ATOMISTIC MODELING OF POINT AND EXTENDED DEFECTS IN CRYSTALLINE MATERIALS

Martin Jaraiz, Lourdes Pelaz, Emiliano Rubio, Juan Barbolla
Dept. de Electronica, Univ. de Valladolid, SPAIN

George H. Gilmer, David J. Eaglesham, Hans J. Gossmann
Bell Labs, Lucent Technologies, Murray Hill, NJ

John M. Poate
NJIT, Newark, NJ.

- INTRODUCTION
- PREVIOUS APPROACHES
- SIMULATION SCHEME
  - SIMULATION BOX
  - TYPES OF DEFECTS
  - SCHEDULER
- EXAMPLES

COMPUTER SIMULATION:

- POWERFUL **ANALISYS & DESIGN** TOOL
- **COMPLEMENTARY** TO **EXPERIMENTAL** TECHNIQUES
- **RAPID GROWTH:**
  - ⇒ A REFLECTION OF THE UNPARALLELED RATE OF INCREASE IN **COMPUTING POWER**

SEMICONDUCTOR PROCESS SIMULATION, IN PARTICULAR, IS NOW WELL ESTABLISHED AS AN ESSENTIAL TOOL FOR:

- STUDYING **NEW MATERIALS/PHENOMENA**.
- DESIGNING **NEW DEVICE STRUCTURES**

UNTIL RECENTLY, **SEMICONDUCTOR DIFFUSION SIMULATORS** WERE ONLY BASED ON **CONTINUUM** TYPE MODELS AND FINITE-DIFFERENCE EQUATION SOLVERS.

TO SIMULATE: $I + V \leftrightarrow 0$

SOLVE: $\delta I/\delta t = D\, \delta I^2/\delta x^2 - R_{Bulk}$

TO ADD NEW MECHANISM:

$I + B_s \leftrightarrow B_I$

ADD AND SOLVE:

$$\delta I/\delta t = D\, \delta I^2/\delta x^2 - K_{IF}\, B_s I + K_{IR}\, B_I - R_{Bulk}$$

$$\delta\, B_I /\delta t = D\, \delta B_I{}^2/\delta x^2 + K_{BIF} B_s I - K_{BIR}\, B_I$$

$$\delta\, B_S /\delta t = - K_{BSF} B_s I + K_{BSR}\, B_I$$

HOWEVER,

THE SHRINKAGE IN DIMENSIONS

THE PERFORMANCE ACHIEVED BY COMPUTERS

IS OPENING THE WAY TO A NEW,

SIMPLER AND **MORE ACCURATE**

TYPE OF SIMULATOR,

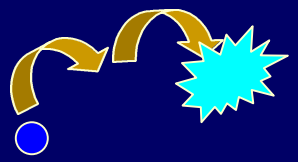
THE ATOMISTIC DIFFUSION SIMULATOR

THE ATOMISTIC DIFFUSION SIMULATOR

SIMULATES THE MOVEMENTS AND INTERACTIONS OF **INDIVIDUAL** POINT DEFECTS:

TO SIMULATE: $I + V \leftrightarrow 0$

PROGRAM:

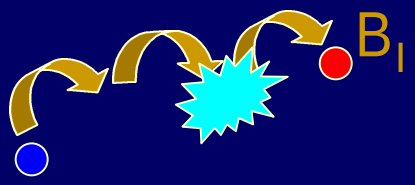


annihilate(I);
annihilate(V);

TO ADD NEW MECHANISM:

$I + B_S \leftrightarrow B_I$

PROGRAM:



annihilate(I);
annihilate(B_S);
create(B_I);

$\Rightarrow$ ALMOST NO ADDITIONAL COMPUTATION TIME

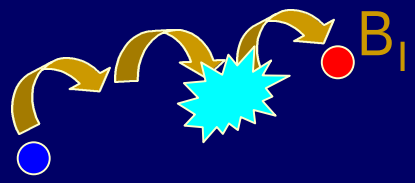
ADVANTAGES

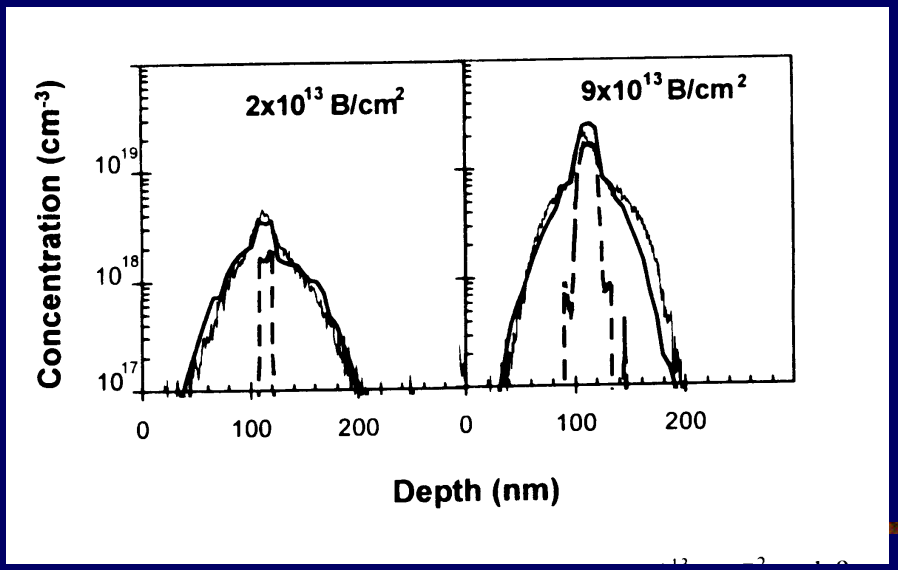
FOR STUDYING **NEW MATERIALS/PHENOMENA**:

ATOMISTIC MODELING PROVIDES A

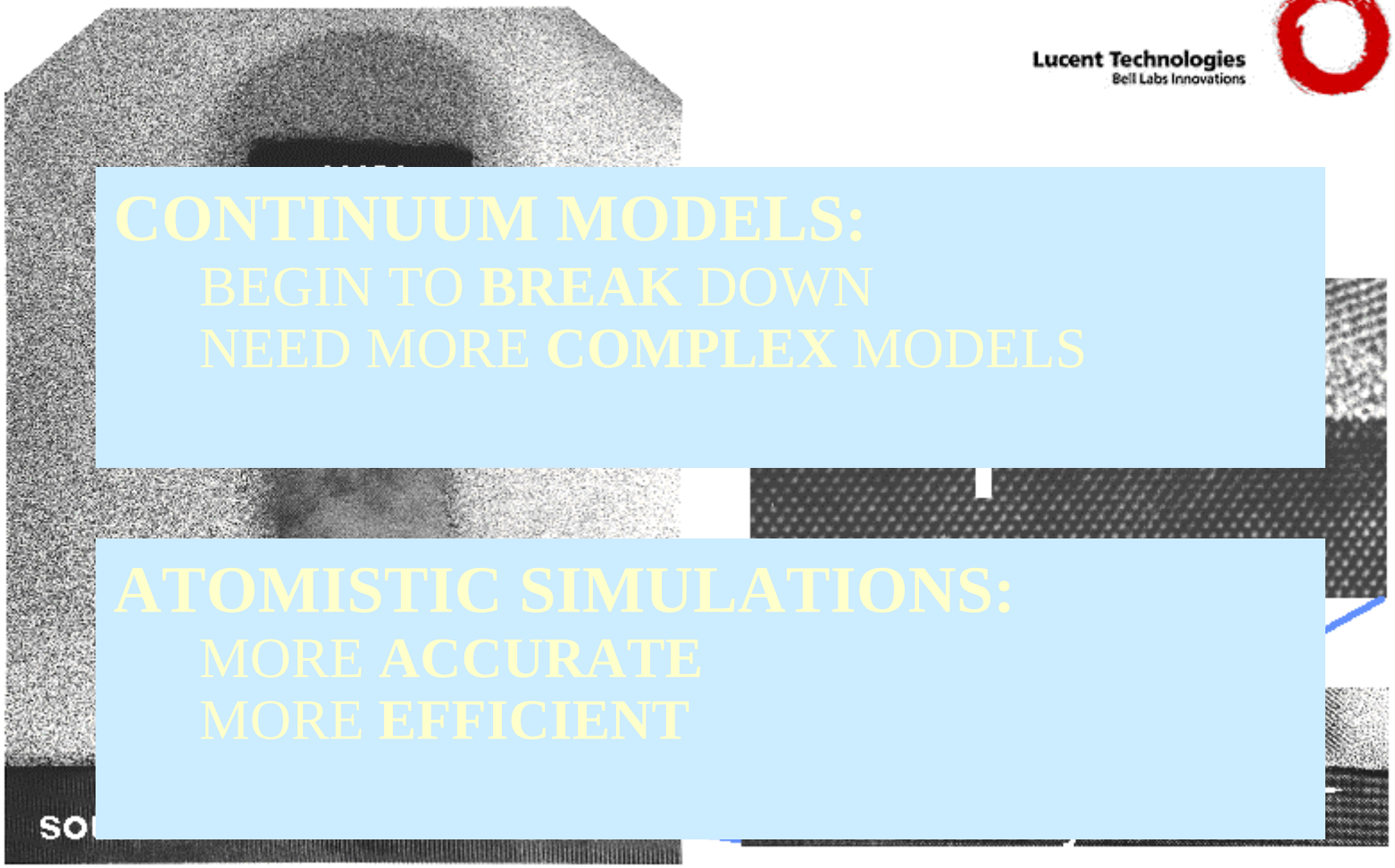
⇒ **SIMPLE AND STRAIGHTFORWARD LINK** BETWEEN

ATOMISTIC MECHANISMS AND **MACROSCOPIC BEHAVIOR**





SEMICONDUCTOR DEVICE DESIGN
AS DEVICE DIMENSIONS SHRINK:



Lucent Technologies
Bell Labs Innovations

CONTINUUM MODELS:

BEGIN TO **BREAK** DOWN

NEED MORE **COMPLEX** MODELS

ATOMISTIC SIMULATIONS:

MORE **ACCURATE**

MORE **EFFICIENT**

TEM micrograph: F. Baumann

ATOMISTIC DIFFUSION SIMULATORS
PREVIOUS APPROACHES:

- **MOLECULAR DINAMICS (MD)**
  - INCLUDES ALL LATTICE ATOMS
  - COMPLEX FORCE CALCULATIONS
    - A few nm
    - A few ps-ns ⇐ **too short** Annealing times

ATOMISTIC DIFFUSION SIMULATORS
PREVIOUS APPROACHES:

- **MONTE CARLO (MC)**
  - CASCADE-SIZE ANNEALS

    T. Muroga and S. Ishino, J. Nucl. Mat. **117**(1983), 36-45 (constant time step)

    H. L. Heinisch, Nucl. Instr. Meth. B**102**(1995), 47-50

THREE YEARS AGO, AT BELL LABS, WE TRIED **A STEP FORWARD**:

" CAN WE USE A KINETIC MONTE-CARLO SIMULATOR TO SIMULATE THE IMPLANTS AND ANNEALS **TYPICALLY PERFORMED** IN SEMICONDUCTOR DEVICE PROCESSING "

?

WE DEVELOPED **BLAST**, AN ATOMISTIC DIFFUSION SIMULATOR, AND THE RESULT WAS:

Implant: 40 keV, 5×10^{13} Si^{+}/cm^{2}

Anneal: 10 min @ 815 °C

$\Rightarrow$ Simulation time: 10 - 20 hours (in 1995)

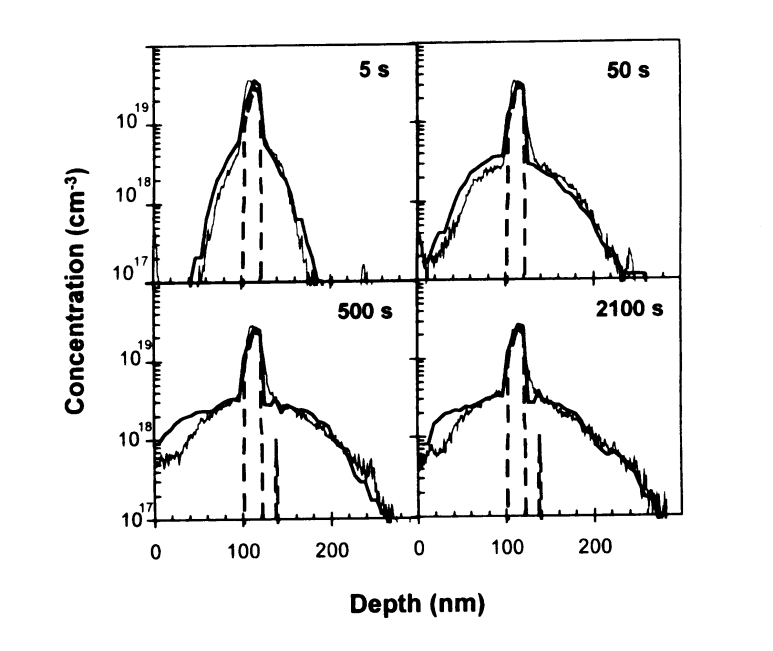
THOSE SIMULATIONS REVEALED (*)

"for the first time, a complete history of the I and V populations, including the formation and ripening of defect clusters"

AS WELL AS

"the mechanisms leading to the success of the (empirical) '+1' model"

(*) Appl. Phys. Lett. **68**, 409 (1996)



"This model provides parameters and simplified mechanisms which can be implemented in continuum process simulators, such as SUPREM-IV or PROPHET" (*)

(*) Appl. Phys. Lett. **70**, 2285 (1997)

The message is:

- ATOMISTIC DIFFUSION SIMULATIONS **ARE FEASIBLE** (at least for research purposes in 1995)

- THEY CAN PROVIDE A UNIQUE INSIGHT INTO THE DOMINANT **MECHANISMS** GOVERNING ION IMPLANTATION AND ANNEALING

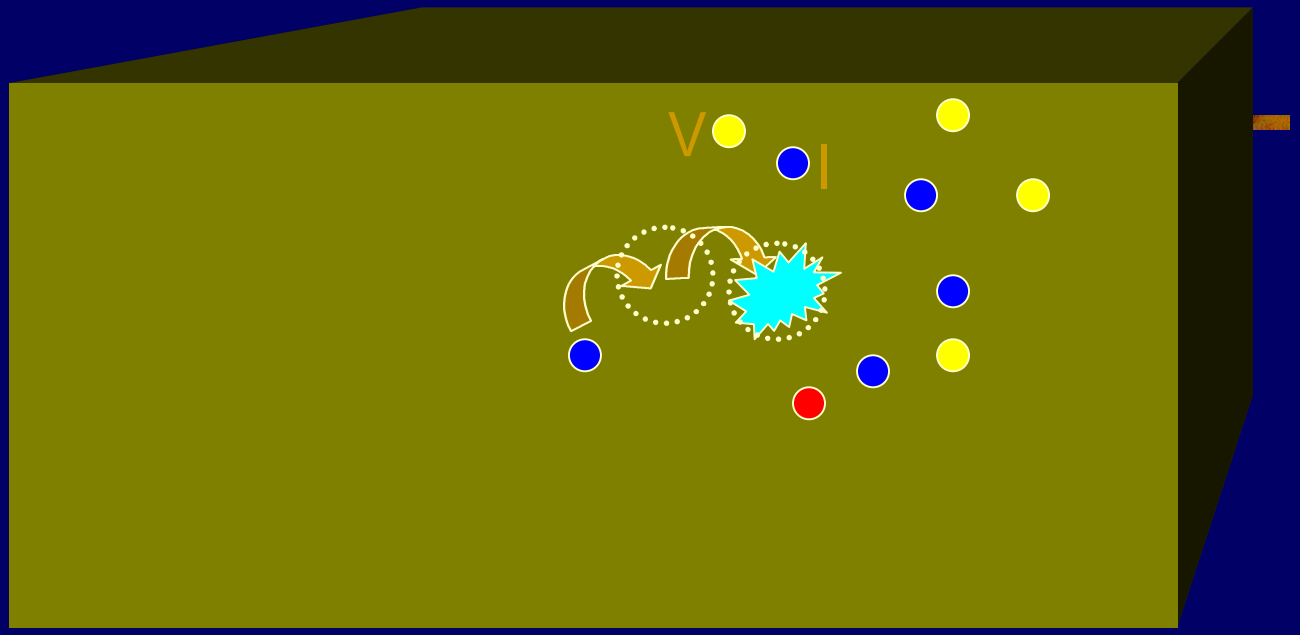
ATOMISTIC DIFFUSION SIMULATION

SIMULATION SCHEME

SIMULATION SCHEME

SIMULATION BOX

FRONT SURFACE



BACK SURFACE

LATERAL BOUNDARY CONDITIONS:

- **PERIODIC**
- **MIRROR**

SIMULATION SCHEME

DEFECT TYPES

1. POINT DEFECTS

- SINGLE POINT DEFECTS: V, I, B, C, ...
  - POSSIBLE EVENT: JUMP
- PAIR POINT DEFECTS: IB, Bi, VO, ...
  - POSSIBLE EVENTS:
    - JUMP: 
    - BREAK UP: IB $\rightarrow$ I + B
    - SWITCH: IB $\rightarrow$ Bi

INTERACTION BETWEEN DEFECTS:

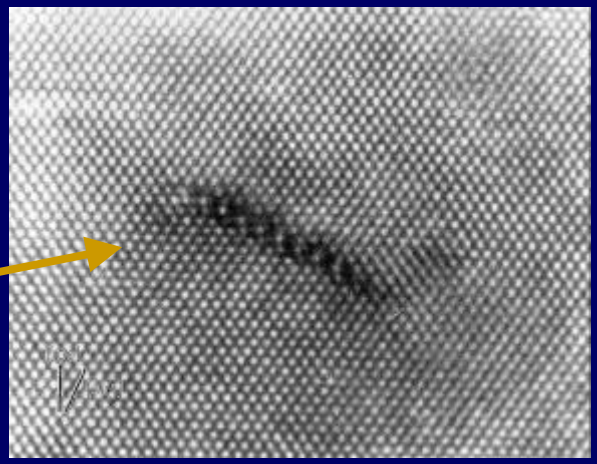
- CAPTURE RADIUS = 3.84 Å
- WITH / WITHOUT AN INTERACTION BARRIER

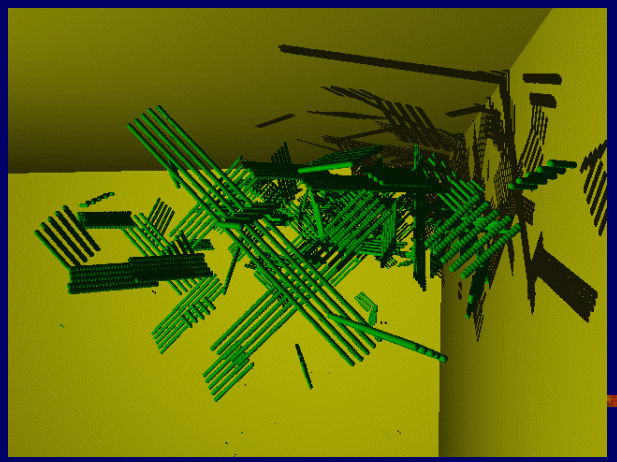
SIMULATION SCHEME

DEFECT TYPES

2. CLUSTERS

- SHAPES:
  - IRREGULAR (blob): V, B, C, ...
  - SPECIFIC:
    - VOIDS
    - {311}'s
    - DISLOCATION LOOPS
    - STACKING FAULTS
- POSSIBLE EVENTS:
  - CAPTURE of a point defect
  - EMISSION of a point defect





SIMULATION SCHEME

DEFECT TYPES

3. COMPLEXES

COMPOSITION:

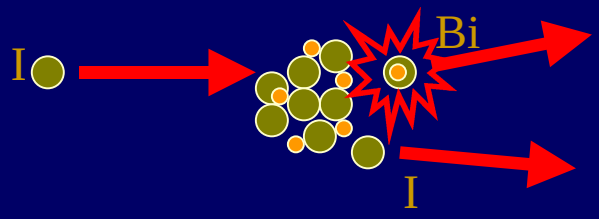
BINARY: I_nB_m, I_nC_m, V_nO_m, ...
TERNARY, ...

SHAPE:

IRREGULAR (small sizes)

POSSIBLE EVENTS:

CAPTURE or EMISSION of a point defect (SINGLE or PAIR)



SIMULATION SCHEME

DEFECT TYPES

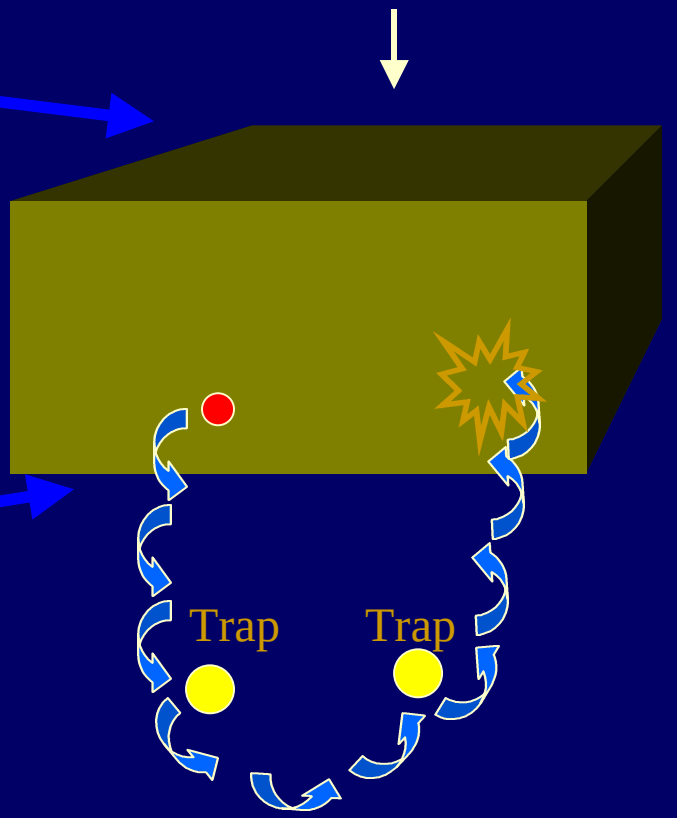
4. SURFACES

FREE SURFACE (Front):

- THERMAL I-V GENERATION
  - Neutral, Oxidation (I),Nitridation (V)
- SINK for point defects:
  - from perfect SINK
  - to perfect MIRROR (energy barrier)

BULK (Back surface):

- DELAYING SURFACE:
  - Random walk
  - Bulk Traps
  - Re-emission from Traps



SIMULATION 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.

simulating ONE EVENT:

FROM CURRENT CONFIGURATION SELECT :

NEXT **EVENT TYPE** (Jump, Emission, ...) AND

INDIVIDUAL **PARTICLE**

SELECT JUMP **DIRECTION**

MOVE PARTICLE TO NEW POSITION

SEARCH FOR INTERACTING NEIGHBORS AT NEW POSITION

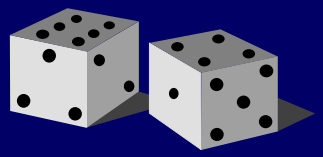
PERFORM **INTERACTION** (Capture, ...)

UPDATE CONFIGURATION

AT THE UNIVERSITY OF VALLADOLID WE HAVE RECENTLY IMPLEMENTED A FAST ATOMISTIC SIMULATOR :

DADOS

(Diffusion of Atomistic Defects, Object-oriented Simulator)



C++, 6000 lines

PERFORMANCE: >**1 Million** events per second

(566 MHz Alpha CPU, Microsoft C++ compiler)

On average, simulates one event in the time it takes to calculate three Jump rates:

$$Jrate = 6 * D_o * \exp(-Ea / kT) / \lambda^2$$

STRATEGY:

- CPU-TIME REDUCTION:

  ⇒ USE ELEMENTAL ARITHMETIC
  (**Bitwise** where possible)

- USER-FRIENDLY, NEAT DESIGN: User can implement new models in a few minutes/hours

  ⇒ USE **OBJECT-ORIENTED** SIMULATION

Object-Oriented Simulation

Class **Interstitial**

{

Private:

Position: x, y, z

Public:

Jump();

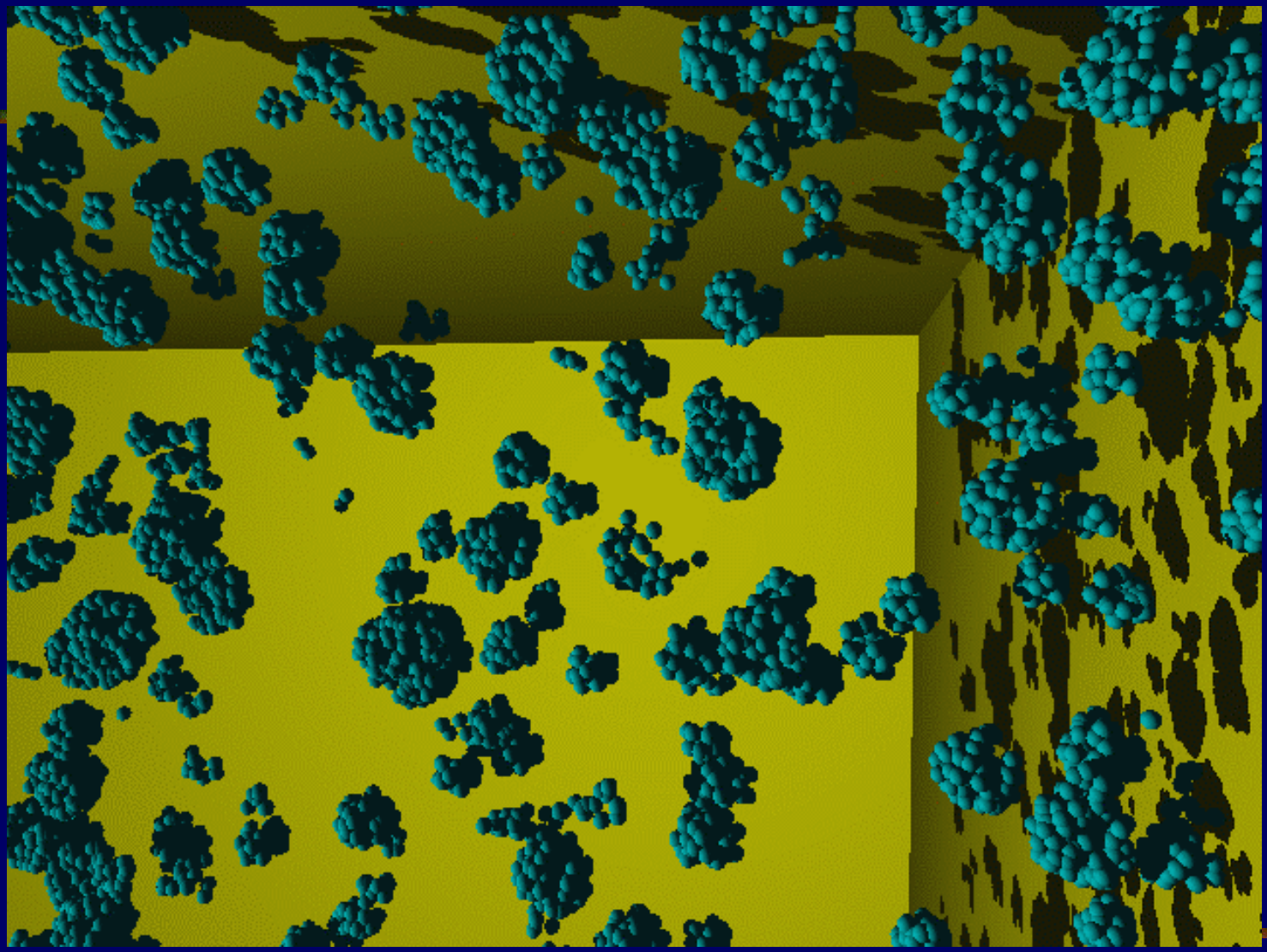
Interact();

}

⇒ Plus: Derived Classes, Virtual functions, Templates, ...

SIMULATION EXAMPLES

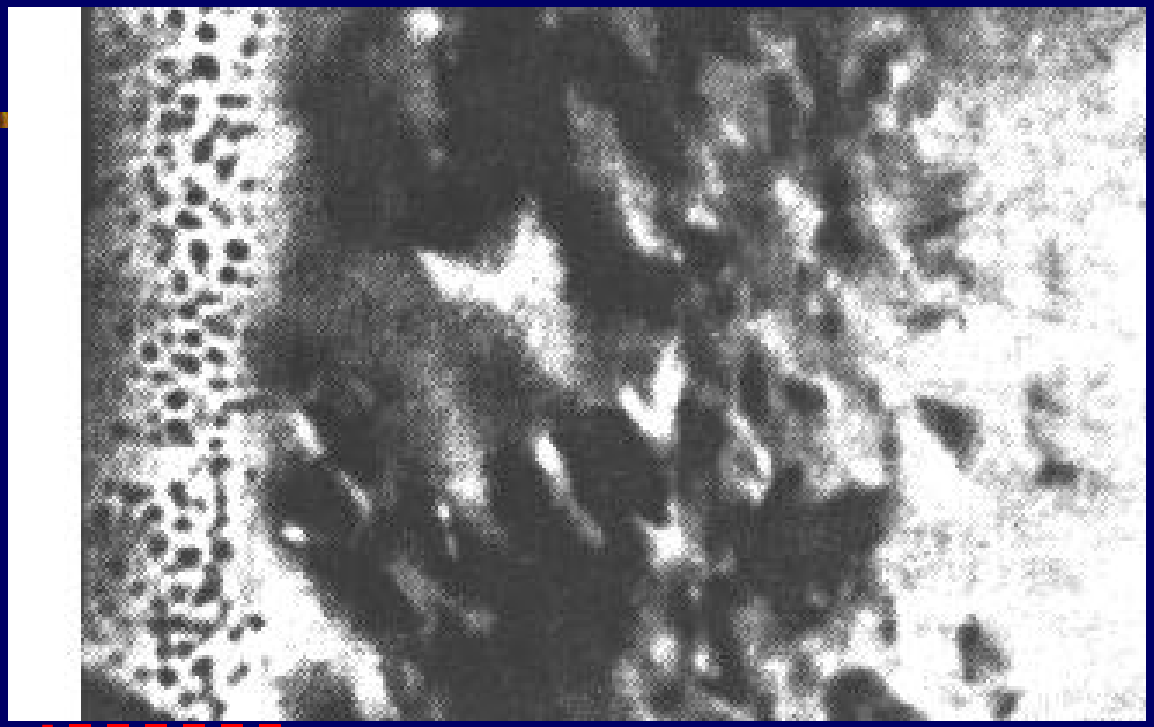
VOIDS



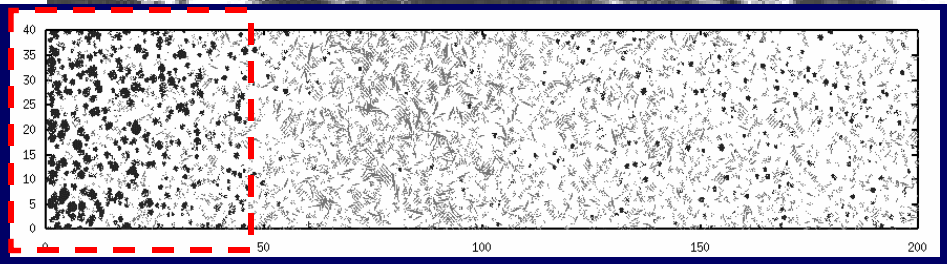
VOIDS

100 keV,
1E16 As/cm^2
beam heating

EXPERIMENT (*)

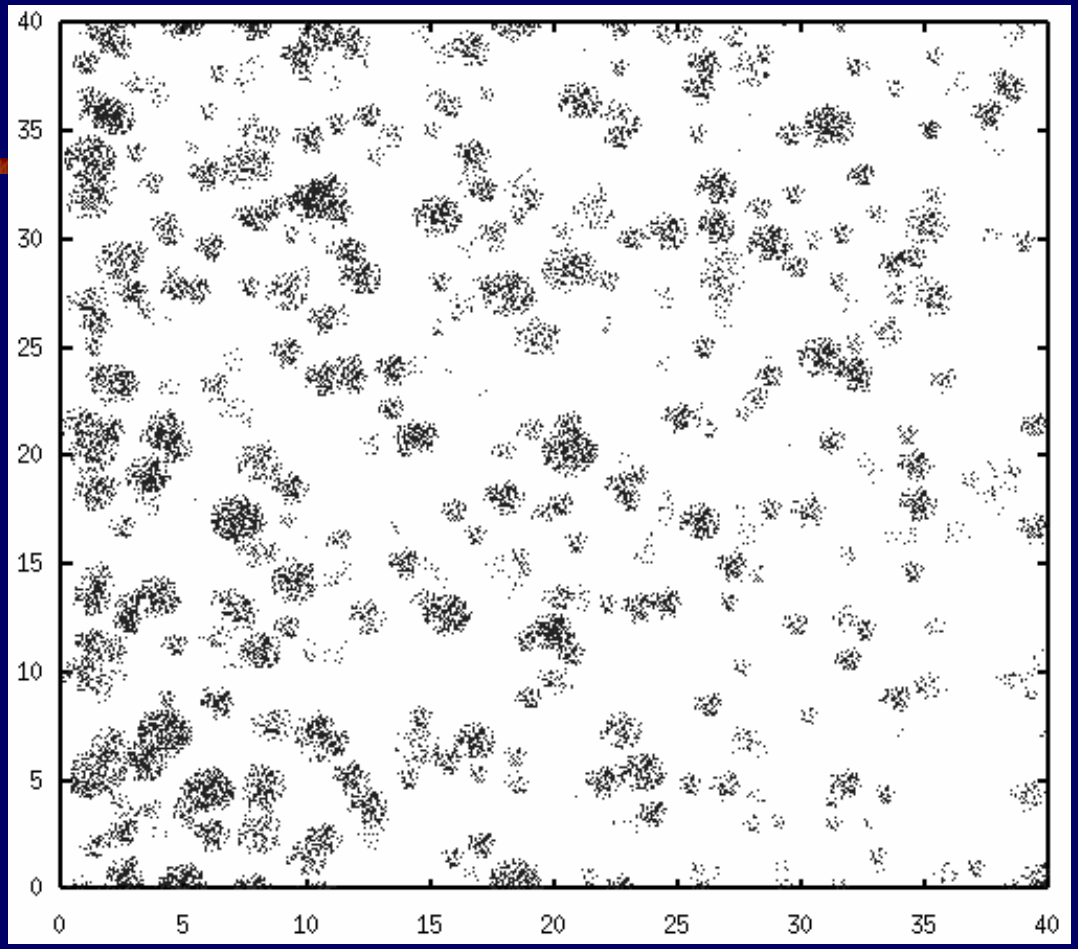


SIMULATION



(*) O. W. Holland and C. W. White, Nucl. Instr. Meth. B59/60(1991), 353-362

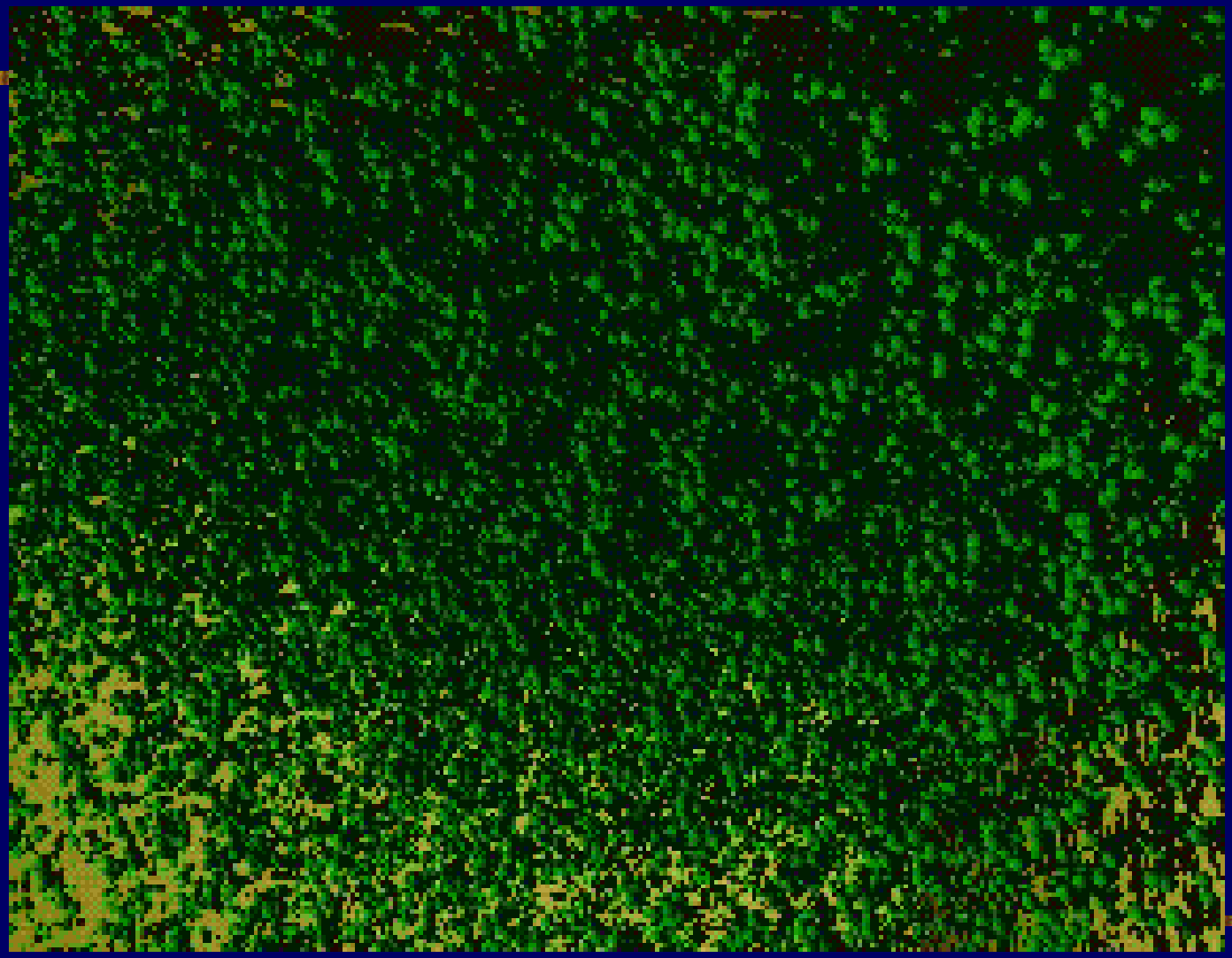
VOIDS



$$E_{bind}(N) = 3.65 - 4.9 \times [\, N^{2/3} - (N-1)^{2/3} \,] \quad eV$$

{311} DEFECTS

{311} FORMATION AND DISSOLUTION



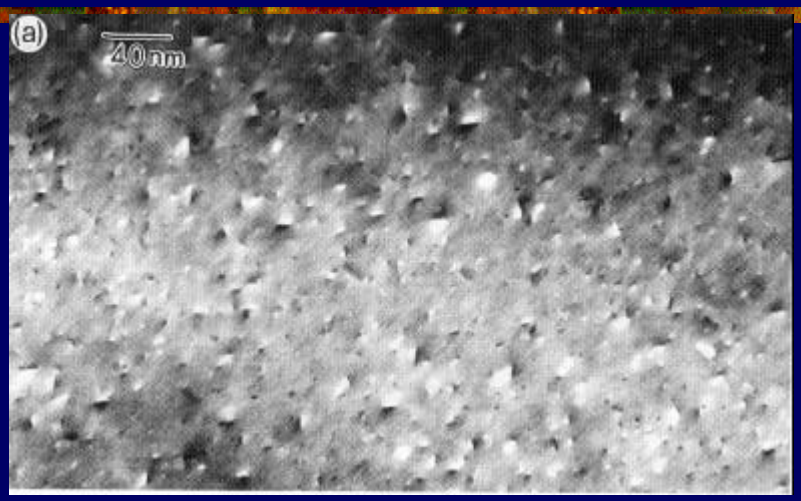
{311} DEFECTS

EXPERIMENT

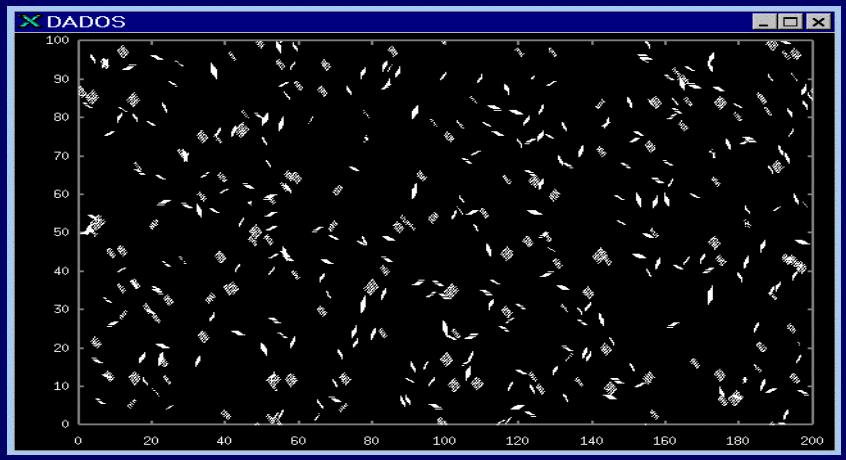
40 keV, 5E13 Si/cm^2
800 C anneal

SIMULATION

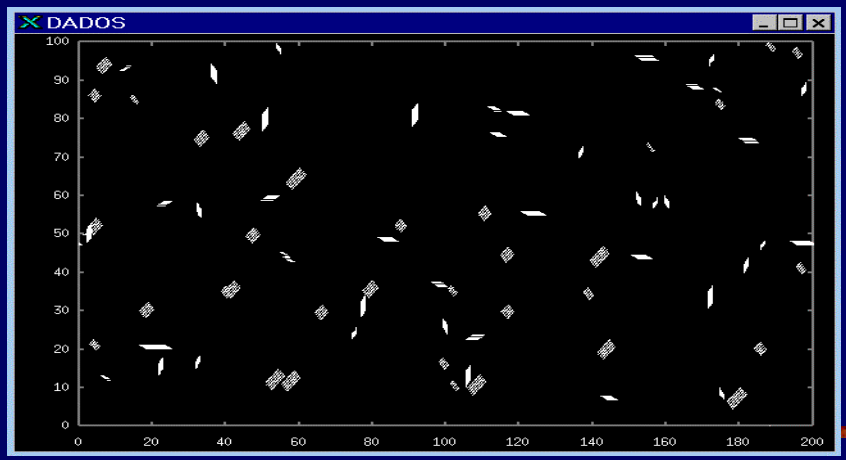
Ebind(n) =2.7 - 2.655[√n - √(n-1)]



5 s

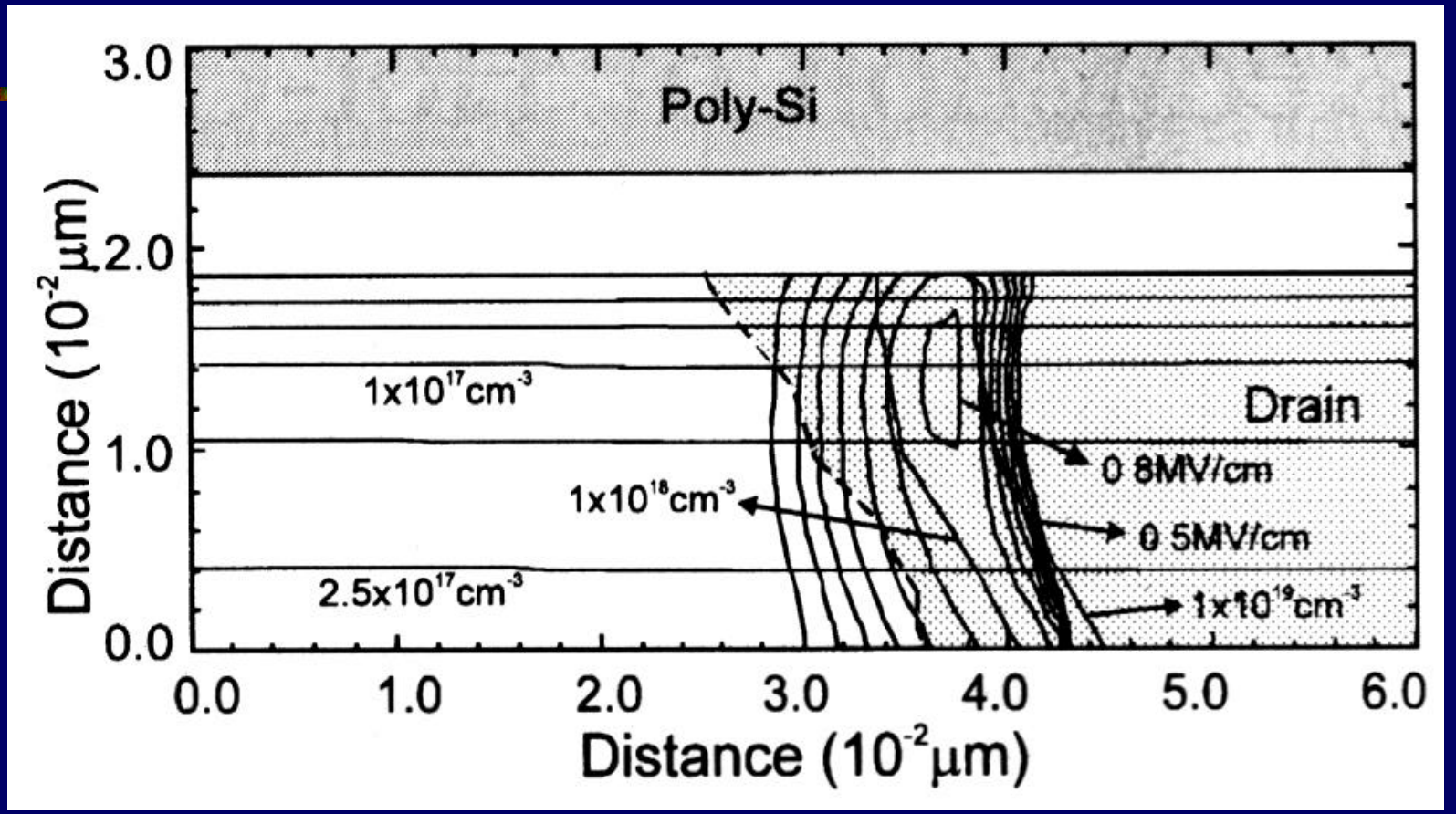


30 s



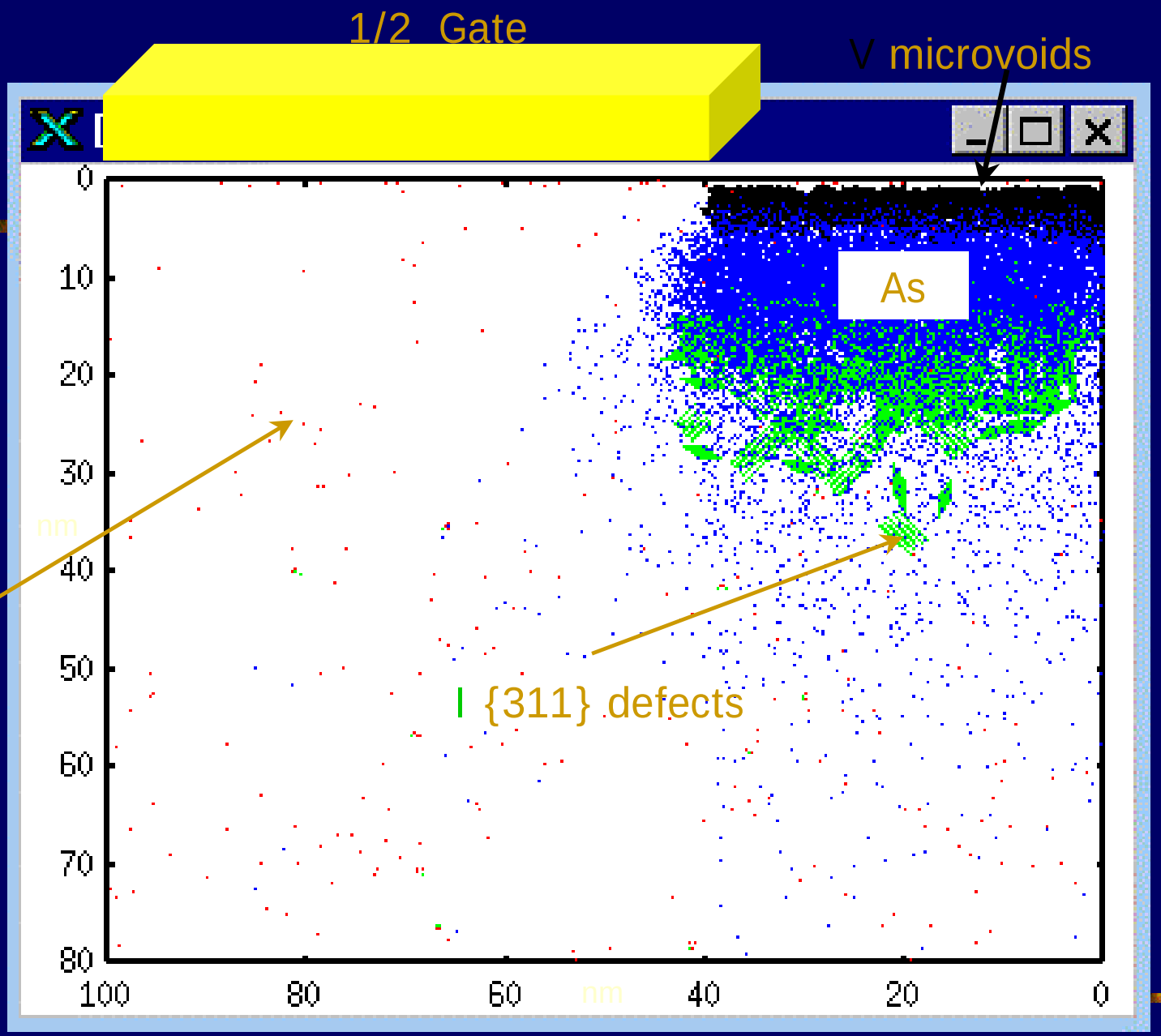
0.12 μm N-MOSFET

0.12 μm nMOSFET



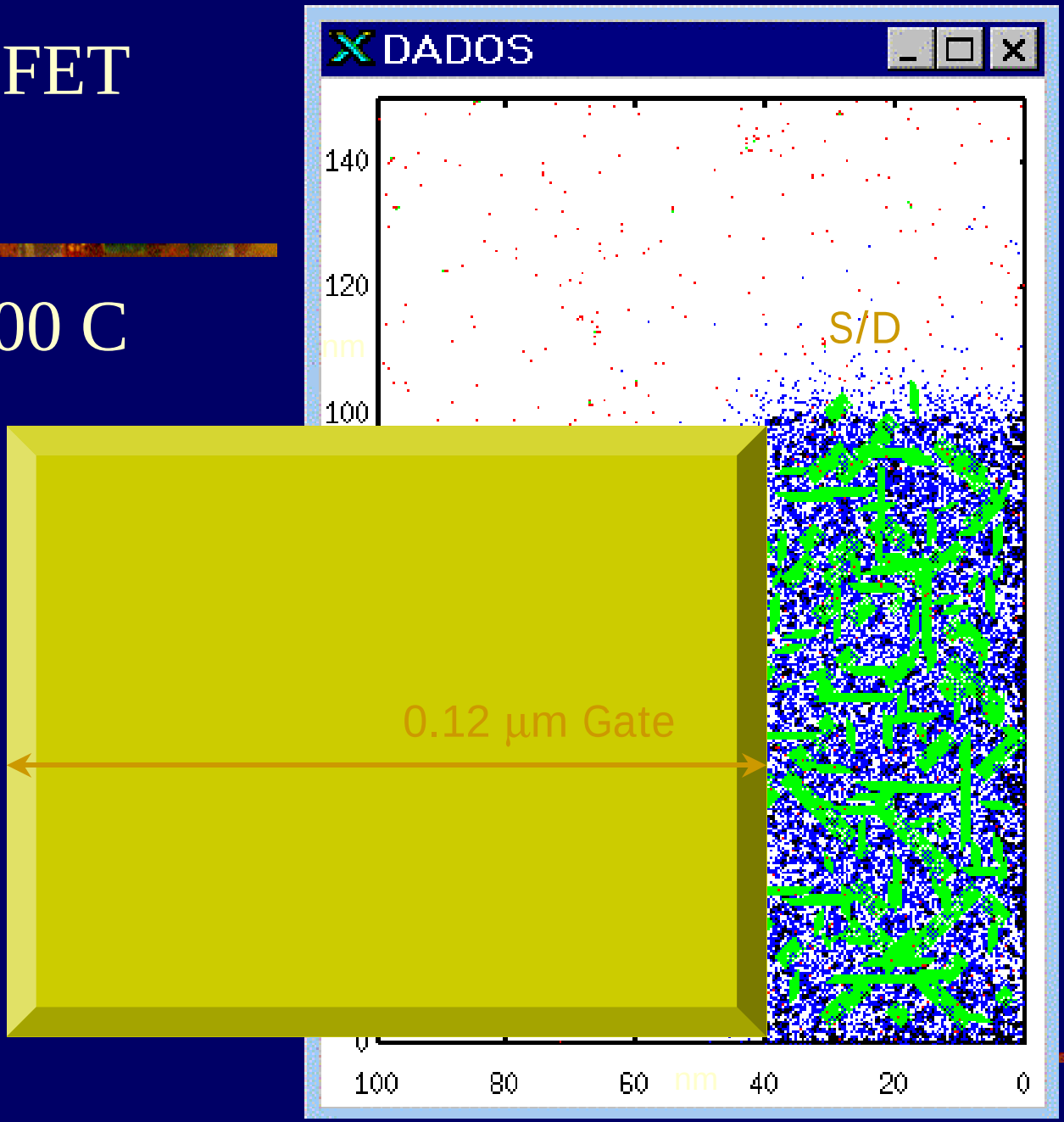
J. Lyu et al, IEEE Electron Device Lett. **18** (1997), 535-537

After
10 s @
800 C

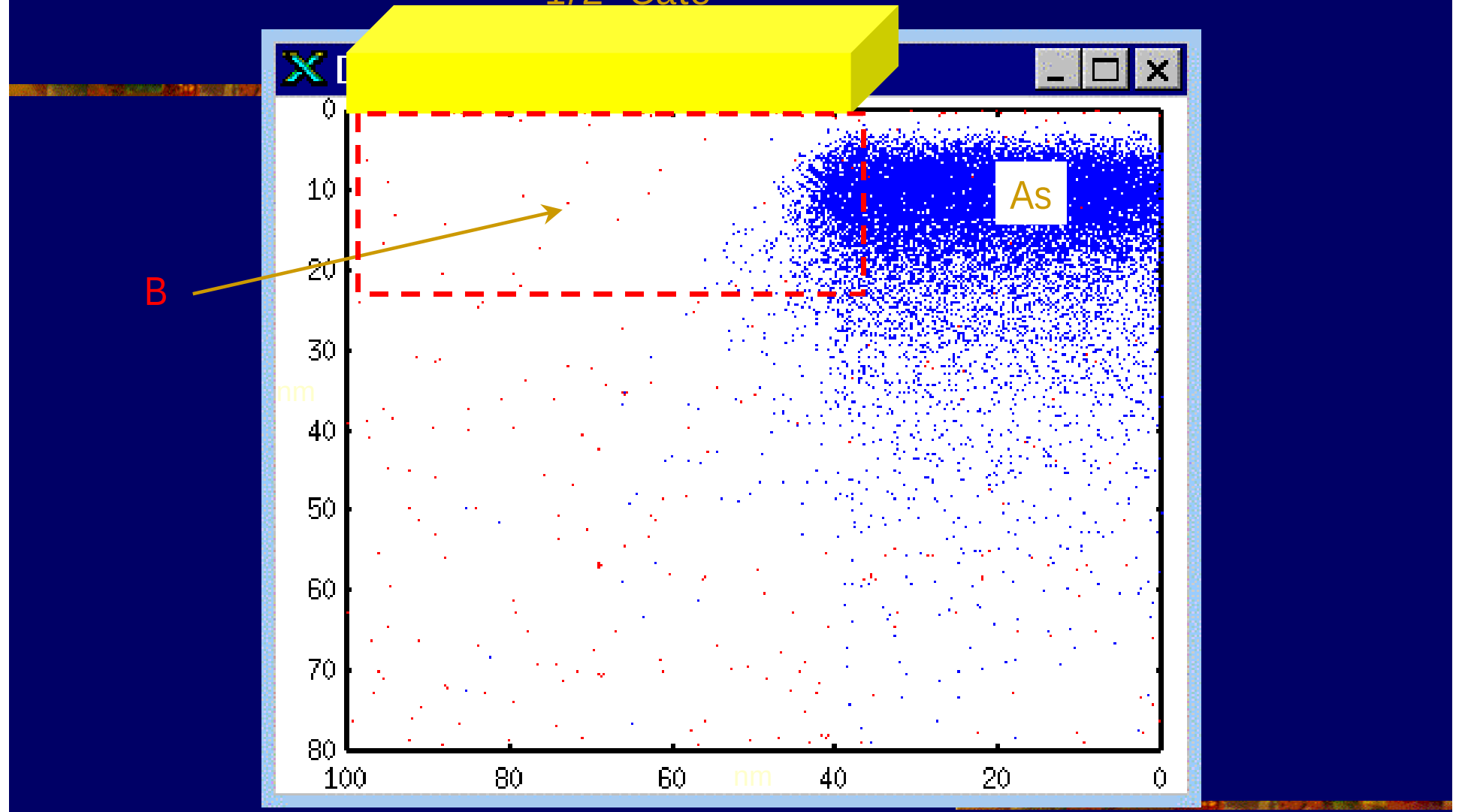


0.12 µm nMOSFET

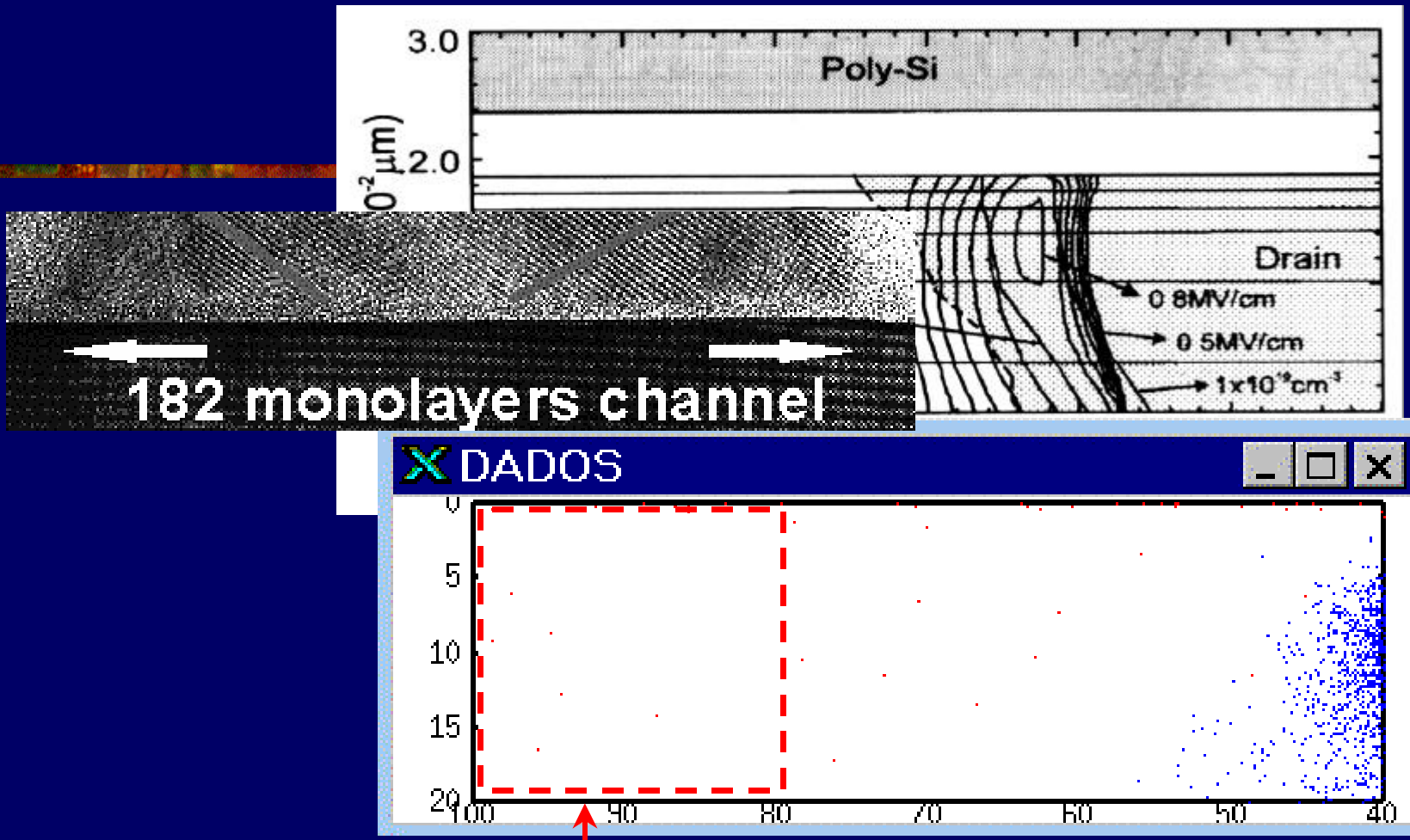
After 10 s @ 800 C



Final configuration (1000s @ 800 C)



SHRINKING DIMENSIONS ⇒ LOCAL **INHOMOGENEITIES**



6 B atoms / (20x20x150 nm^3) = 1x10^{17} cm^{-3}