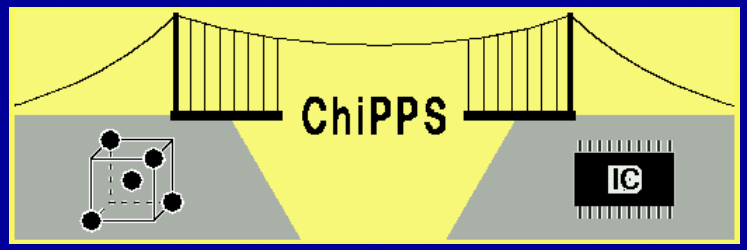
Building a bridge between *ab-initio* calculations and process simulation



Martin Jaraiz

University of Valladolid, Spain

mjaraiz@ele.uva.es

Thanks to:

E. Rubio, P. Castrillo, R. Pinacho,
L. Pelaz, J. Barbolla

University of Valladolid, Spain

G. Gilmer, C. Rafferty

Bell Labs Lucent Tech., USA

Outline

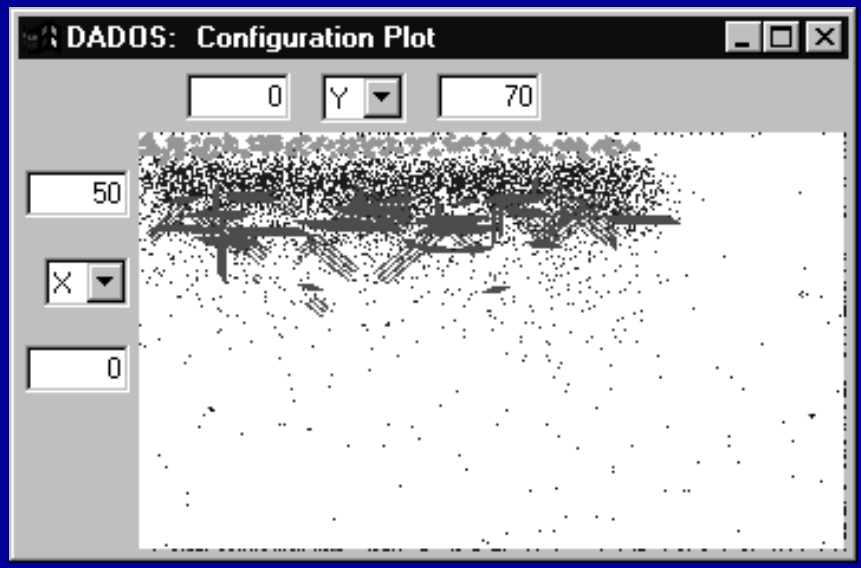
- The Problem: Complex Processing
- The Solution: Atomistic Kinetic Monte Carlo
- The Challenge: Obtaining the Parameters
- Looking Ahead: Genetic Algorithms, Neural Networks, …

The Problem

Complex Materials Processing Scenarios

The Problem:
Complex Processing Scenarios

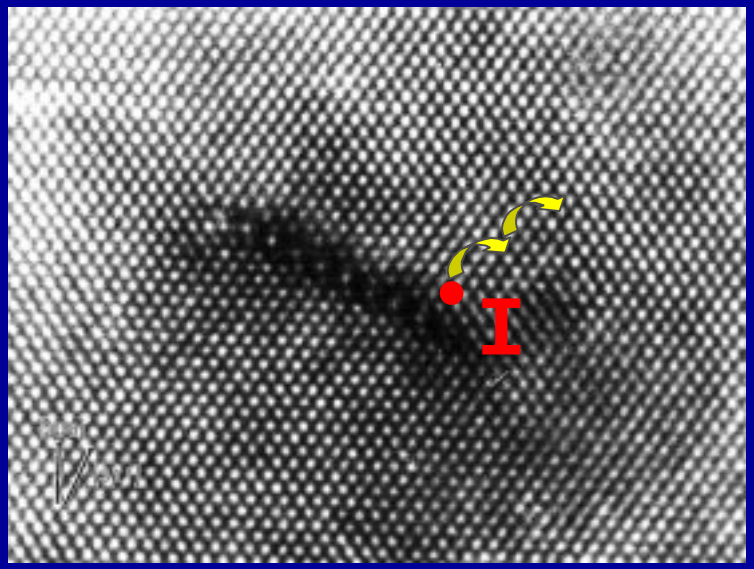
1. Many different species
   (V, I, As, C, O, B, …)
1. … and interactions
   (I-B, V-O, I-C-O, …)
1. Highly non-equilibrium conditions
   (Pair reactions, …)
4. Extended defects
   (voids, {311}'s, loops, …)
   - Emission/Capture rates dependent on Size & Shape
5. Low thermal budget
   (electrical activation?)



6. Ever smaller device dimensions
   - 2D: short channel effect
   - 3D: narrow channel effect
   - Local inhomogeneities (dopant discreteness)

The Problem:
Complex Processing Scenarios

- Molecular Dynamics (MD) is most accurate, but limited to <1 nanosecond:
  - Follows all the atoms
  - 'Fixed' time step $\cong 10^{-15}$ s
- We use MD (off-line) to calculate the KMC event rates.



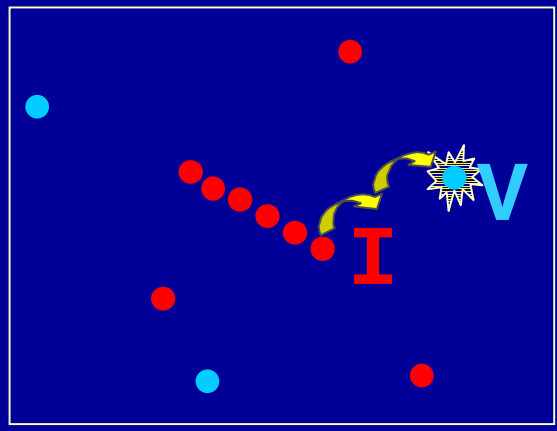
The Solution

Atomistic Kinetic Monte Carlo (KMC)

KMC vs. Molecular Dynamics

- Uses event rates obtained from DFT, classical MD or experiments
- KMC follows only the defect atoms
- Self-adjusts the timestep during the course of the simulation

Δt: ps … hours



KMC simulates real processing times using atomistic mechanisms

KMC vs. Continuum Models

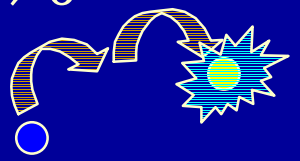
Continuum

TO SIMULATE:

SOLVE:

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

$$I + V \leftrightarrow 0$$



PROGRAM:

annihilate(I);
annihilate(V);

Atomistic

TO ADD NEW MECHANISM:

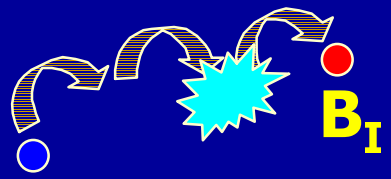
SOLVE:

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

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

$$dB_S/dt = \ldots$$

$$I + B_s \leftrightarrow B_I$$



PROGRAM:

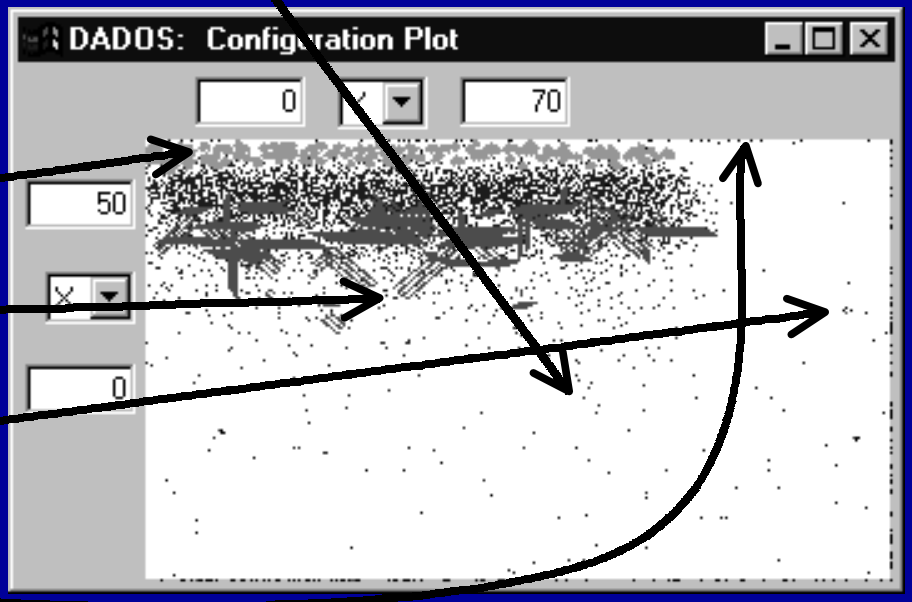
annihilate(I);
annihilate(B_S);

computation time ↑↑↑

⇒ almost no additional computation time

KMC: Accurate description of Defects

- Point defects (V, I, B, As, …)
- Extended defects (actual geometry)
  - Small clusters
  - V: Voids
  - I: {311}'s, Loops
  - Dopant clusters (B_nI_m, …)
- Surfaces



KMC: Easy definition of Defect Interactions

```
…
case Vacancy:
   switch ( neighbor )
   {
         case Vacancy:
               return new Cluster<Vacancy>;
         case Bi:
               neighbor->delete();
               this->delete();
               return new PointD<Boron>;
   }
…
```

- Execution speed independent of number of interactions

The KMC core:
The Event Scheduler

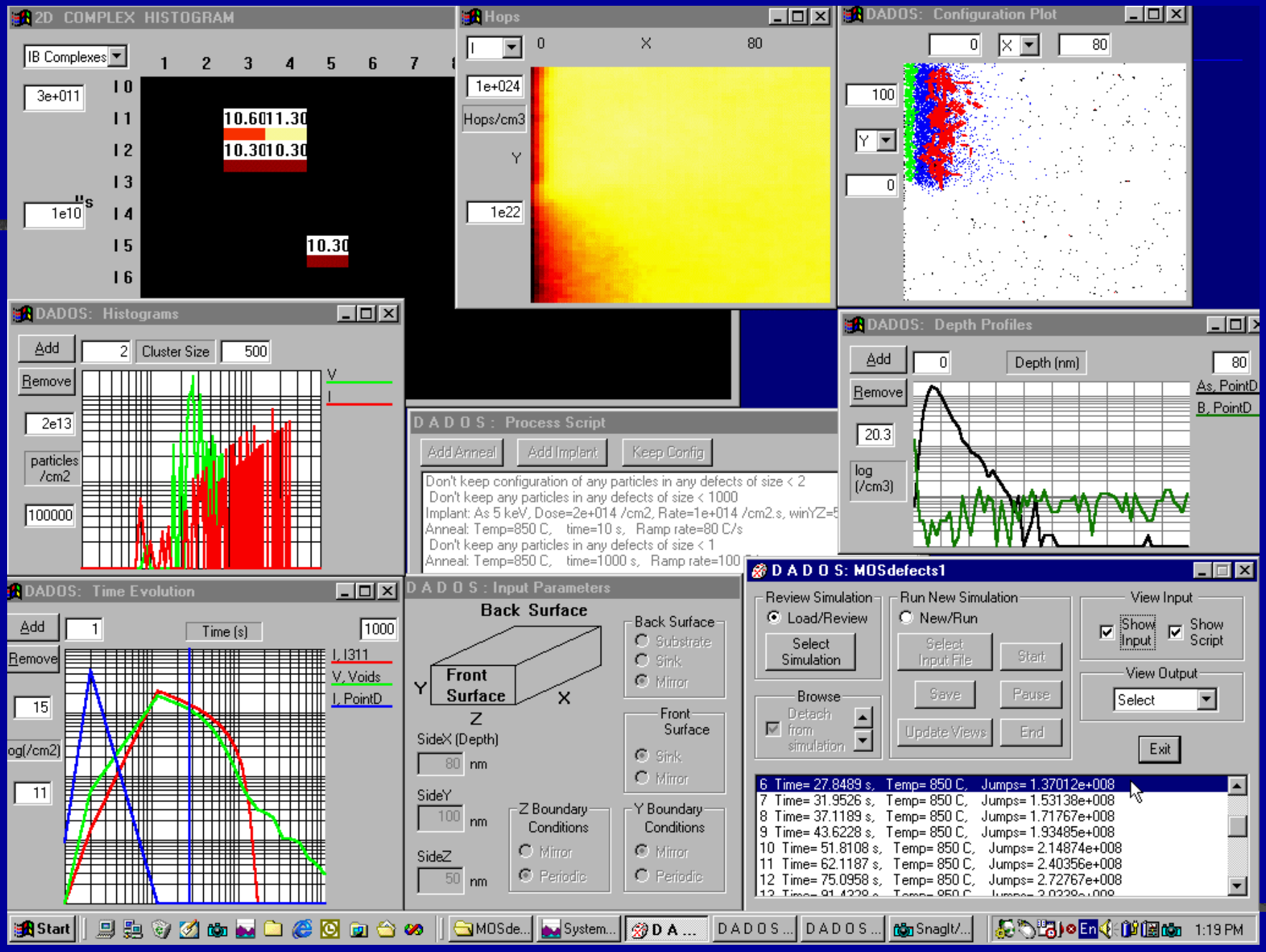
EXAMPLE:

	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


2D COMPLEX HISTOGRAM
IB Complexes
3e+011
1e10
10.60
11.30
10.30
10.30
10.30
Hops
1e+024
Hops/cm3
1e22
DADOS: Configuration Plot
100
0
80
DADOS: Histograms
Add
Remove
2
Cluster Size
500
2e13
particles /cm2
100000
V
I
DADOS: Depth Profiles
Add
Remove
Depth (nm)
20.3
log (/cm3)
As, PointD
B, PointD
DADOS: Process Script
Add Anneal
Add Implant
Keep Config
Don't keep configuration of any particles in any defects of size < 2
Don't keep any particles in any defects of size < 1000
Implant: As 5 keV, Dose=2e+014 /cm2, Rate=1e+014 /cm2.s, winYZ=5
Anneal: Temp=850 C, time=10 s, Ramp rate=80 C/s
Don't keep any particles in any defects of size < 1
Anneal: Temp=850 C, time=1000 s, Ramp rate=100
DADOS: Time Evolution
Add
Remove
Time (s)
15
og(/cm2)
11
I, I311
V, Voids
I, PointD
DADOS: Input Parameters
Back Surface
Front Surface
SideX (Depth)
80 nm
SideY
100 nm
SideZ
50 nm
Back Surface
Substrate
Sink
Mirror
Front Surface
Sink
Mirror
Z Boundary Conditions
Mirror
Periodic
Y Boundary Conditions
Mirror
Periodic
DADOS: MOSdefects1
Review Simulation
Load/Review
Select Simulation
Run New Simulation
New/Run
Select Input File
Start
Save
Pause
Update Views
End
Browse
Detach from simulation
View Input
Show Input
Show Script
View Output
Select
Exit
6 Time= 27.8489 s, Temp= 850 C, Jumps= 1.37012e+008
7 Time= 31.9526 s, Temp= 850 C, Jumps= 1.53138e+008
8 Time= 37.1189 s, Temp= 850 C, Jumps= 1.71767e+008
9 Time= 43.6228 s, Temp= 850 C, Jumps= 1.93485e+008
10 Time= 51.8108 s, Temp= 850 C, Jumps= 2.14874e+008
11 Time= 62.1187 s, Temp= 850 C, Jumps= 2.40356e+008
12 Time= 75.0958 s, Temp= 850 C, Jumps= 2.72767e+008
Start
MOSde...
System...
D A ...
DADOS...
DADOS...
SnagIt/...
1:19 PM

KMC: Example 1

Local Inhomogeneities:

- Dopant Discreteness
- Clusters

Dopant Distribution Models

Continuum Models

↓

Dopants: Discrete Random (?)

↓

Possible Spatial correlation due to:

- Dopant charge states
- Clusters

Dopants: Possible spatial correlation

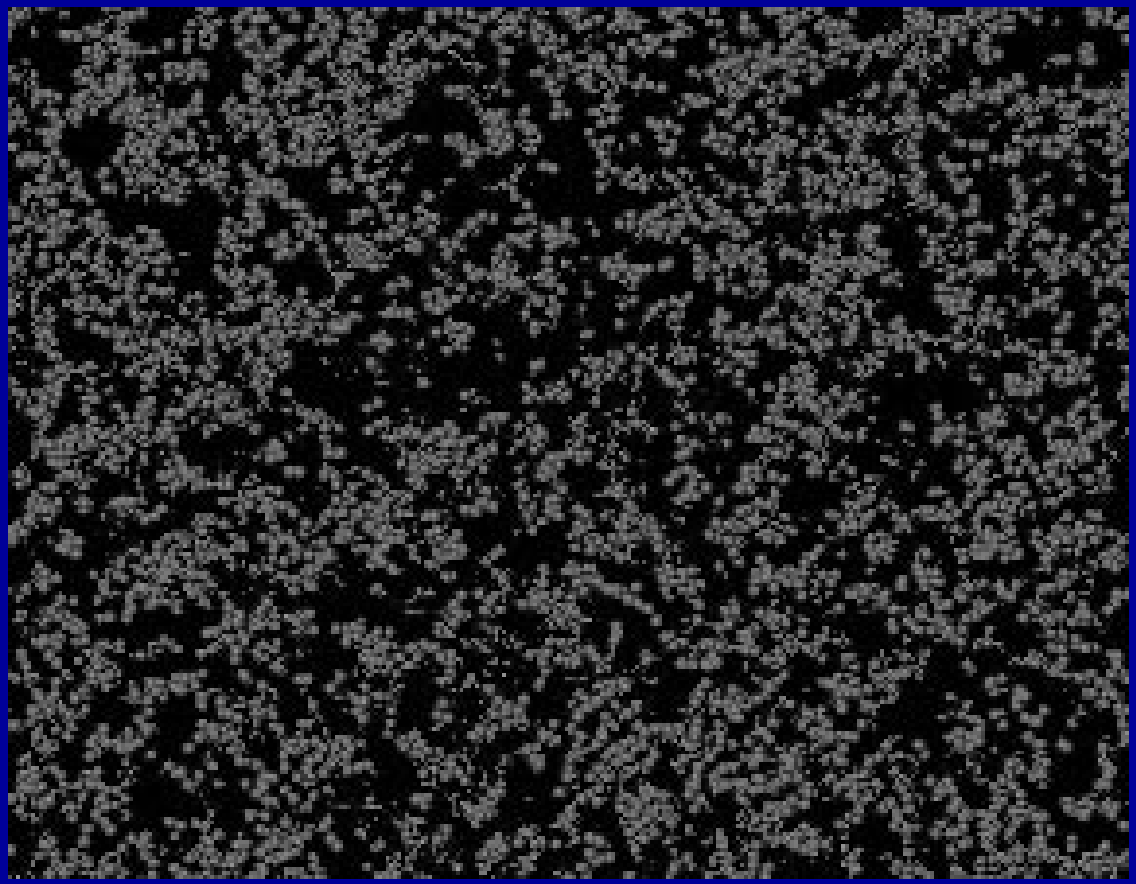
Diffusion of charged point defects could give rise to spatial correlation (they cannot be arbitrarily close to each other).

In fact, similar effects have been shown to occur in the oxide charge distribution in MOS structures

$\Rightarrow$change in the effective mobility.

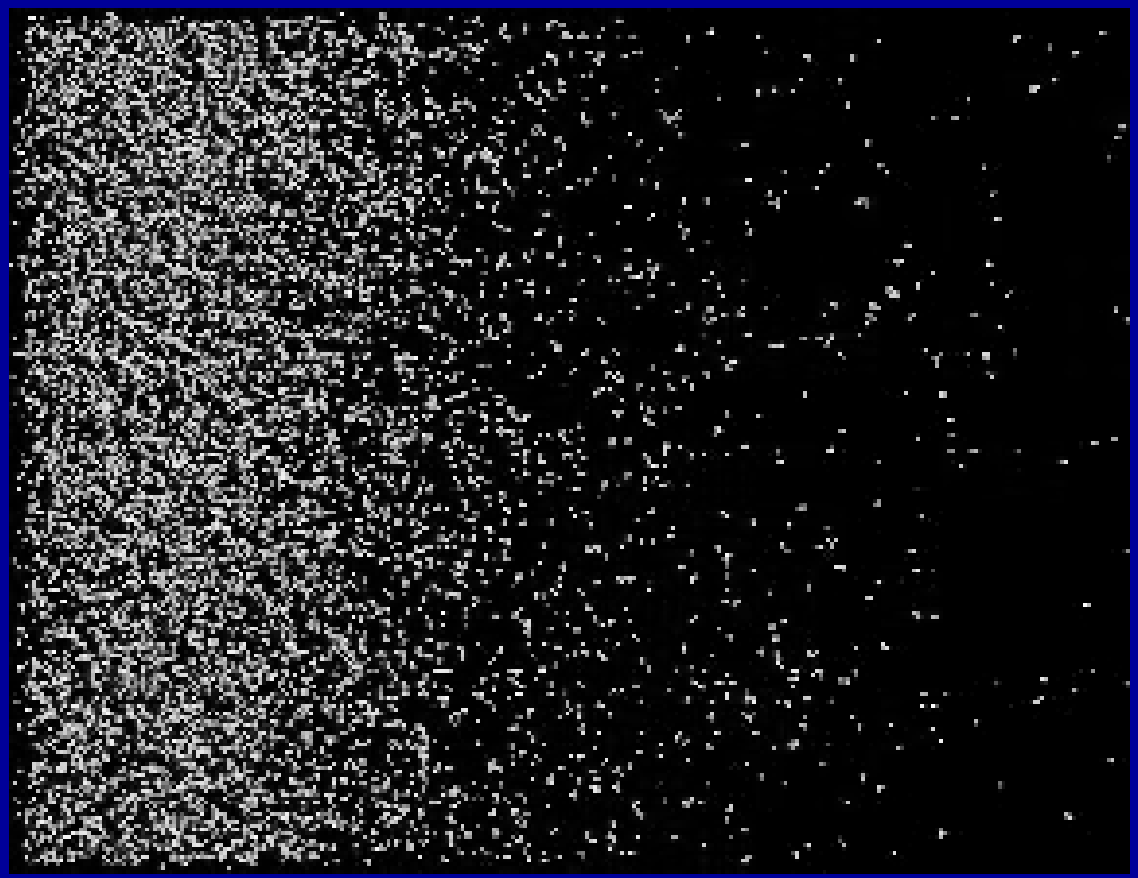
F. Gamiz et al., Semic. Sci. & Technol, (1994)

Local Inhomogeneities: Clusters



Front View

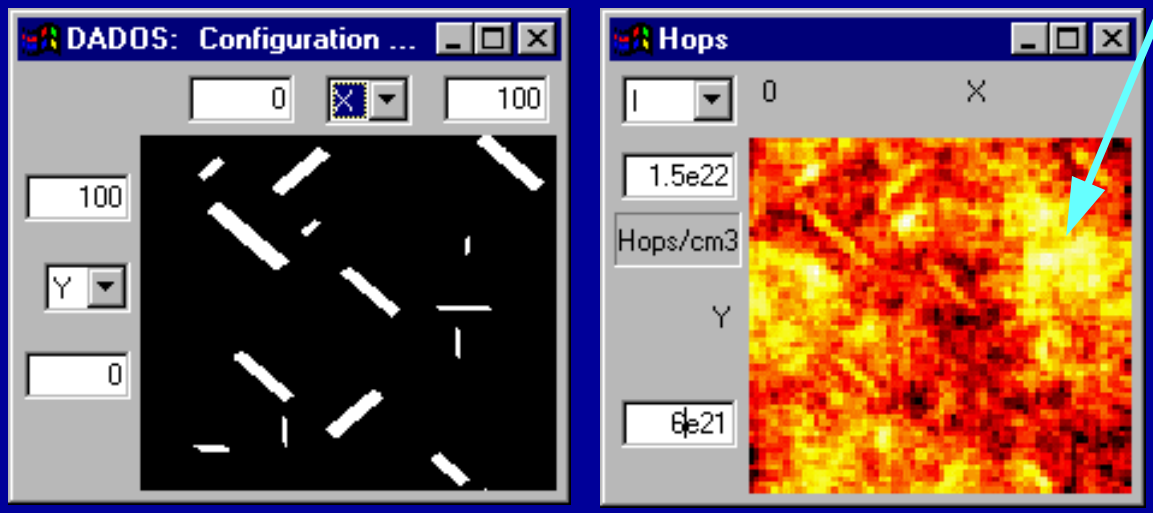
Local Inhomogeneities: Clusters



Cross-section

Local Inhomogeneities: Clusters

High B diffusivity



{311} defects

Interst. hops

KMC: Example 2

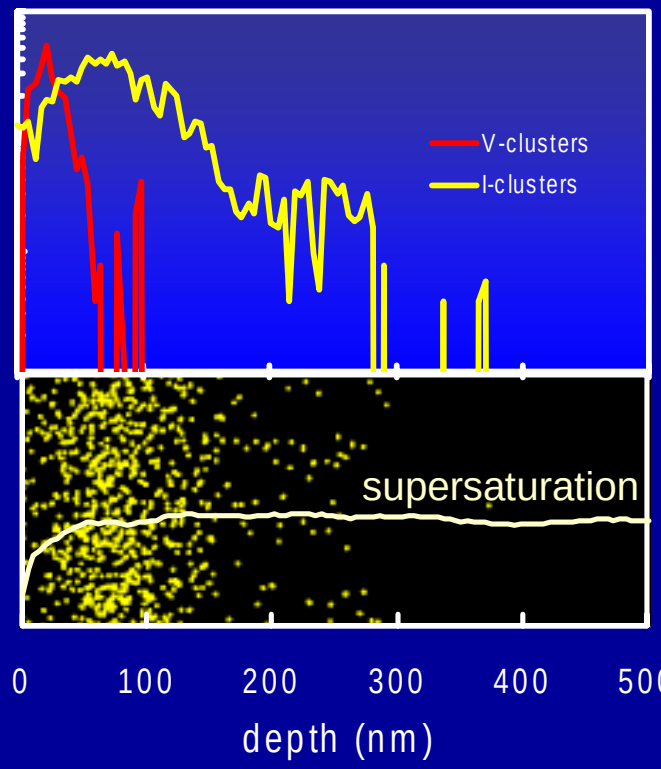
KMC used to validate Simplifying Assumptions

KMC used to validate simplifying assumptions

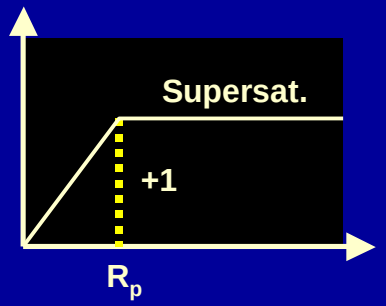
Emission energies of I-clusters:
Cowern et al., Phys. Rev. Lett. **82**, *4460 (1999)*

Implant + Anneal

600 ºC, 1000 s



Simplified model



- No V's ("+1" model)
- ...

$$\frac{dN_n}{dt} = F_{n-1}N_{n-1} - F_nN_n - R_nN_n + R_{n+1}N_{n+1}$$

$$S = \frac{\sum_{n=2}^{\infty} \beta_n R_n N_n}{D_I C_I^* (\sum_{n=2}^{\infty} 4\pi a_n N_n + 1/r_p)},$$

where

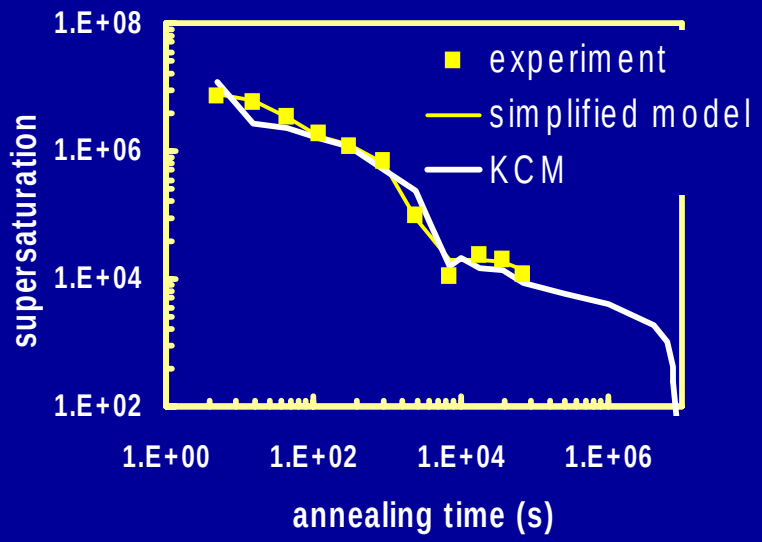
$$F_n = 4\pi a_n D_I C_I^* S,$$

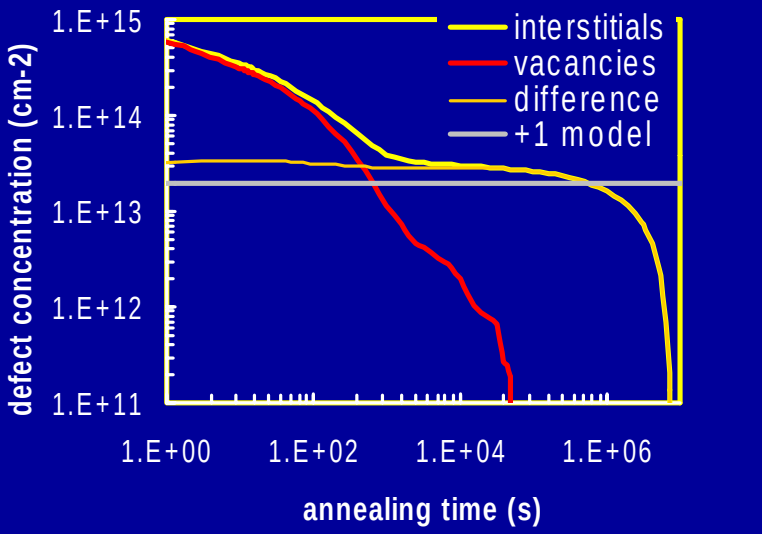
$$R_n = (6D_{0n}a_n/\lambda^3)\exp -[E_{\text{diss}}(n)]/kT$$

How accurate is the Simplified model ?

- **Very good agreement with full simulation …**

… in spite of the presence of Vacancies and other assumptions





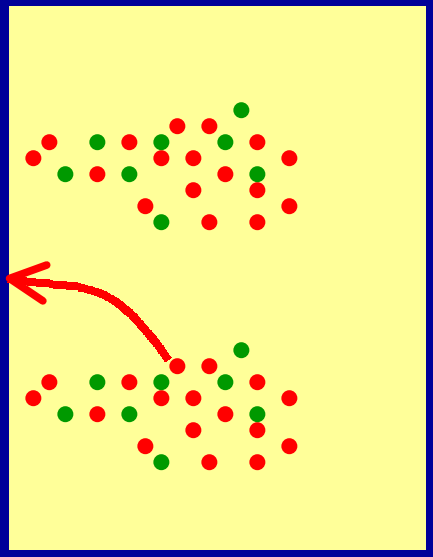
KMC: Example 3

Implantation Damage and the "+N" Number

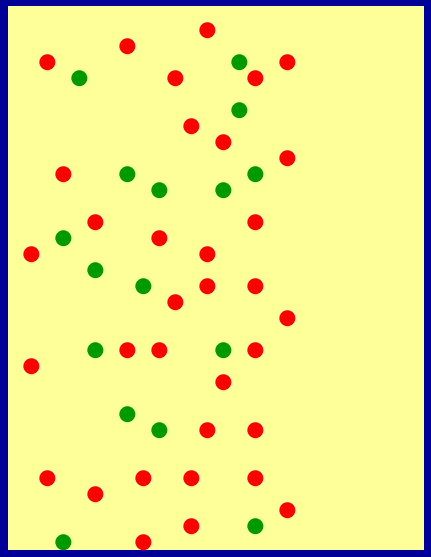
KMC can yield an accurate “+N” :

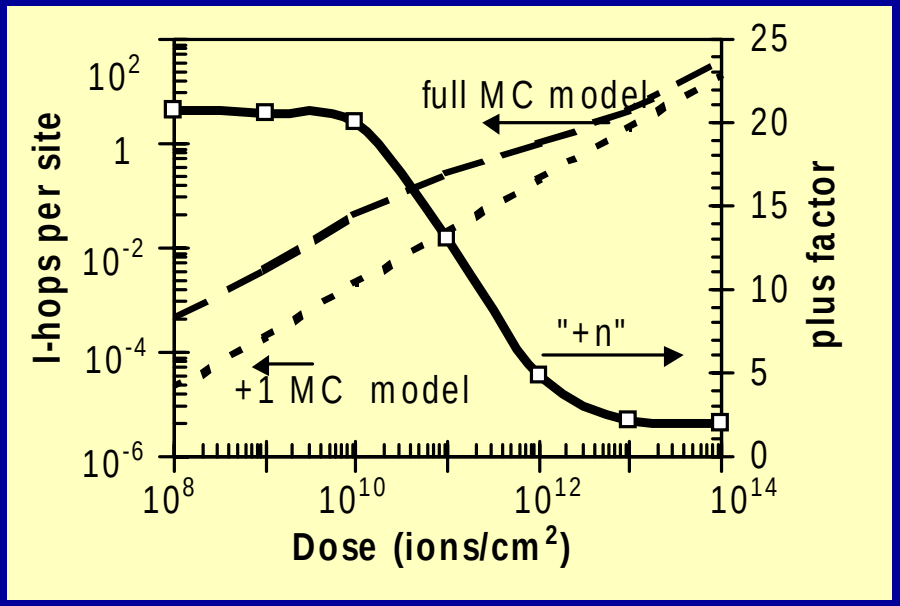
Low Dose Implant → Non-overlapping Cascades (Spatial Inhomogeneities)

Atomistic



Continuum





Pelaz et al., APL. **74** (1999) 2017

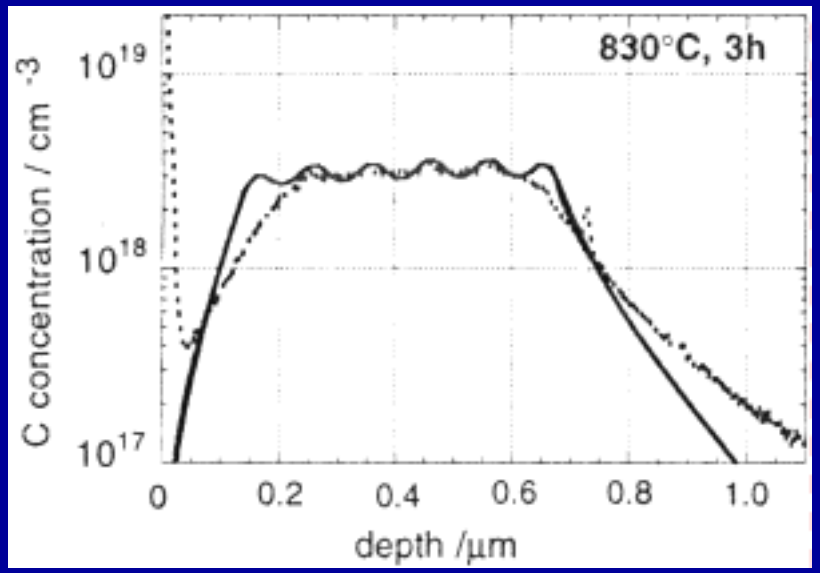
KMC: Example 4

Extraction of parameters for Carbon diffusion in Silicon

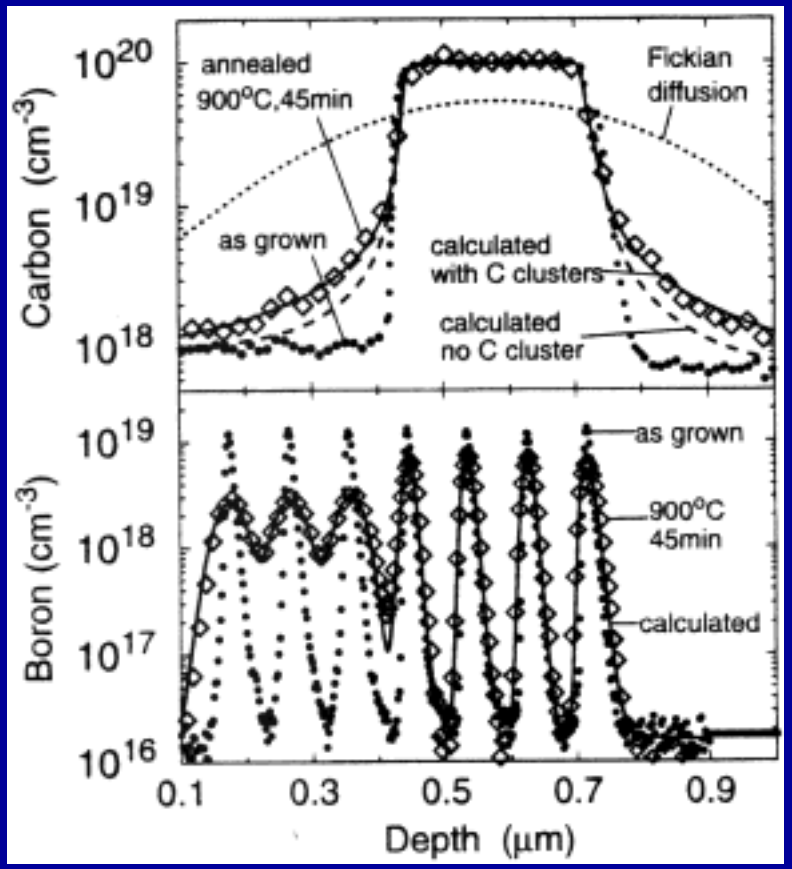
Importance of Carbon in Silicon processing

- Reduction of the diffusion of B and P
  - C traps self-Interstitials
- Unintentional impurity
  - Introduced during crystal growth.
- High concentration (10^{16} -10^{18}cm^{-3})
  - Above its solubility at annealing temperatures

Carbon diffusion: the state of the art



Werner et al., Appl. Phys. Lett. (1998)



Rücker et al.
Appl. Phys. Lett. (1998)

Improving the model with Carbon clustering mechanisms

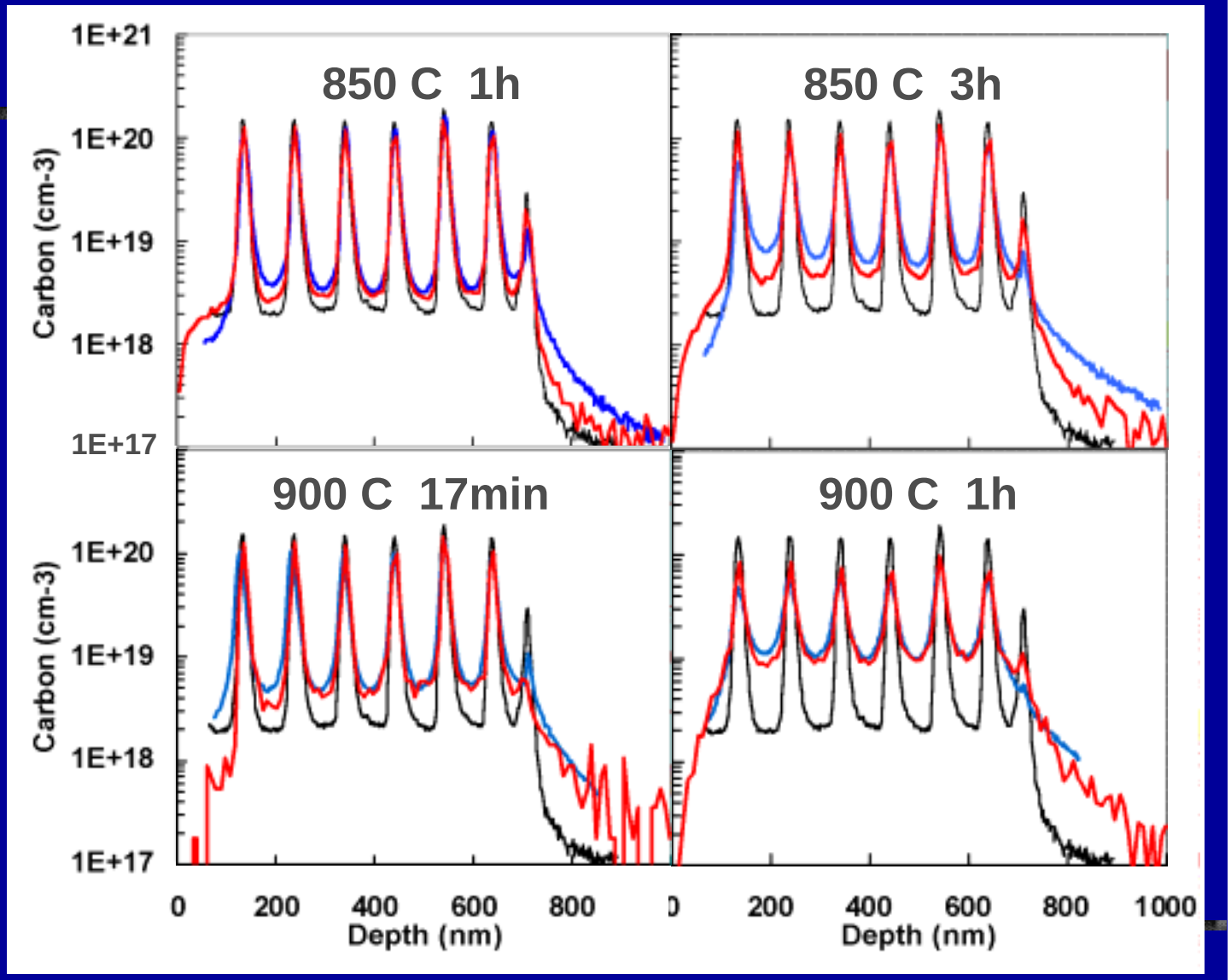
$$I + C_s \leftrightarrow C_i$$
$$C_i + C_s \leftrightarrow C_2I \equiv C_iC_s$$
$$C_2I \leftrightarrow C_2 + I$$
$$C_i + C_2 \leftrightarrow C_3I$$
$$I + C_2I \leftrightarrow C_2I_2$$
$$C_i + C_2I \leftrightarrow C_3I_2$$
$$\circ\circ\circ$$

C (+I, +C_i)	C_2	C_3	C_4	$\circ\circ\circ$
$CI \equiv C_i$	C_2I	C_3I	C_4I	
CI_2	C_2I_2	C_3I_2	C_4I_2	
CI_3	C_2I_3	C_3I_3	C_4I_3	
CI_4	C_2I_4	C_3I_4	C_4I_4	

$\circ\circ\circ$

- Continuum approach: many rate equations
- KCM: Easy modeling

KMC Simulation of Carbon diffusion



as grown
experiment
KMC simulation

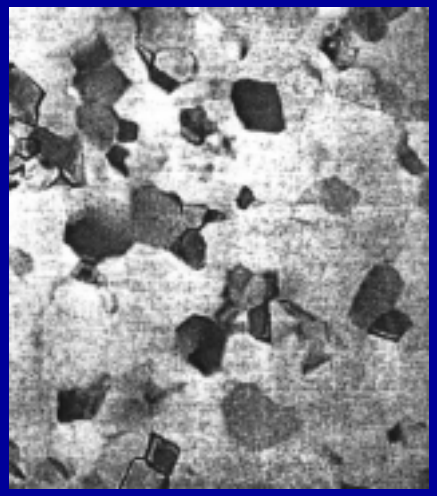
Pinacho et al. MRS 2000

Lattice Kinetic Monte Carlo

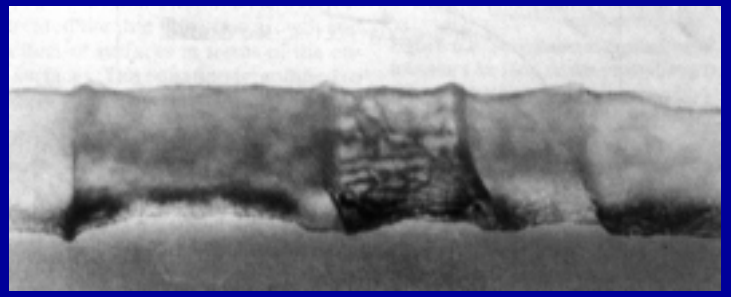
Polycrystalline Materials

Why **Lattice** KMC?

Aluminum, Polysilicon, …: Polycrystalline structure



100 nm



0.5 µm

- Kang et al, J. Electron. Mater. , 1997
- Murarka, “Metallization”, 1993

- Surface texture
- Grain Boundary diffusion
- Electromigration

Simulation approaches

- Continuum equations:

  SPEEDIE, SAMPLE, EVOLVE, DEPICT

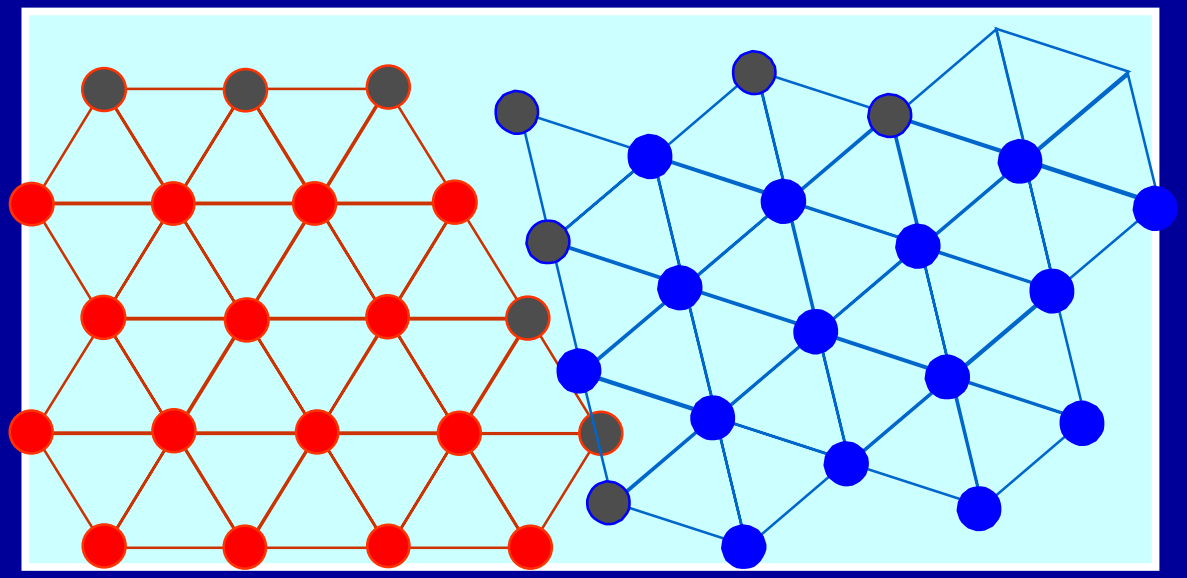
- 2-D ballistic simulator:

  SIMBAD, GROFILMS

- 3-D atomistic approach: ADEPT

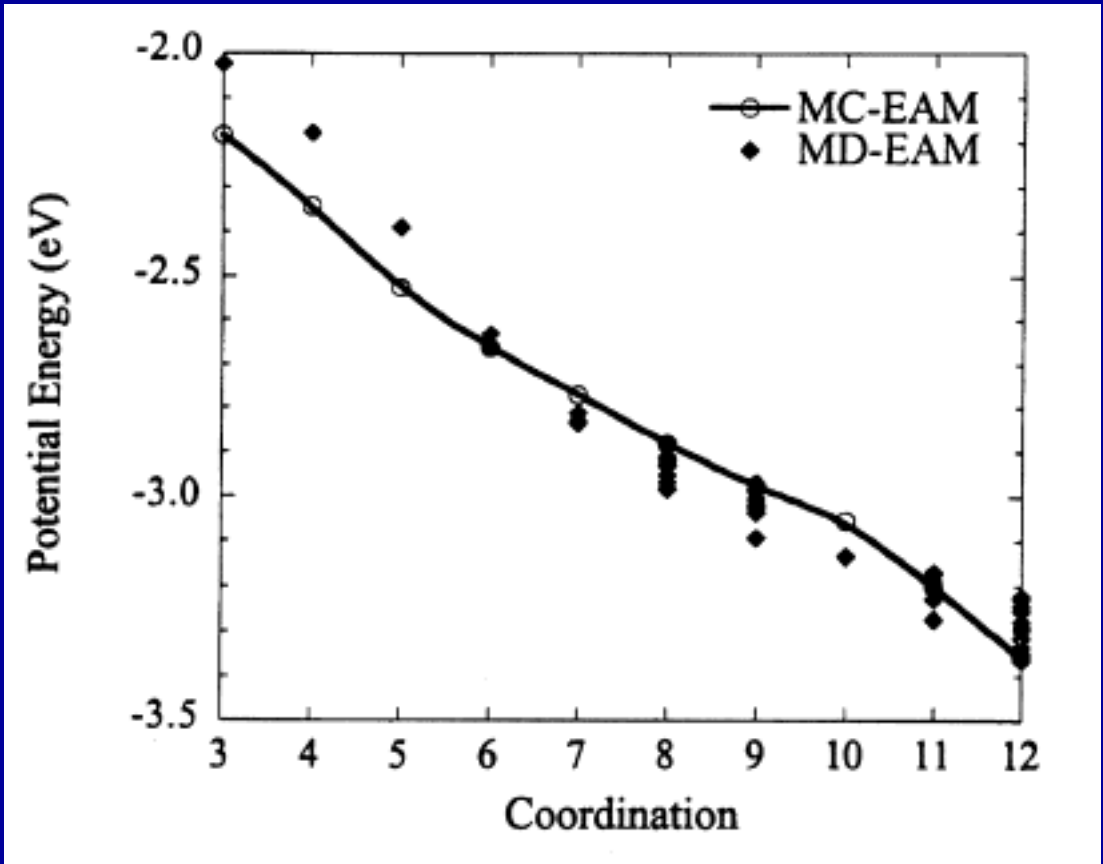
This Work: Polycrystalline 3-D atomistic approach

Simulation Box

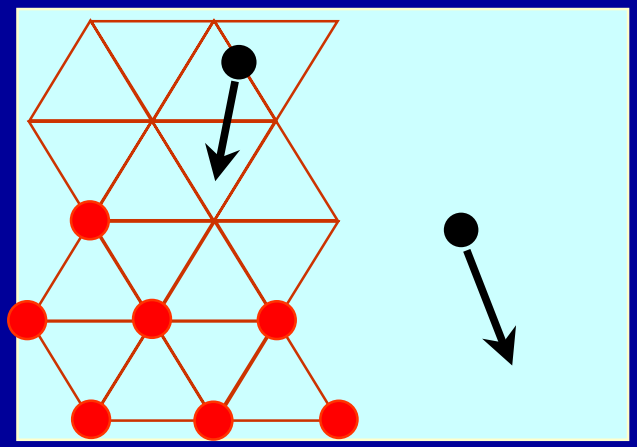


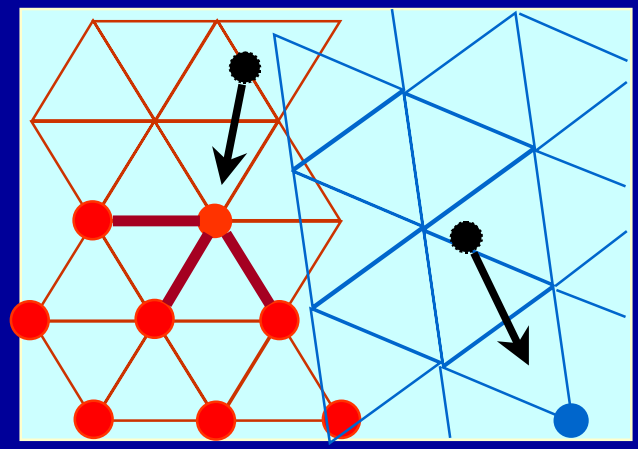
- Atoms are attached to the sites of a perfect fcc lattice.
- As a first approximation, the binding energy of each site depends on the number of occupied nearest neighbors

Energies from MD Embedded Atom Method using Gupta Potential



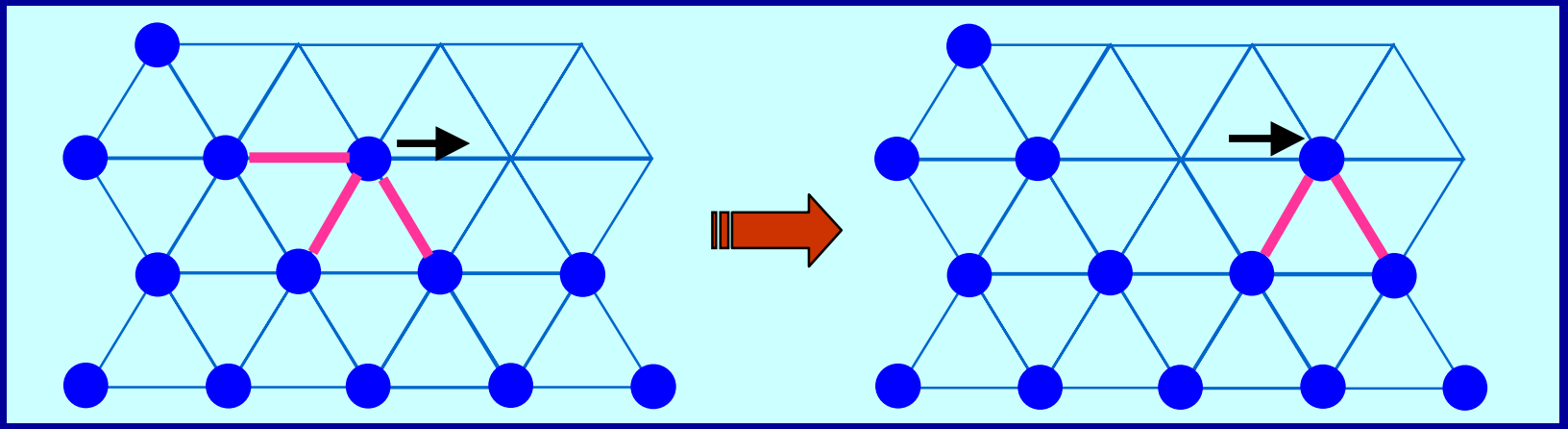
Deposition





- Initial position and velocity according to desired distribution
- Atom travels in a straight line until it either:
  - Finds some neighbors: gets attached to that grain
  - Finds no neighbors: starts a new grain (orientation).

Surface Diffusion



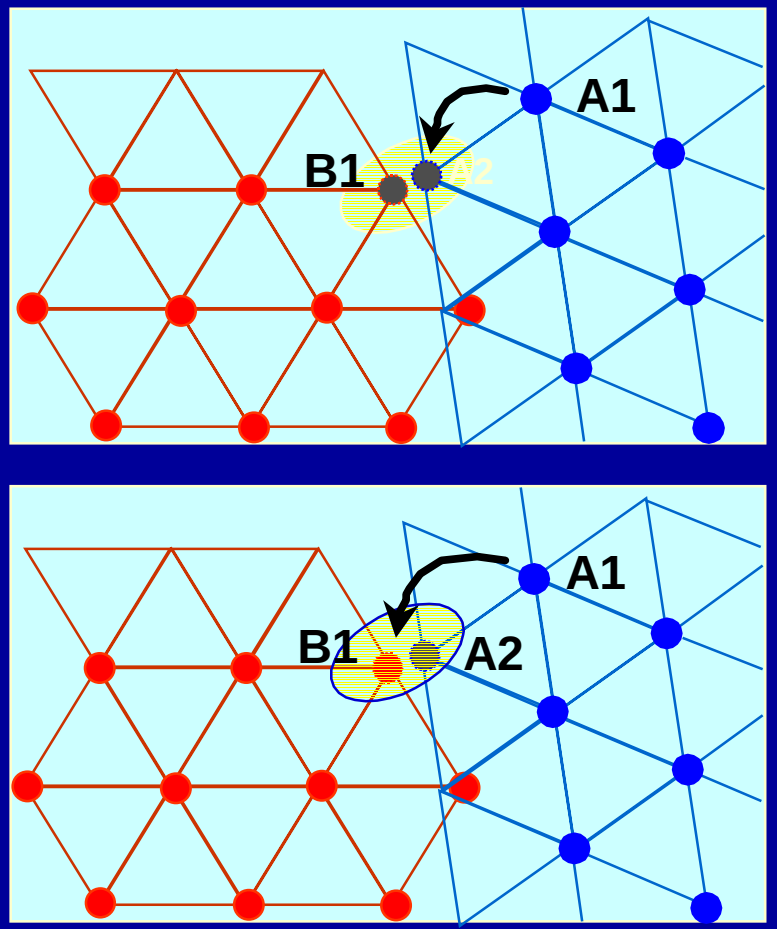
- Atoms not fully coordinated can jump to a neighboring empty site.
- The jump probability depends on the number of nearest neighbors and on the migration energy.

Grain Boundaries

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

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

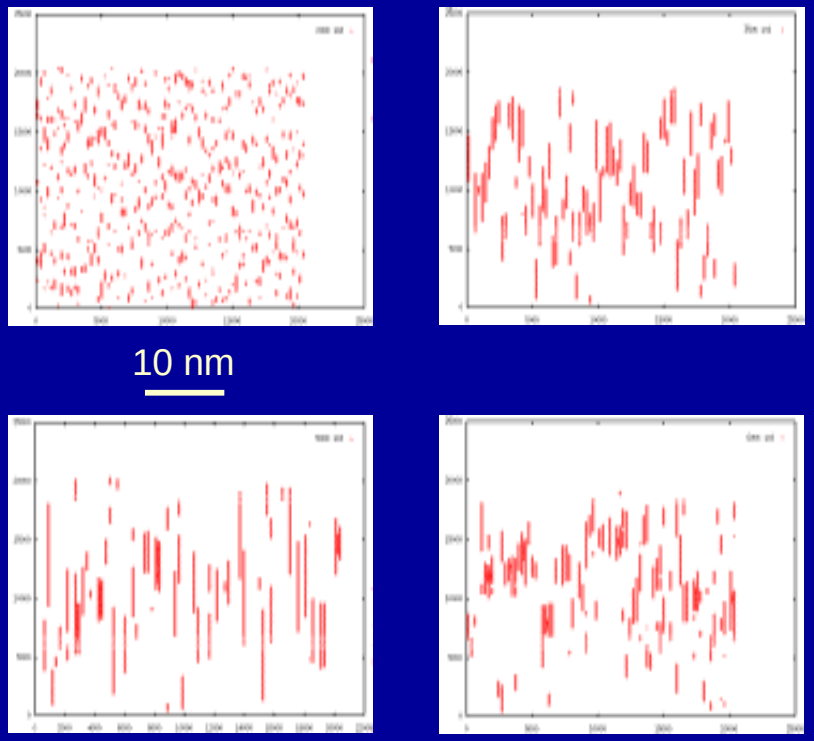
2. If energy (B1) < energy(A2) then the jump final site is B1.



Lattice KMC: Simulation Examples

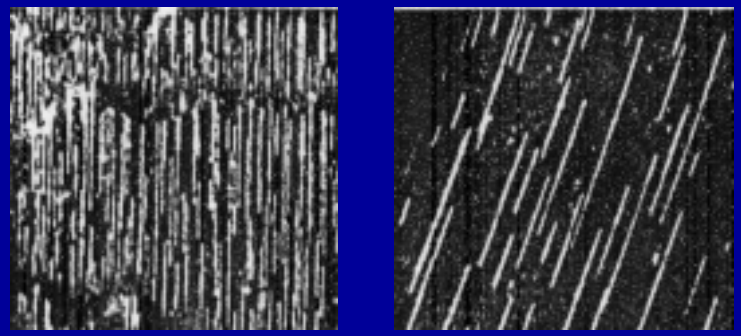
- Nucleation
  - Crystalline Substrates: Orientation
  - Amorphous Substrates: Wetting
- Annealing:
  - Texture evolution

Nucleation on Al (110)



10 nm

Simulation:
Al on Al (110) @ 200K, 350K, 500K, 600K
Coverage=0.1 ML

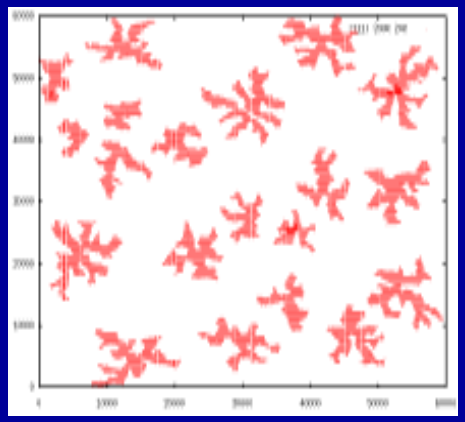


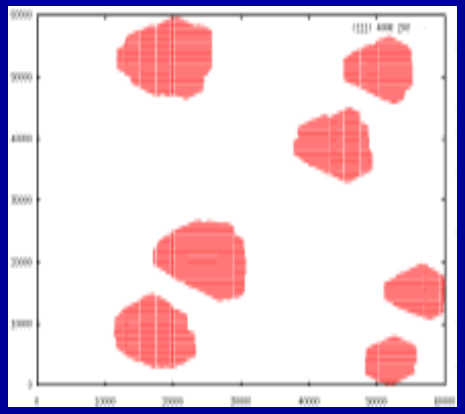
50 nm

STM images of Cu islands on Pd(100) at 265K and 300 K and coverage of 0.1 ML and 0.07 ML

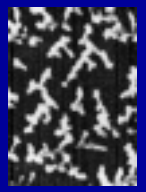
Nucleation on Al (111)

Simulation:
Al on Al (111)
@ 200K and 400K

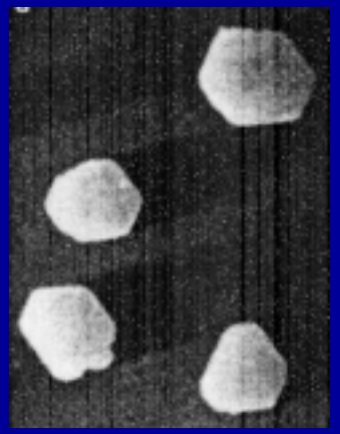




STM measurements:
Pt on Pt(111)
@ 200K and 455K



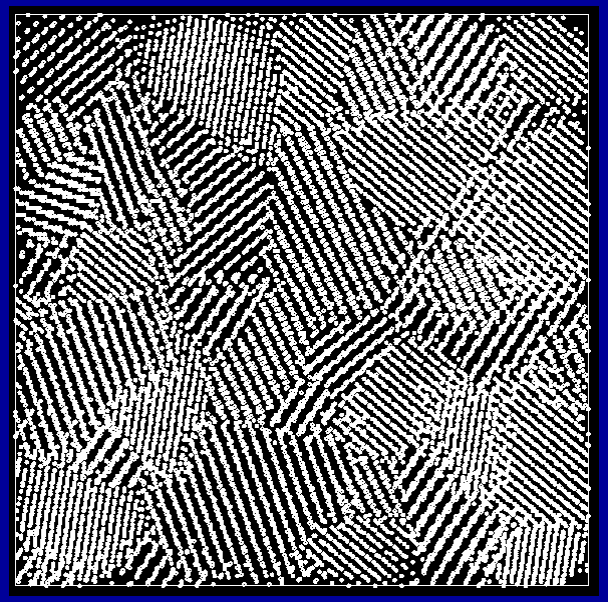
20 nm



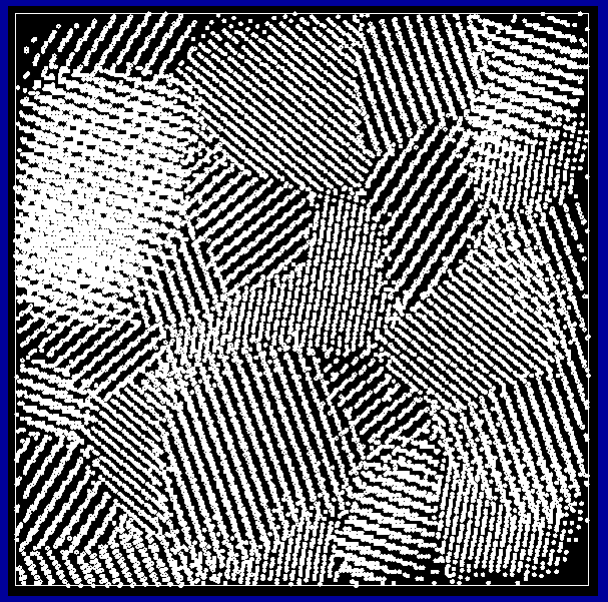
20 nm

Nucleation on Amorphous Substrates

Bonding to substrate**:** effect on the grain size



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

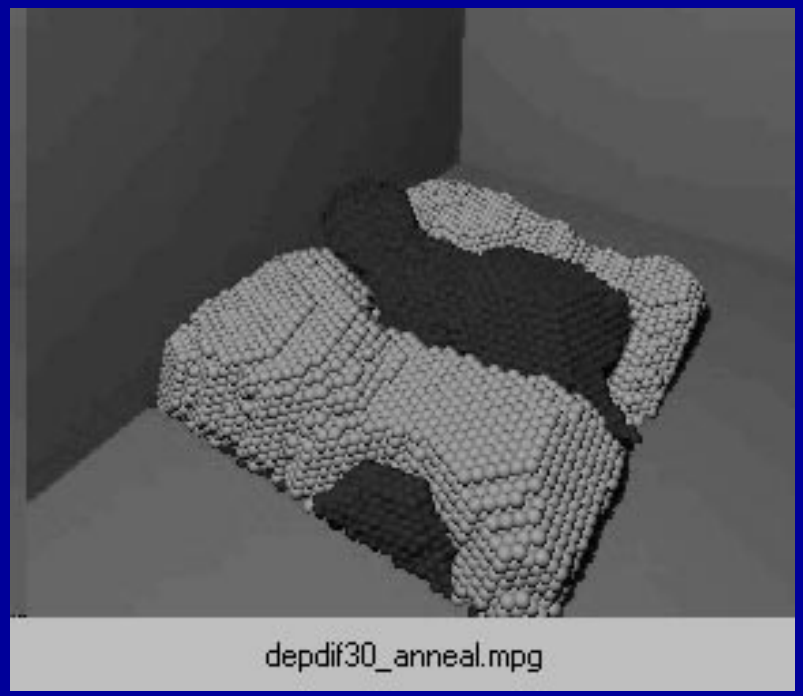


"Non-wetting" substrate
(Weak bonding)

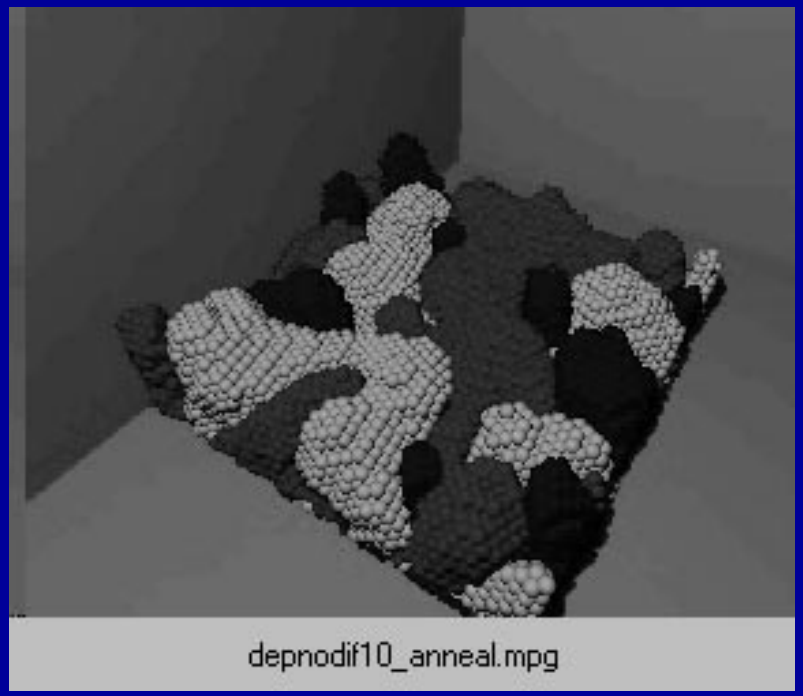
Annealing: Texture Evolution

Number of atoms: 20000
Simulation size: 0.012 µm
⇒ Actual size: 0.25µm

$T_{dep} = T_{ann} = 663$ K
Annealing time = 2.7 ms



$T_{dep} = T_{ann} = 513$ K
Annealing time = 0.18 s



The Challenge

Obtaining KMC Input Parameters

In Complex Scenarios

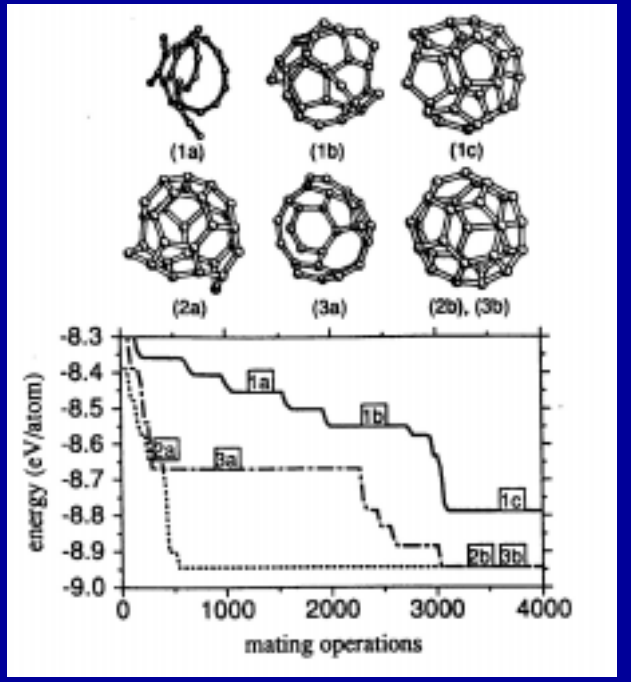
Obtaining KMC Parameters from MD with a Genetic Algorithm

Problem: Find minimum energy configuration of 60 Carbon atoms, starting from random coordinates.

60 x 3 coords. = 180 unknowns

Assuming only 10 possible values for each coordinate: $\sim 10^{180}$ configs. ! (the Universe is about 10^{18} s old)

- The GA found the solution in ~ 5000 steps (configs.)
- It had not been solved by any other technique before



Deaven and Ho, PRL **75** (1995) 288

Free-standing Si clusters: Ho et al., *Nature* **392** *(1998) 582*

Evolutionary Computation (Genetic Algorithms, …)

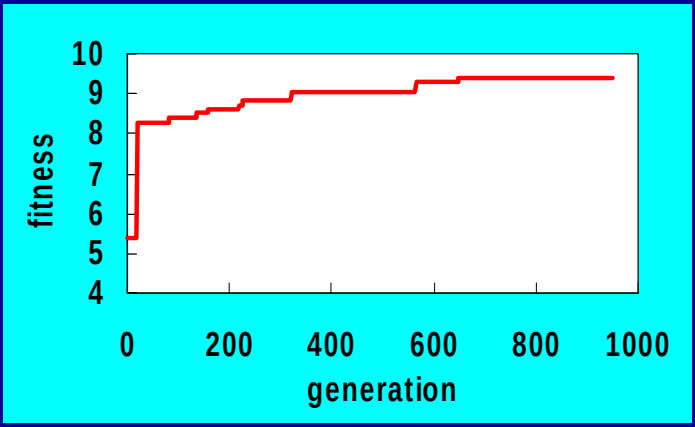
D. B. Fogel, IEEE Spectrum, Feb. 2000:

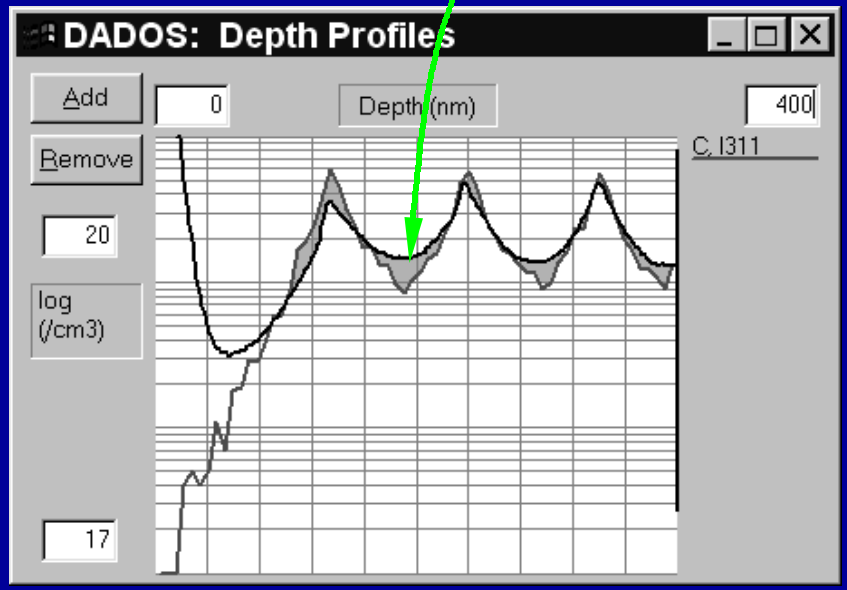
- "… is one of the fastest growing areas of Computer Science"
- "It is addressing **complex engineering** problems that were previously beyond reach"

Using a GA To Extract KMC Parameters From Experimental Data

"Genes" →	E_{mI}	E_{bCi}	E_{C2}	…	Fitness
"Chromosome":	1.3	2.0	1.9	3.1	4.2 → 8.331

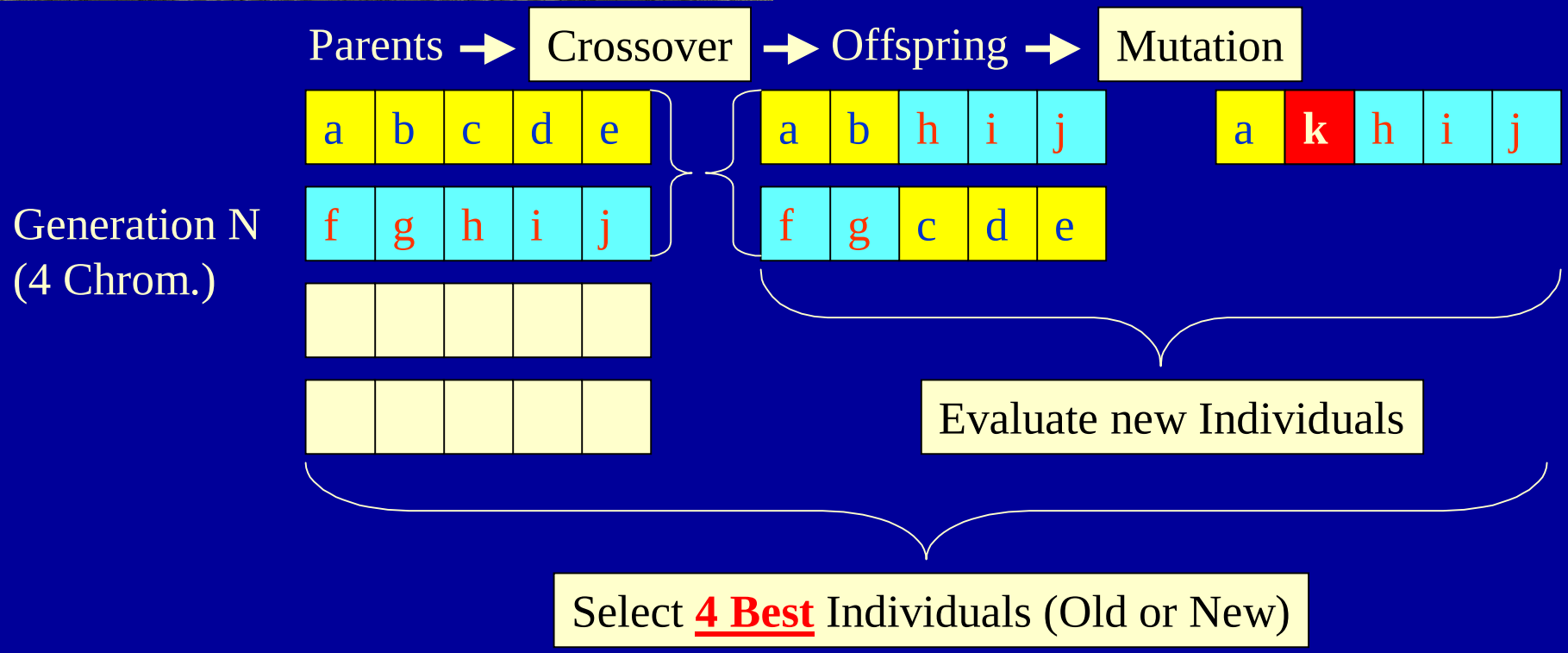
Fitness Evaluation: DADOS simulations
(just a rough estimate)
done in ~ 3 minutes / simulation





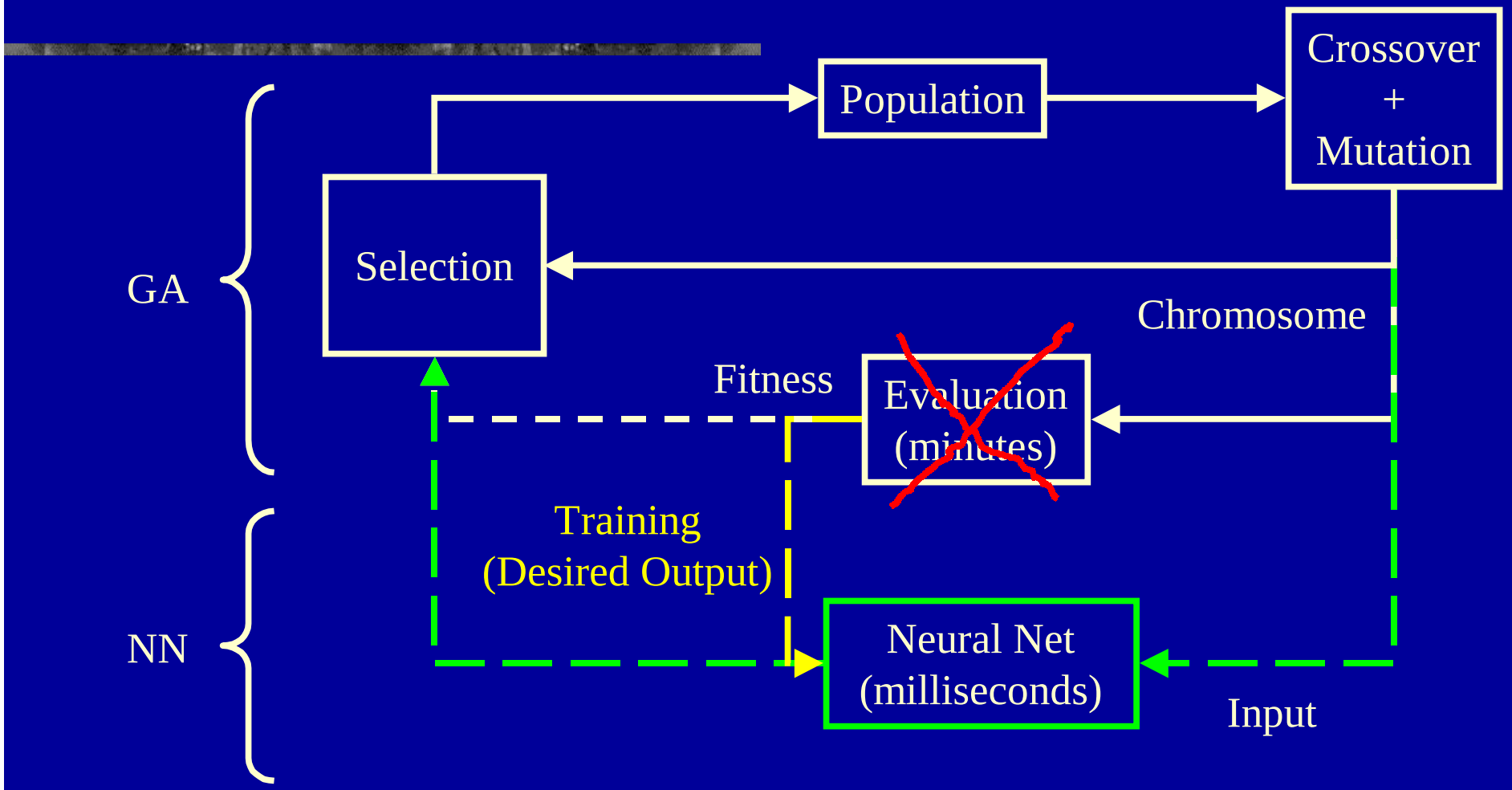
Genetic Algorithm from: http://lancet.mit.edu/ga/

What Is a Genetic Algorithm?



Looking Ahead

Looking Ahead: GA + Neural Networks



Looking Ahead

- Genetic Programming
  - Symbolic Regression:

    Set of symbols: { +,-,/,•, exp, cos, X,Y,Z, … }

    Find best fitting **function**: f = X - Z • exp(Y)
  - Materials Processing:

    Set of mechanisms: { Frank-Turnbull, Interstitialcy, Surface emission, E_1, E_2, … }

    Find best mechanisms and energies
  - …

In Summary:

Materials Research can benefit from:

- Atomistic KMC Process Modeling
  - Detailed and Accurate
  - Straightforward to Implement / Modify new Models
  - Can handle complex Processing scenarios
- AI methods (Genetic Algorithms, Neural Nets, …)
  - Opening a whole new range of capabilities
  - Currently under intense exploration. Looks most promising