Atomistic Process Modeling

An Accurate and Straightforward Approach for Complex Processing Scenarios

Martin Jaraiz

University of Valladolid, Spain

Thanks to:

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

University of Valladolid, Spain

George Gilmer, Conor Rafferty

Bell Labs Lucent Tech., USA

Outline

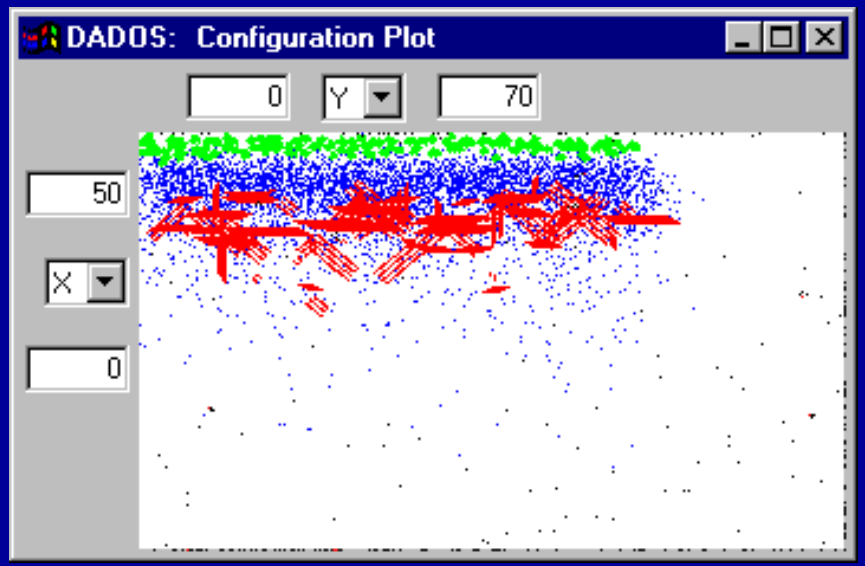
- The Problem: Complex Processing
- The Solution: Atomistic Kinetic Monte Carlo
- The Challenge: Obtaining the Parameters
- Looking Forward: Genetic Algorithms, Neural Networks, …

The Problem

Complex Materials Processing Scenarios

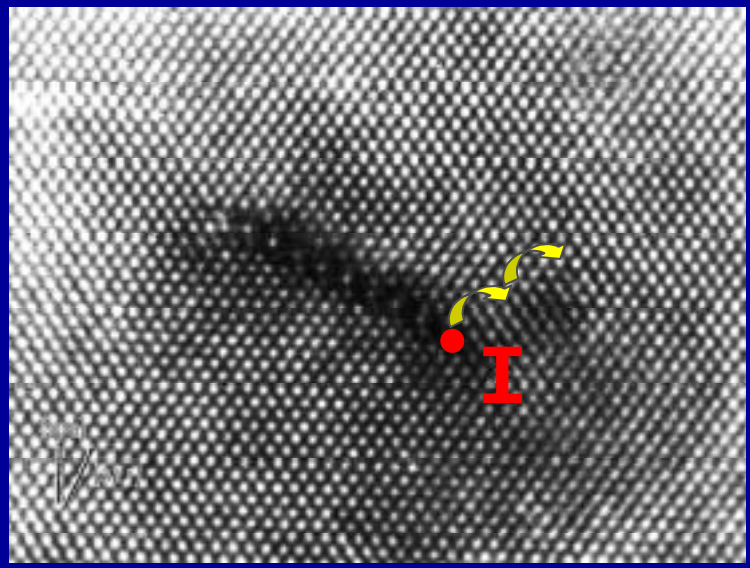
The Problem:
Complex Processing Scenarios

1. Many different species (V, I, As, C, O, B, …)
2. … and interactions (I-B, V-O, I-C-O, …)
3. 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:

  time step $\cong 10^{-15}$ s

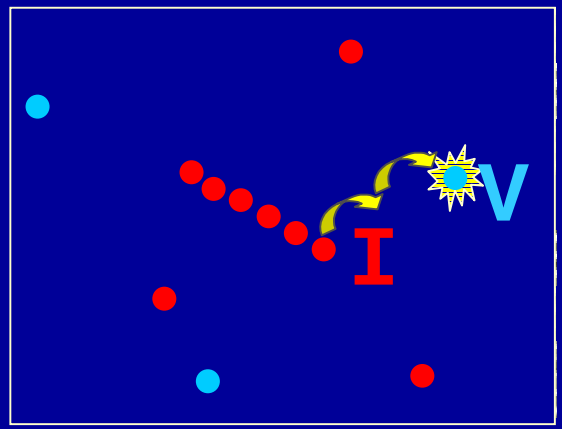
- We use it (off-line) to calculate the KMC event rates.

The Solution

Atomistic Kinetic Monte Carlo (KMC)

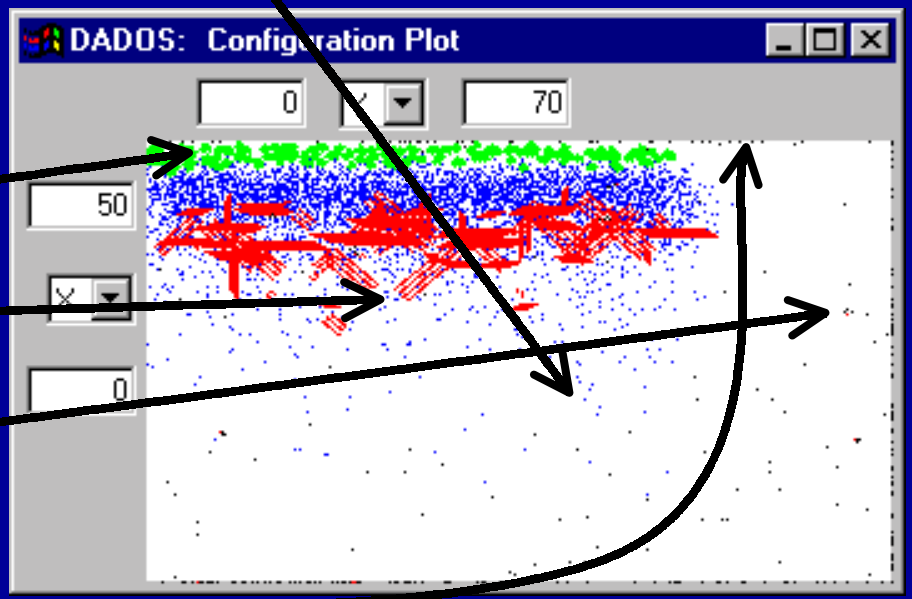
The Solution:
Atomistic Kinetic Monte Carlo (KMC)

- KMC follows only the defect atoms
- Self-adjusts time step during the course of the simulation (Δt: $10^{-9} \rightarrow 10^{3}$ s)
- Uses event rates obtained from MD or experiments



Atomistic Modeling 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



Defect Interactions

- Easy definition / modification :

```
…
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 Event Scheduler

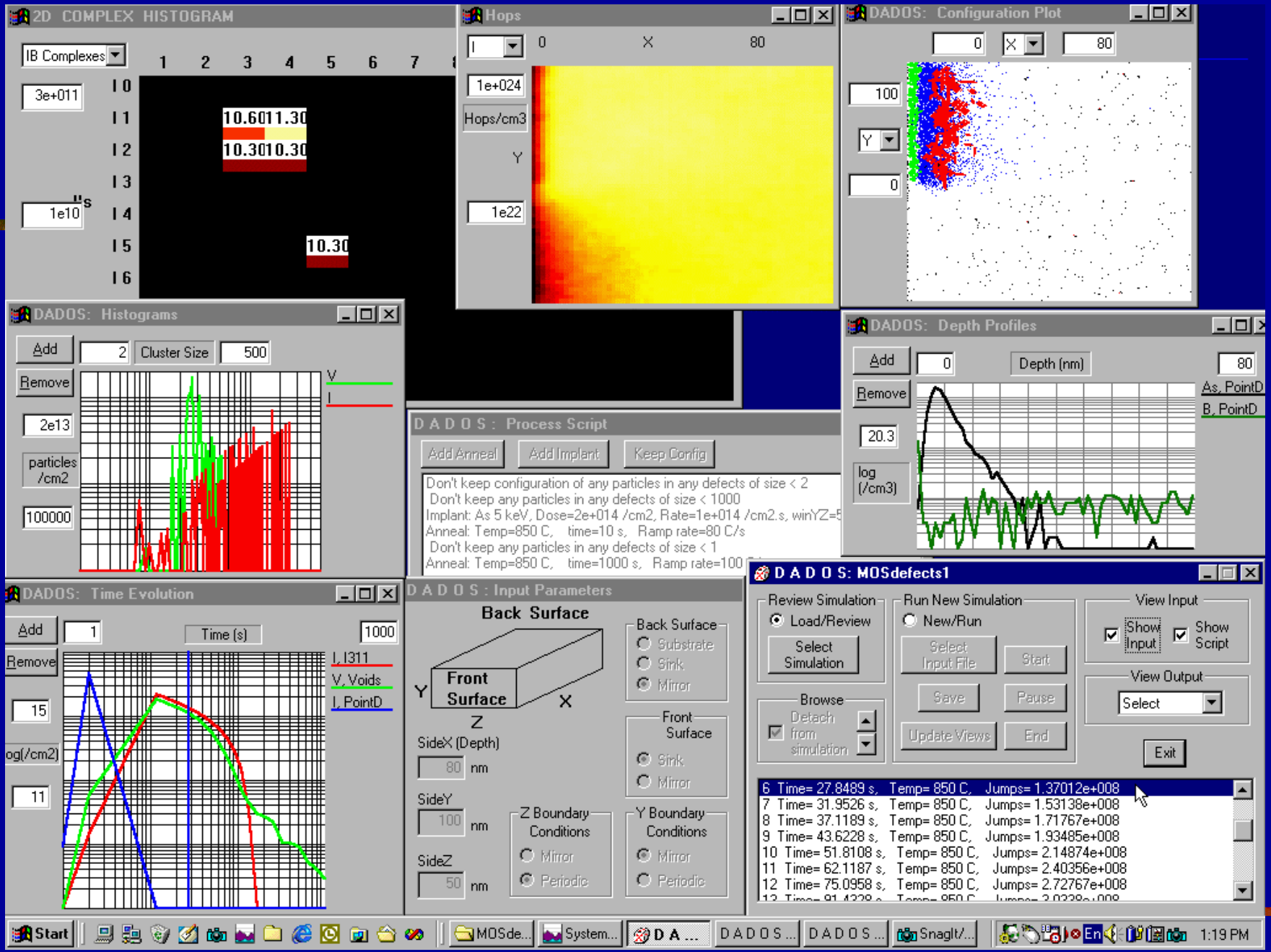
EXAMPLE:

	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
μs
10.6011.30
10.3010.30
10.30
Hops
1e+024
Hops/cm3
1e22
DADOS: Configuration Plot
100
DADOS: Histograms
Add
Remove
Cluster Size
500
2e13
particles /cm2
100000
DADOS: Depth Profiles
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
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
Time (s)
I, I311
V, Voids
I, PointD
DADOS: Input Parameters
Back Surface
Front Surface
SideX (Depth)
SideY
SideZ
Z Boundary Conditions
Y Boundary Conditions
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
1:19 PM

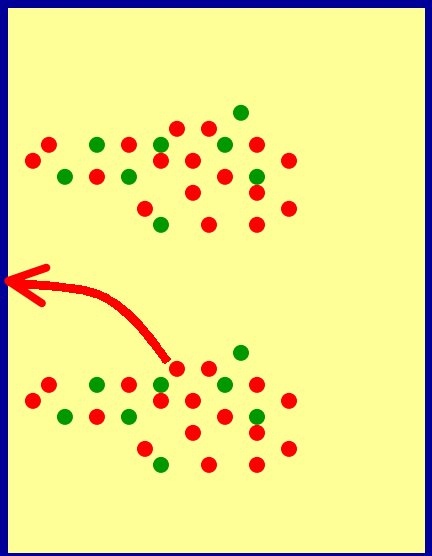
KMC: Feature Example 1

Implantation Damage and the "+N" Number

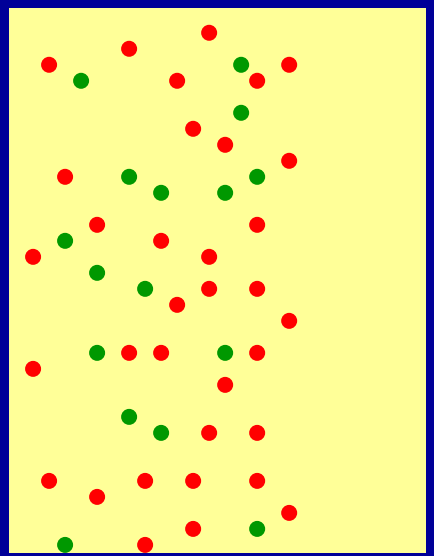
KMC can yield an accurate “+N” :

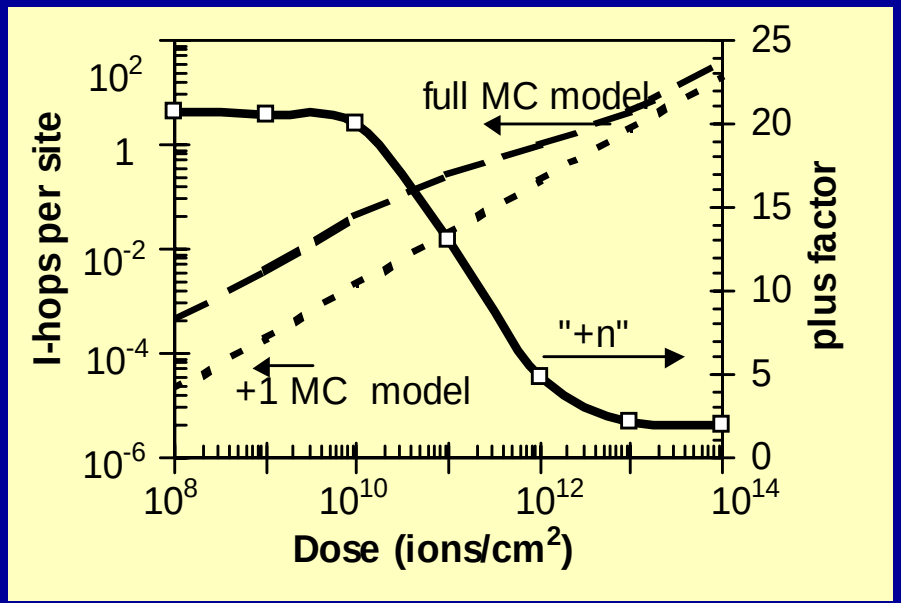
Low Dose Implant → Non-overlapping Cascades (Spatial Inhomogeneities)

Atomistic



Continuum





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

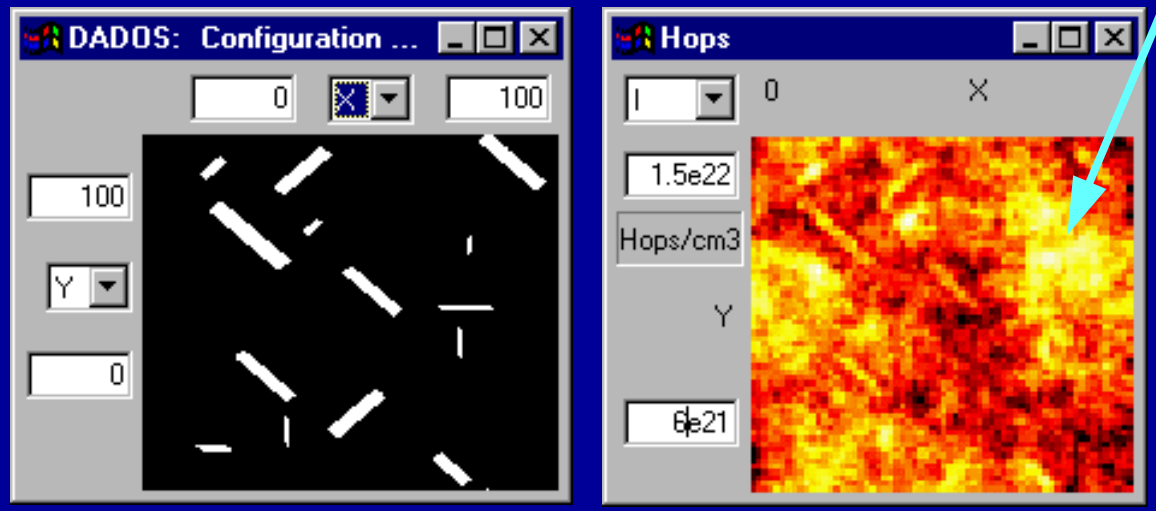
KMC: Feature Example 2

Local Inhomogeneities:

- Dopant Discreteness
- Clusters

Local Inhomogeneities: Clusters

High B diffusivity



{311} defects

Interst. hops

KMC: Feature Example 3

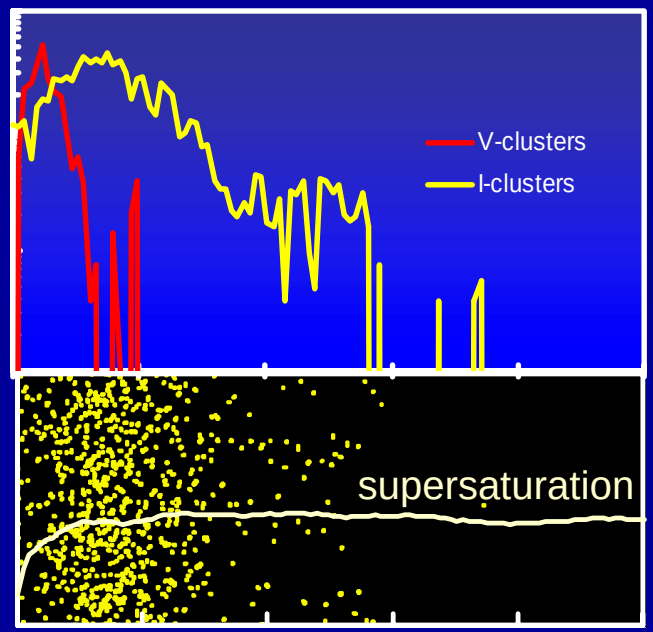
KMC used to validate Simplifying Assumptions

KMC used to validate simplifying assumptions

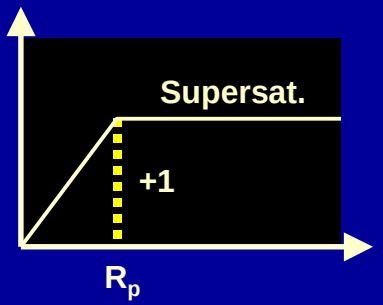
Emission energies of I-clusters:
Cowern et al., Phys. Rev. Lett. **82**, *4460 (1999)*

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

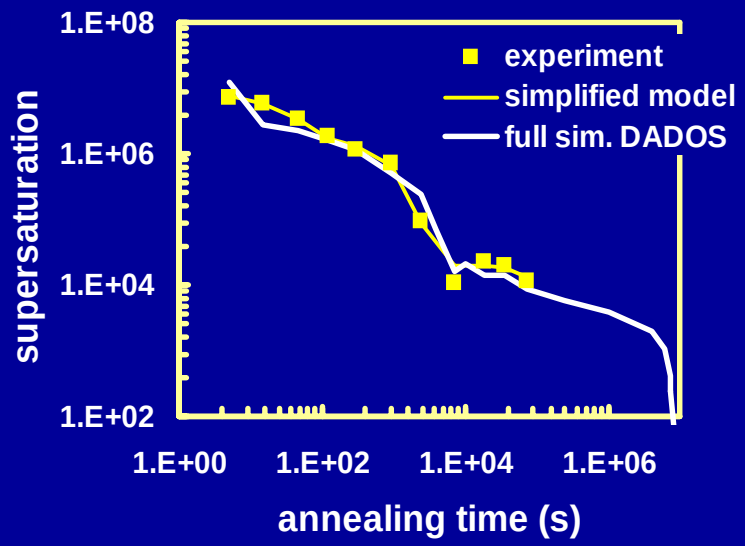
$$F_n = 4\pi a_n D_I C_I^* S,$$

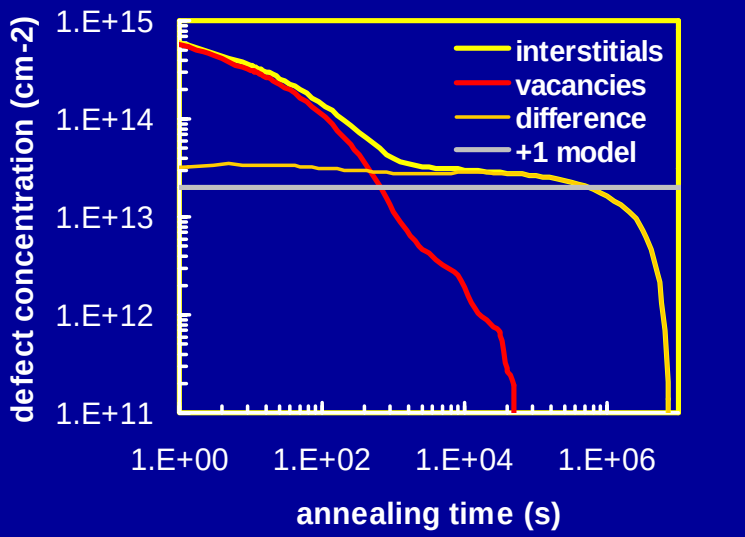
$$R_n = (6D_{0n}a_n/\lambda^3) \exp -[E_{\text{diss}}(n)]/kT$$

How accurate is the Simplified model ?

- **Very good agreement with <u>full</u> simulation …**

… in spite of the presence of Vacancies and other assumptions





The Challenge

Obtaining KMC Input Parameters
In Complex Scenarios

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"

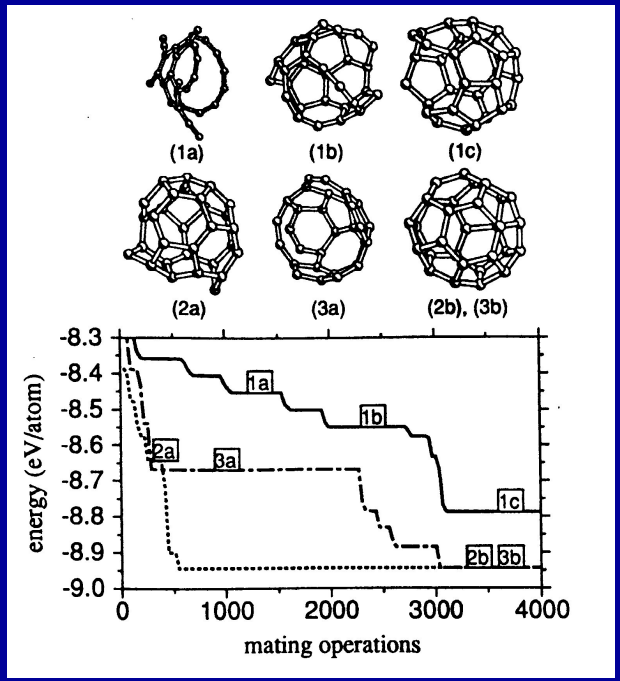
Obtaining KMC Parameters from MD with a Genetic Algorithm

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



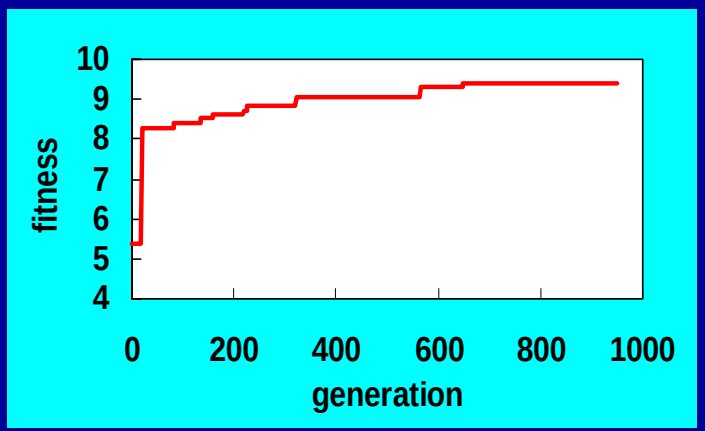
Deaven and Ho, PRL **75** (1995) 288

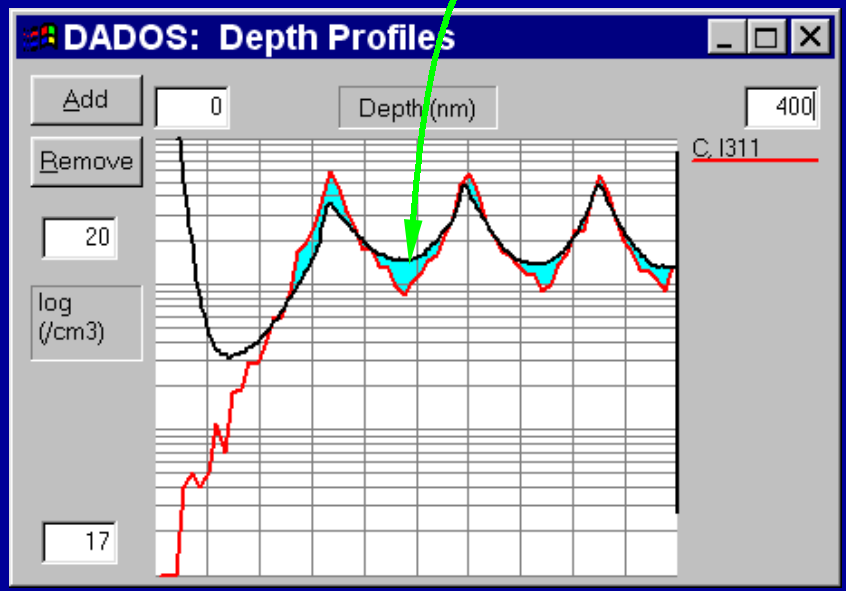
Free-standing Si clusters: Ho et al., *Nature* **392** *(1998) 582*

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

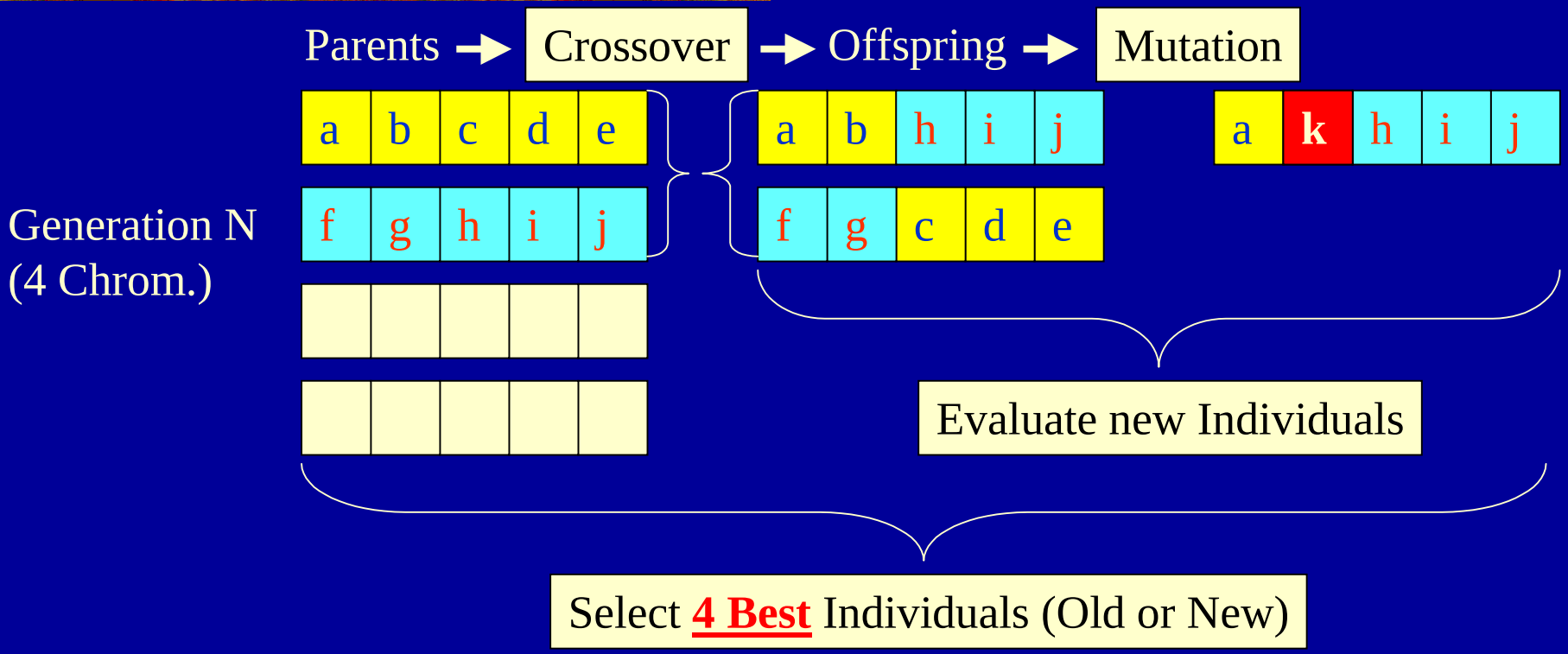
Fitness Evaluation: DADOS simulations
(just a rough estimate)
done in ~ 3 minutes / simulation





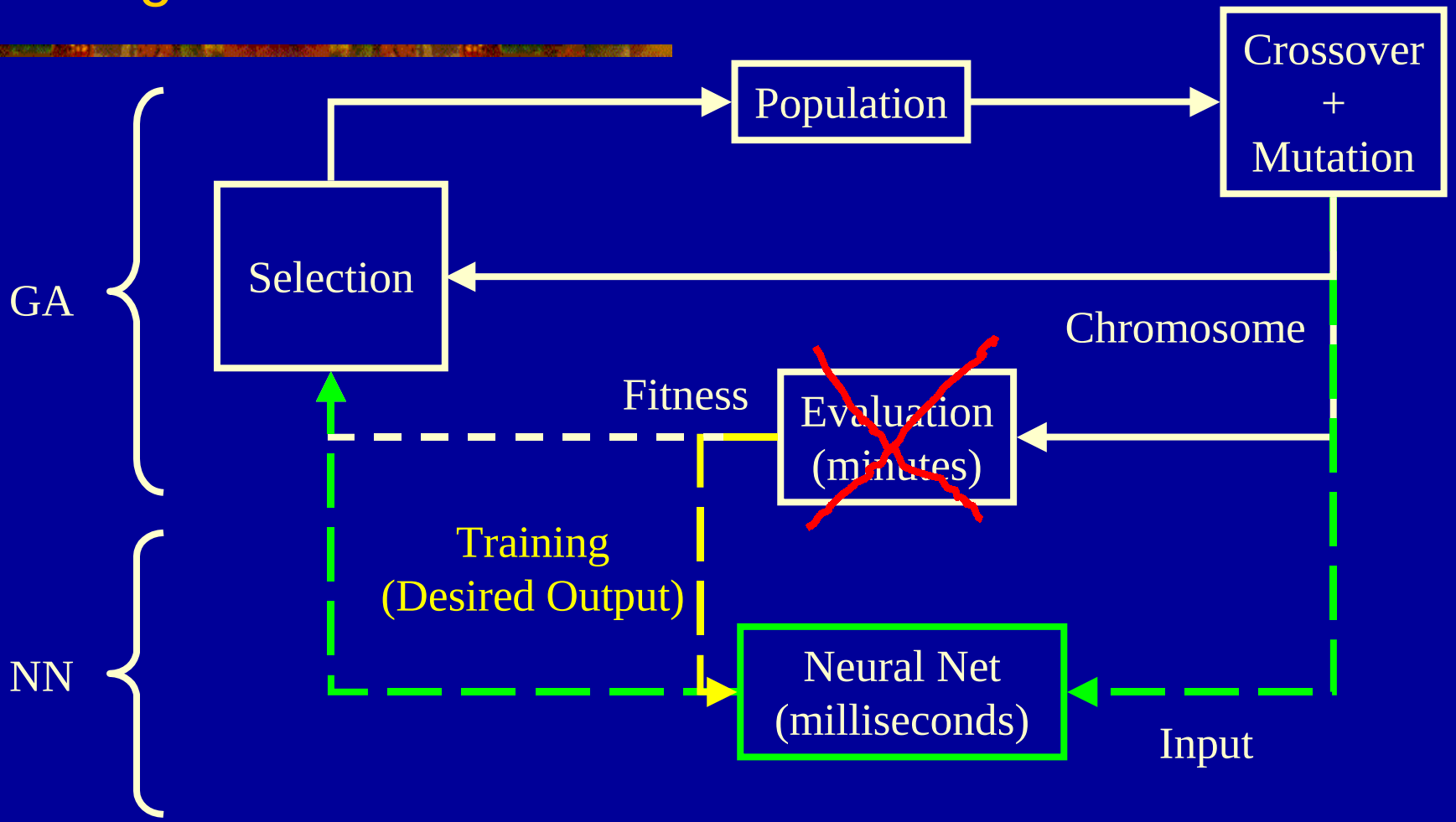
Genetic Algorithm from: http://lancet.mit.edu/ga/

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