Predictive Front-End Process Simulation

*The **kinetic Monte Carlo** Approach*

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Crolles, 12 April 2005

Acknowledgments

Recent collaborators:

- I. Martin-Bragado
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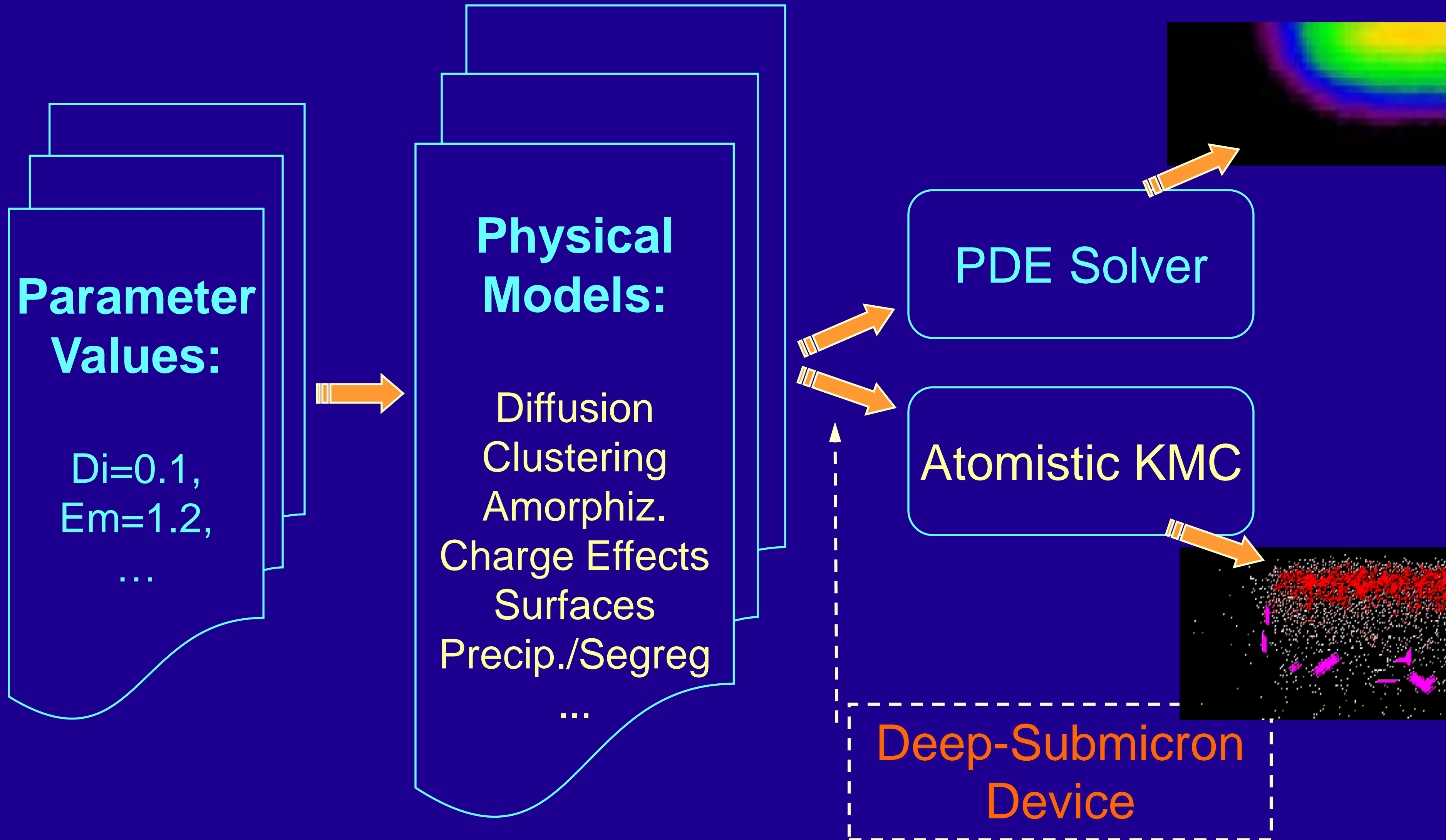
Outline

- *DADOS kMC: Brief history*
- Model overview
  - Point defects: Charge model
  - Extended defects (small clusters, {311}s, Disloc. loops, Voids)
  - Damage, Amorphiz. & Recrystallization
  - Impurities & Impurity clusters
  - Other Materials (Oxides, Nitrides) & Interfaces
  - SiGe & Strain effects
- Next improvements
- Conclusions

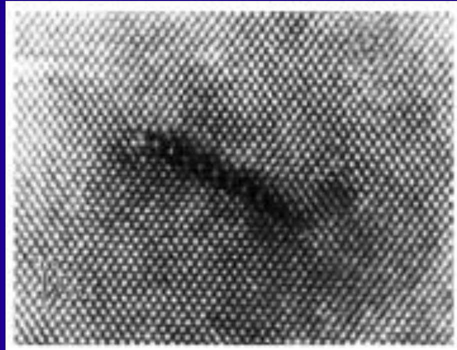
DADOS: Brief history

- Summer 1994, Bell Labs : First kMC code (BLAST) was begun by Jaraiz & Gilmer.
- 1996, Univ. of Valladolid: Based on the accumulated experience, Jaraiz rewrote the code completely and named it DADOS.
- 1996 to 2001: DADOS improved at the Univ. of Valladolid, and source code distributed to some Research Centers and Universities.
- 2001: License agreement signed with Avant! to include DADOS into Taurus™
- 2002: Synopsys acquires Avant!
- At present, there are nearly 40 journal papers published with DADOS results (16 APL, 5 JAP, 2 PRB, 2 PRL among others)

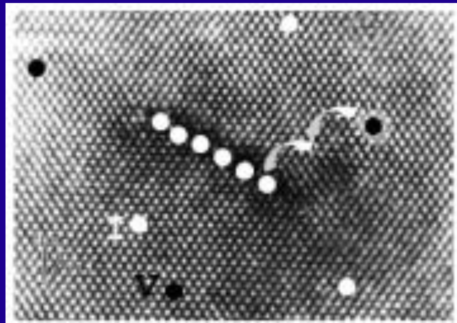
Front-End Process Modeling



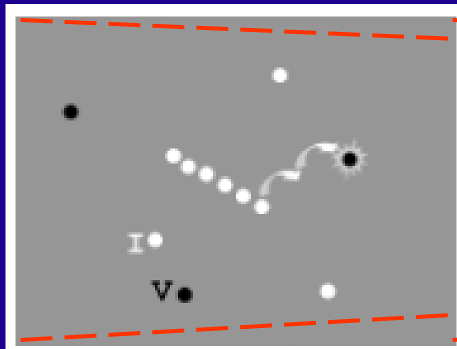
The Atomistic KMC Approach



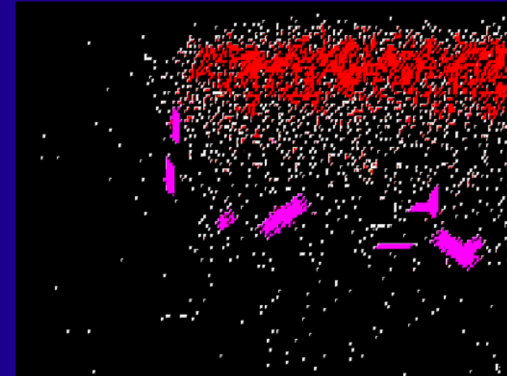
Lattice Atoms are just vibrating



Defect Atoms can move by diffusion hops

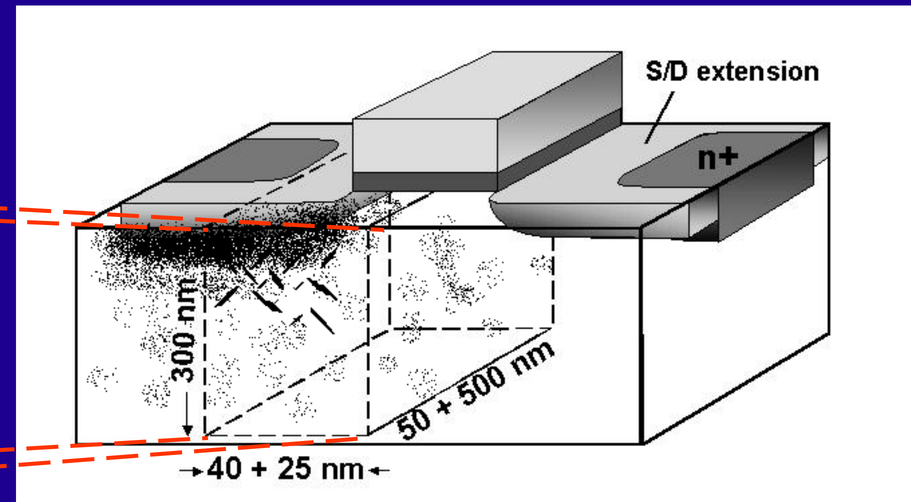


KMC simulates Defect Atoms only



Output

3D Atomistic kMC Simulator



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Point defects and Impurities

$I \begin{cases} I^+ \\ I^0 \\ I^- \end{cases}$	$V \begin{cases} V^{++} \\ V^+ \\ V^0 \\ V^- \\ V^{--} \end{cases}$	$As \{ As^+$	$As_i \begin{cases} As_i^+ \\ As_i^0 \end{cases}$	$As_v \begin{cases} As_V^+ \\ As_V^0 \\ As_V^- \end{cases}$
$B \{ B^-$	$B_i \begin{cases} B_i^+ \\ B_i^0 \\ B_i^- \end{cases}$	$C \{ C^0$	$C_i \{ C_i^0$	$In \{ In^-$
$In_V \begin{cases} In_V^0 \\ In_V^- \end{cases}$	$In_i \begin{cases} In_i^0 \\ In_i^- \end{cases}$	$P \{ P^+$	$P_i \begin{cases} P_i^0 \\ P_i^+ \end{cases}$	$P_V \begin{cases} P_V^+ \\ P_V^0 \\ P_V^- \end{cases}$

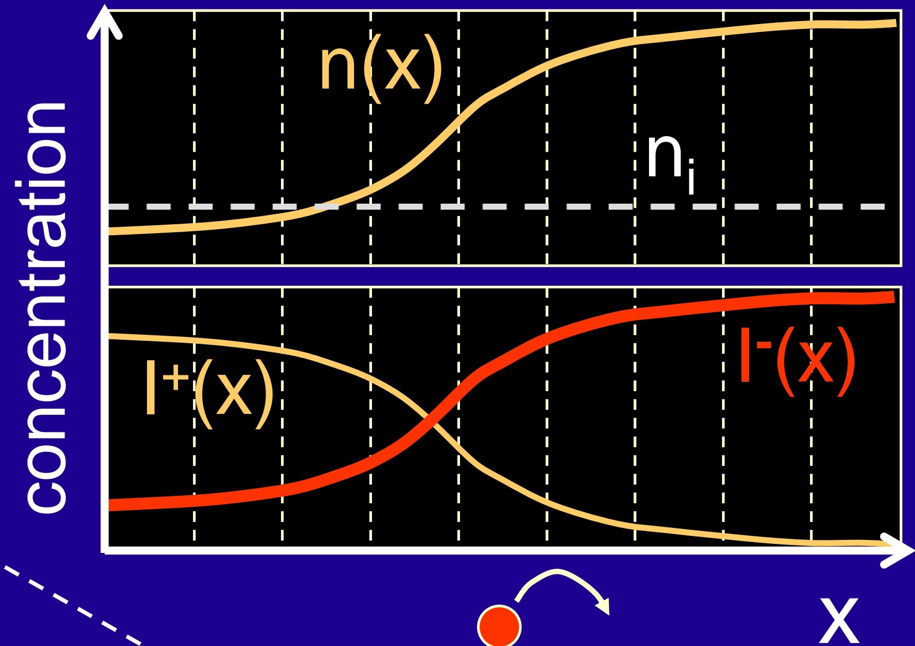
Table 8.21: Example of charge species in DADOS

- Egap(T) + Renormalization (high doping)
- Nc(T), Nv(T)
- Fermi-Dirac statistics

Charge Effects: Implementation

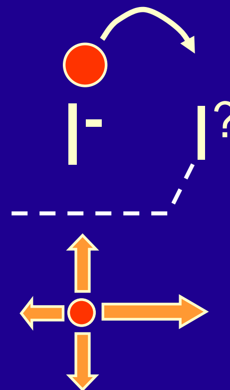
- Charge state update
  - static (immobile species)
  - dynamic (mobile species)

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



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

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

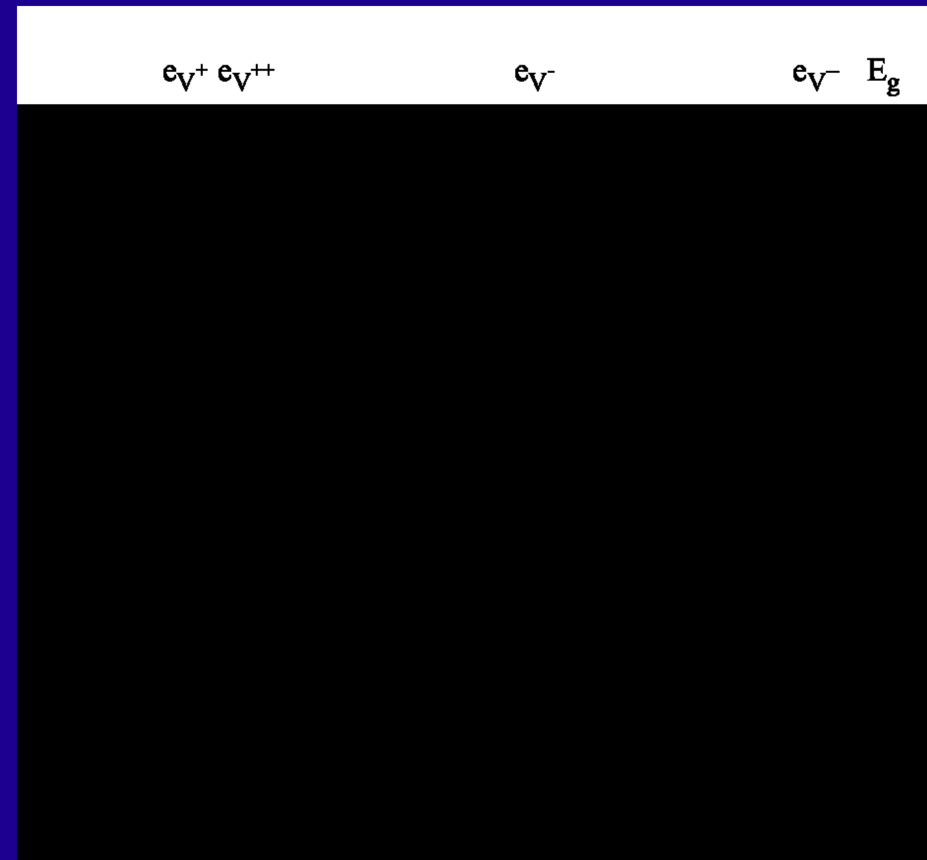


- n(x): from charge neutrality + Debye **smoothing**
- no interaction between repulsive species

Fermi-level Dependencies (I, V)

- Example: Vacancy charge states (V0,V-,V--,V+,V++)

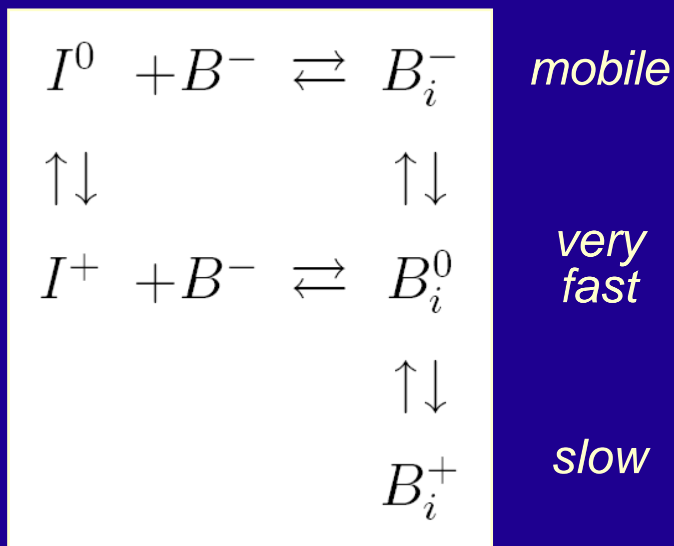
$$\frac{[V^j]}{[V^{j-1}]} = \exp\left(\frac{e_V(j,j-1) - e_F}{kT}\right)$$

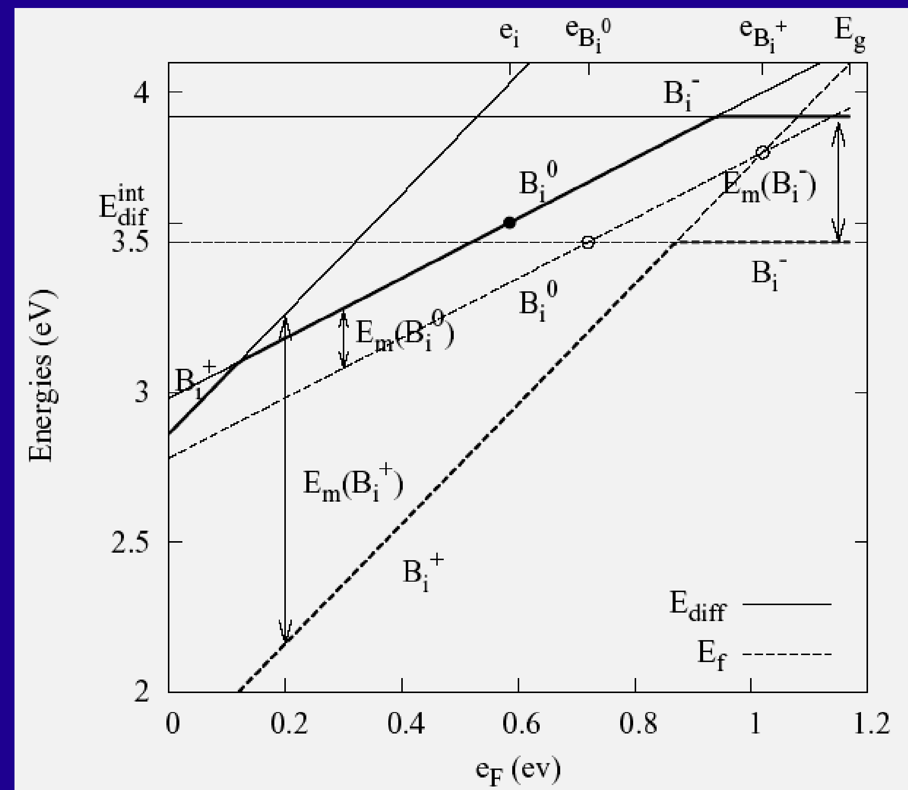


Dominant V charge state as a function of local Fermi-level $e_F(x,y,z)$

Fermi-level Dependencies (Impurities)

- Example: Boron charge states

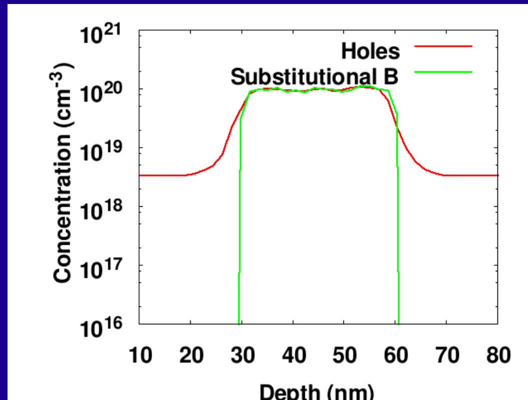




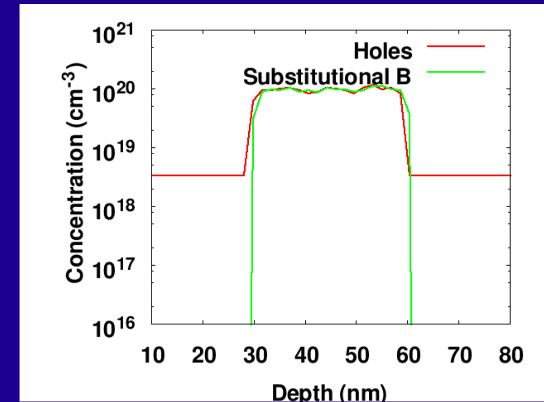
3D charge model (tests)

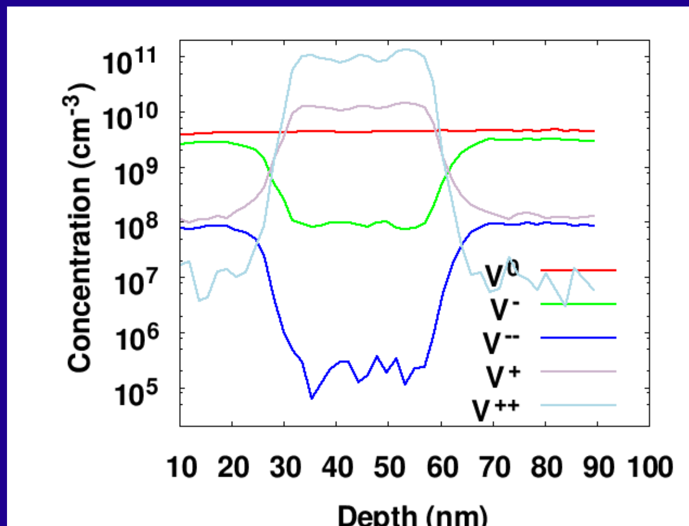
*Efficient **smoothing** algorithms for **point** charges, based on charge neutrality + local **Debye estimates***

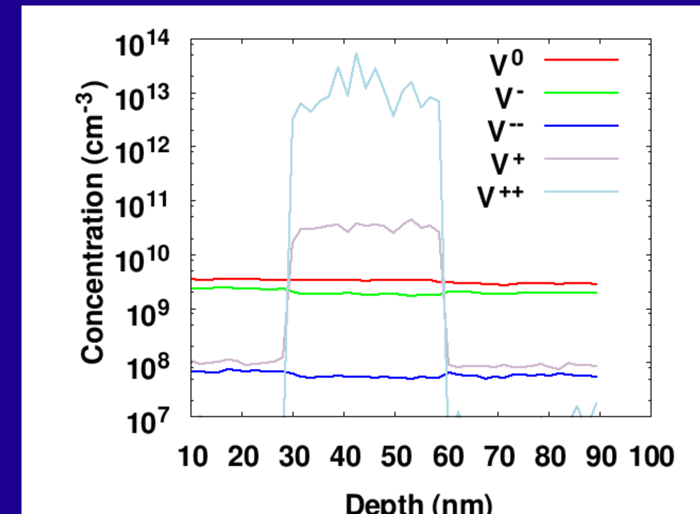
With smoothing:



Without:

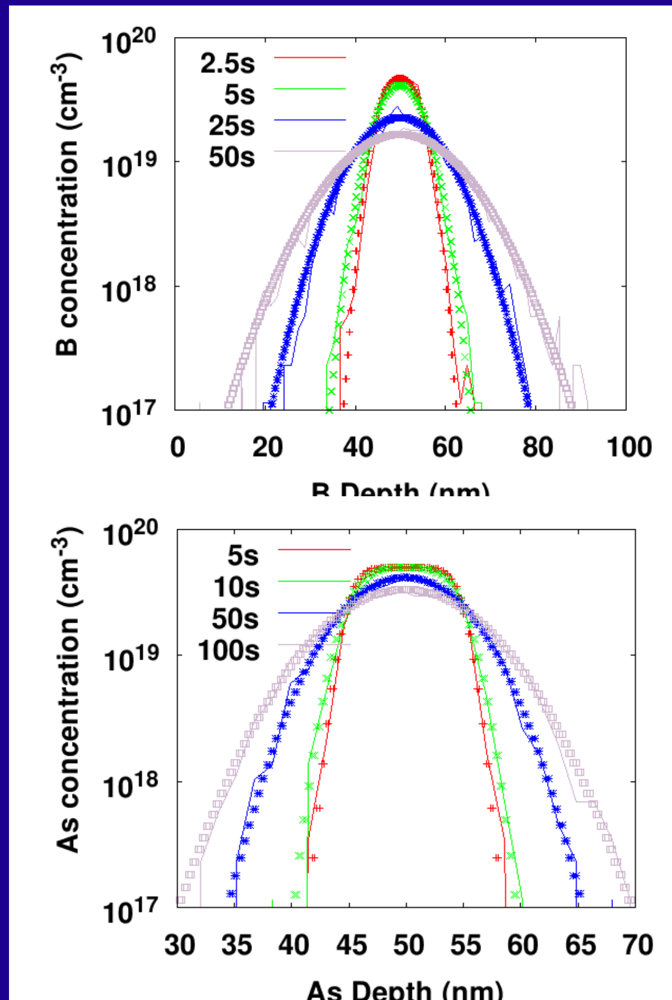






Intrinsic/extrinsic diffusion (tests)

Intrinsic



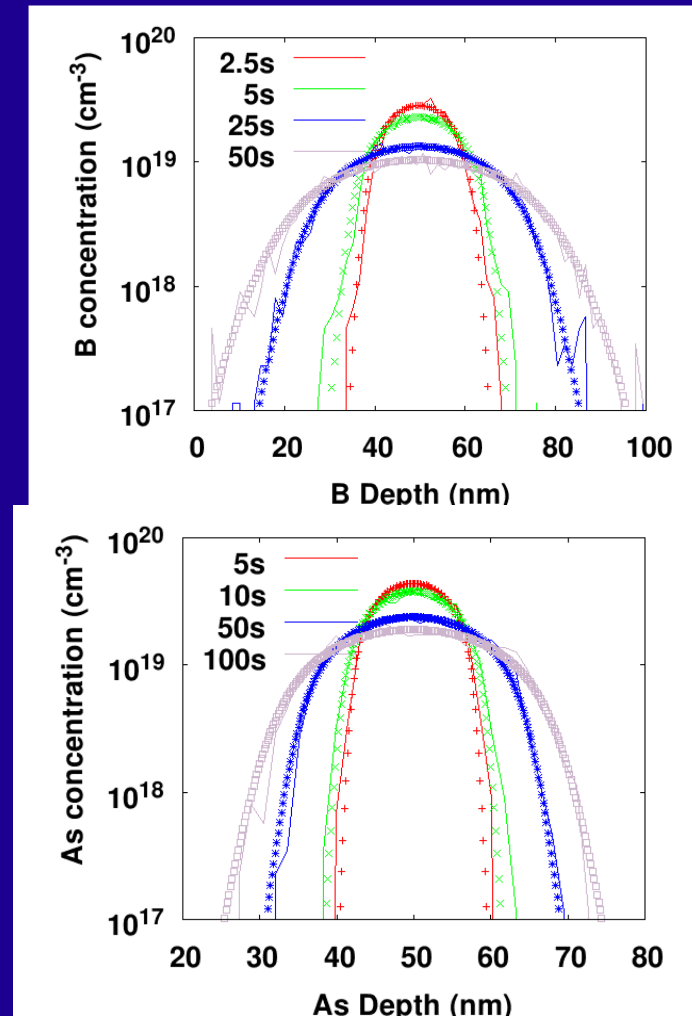
Lines:

Simulation

Symbols:

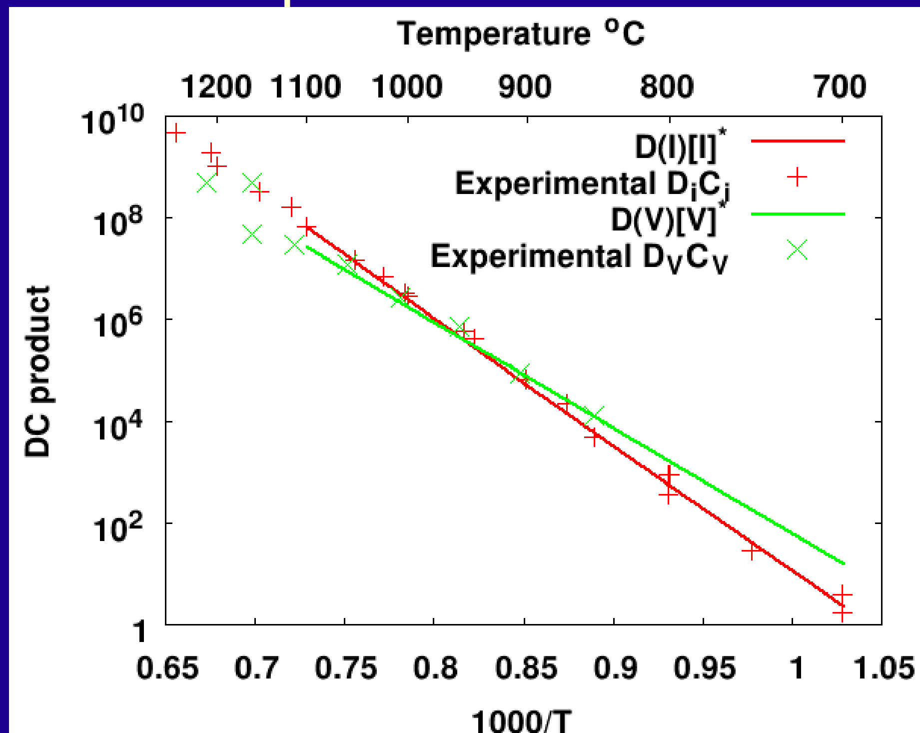
Continuum

Extrinsic



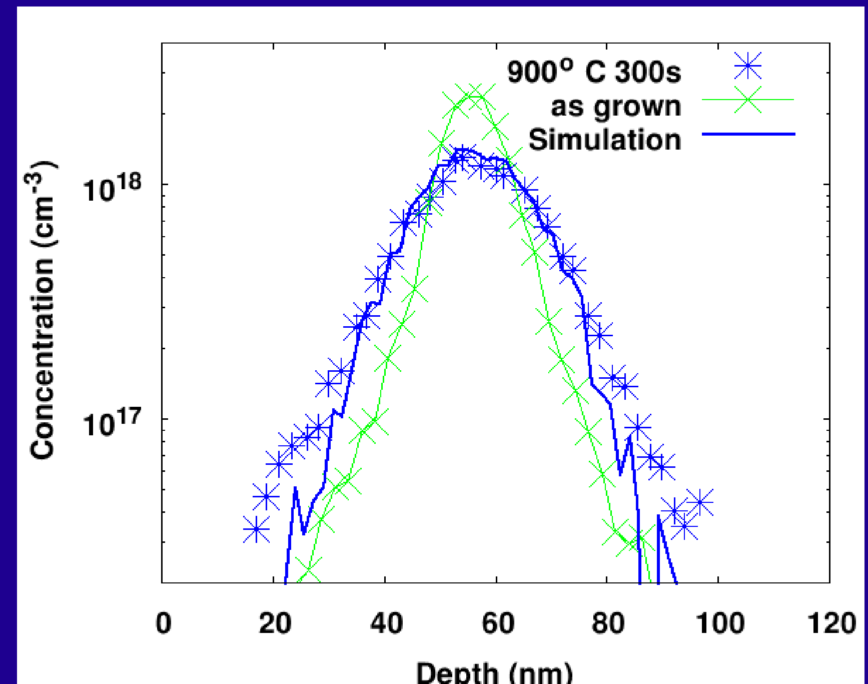
Point defects: Some tests under equilibrium conditions.

I and V equilibrium transport



Bracht et al,98;Cowern et al, 99; Giese et al, 00

Dopant spike diffusion (boron) in equilibrium



Cowern et al, 91

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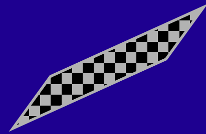
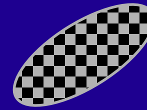
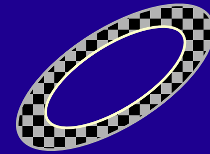
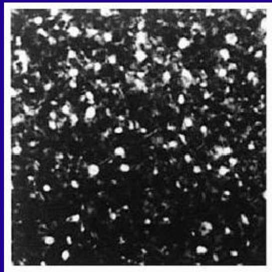
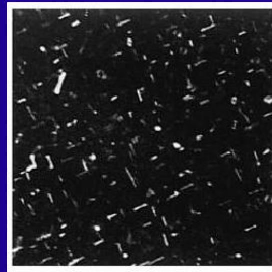
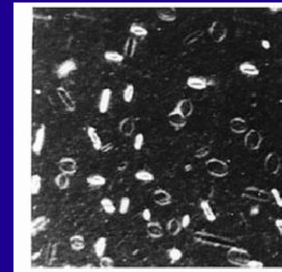
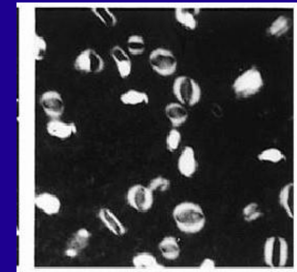
Extended Defects: Interstitials

Small clusters | {311} defects | Faulted loops | Perfect loops

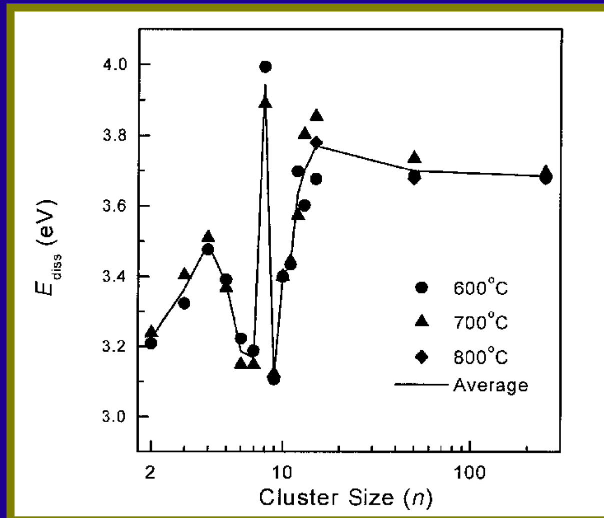




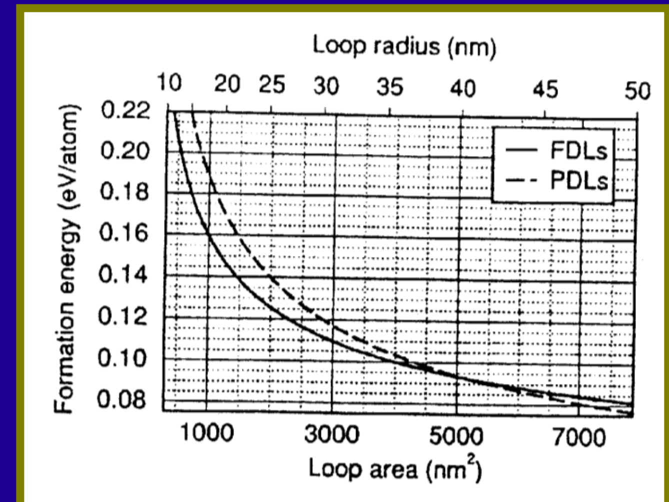


TEM images from Claverie et al.



Cowern et al.



Cristiano et al.

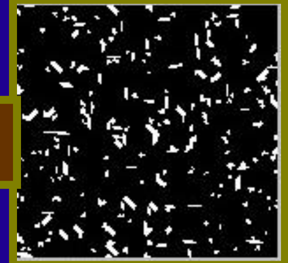
311-defects dissolution

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

Simulation

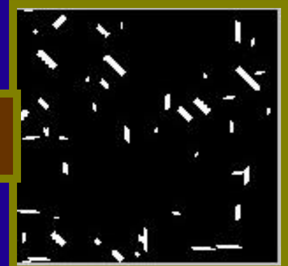
738ºC

200 s



600 s

1200 s



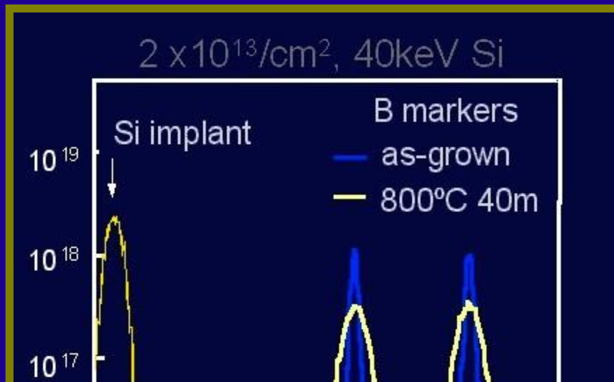
1800 s

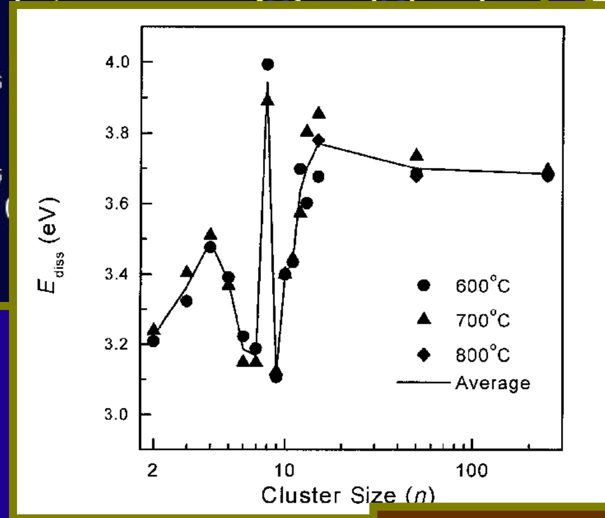
1.E+15
1.E+14
1.E+13
1.E+12
1.E+11
interstitials in defects (cm-2)
1
10
100
1000
10000
100000
Anneal time (s)
Experimental:
815ºC
738ºC
705ºC
670ºC
Lines: simulation

Data: Eaglesham et al.

Interstitial Supersaturation

Controls dopant diffusivity





Cowern et al.

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

Interstitial supersaturation

Experimental

◆ 600ºC

■ 700ºC

▲ 800ºC

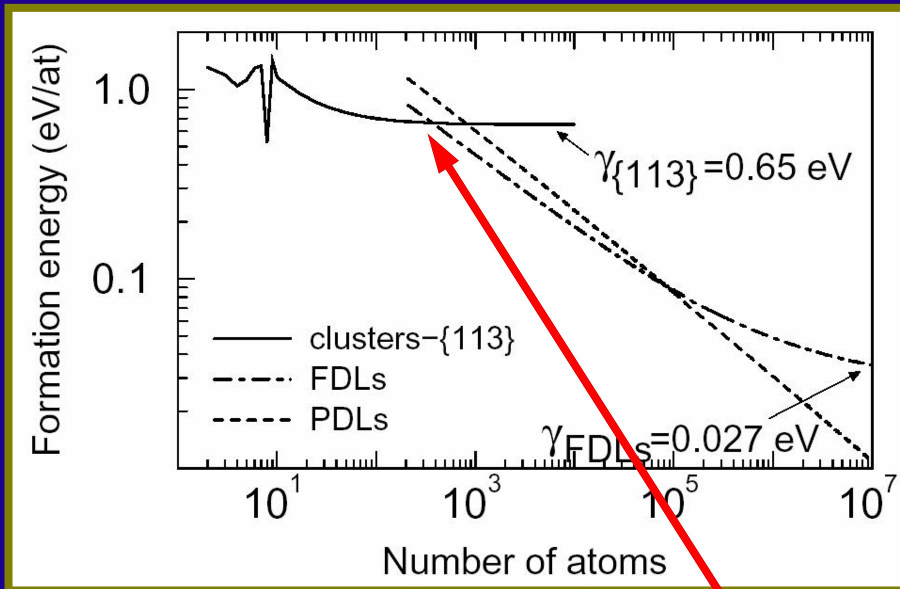
Lines: Simulation

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

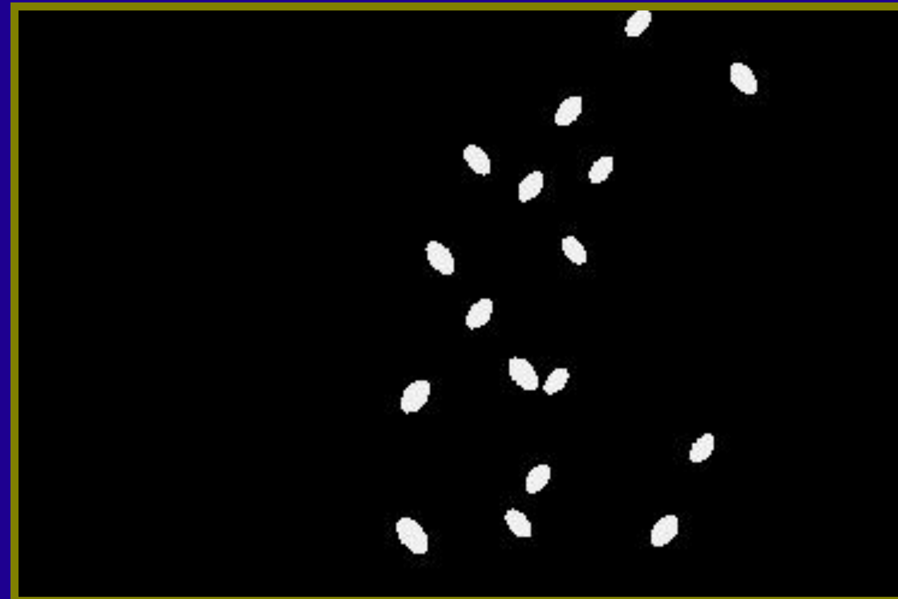
Anneal time (s)

Data: 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.

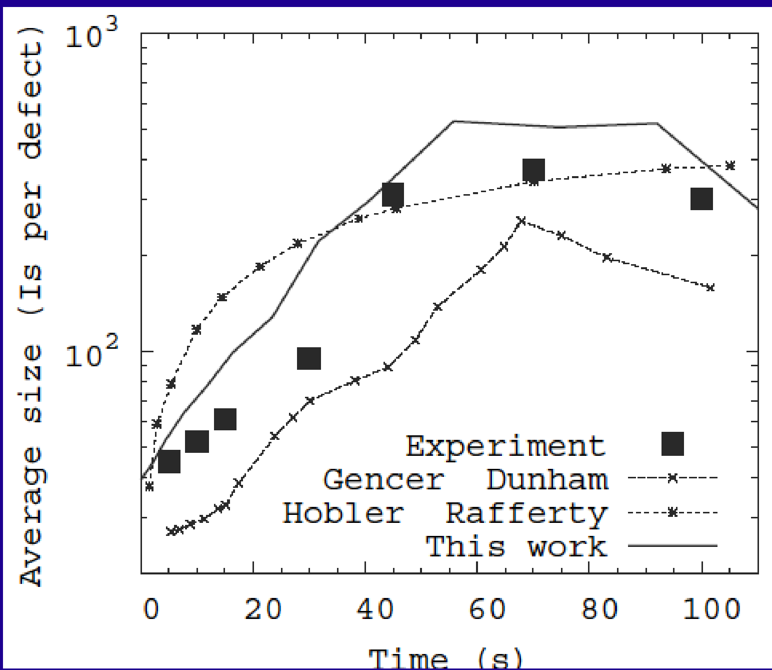
Transitition {311}→Loop: Activation Energy = 0.7 eV

{311} → Disloc. Loop transition

Thermally activated (0.7 eV)

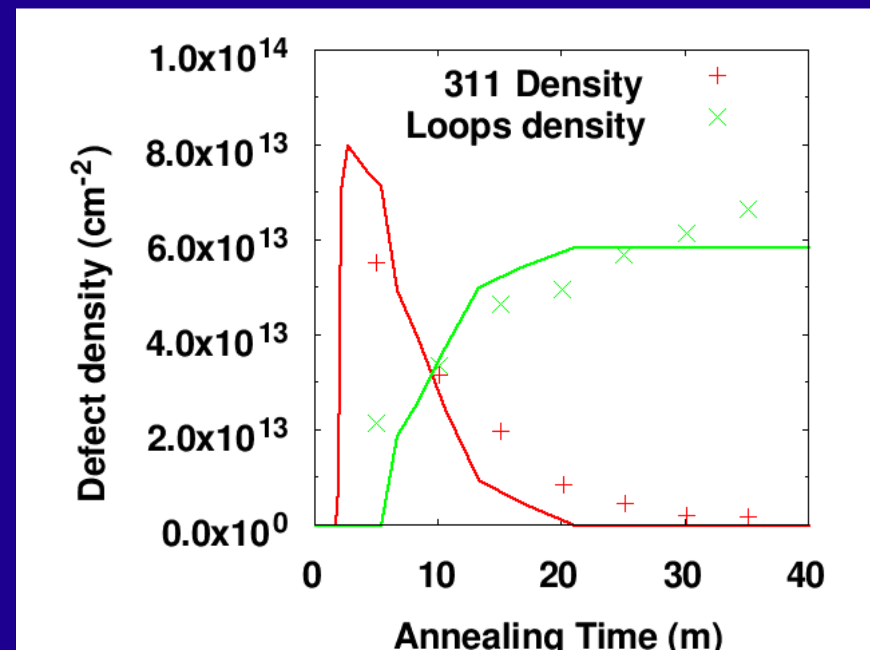
{311} size needs to be predicted, for correct transition to DLoop

{311} mean size evolution



Eaglesham et al, 94

{311} to dislocation loops transition.



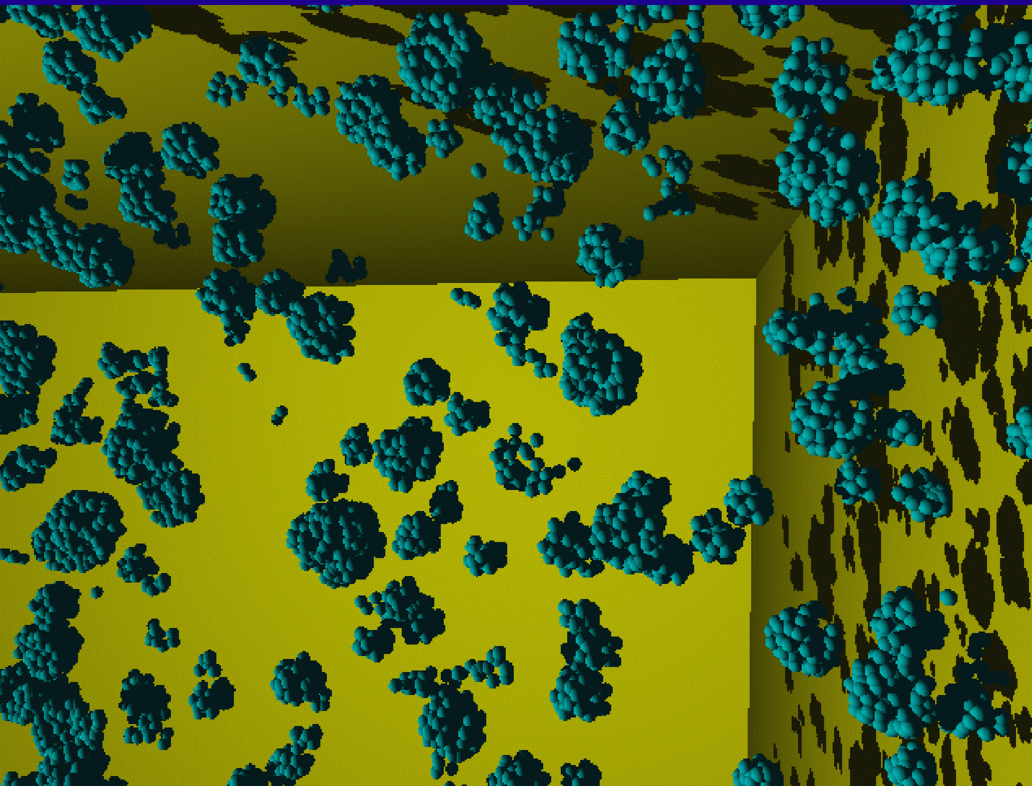
Li and Jones, 98

Lines: **Simulation**

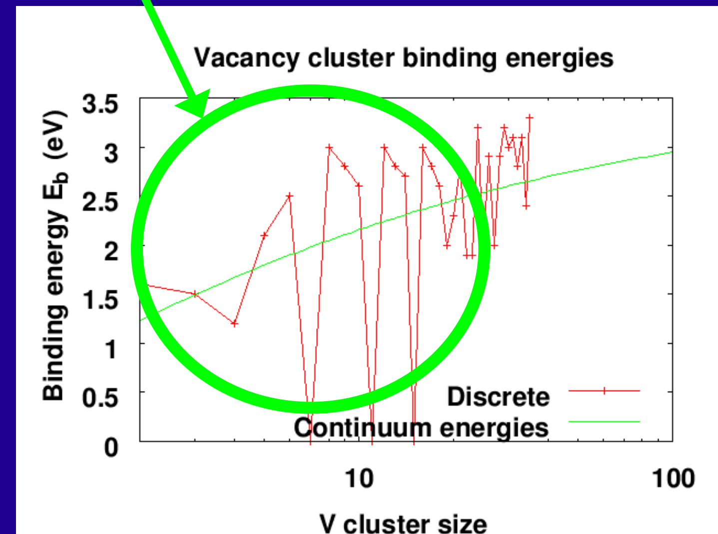
Symbols: **Experiment**

Vacancy Clusters & Voids

- Agglomeration of V's with an irregular shape (small clusters) or spherical (Voids) with the Si atomic density



Binding energies for V clusters and Voids



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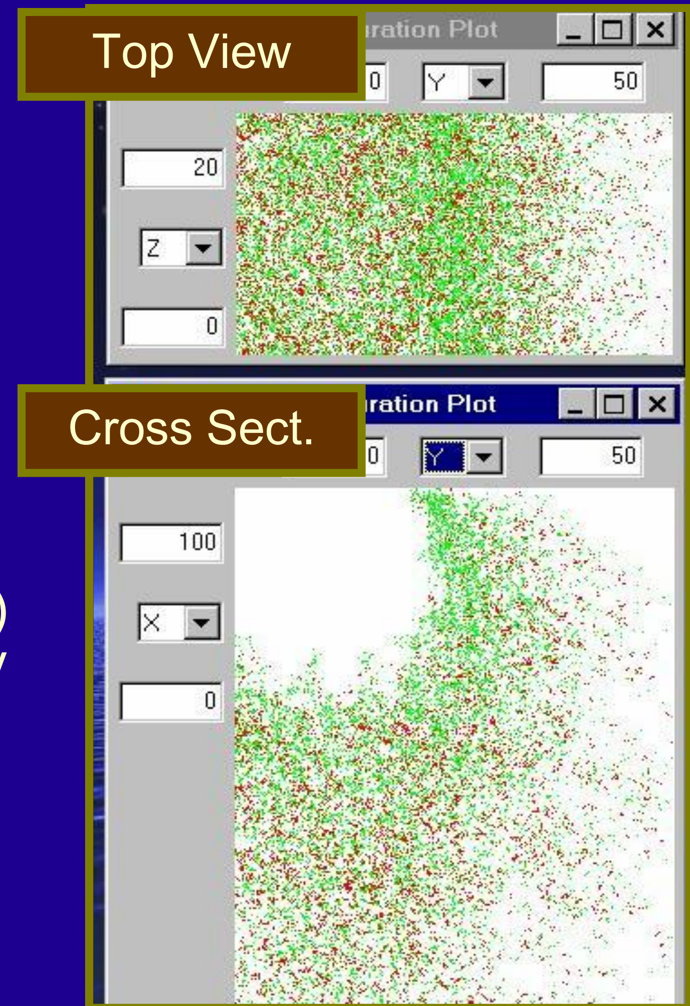
Damage accumulation - Amorphization

Implementation (3D):

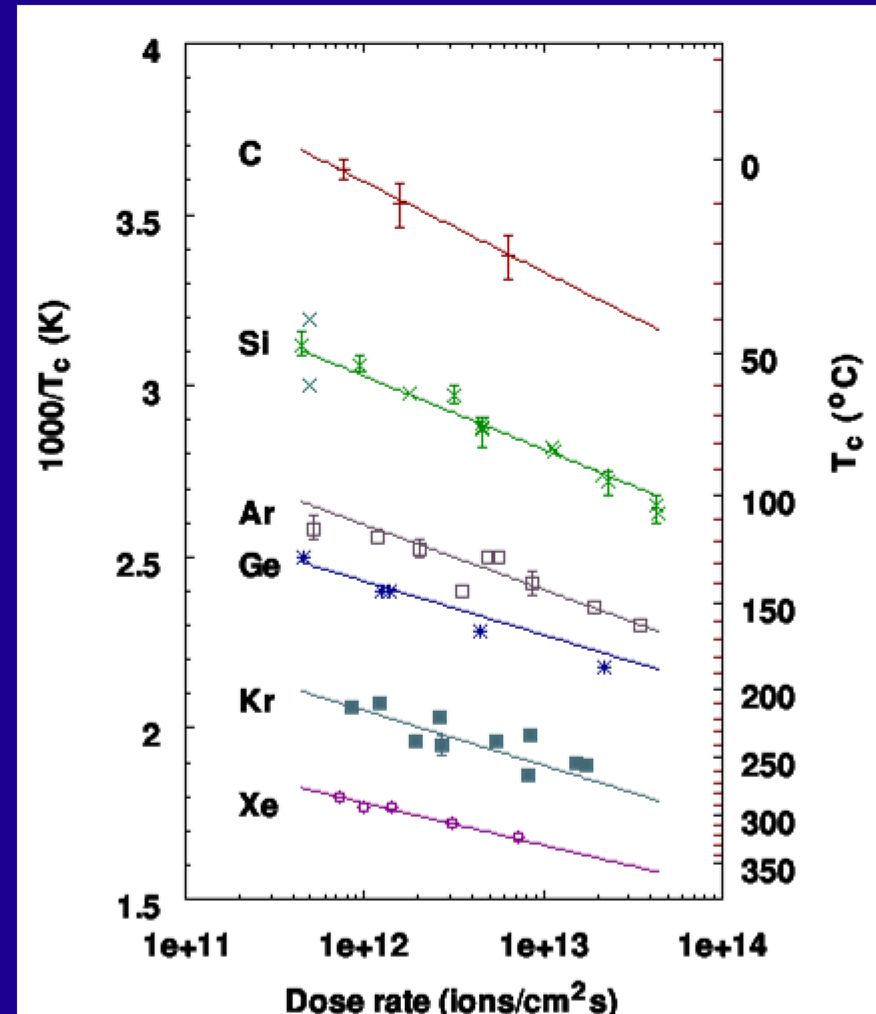
- Accumulate I's & V's into **Amorphous Pockets** (AP).
- **AP**'s have irregular shape, like clusters.
- **AP**'s allow for dynamic anneal between cascades.
- **AP**'s activation energy (for recrystallization) is a function of AP size (equiv. number of IV pairs).



Amorphization: Results (I)

Lines: Simulation

Symbols: Experiment
Golbderg et al, 95



Amorphization is **predictive** for a wide range of experimental conditions:

- Ion mass
- Dose rate
- Temperature

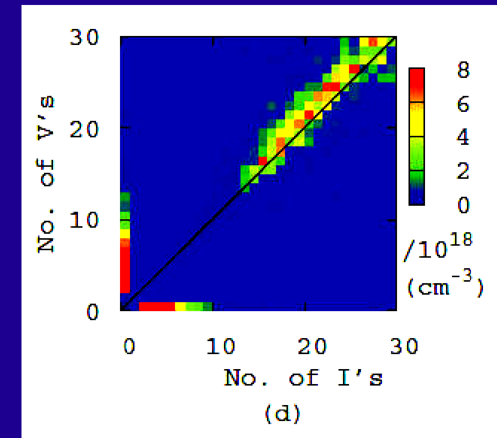
Amorphization: Results (II)

Amorphization is **predictive** for a wide range of experimental conditions:

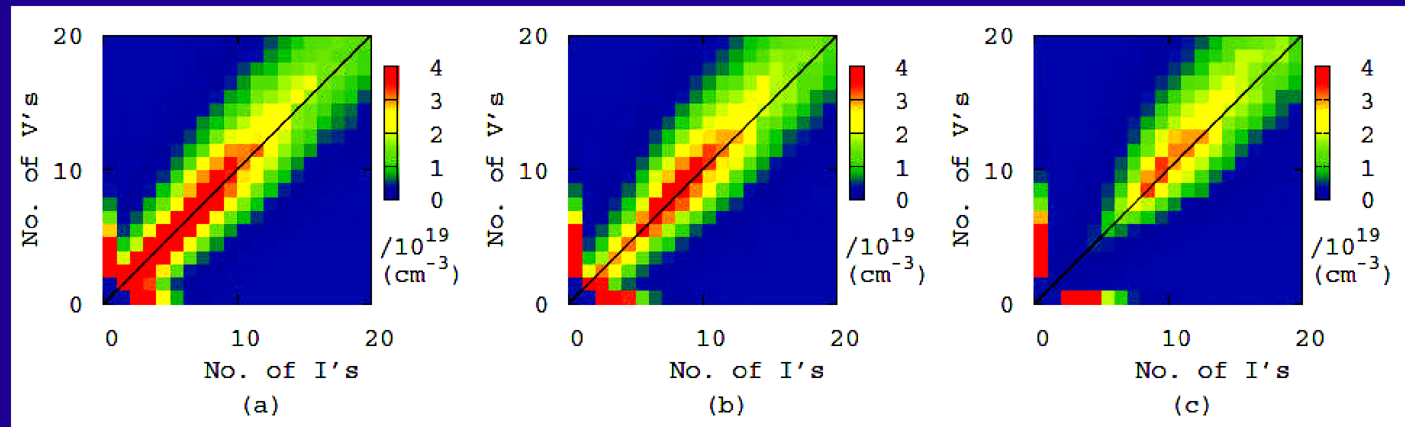
•**V-rich** Amorphous Pockets: more free I's (in agreement with MD)

•**Polyatomic** ions

Silicon



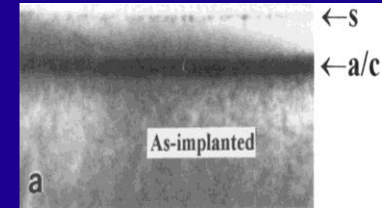
Carbon sequence

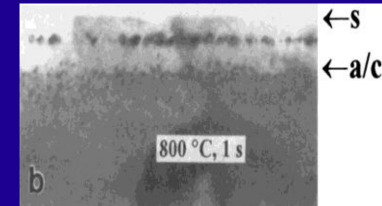


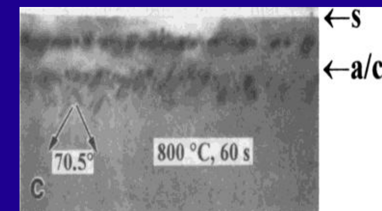
Recrystallization: Defects sequence

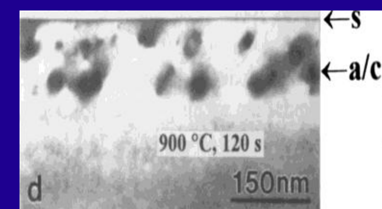
Implant: 50 KeV, 3.6×10^{14} Si/cm^2
(Pan et al., APL 1997)

100 nm







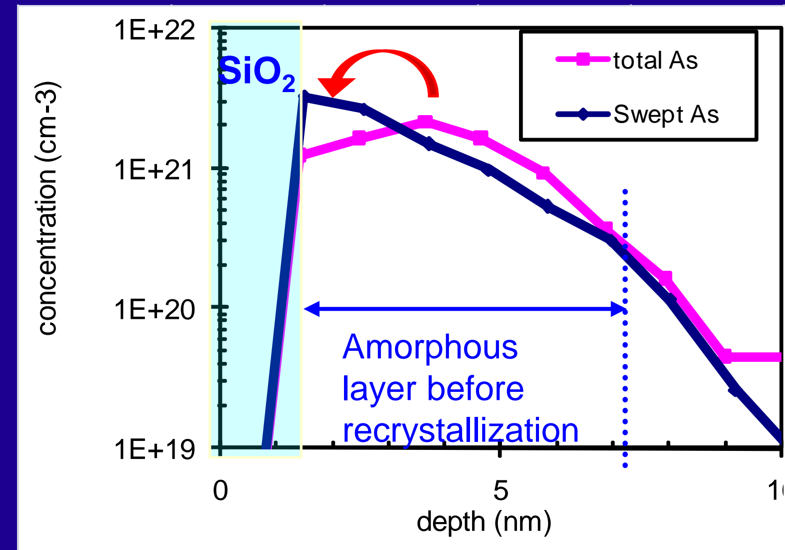


DADOS Simulation

*Recrystallization: Impurity **sweep**/deposit.*

- Dopants have a probability to be **swept** by the recrystallization front.
- Otherwise they are left as **active dopants** or
- If they exceed the solubility limit they can be deposited as **impurity clusters**.

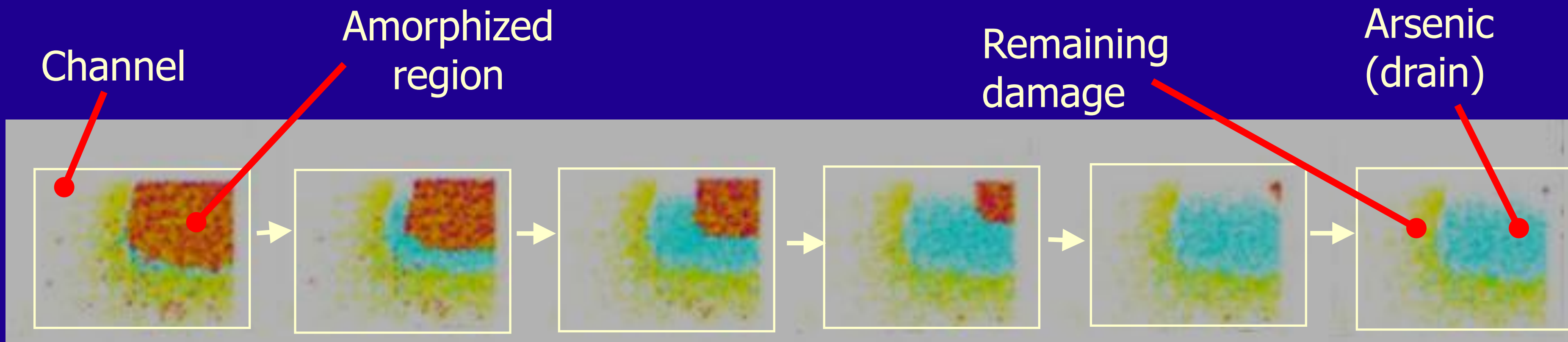
Implant (As 2keV, 10^{15} cm^{-2})
Annealing (700ºC, 2h)



3D-Recristalization Front

Velocity:

$$v_{recrys} = V_{0,recrys} * \exp\left(-\frac{E_{recrys}}{k_B T}\right)$$



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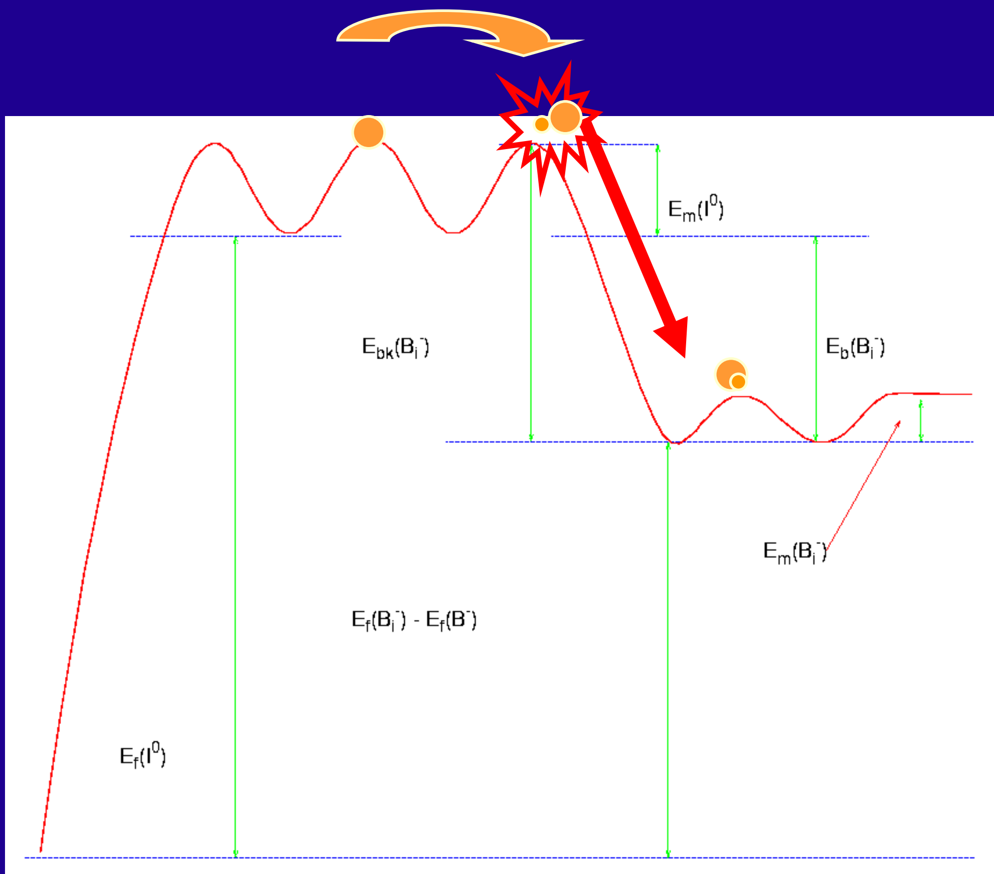
Impurity-related problems

- Complex relationships between:
  - Damage
  - Recrystallization: Sweep/Deposition
  - Charge
  - extended defects interactions
    - {311}-Indium
    - DLoops-Boron
  - generalized Frank-Turnbull (self-consistent)
  - … everything affects dopant diffusion and activation/deactivation!

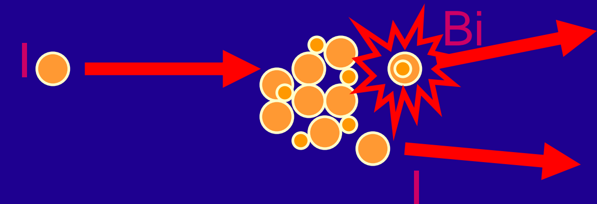
Impurities: mobile species & clusters

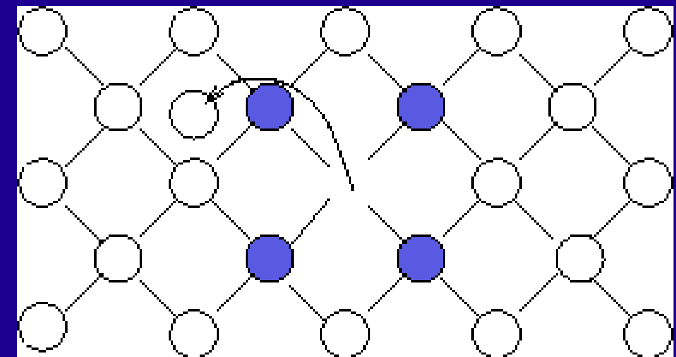
kick-out mechanism



Cluster

capture & emission



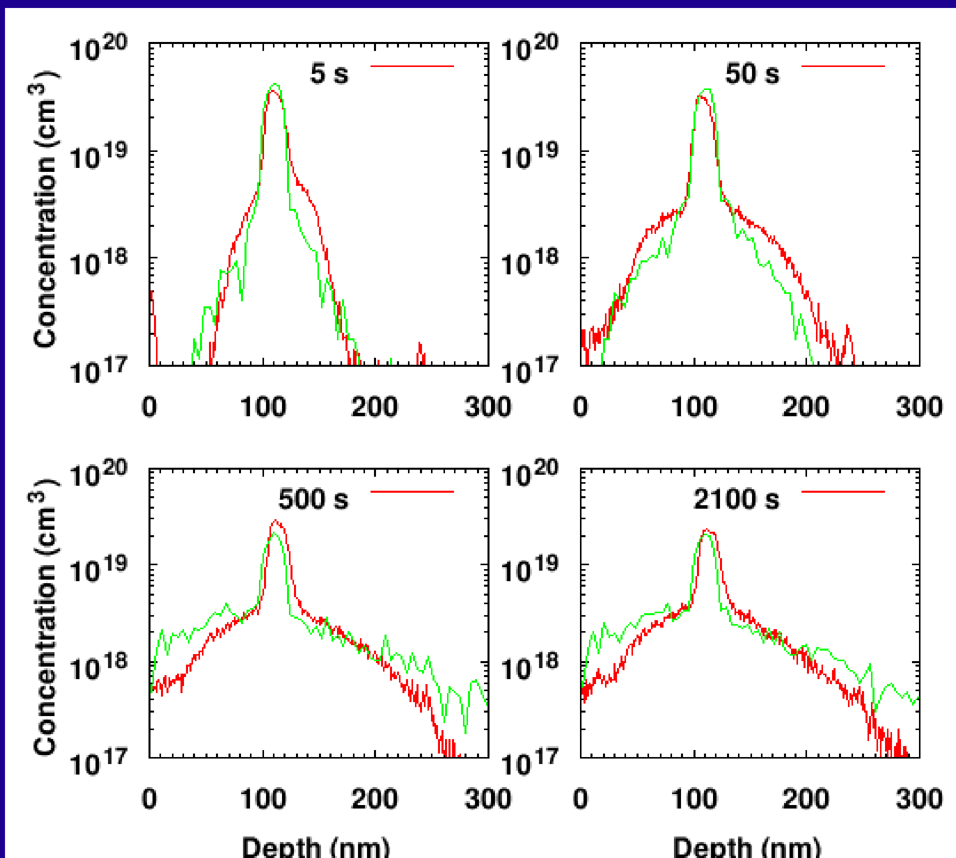


Frank-Turnbull mechanism

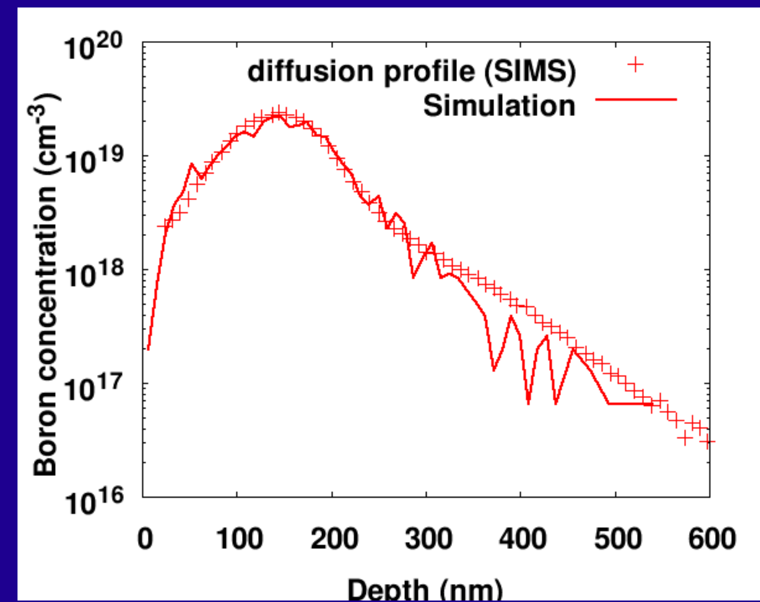
Boron (I)

Boron clustering and diffusion

Silicon implant,
Boron spike



Boron implant



Huang et al, 97

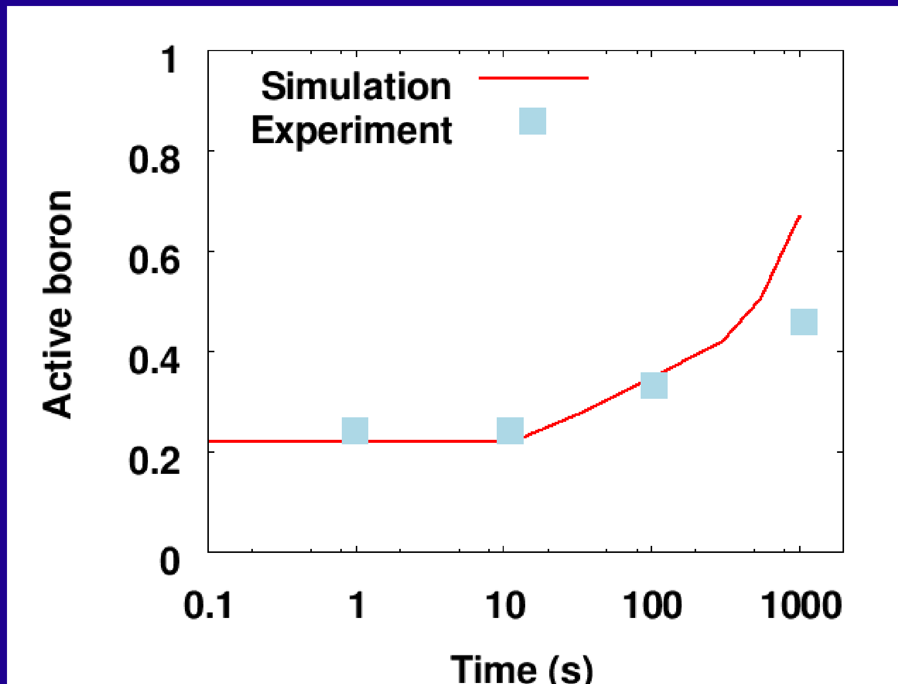
Pelaz et al, 97

Boron (II)

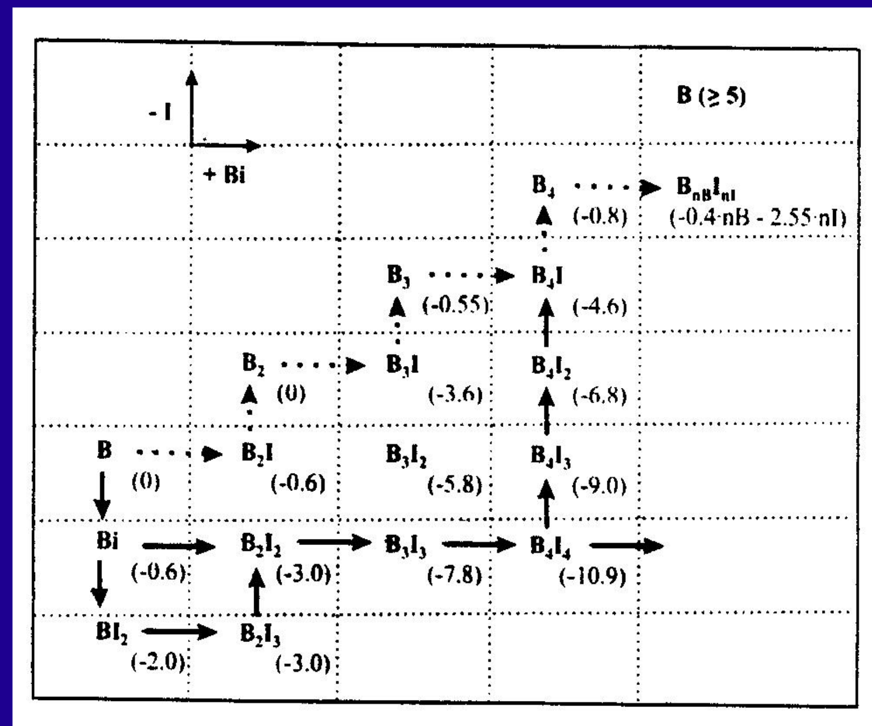
Boron activation

40 keV, $2x10^{14}$ cm^{-2} B implant

1000 s at 800^{0}C annealing



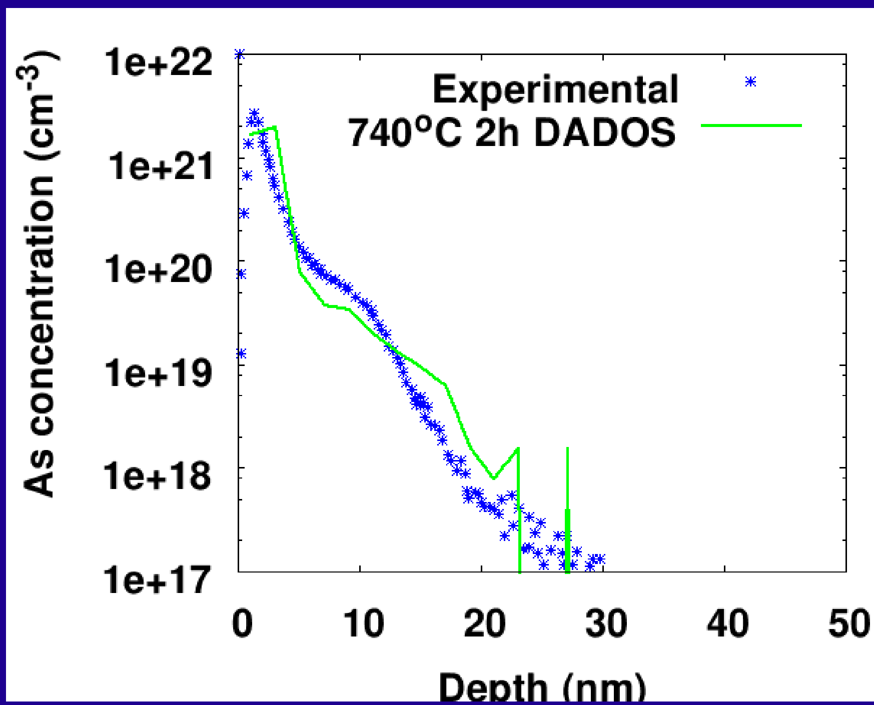
I_nB_m Pathway



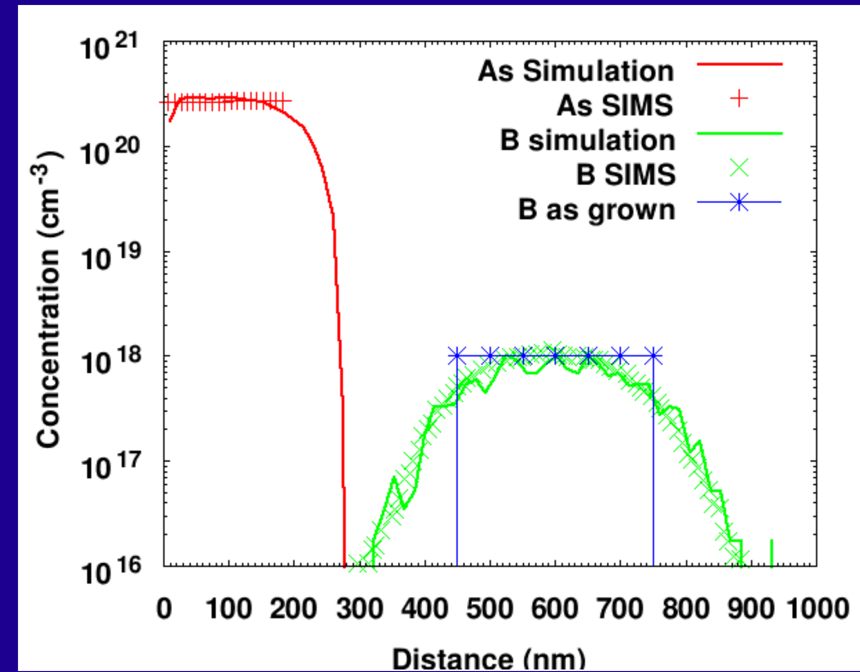
Pelaz et al. 99

Arsenic

Arsenic diffusion, clustering & activation/deactivation



Chakravarthi et al, 02



Rousseau et al, 98

Outline

- DADOS kMC: Brief history
- Model overview
  - Point defects: Charge model
  - Extended defects (small clusters, {311}s, Disloc. loops, Voids)
  - Damage, Amorphiz. & Recrystallization
  - Impurities & Impurity clusters
  - ***Other Materials (Oxides, Nitrides) & Interfaces***
  - SiGe & Strain effects
- Next improvements
- Conclusions

Materials Interfaces

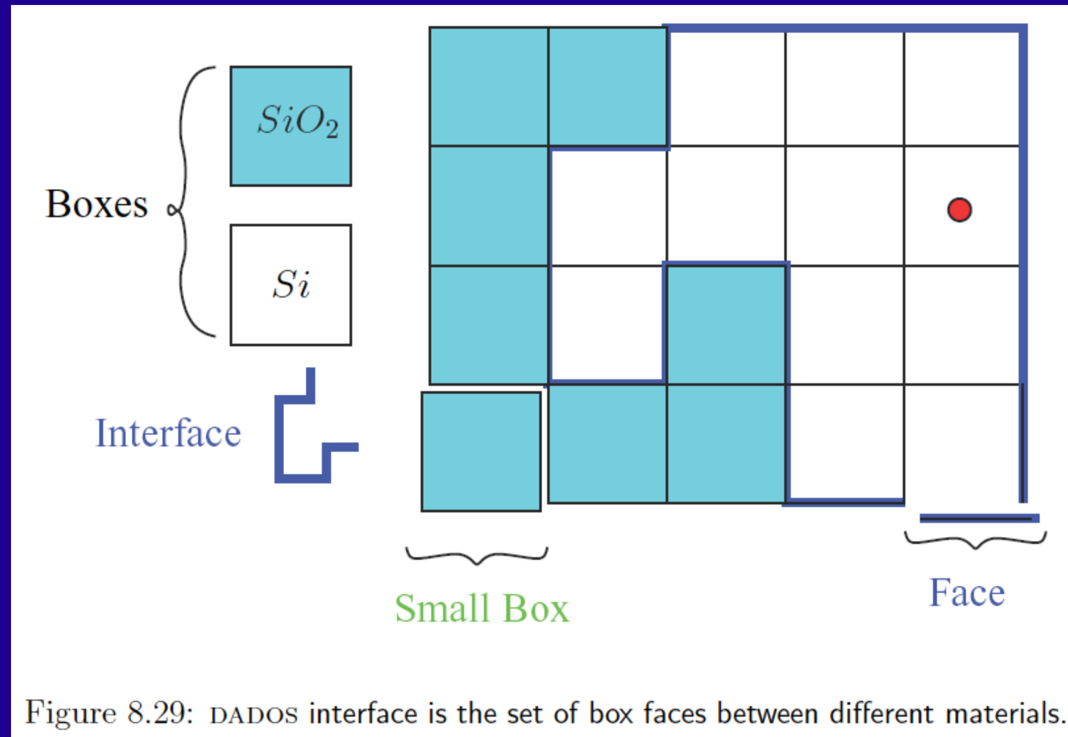


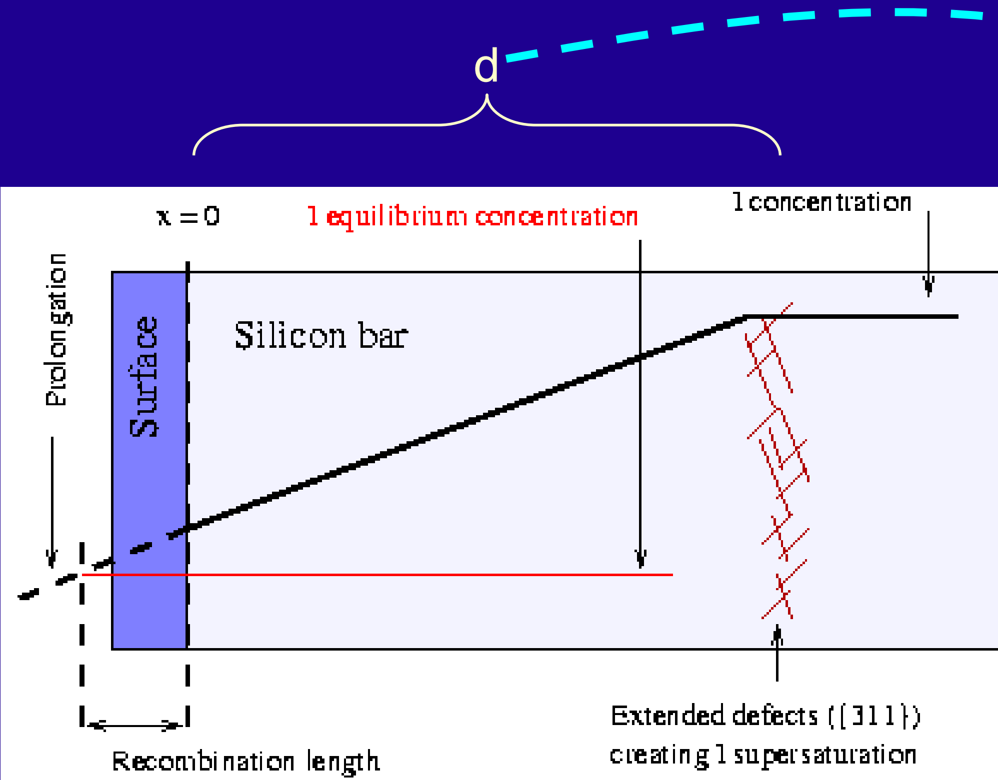
Figure 8.29: DADOS interface is the set of box faces between different materials.

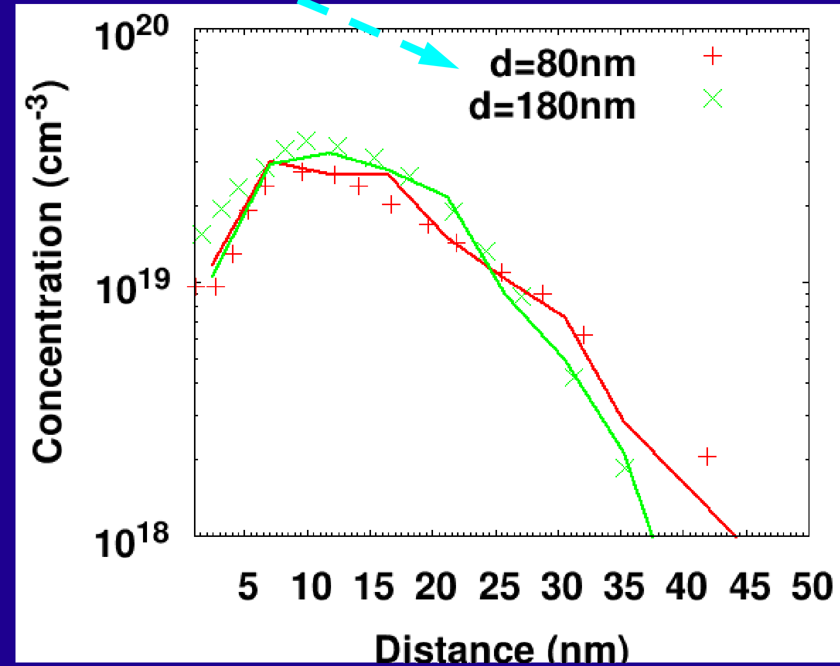
- Oxides, Nitrides: simple (B, As...) **Diffusion**.
- Impurity **Trapping** at the Interface
- Impurity **Segregation** into the other material

Materials Interfaces : I, V

Surface Recombination length

d





Lines: **Simulation**

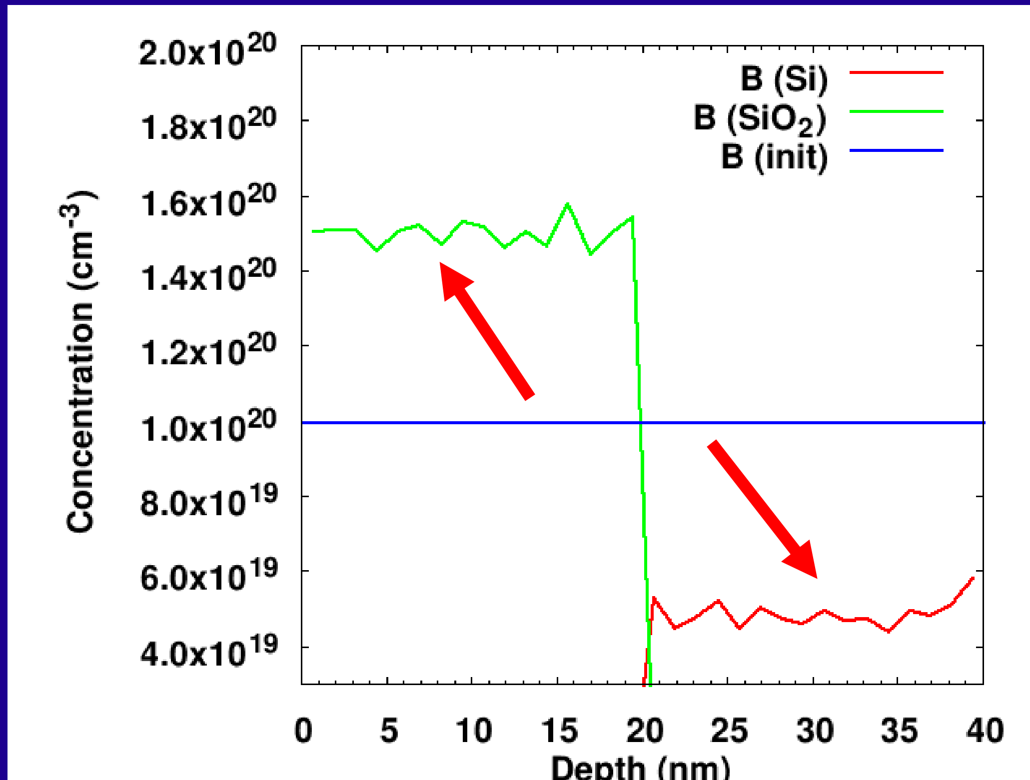
Symbols: **Experiment, Cowern et al, 99**

Materials Interfaces : Impurities

Oh-Ward model (IEDM'98): $F = C_s h \left(1 + \frac{e}{a}\frac{\sigma_F}{\sigma_{max}} - \sum_{\text{species}} \frac{\sigma_F}{\sigma_{max}}\right) - h\kappa\sigma_F,$

Trapping — Emission

SiO_2/Si: B trapping/segregation/diffusion



SiO_2 — Si

← Initial boron profile: 1×10^{20} cm^{-3}

Subsequent annealing: 2000 s at 1000 ºC

Outline

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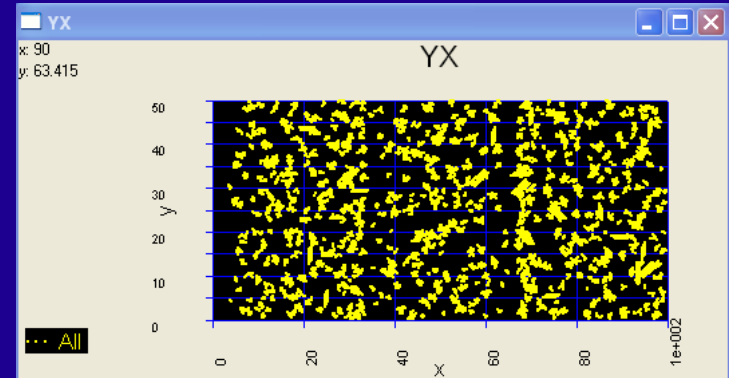
Modeling SiGe & strain

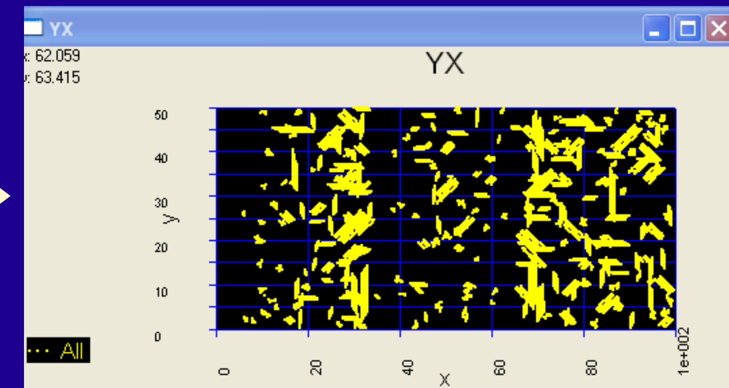
Self-Interstitials:

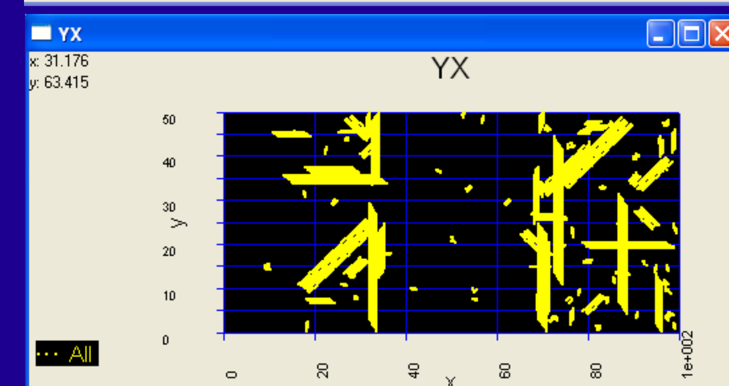
Higher $E_{act}(I) = E_{form} + E_{mig}$

We take same E_{mig}

$\Rightarrow$ Higher E_{form} $\Rightarrow$ **Lower I conc.**







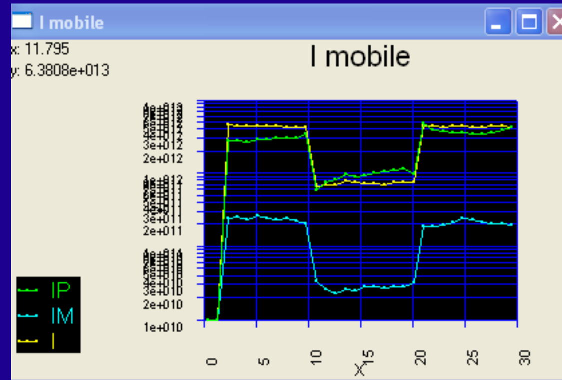
SiO_2/Si interface

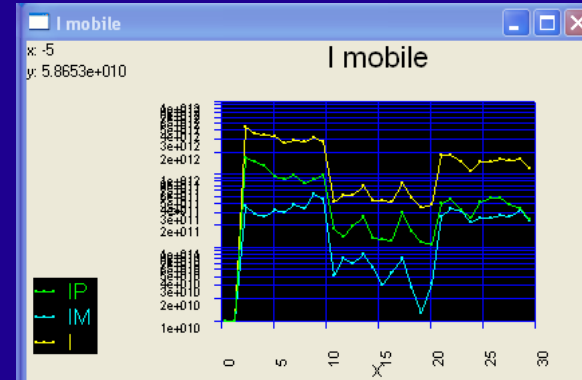
Unrelaxed $Si_{0.8}Ge_{0.2}$

B, As Diffusion in strained SiGe

Higher $E_{act}(I)$

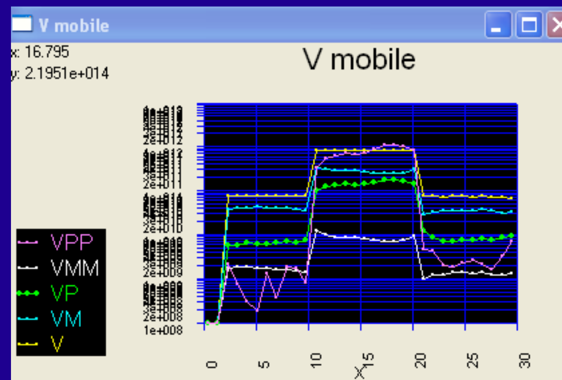
Lower I conc.

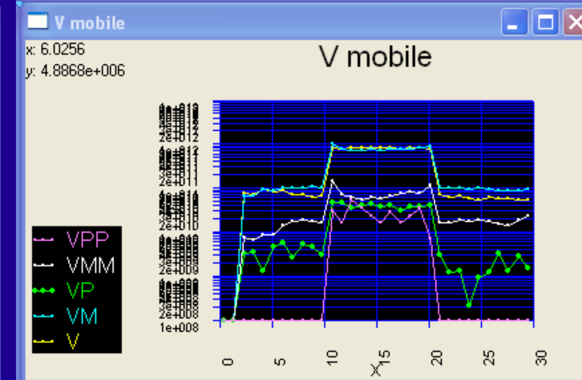




Lower $E_{act}(V)$

Higher V conc.

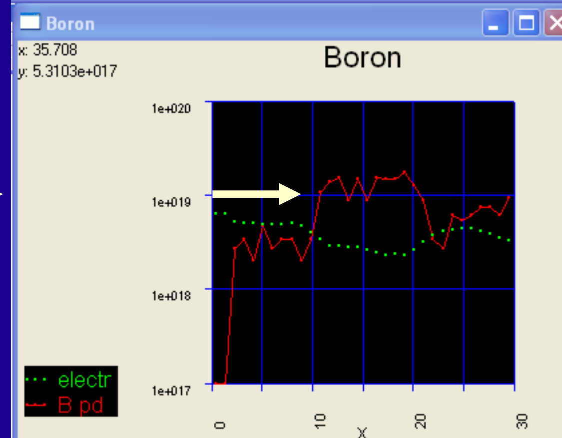


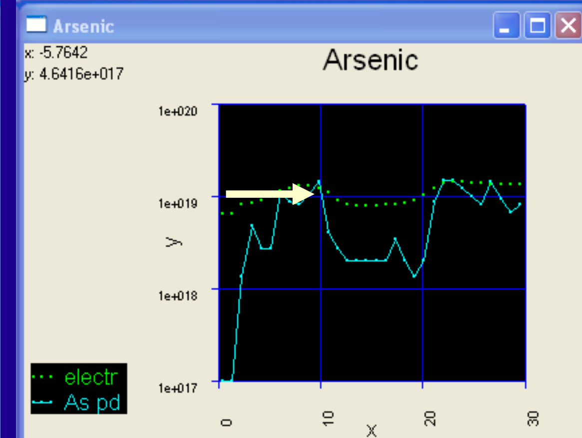


Initial uniform conc. 1e19 cm^{-3} →

Lower B diffusivity

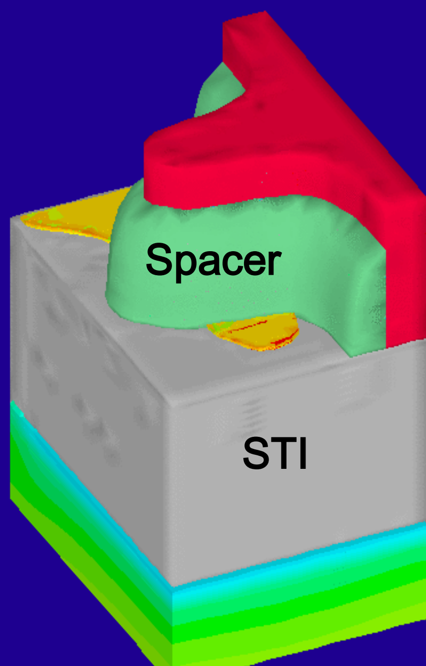
Higher As diffusivity

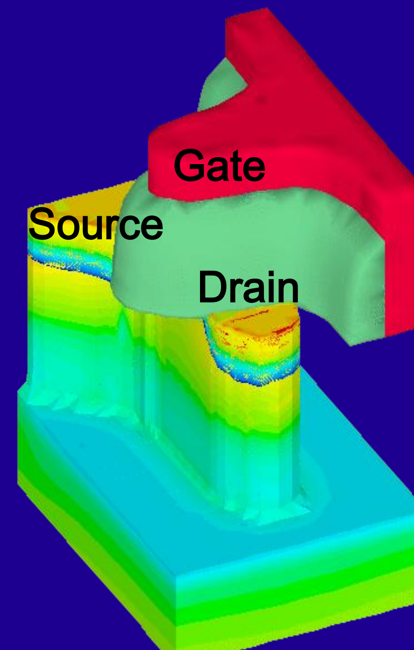




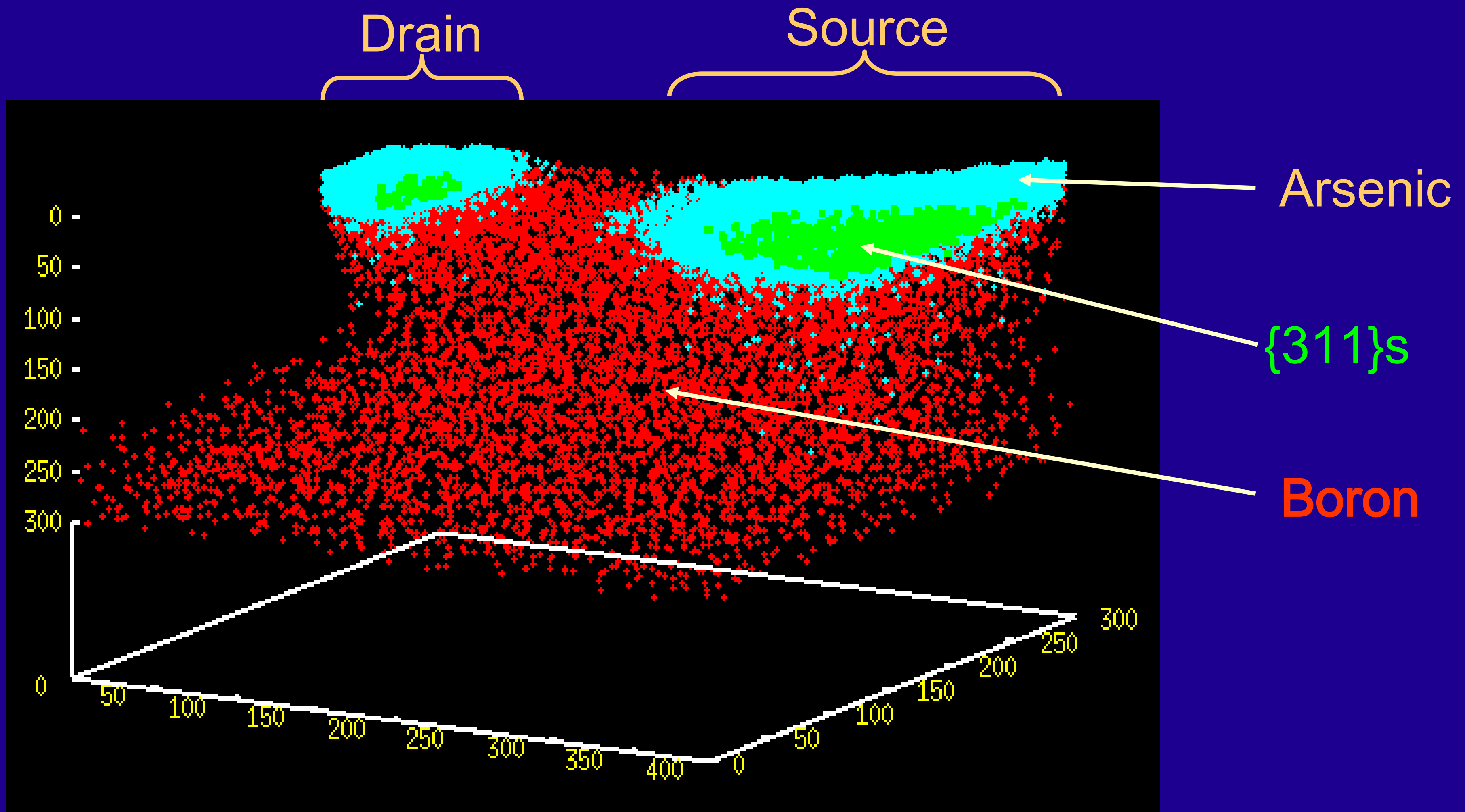
3D-Atomistic Simulation in Taurus

- TPA (Taurus Process Atomistic) uses DADOS to perform atomistic simulation of diffusion and defects.
- Taurus handles the rest of the processing (deposition, etching…) in the conventional way.

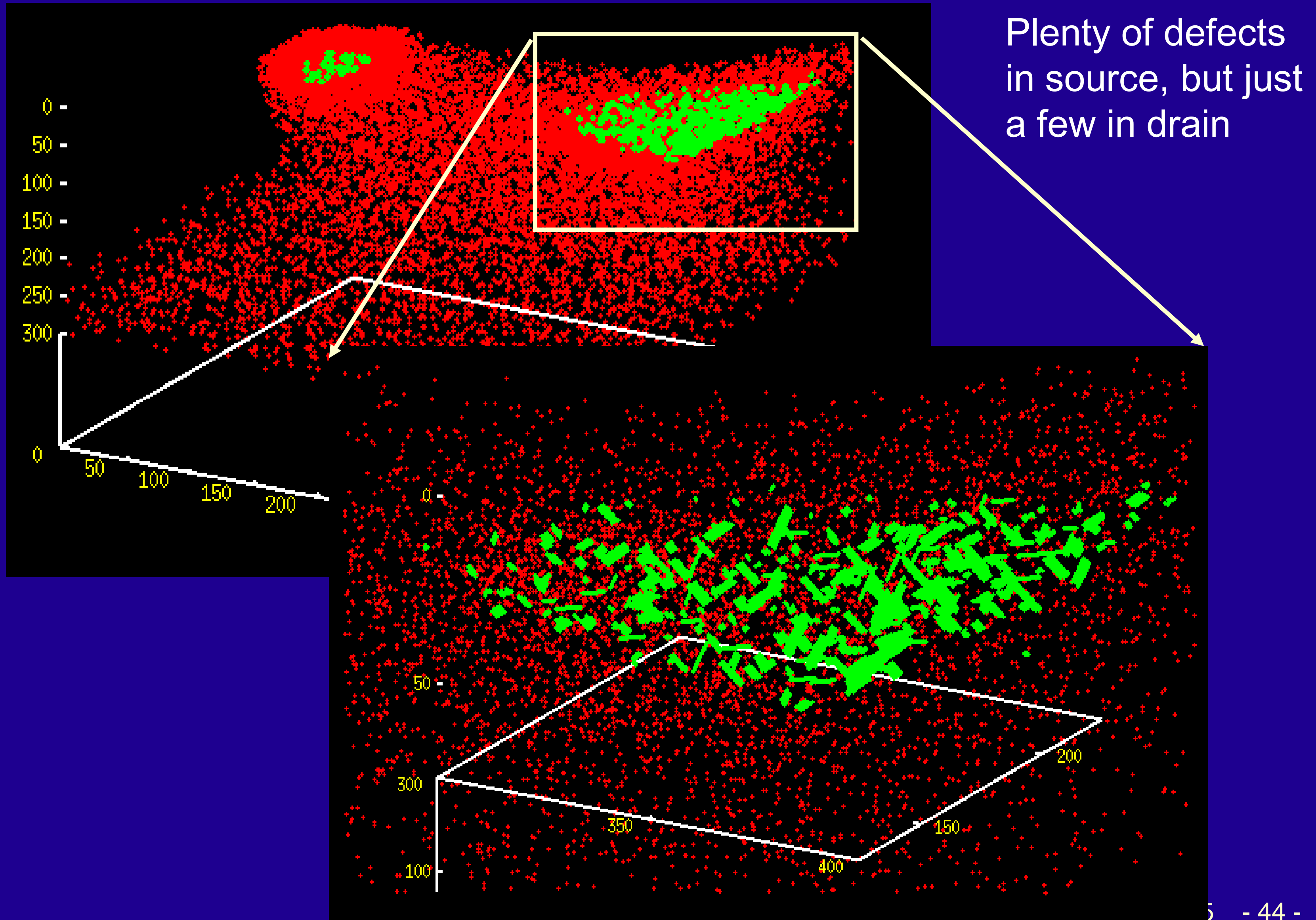




Dopants and Defects in DADOS



{311} Extended Defects: Zoom-In



Plenty of defects in source, but just a few in drain

What can be improved next?

- Other dopants: C,P,F,In… (mechanisms ready, calibration needed)
- Efficiency (CPU time and memory)
- Flexibility in the models: Models defined by the user (partially done)
- Diffusion in amorphous layers
- Moving boundaries (materials interfaces).
- Include Si-Ge alloys (in progress).
- Include stress (in progress).

Conclusions

- The strength of kMC is that it can handle many mechanisms **simultaneously**, as needed in complex processing.
- As a consequence it can be highly **predictive**, as already shown in several publications.
- It is not meant to compete in **accuracy** with ad-hoc simulation approaches, 'tabulated' for specific conditions.
- The goal, instead, is to attain a kMC simulator that, although not highly accurate for any particular simulation, **it never gives a totally wrong result**, even for previously unexplored simulation conditions.
- kMC is a predictive process simulation technique, intended to replace **time/money** costly **experiments** to explore **unknown** new conditions, for which conventional simulators can be highly unreliable.