1.E+00 1.E+01 1.E+02 1.E+03 1.E+04 1.E+05
Anneal time (s)

Experimental data from Cowern et al.

Dislocation Loops



From Claverie et al.



DADOS Simulation

Loop energy < {311} energy
if Number of atoms > 345

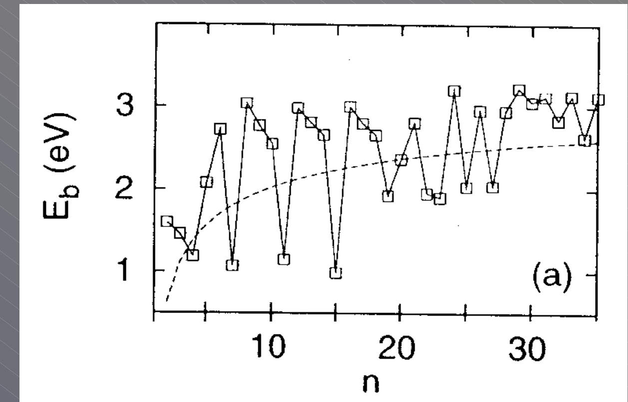
However, {311} can in fact reach sizes >> 345

Therefore, the {311} → Loop transformation cannot be based just on minimum configurational energy.

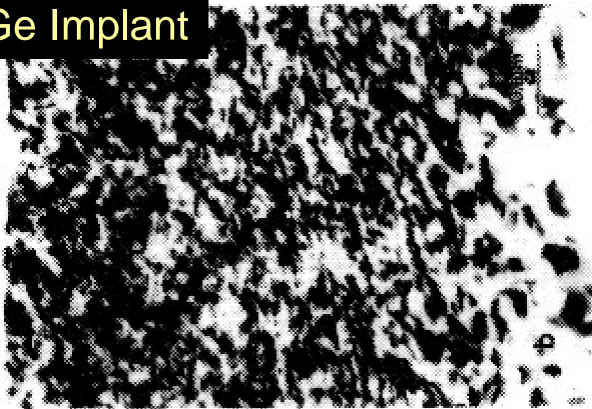
{311}→Loop: Activation Energy?

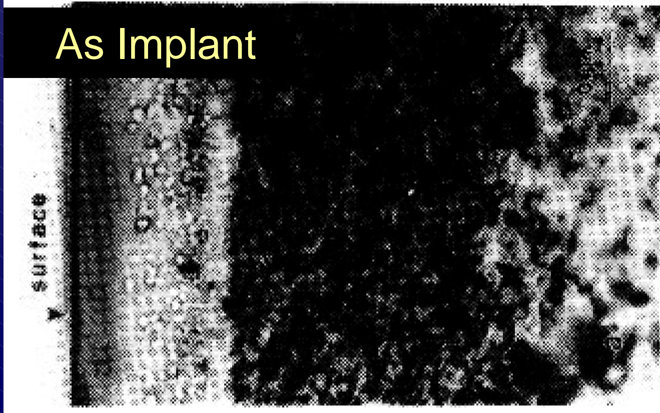
Extended Defects: Vacancies

- Big V-clusters are spheroidal (Voids)
- Energies from Bongiorno et al. (Tight-Binding)



⇒ But chemical / electrical effects are evident from experiments (Holland et al.):

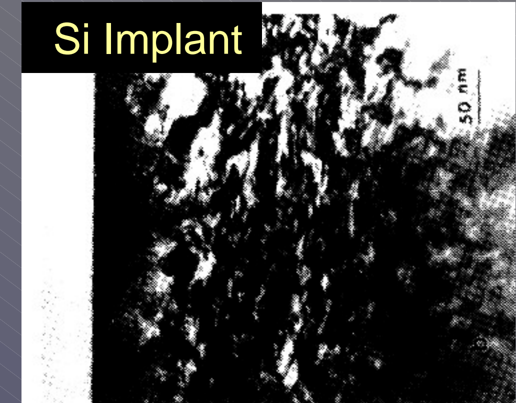


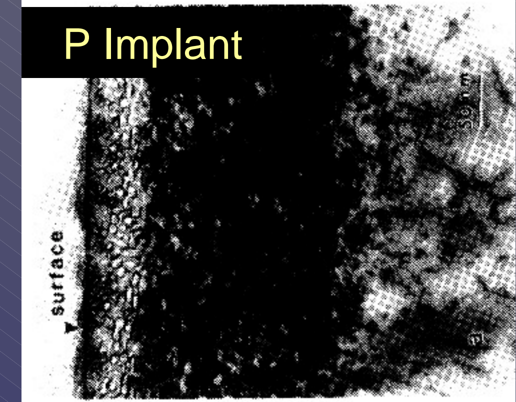


← Isoelectric →

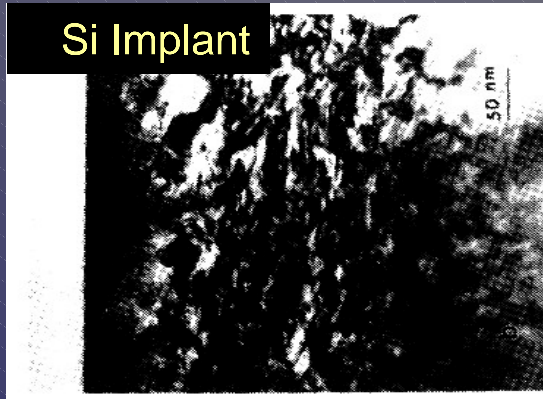
Nearly same atomic Number & Mass

← Dopants →

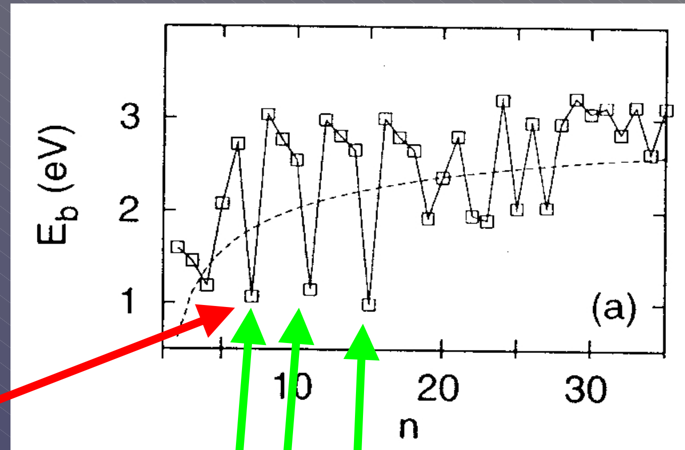


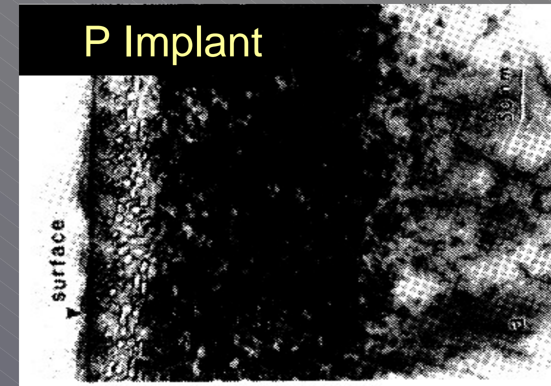


Extended Defects: Vacancies (II)



Chemical / electrical effects





No negative Eb at n=7

Simulation with negative Eb at sizes 7, 11, 15

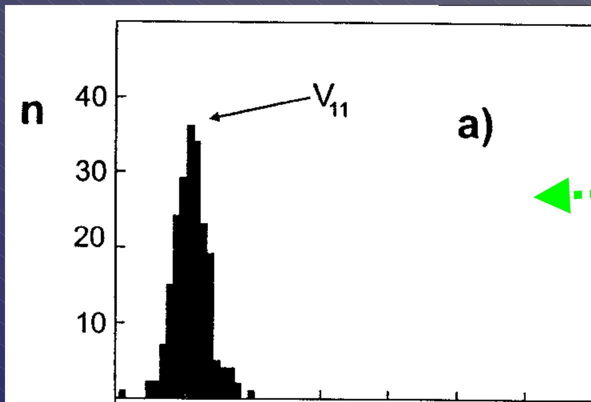
Lattice / Non-Lattice KMC

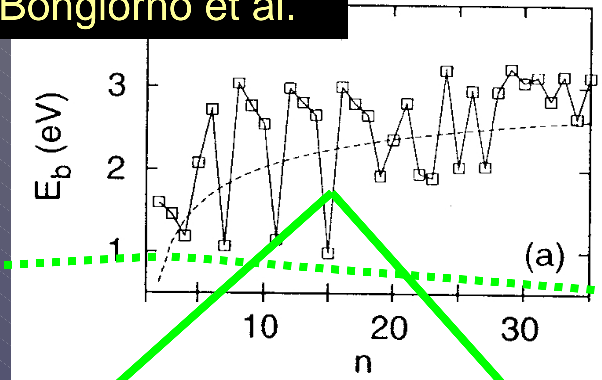
Do we **need** Lattice KMC?

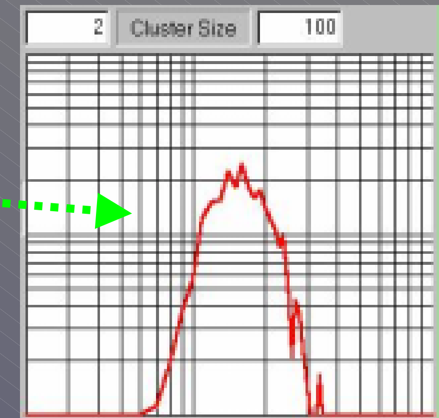
Lattice KMC

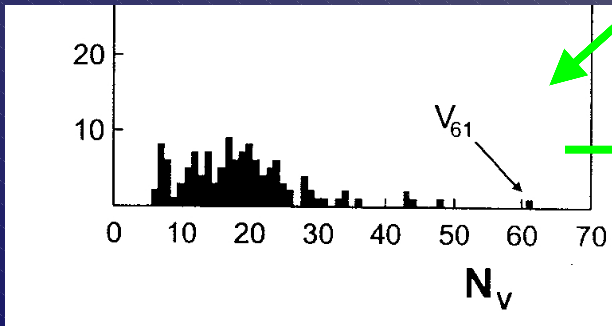
Bongiorno et al.

Non-Lattice KMC

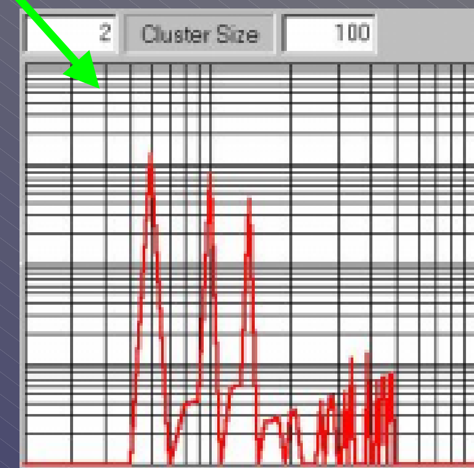








Attributed to the mobility of small clusters in Lattice-KMC



The dominant factor seems to be the **energetics**.

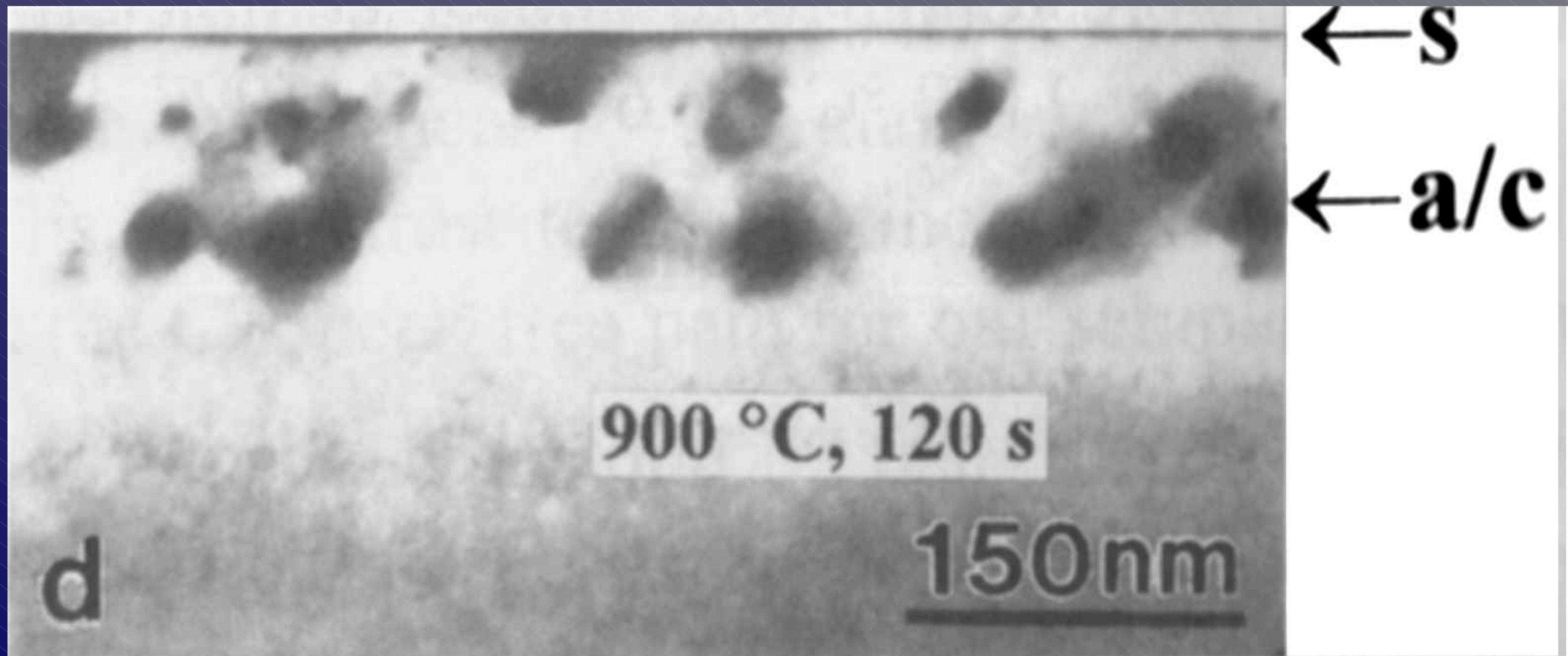
It is not clear the need for Lattice KMC

Amorphization / Recrystalization

Amorphization:

- Massive lattice disorder
- Continuum spectrum of time-constants and atomic configurations involved

Not amenable to atomic-scale KMC description for device sizes.

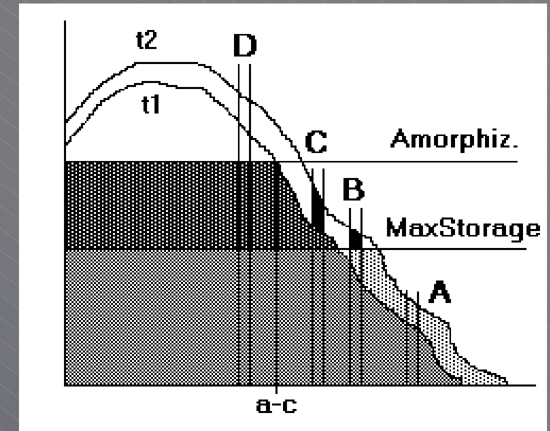


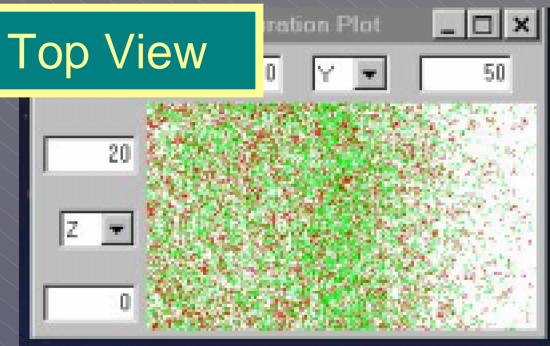
Implant: 50 KeV, 3.6×10^{14} Si/cm^2 (Pan et al., APL 1997)

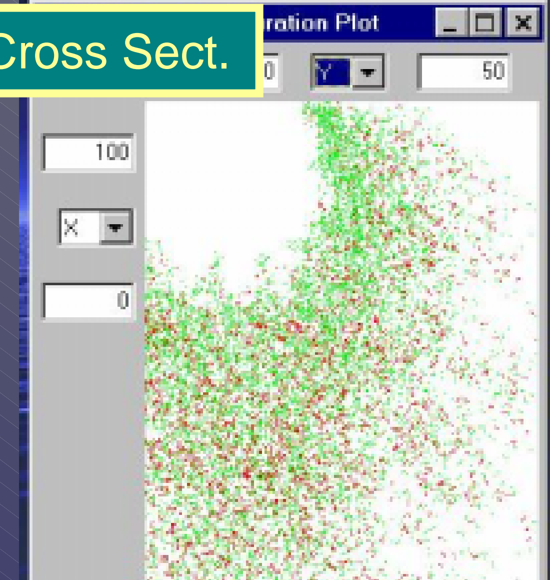
Amorphization / Recrystalization

Implementation (3D):

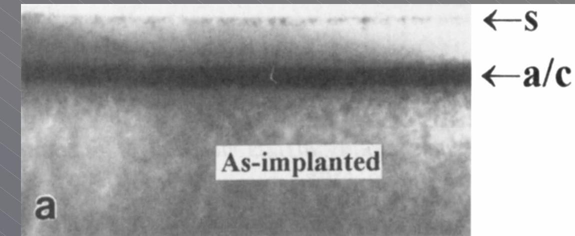
- Small (2nm-side) "damage boxes"
- Accumulate Interst. & Vacs. ("disordered pockets") up to a maximum number per box (MaxStorage)
  - This allows for dynamic anneal between cascades
  - Maintain the correct I-V balance in each box
- When a box reaches a given damage level becomes an "Amorphous region"
- Amorphous regions in contact with the surface or with a crystalline region recrystalize with a given activation energy.
- Any I-V unbalance is accumulated as the amorphous region shrinks ("dumped" onto adjacent amorphous boxes).

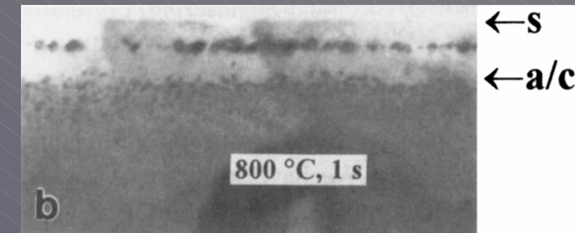


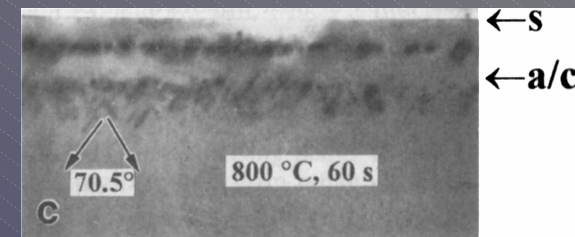


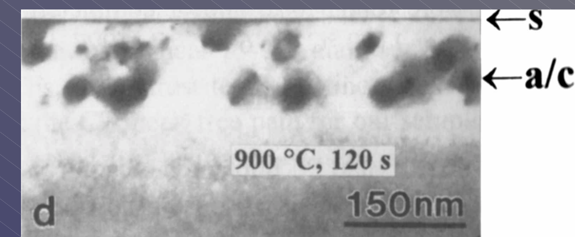


Amorphization / Recrystalization







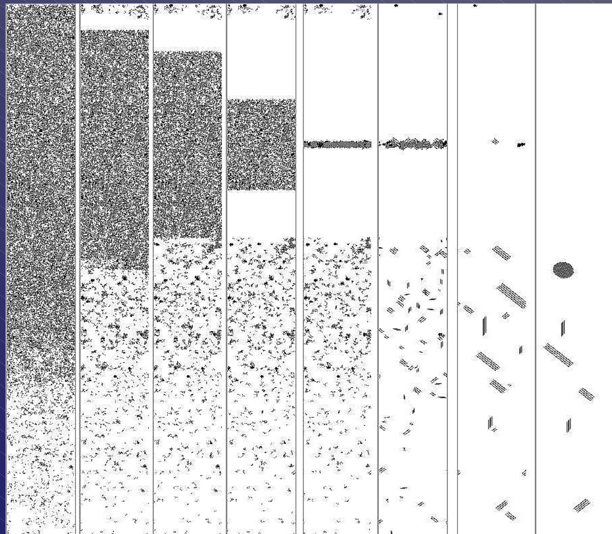


KMC Simulation

Implant: 50 KeV, $3.6x10^{14}$ Si/cm^2
(Pan et al., APL 1997)

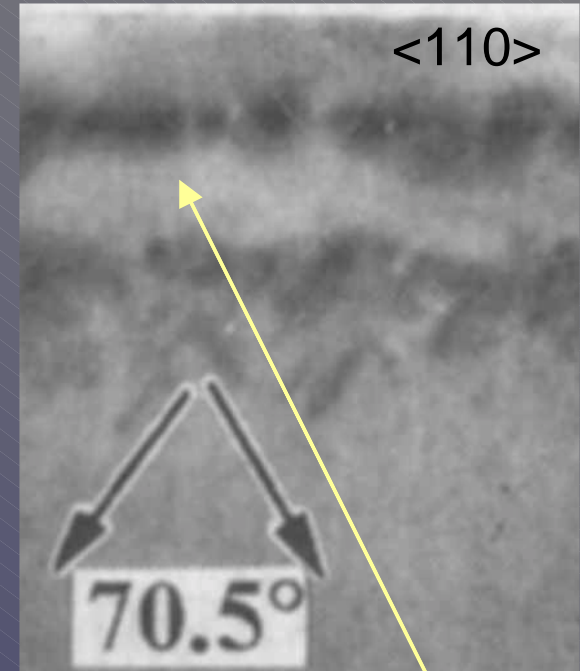
Amorphization / Recrystalization

800 C, 60 s



Simulation

(Pan et al., APL 1997)



No net I excess within the amorphised layer

⇓

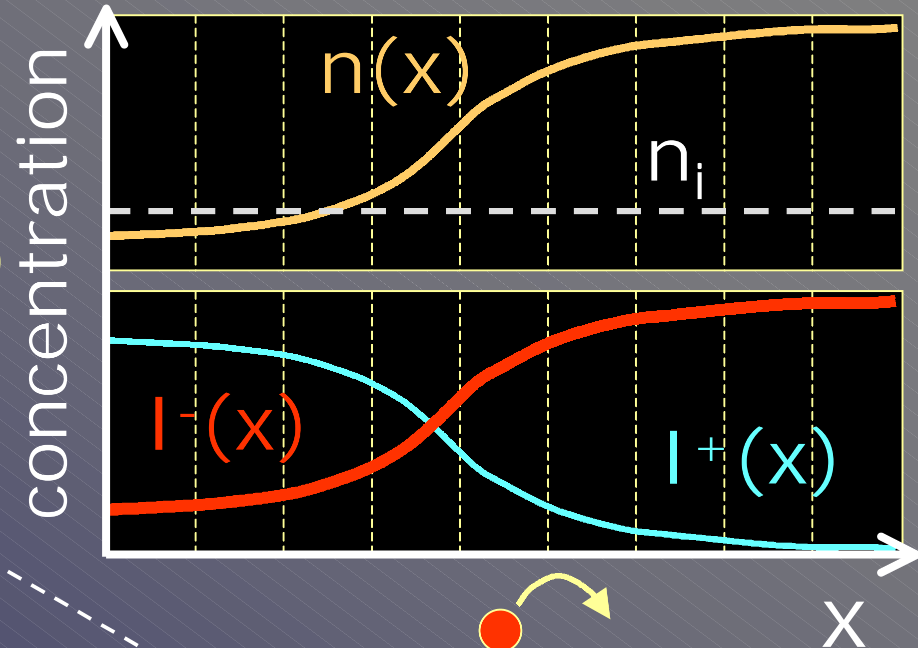
I,V recombination dissolves {311} and Loops

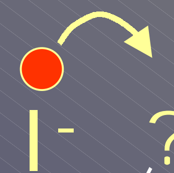
Are V's being held in small, stable clusters, that prevent recombination?

Charge Effects: Implementation

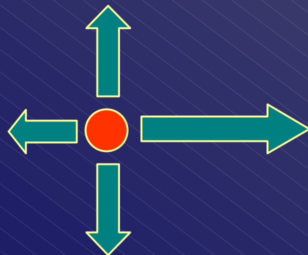
- Charge state update
  - static (immobile species)
  - dynamic (mobile species)

$$\frac{[I^-]}{[I^o]} = \frac{n(x)}{n_i} \cdot \delta_{I^-}$$





- Electric field(ξ) drift
  - modeled as biased diffusion

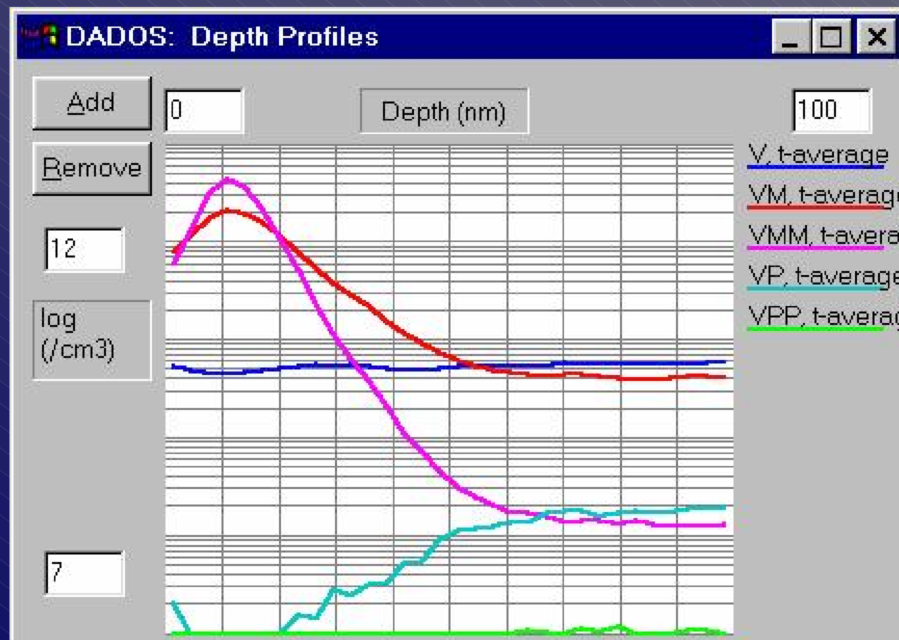


$$\frac{P(+x)}{P(-x)} = \exp\left(\frac{q \cdot \xi \cdot \lambda}{kT}\right)$$

- n(x) calculated from charge neutrality approximation
- no interaction between repulsive species

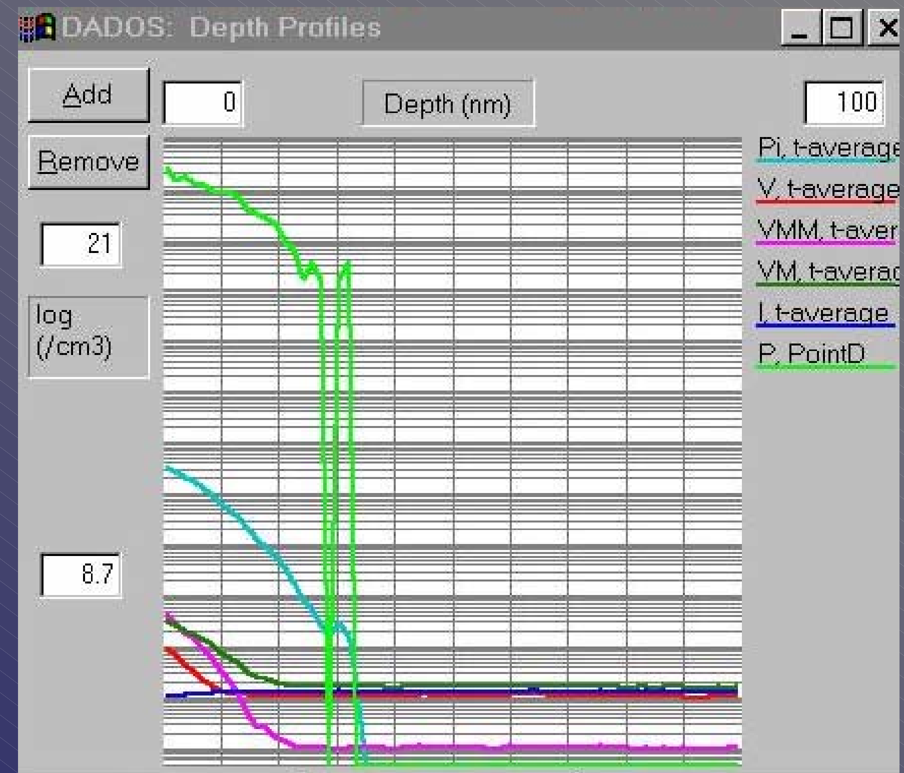
Charge Effects: Examples

- Equilibrium conditions



- Non equilibrium

  Phosphorous in-diffusion



Surface: I,V

- Inert
  - Emission Rate = $D0 * \exp(-(Ef+Em)/kT)$
  - Recomb. Probability = $\frac{\text{Recomb. Length}}{\text{Jump Distance}}$

- Oxidation:
  - I-supersaturation
- Nitridation:
  - V-supersaturation

⇒ Atomistic KMC can incorporate any currently available injection rate model (from SUPREM, etc)

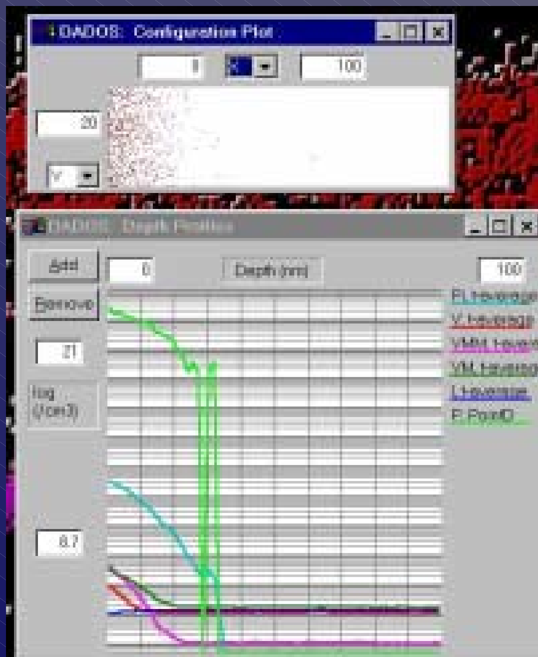
Surface: Impurity Atoms

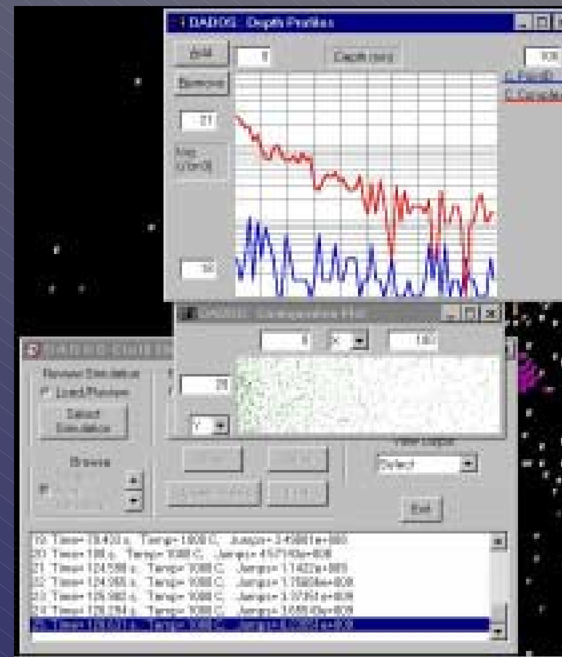
- Surface-to-Bulk: (Diffusion from the Surface)

  Given the Surface concentration calculate the corresponding mobile species emission rate.

- Bulk-to-Surface: (Grown-in, Implant,…)

  1. Monitor the number (N_A) of Impurity atoms that arrive at the surface.
  2. Emit the mobile species at a rate proportional to N_A up to the solubility limit.





In Atomistic KMC **all** mechanisms are operative **simultaneously**

Unforeseen effects can show-up when all mechanisms are included simultaneously

Examples:

1. Nominally "non-amorphising" implants (e.g. 40 KeV, 8×10^{13} cm^{-2} Si) can still generate small, isolated amorphous regions due to cascade overlapping.

2. Self-diffusion Data (Bracht, Phys. Rev. B **52** (1995) 16542):

   $\Rightarrow$ V parameters (Formation + Migration)

   The split (Formation, Migration) was chosen such that (together with the V cluster energies from Bongiorno, PRL) V clustering spontaneously generates Voids.

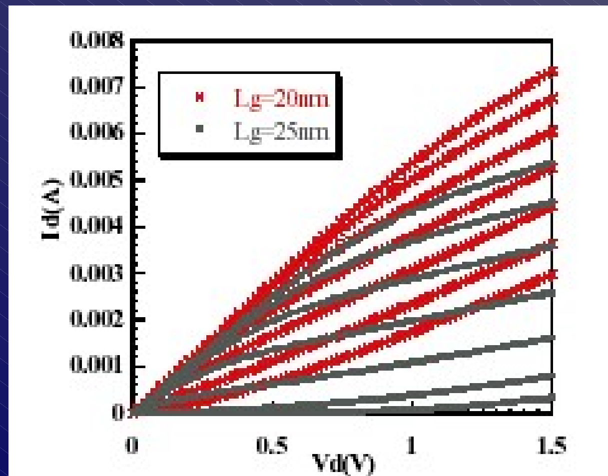
$\Rightarrow$ Missing mechanisms can lead to missed **side-effects**.

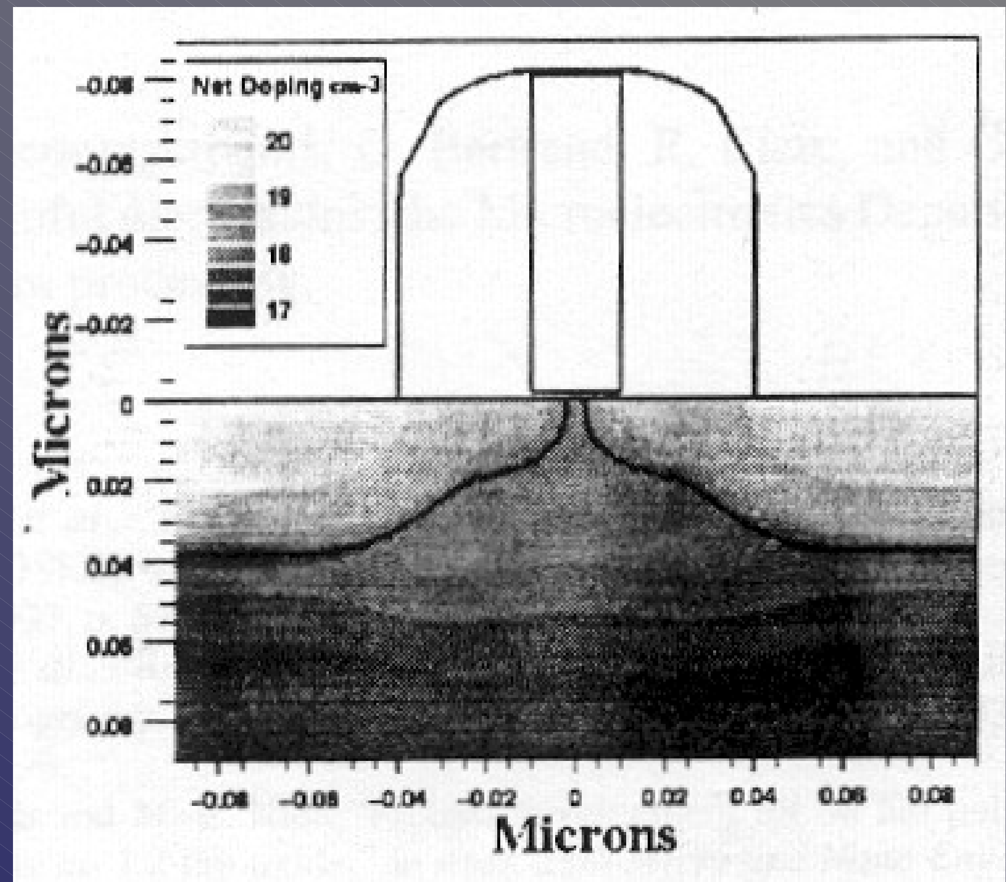
Device Processing

Example:

A 20-nm NMOSFET

(Deleonibus et al., IEEE Electron Dev. Lett., April 2000)





Device Processing

DADOS Simulation

As Implanted

1s @ 950 C

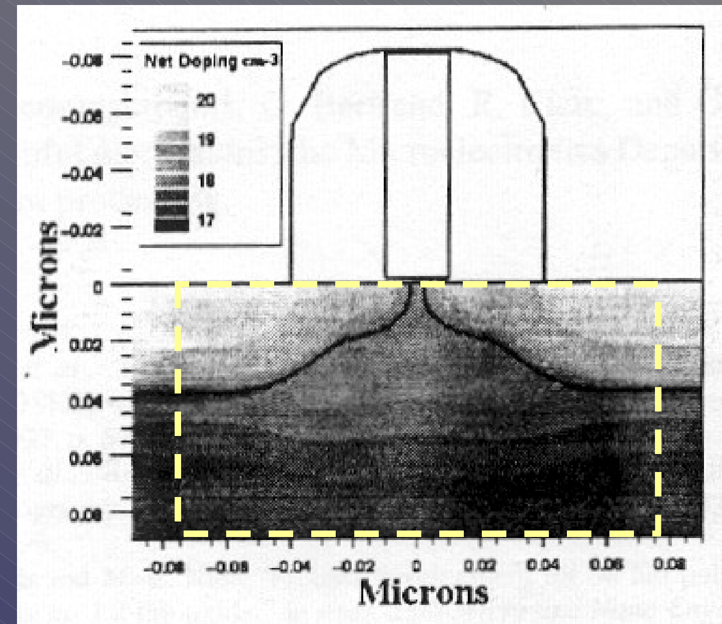
Calculation region: 100x70x50 nm^3

S/D Extension: 3 KeV, 10^{14} As/cm^2

S/D Deep-Implant: 10 KeV, 4×10^{14} As/cm^2 (?)

Anneal: 15 s @ 950 C

15s @ 950 C



Deleonibus et al.,
IEEE Elec. Dev. Lett., April 2000

Anneal CPU time on a 400 MHz Pentium-II:

32 min

Deep-Implant also simulated

(Extension only: 5 min)

Conclusions

Atomistic KMC can handle:

- **All** these mechanisms
- **Simultaneously**
- Under highly **non-equilibrium** conditions
- In **3D**

Atomistic Front-End Process Simulation can **advantageously** simulate the processing steps of current **deep-submicron device** technology.