

Fys4310

DOPING

DIFFUSION

Diffusion program I

phenomenological

Ficks laws

Intrinsic diffusion - extrinsic diffusion

Solutions of Fick's laws

'predeposition', 'drive-in'

electrical field enhancement

Concentration dependant diffusion (As)

atomistic

Si-Self diffusion

Vacancy diffusion

Charged vacancy model

Impurity diffusion

Vacancy -dopant interactions

Diffusion program II

Math & practical

Numerical solutions of Ficks laws

Computer packages

Materials science

High concentration effects

Pairs, quartets, defects

experimental./ref.reading

Measurements of diffusion

SIMS, Radio tracer, RBS

Differential Hall, SRM, CV, stain etch

Bolzman Matano method

Diffusion equipment, furnaces, boilers, sources

Diffusion program III

Examples

B in Si

As in Si

P in Si, high concentration

Emitter push

Zn in GaAs

etc.

These points/topics are woven into other headings

High doping effects

Solubility, Metastable doping

Dopant interactions

Defects introduced in diffusion doping, Stresses

Defining doping areas, masking, Diffusion in SiO_2 vs Si

Diffusion of metallic impurities

Diffusion phenomenological

Ficks laws

Ficks 1st law $J = -D\nabla C \stackrel{1D}{=} -D \frac{\partial C}{\partial x}$ Defines D
phonomenologic

Continuity equation $\frac{\partial C}{\partial t} = -\nabla J = \nabla(D\nabla C) \quad \begin{matrix} \uparrow \\ = D\nabla^2 C \end{matrix} \quad J: \text{flux}$
 $\nabla D = 0$

Ficks 2nd law $\frac{\partial C}{\partial t} = D\nabla^2 C \stackrel{1D}{=} D \frac{\partial^2 C(x,t)}{\partial x^2}$

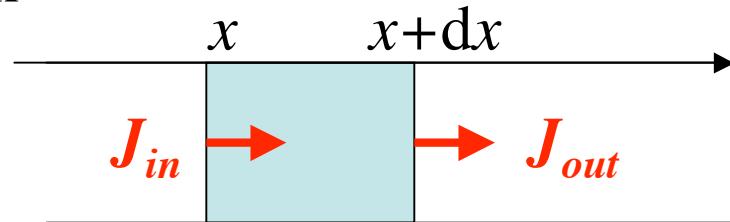
Continuity equation should be well known

$$\frac{\partial C}{\partial t} = -\nabla J$$

One dimensional $\frac{\partial C(x,t)}{\partial t} = -\frac{\partial J(x,t)}{\partial x}$

J : flux
 C : concentration
 t : time

Derivation



$$(J_{in} - J_{out})A = A \cdot dx \cdot \dot{C}$$

$$-(J_{out} - J_{in}) = dx \cdot \frac{\partial C}{\partial t}$$

$$\frac{\partial C}{\partial t} = -\frac{(J_{out} - J_{in})}{dx}$$

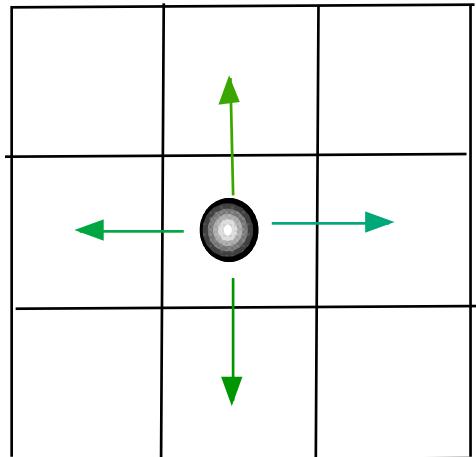
$$\Rightarrow -\frac{(J(x + dx) - J(x))}{dx} \underset{dx \rightarrow 0}{=} \boxed{\frac{\partial J}{\partial x} = \frac{\partial C}{\partial t}}$$

qed

Diffusion in general microscopically

Random walk
Brownian motion

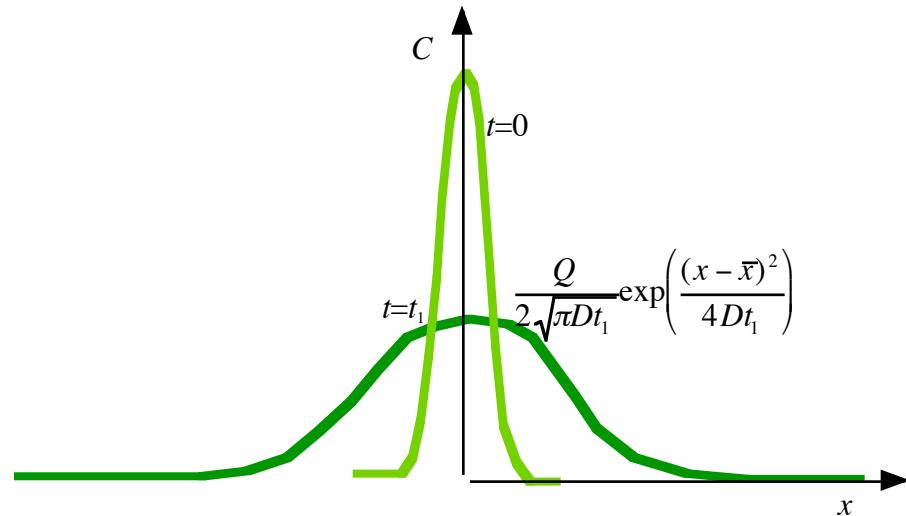
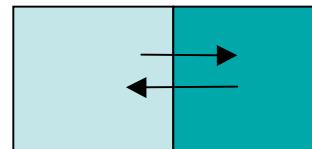
Microscopic lattice modelling



Comparison gives D

$$D = Z \frac{a^2 v}{6} \exp\left(-\frac{E_a}{kT}\right)$$

a : jump distance
 v : trial rate
 Z : geometry



Phenomenologically Ficks 1. og 2.

$$E_a = E_m + E_v \cdot \text{migr.} + \text{vac}$$

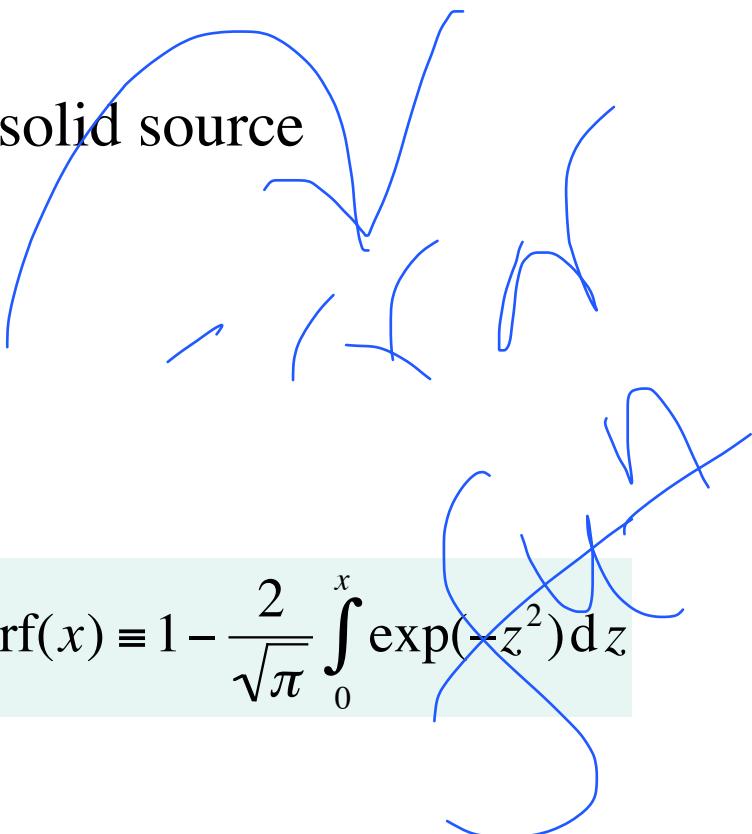
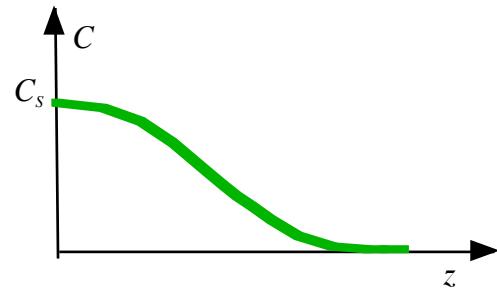
6: std for cubic

Analytic solution diffusion equation 1

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial z^2}$$

Boundary cond. - "predeposition" from gas or solid source

$$\begin{aligned}C(z,0) &= 0 \\C(0,t) &= C_s \\C(\infty,t) &= 0\end{aligned}$$



Solution

$$C(z,t) = C_s \operatorname{erfc}\left(\frac{z}{2\sqrt{Dt}}\right)$$

$$\operatorname{erfc}(x) \equiv 1 - \operatorname{erf}(x) \equiv 1 - \frac{2}{\sqrt{\pi}} \int_0^x \exp(-z^2) dz$$

Total amount $Q_T = \frac{2}{\sqrt{\pi}} C_s \sqrt{Dt} \quad t > 0$

Analytic solution diffusion equation 2

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial z^2}$$

Boundary cond. - "drive - in"

$$C(z,0) = 0, z \neq 0 \quad \delta \text{ on surface}$$

$$\frac{\partial C(0,t)}{\partial z} = 0 \quad \text{no flux}$$

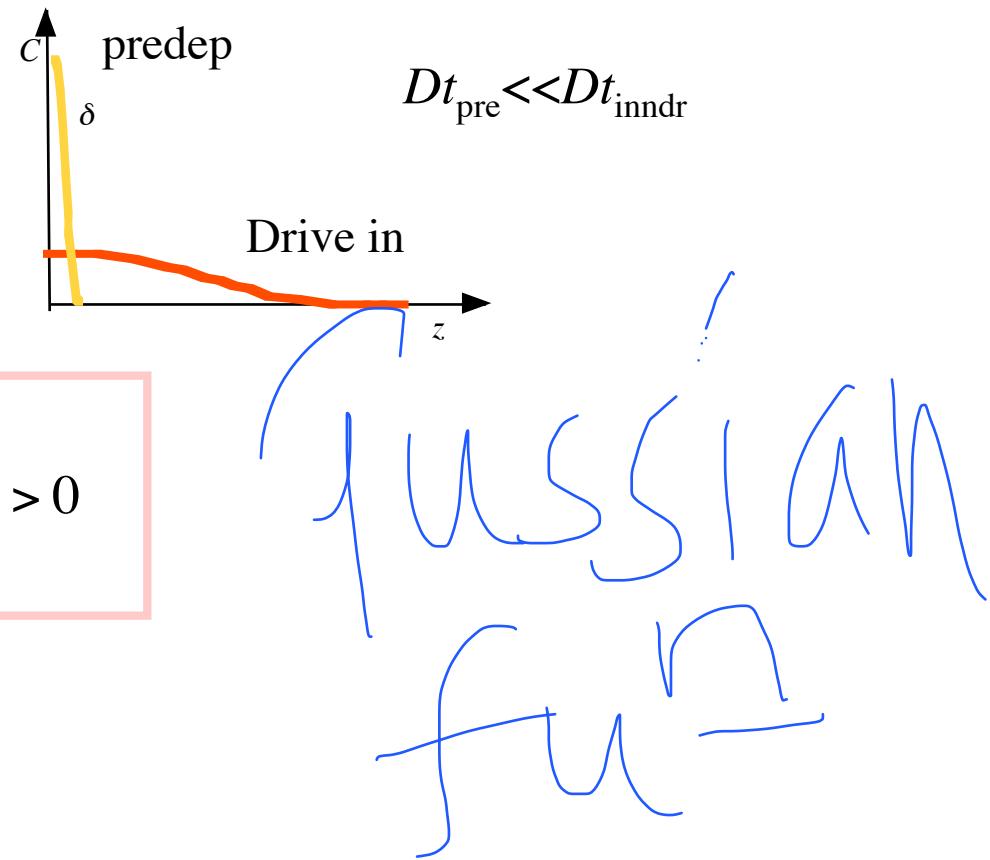
$$C(\infty, t) = 0$$

$$\int_0^\infty C dz = Q_T = \text{konst}$$

Solution

$$C(z,t) = \frac{Q_T}{\sqrt{\pi D t}} \exp\left(-\frac{z^2}{4 D t}\right) \quad t > 0$$

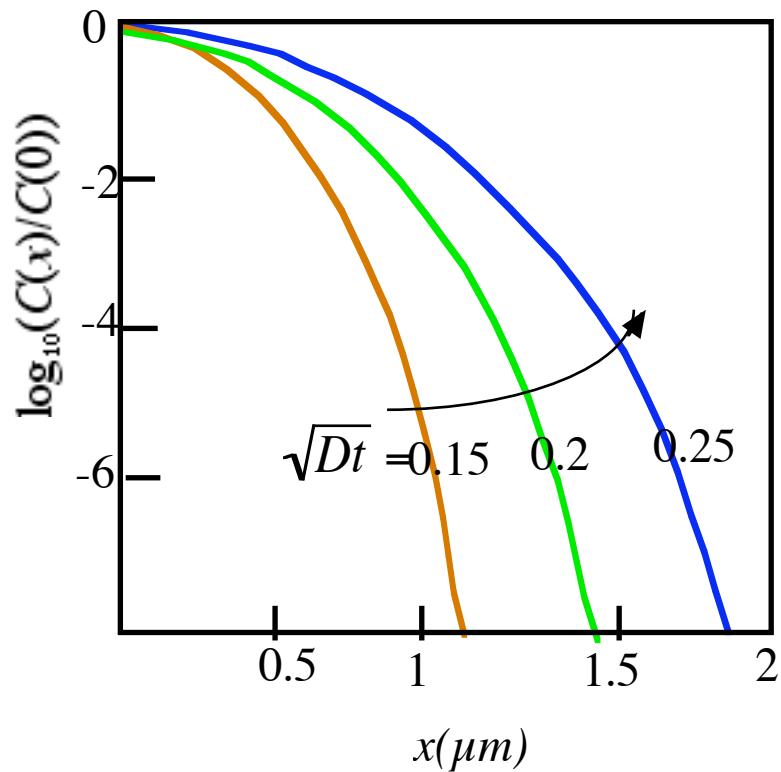
$$C_s(t) = C(0,t) = \frac{Q_T}{\sqrt{\pi D t}}$$



Curve shape for idealized case

INTRINSIC Diffusion

Pre deposition



Drive in

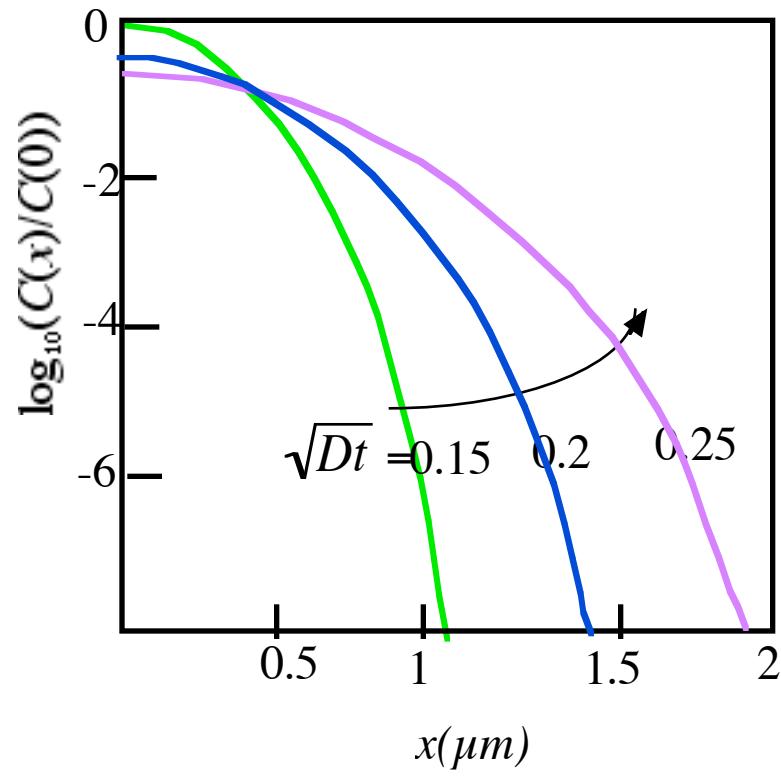
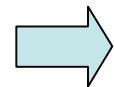


Fig. 3-7 a b, Cambell

Electric field assisted diffusion - doping

$$\frac{\partial C}{\partial z} \neq 0$$



$$\mathcal{E} \neq 0$$

Elec field

$$\begin{aligned}\text{Flux } J &= -D \frac{\partial C}{\partial z} + \mu^* C \mathcal{E} \\ &= -D(1 + \eta) \frac{\partial C}{\partial z}\end{aligned}$$

$$\eta = 0..1$$

$$C \approx n$$

$$n \propto \exp\left(-\frac{E_c - E_F}{kT}\right)$$

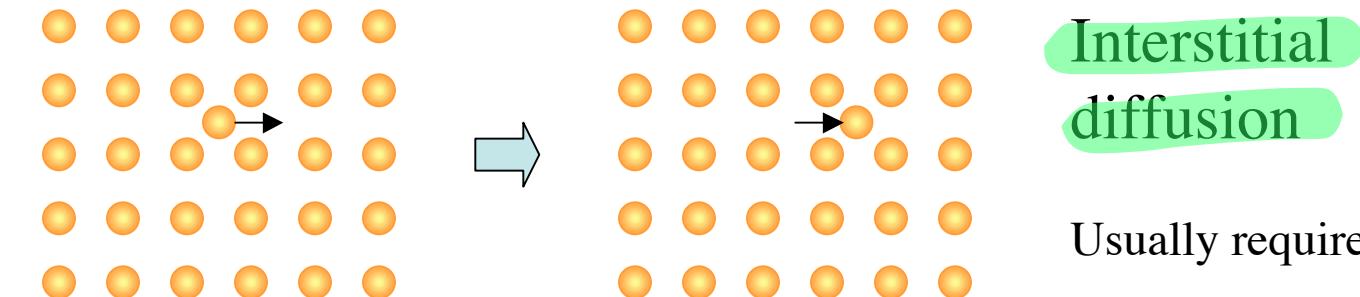
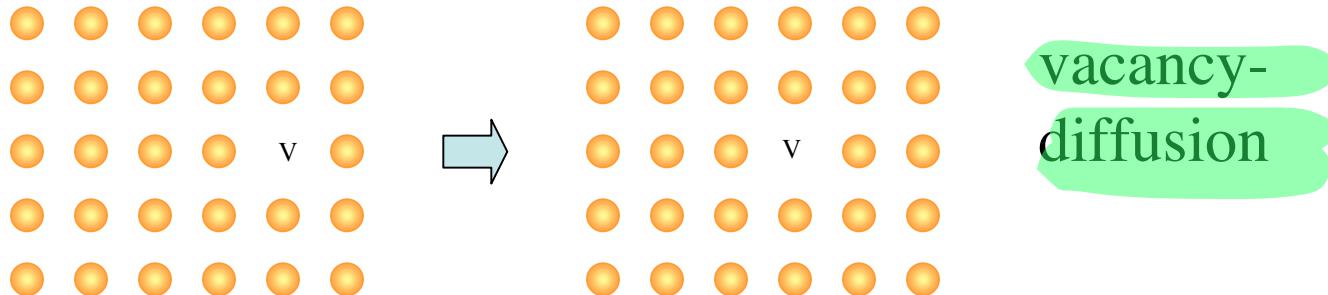
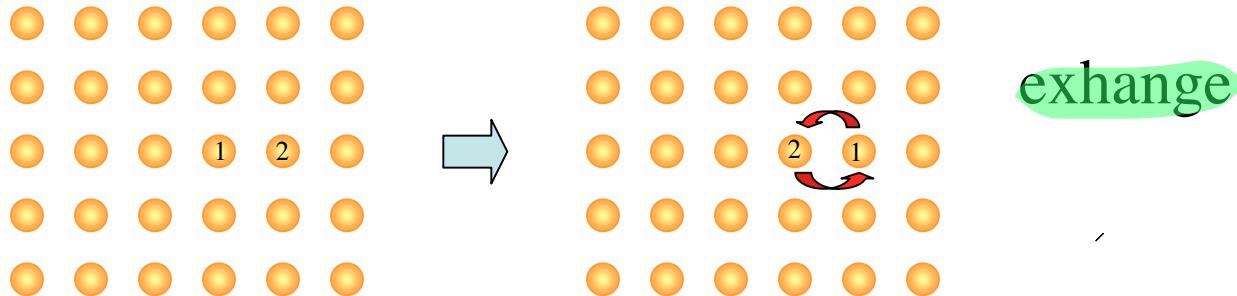
$$\frac{dE_F}{dz} = 0 !!$$



$$\frac{dE_c}{dz} \neq 0$$

$$\mathcal{E} \propto \frac{\partial E_c}{\partial z}$$

Atomic diffusion -self diffusion



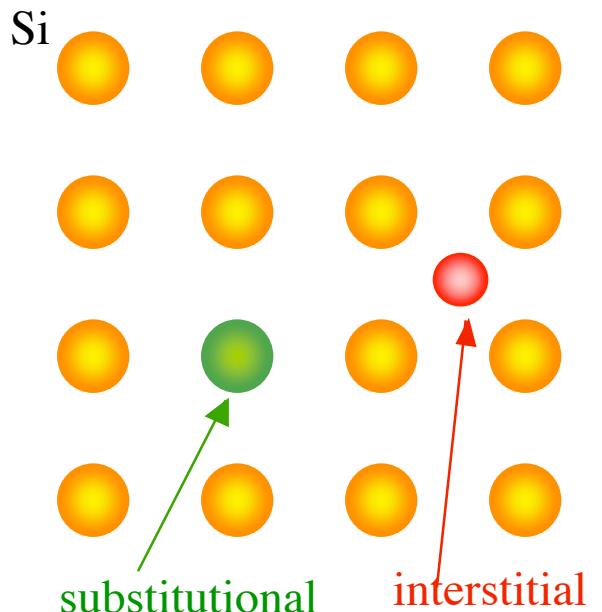
Usually requires little energy

Interstitials can knock
out regular atoms -
interstitialcy

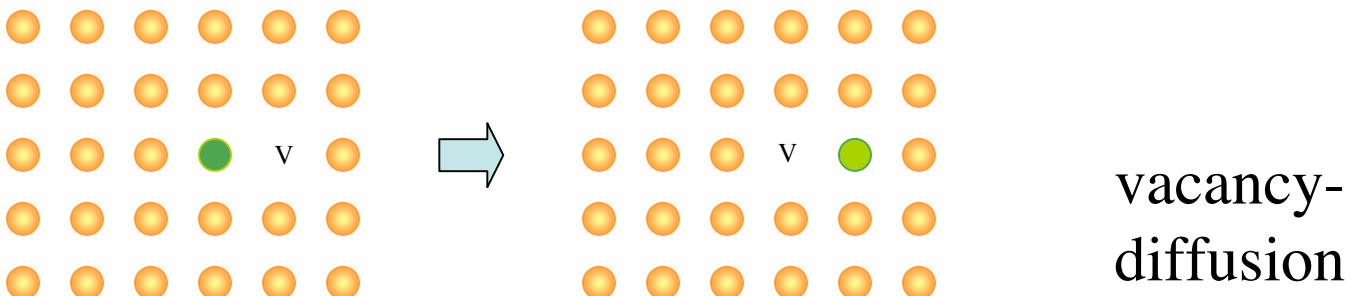
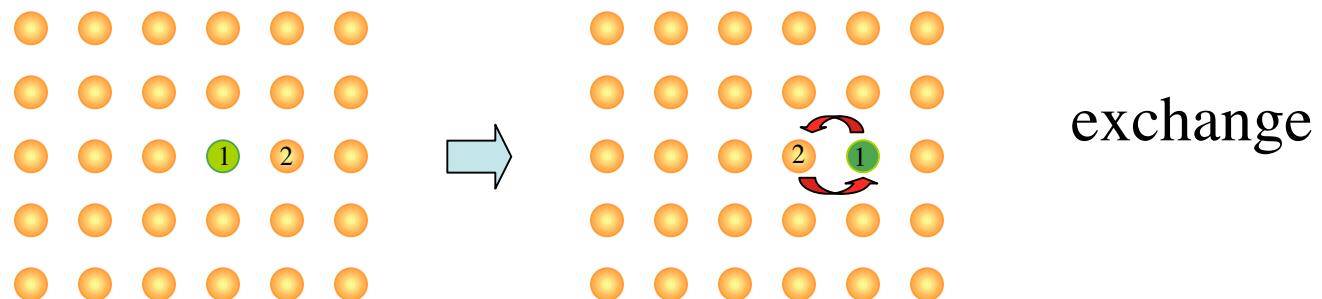
Atomic diffusion

Int	O, Fe, Cu, Ni, Zn
Sub	P, B, As, Al, Ga, Sb, Ge

Interstitials can move from on interstitial position to the next-
Interstitial diff. Usually requires little energy



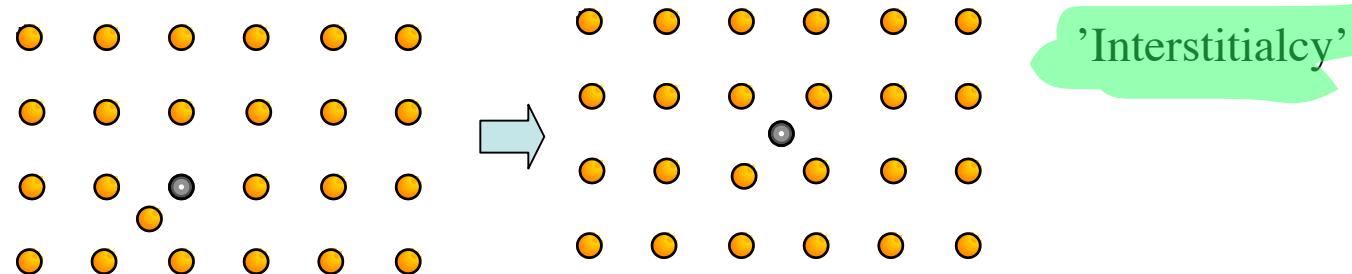
Substitutionals may move in various ways



Atomic diffusion

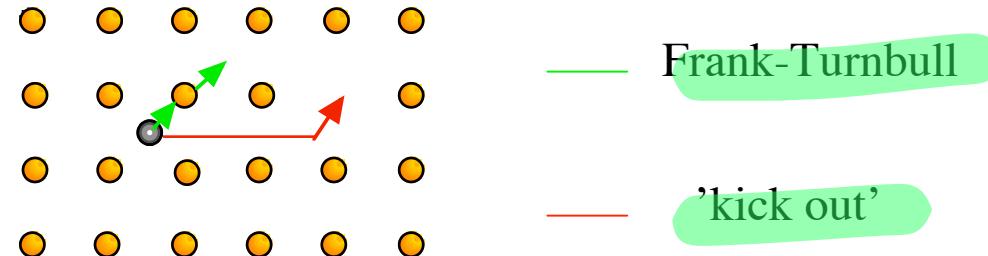
Various diffusion mechanisms for doping atoms

Fig 3.5



B and P may diffuse this way -also depends whether have Si(I) or V

Fig 3.6

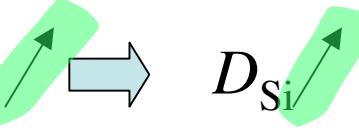


Atomic diffusion

Si self diffusion - guess vacancy diffusion

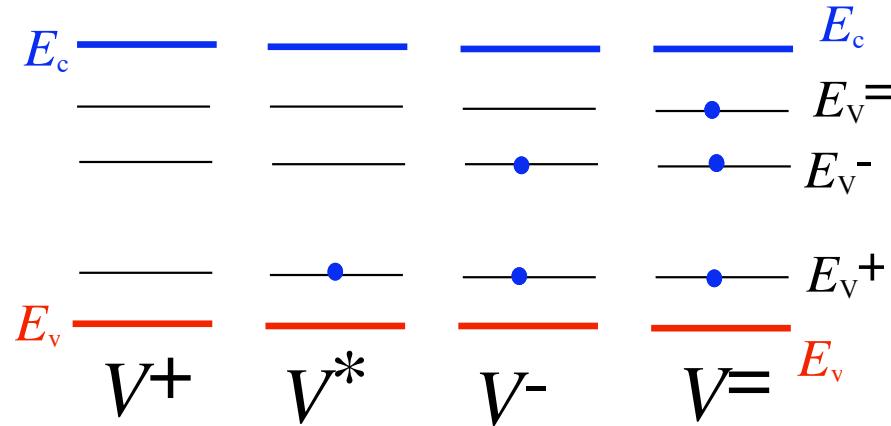
Can be measured by labeling the Si atoms by radioactive Si*

Assume D_{Si} can be
measured
Finds:

P conc.  D_{Si}  dependant on the doping density

Why?

Atomic diffusion Vacancy diffusion



Vacancy concentration depends on doping concentration

Probability for jump via vacancy depends on vacancy concentration

i.e. Diffusivity D depends on doping concentration

$$D = D_i^* + D_i^+ \left(\frac{p}{n_i} \right) + D_i^- \left(\frac{n}{n_i} \right) + D_i^= \left(\frac{n}{n_i} \right)^2$$

D_i^y : diffusivity
of Si by vac.
w. charge y

atomistic diffusion consequences

For dopant atoms

$$n=n(C) \quad n: \text{electron concentration}$$

$$p=p(C) \quad C: \text{doping concentration}$$

i.e.

$$D=D(C) \text{ and } C=C(x)$$

ie **EXTRINSIC DIFFUSION**

Diffusion equation $\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right)$ Must be solved numerically

Diffusion, atomistic model consequences

Assume can measure D

How?

From

$$D = D_i^* + D_i^+ \left(\frac{p}{n_i} \right) + D_i^- \left(\frac{n}{n_i} \right) + D_i^= \left(\frac{n}{n_i} \right)^2$$

Measure D vs. n the we can determine D^* , D^- and $D^=$

Fit to $D^y = D_0^y \exp\left(-\frac{E_a^y}{kT}\right)$ $y:$ charge $*, -, +, =$

Diffusion, atomistic model consequences

Assume D can be measured, How?

From

$$D = D_i^* + D_i^+ \left(\frac{p}{n_i} \right) + D_i^- \left(\frac{n}{n_i} \right) + D_i^= \left(\frac{n}{n_i} \right)^2$$

With measurements of D vs. n you can determine D^* , D^- , $D^=$

Fit to

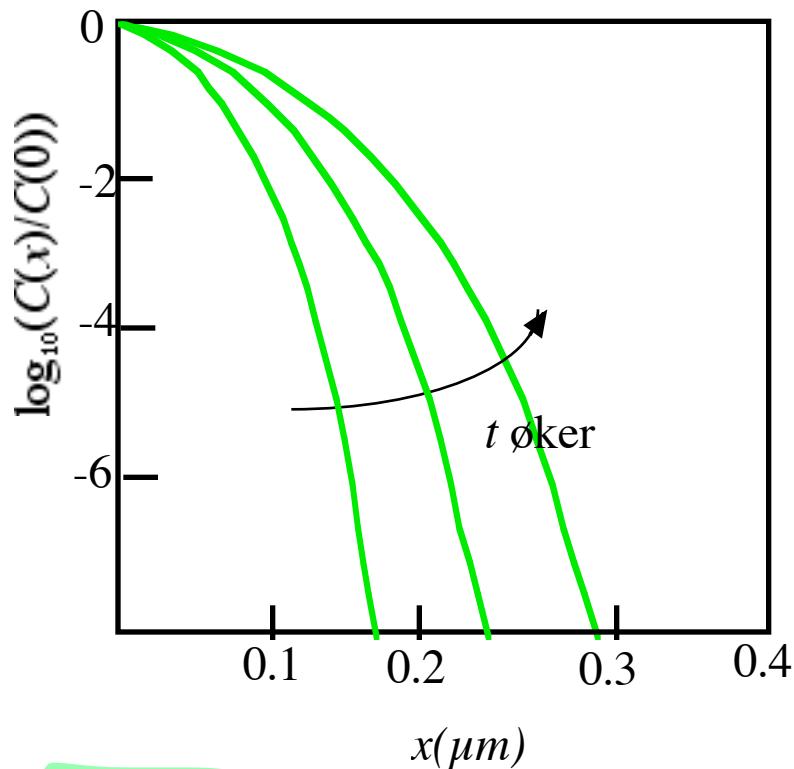
$$D^y = D_0^y \exp\left(-\frac{E_a^y}{kT}\right) \quad y: \text{charge state } *, -, +, =$$

Measured

Atom	Do+	Ea+	Do*	Ea*	Do-	Ea-	Do=	Ea=
As			7e-3	3.44	12	4.05		
P			3.9	3.66	4.4	4	44	4.4
B	0.41	3.46	4e-2	3.46				

Diffusion, typical profiles

Fig 3.8 B high conc.

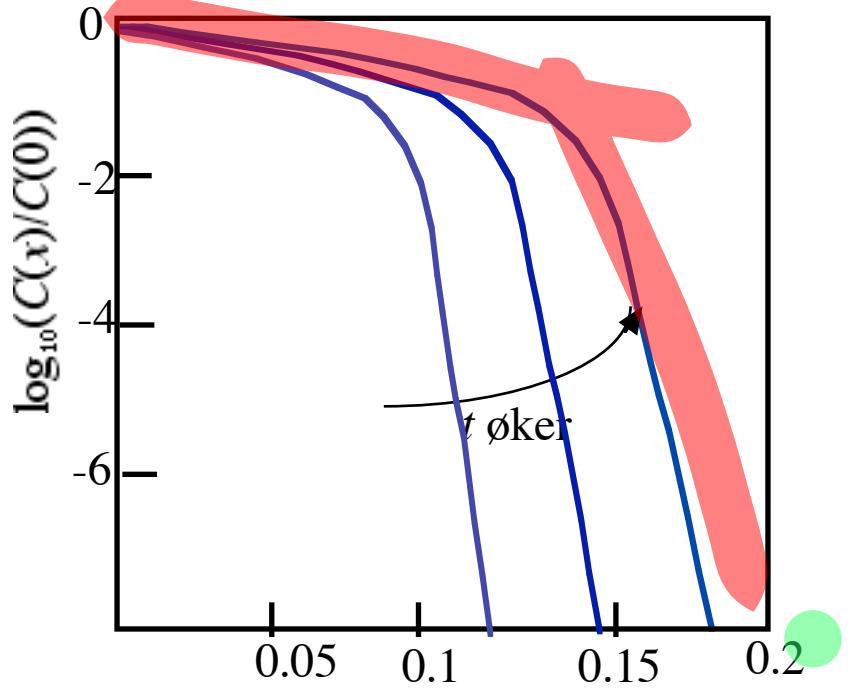


B acceptor

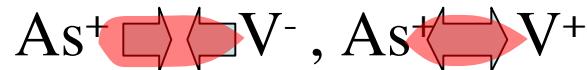


$$D_B = \left(D^* + D^+ \frac{p}{n_i} \right) \cdot h$$

Fig 3.9 As high conc.



As donor, As^+



$$D_{As} = \left(D^* + D^- \frac{n}{n_i} \right) \cdot h$$

$n \gg n_i : h=2,$

$$D_{As} \approx 2 \frac{n}{n_i} D^-$$

Diffusion, High doping effects

Dislocations

Band gap shrinkage

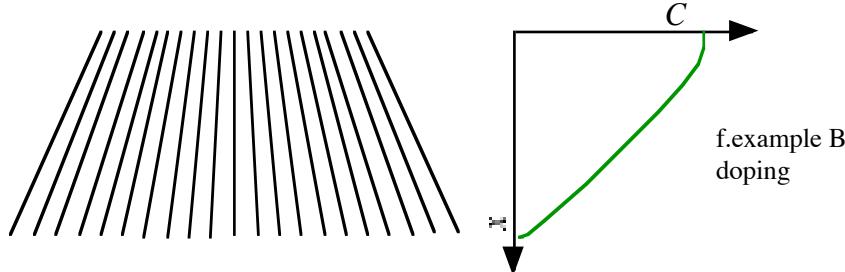
Cluster formation

Segregation

Diffusion, High doping effects

Dislocations

Stress-no disloc.



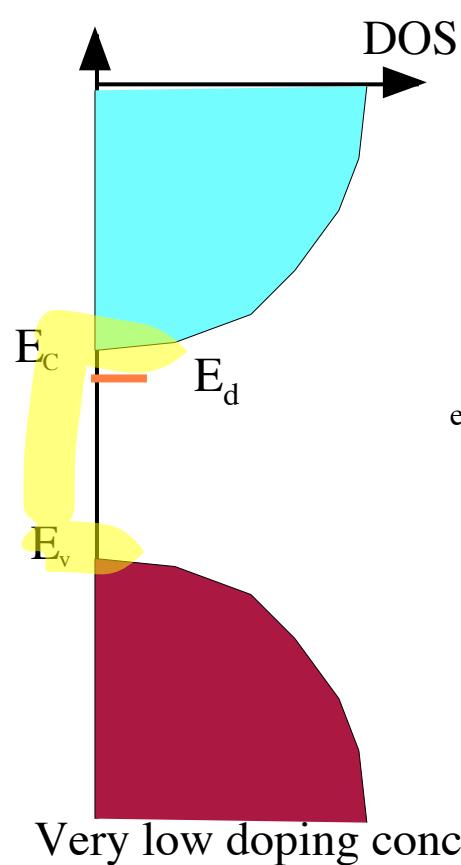
Disadvantage for stress in membranes for MEMS, ie for pressure sensors

Elastic energy released by creating a dislocation

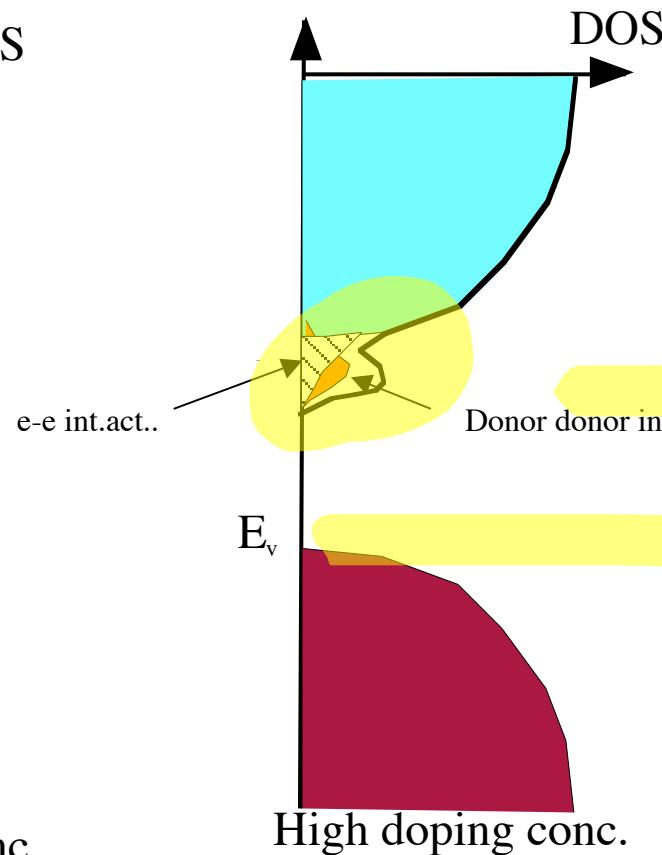
Stress in heavy B doping of Si tried compensated by adding Ge

Diffusion, High doping effects

Band-gap narrowing



Very low doping conc.

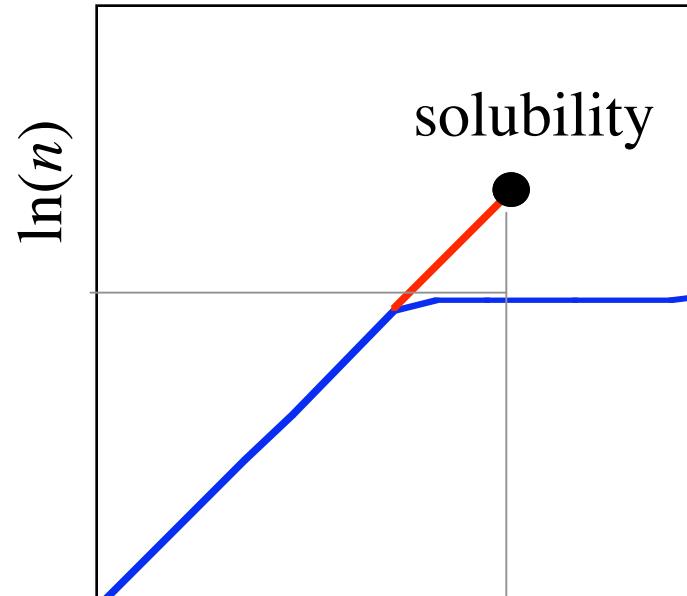


High doping conc.

E_g varies
 n_i varies
[V] varies.

Diffusion, High doping effects

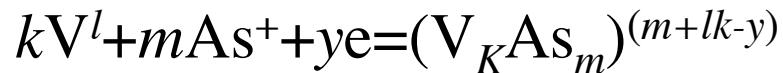
Cluster formation



Complexes/clusters

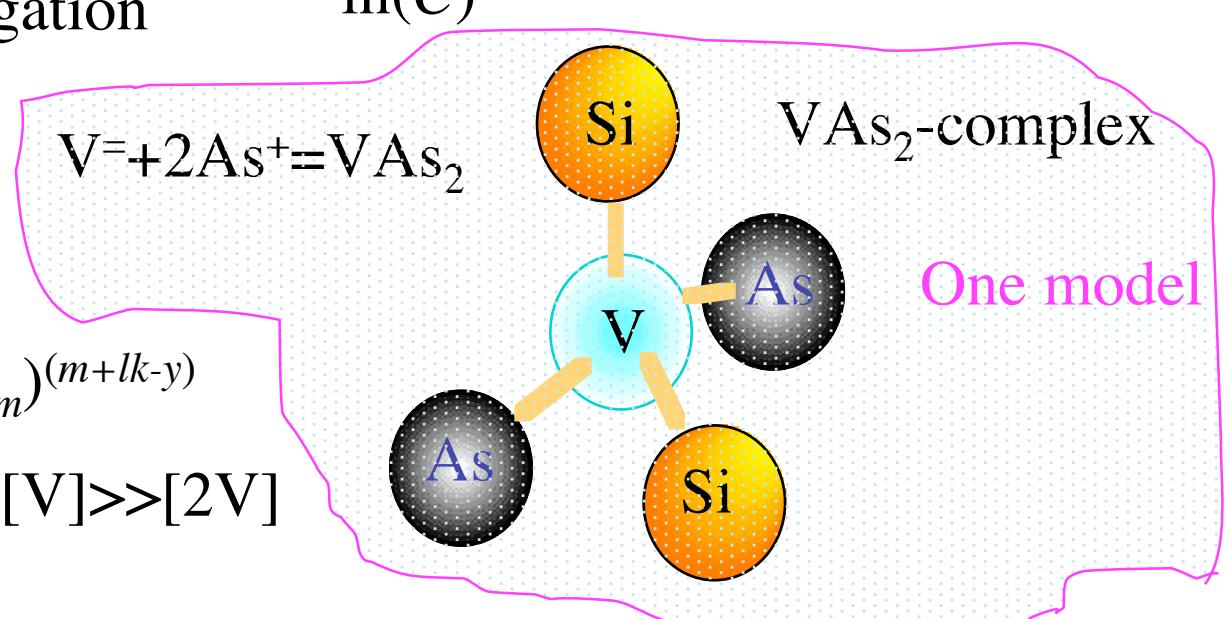
Maybe precursor to segregation

Various reactions



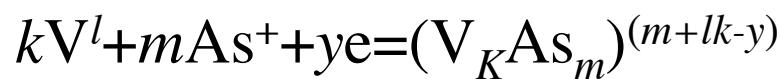
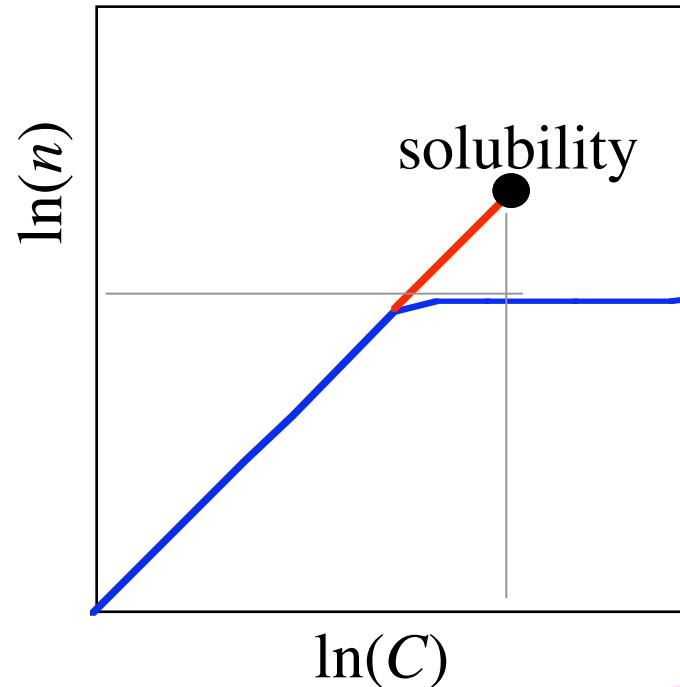
Complex neutral, el.neg, $[V] \gg [2V]$

Gives $k=1$ and $m=1,2,4$



Diffusion, High doping effects

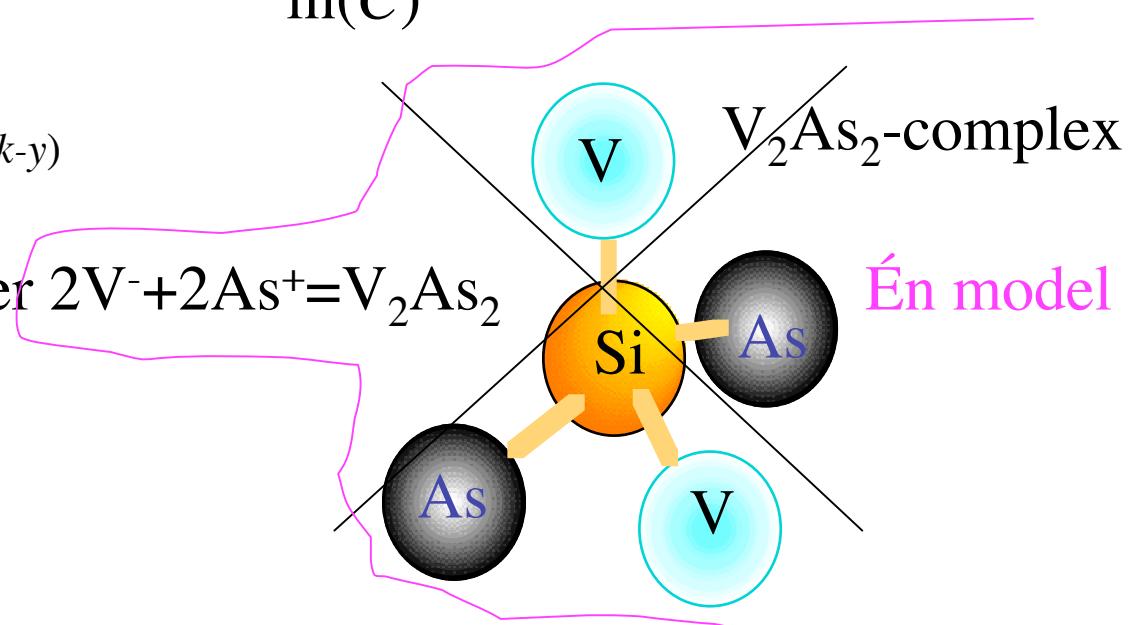
Cluster formation



How to find out about cluster $2V^- + 2As^+ = V_2As_2$ models.?

V_2As_2 -complex

Én model

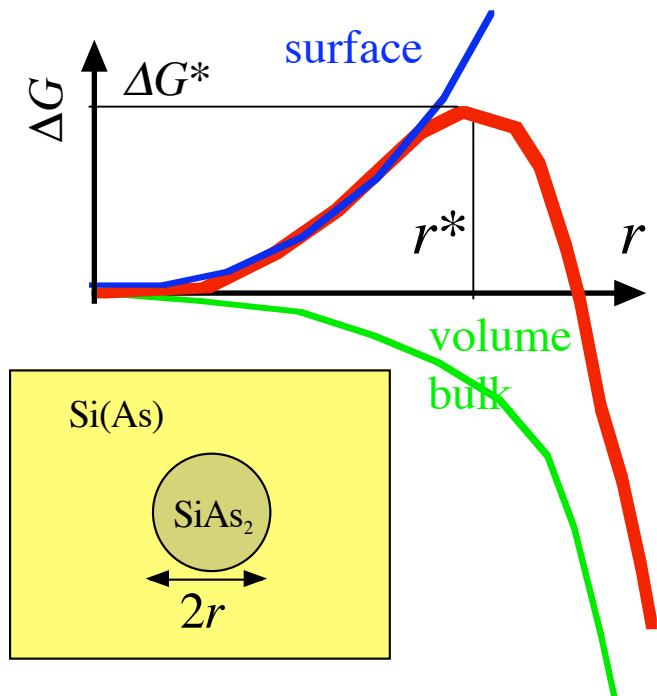


Diffusion, High doping effects

Segregation

Requires nucleation of new phase,

i.e. the concentration must correspond to super saturation before precipitation occurs. The density of precipitates depends upon nucleation rate and upon diffusion. It means measurements of solubility can require patience particularly at low temperatures.



Diffusion, Numerical calculation considerations

Solving the diffusion equations (by simulations)

General methods

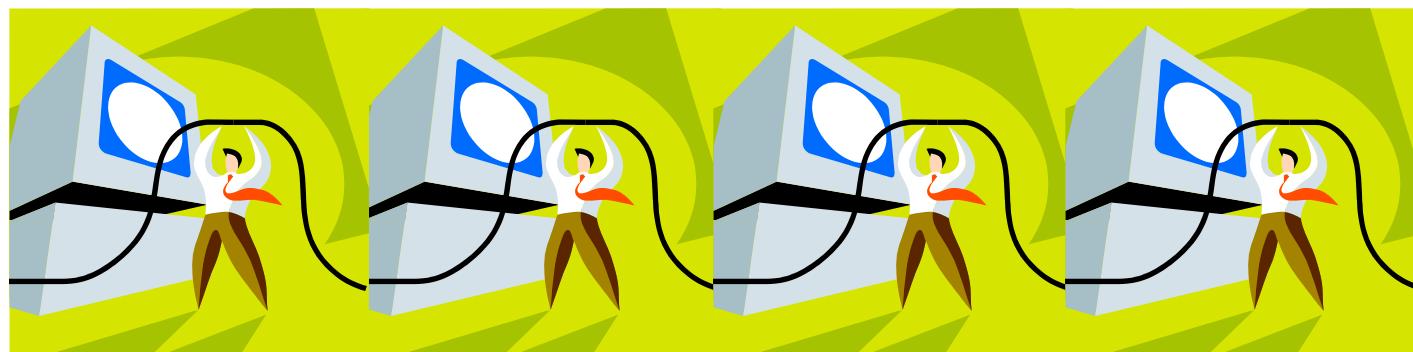
→ Finite differencing

Finite element

Monte Carlo

Spectral

Variational



Diffusion, numeric 'finite difference'



Representations of time and space differentials

$$x_j = x_0 + j\Delta x$$

$$t_n = t_0 + n\Delta t$$



$$\frac{\partial u}{\partial t} \Big|_{j,n} = \frac{u_j^{n+1} - u_j^n}{\Delta t} + O(\Delta t)$$

Forward Euler differentiation,
Accuracy to 1ste order Δt



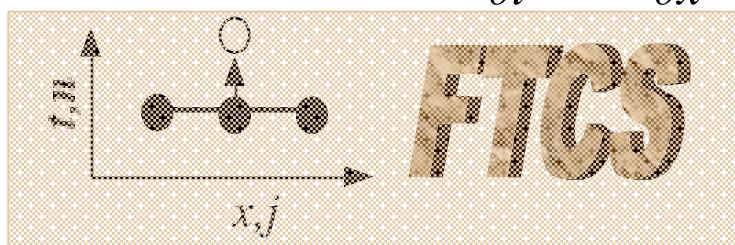
$$\frac{\partial u}{\partial x} \Big|_{j,n} = \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} + O(\Delta x^2)$$

Combining **a** and **b** give representation FTCS Forward Time Centered Space

example. diff.eq. $\frac{\partial u}{\partial t} = -v \frac{\partial u}{\partial x}$

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -v \left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} \right)$$

NB Unstable*



FTCS explicit so U_j^{n+1} can be calculated for each j from known points

Stability achieved by

$$u_j^n \rightarrow \frac{1}{2} (u_{j+1}^n + u_{j-1}^n)$$

Stability just as much art as science

Diffusion, numeric 'finite difference'

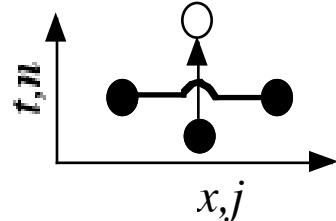


$$\frac{\partial C}{\partial t} = -\frac{\partial F(C)}{\partial x}$$

F: Flux
C: Flux

Leapfrog

$$\frac{C_j^{n+1} - C_j^{n-1}}{2\Delta t} = -\frac{F_{j+1}^n - F_{j-1}^n}{2\Delta x}$$



Here $\frac{\partial C}{\partial t}$
accuracy 2nd order in Δt

Diffusion equation in simple case

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

FTCS:
(explicitly)

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} = D \left(\frac{C_{j+1}^n - 2C_j^n + C_{j-1}^n}{\Delta x^2} \right)$$

Often stability means many time steps

Stab. criteria: $\frac{2D\Delta t}{\Delta x^2} \leq 1$

Diffusion, numeric 'finite difference'



(explicit)

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

FTCS:

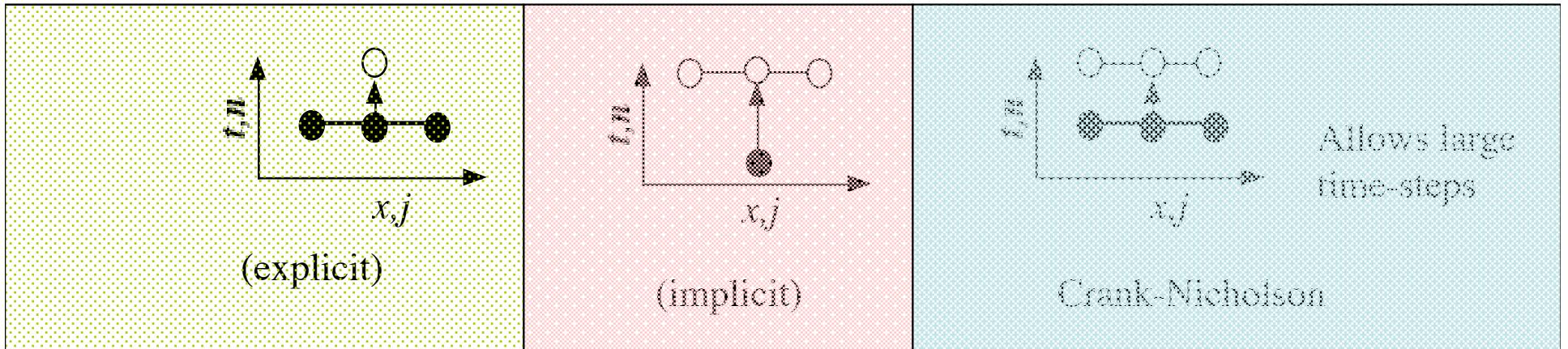
$$\frac{C_j^{n+1} - C_j^n}{\Delta t} = D \left(\frac{C_{j+1}^n - 2C_j^n + C_{j-1}^n}{\Delta x^2} \right)$$

(implicit) Backward time

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} = D \left(\frac{C_{j+1}^{n+1} - 2C_j^{n+1} + C_{j-1}^{n+1}}{\Delta x^2} \right)$$

Combining the two

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} = \frac{D}{2} \left(\frac{(C_{j+1}^{n+1} - 2C_j^{n+1} + C_{j-1}^{n+1}) + (C_{j+1}^n - 2C_j^n + C_{j-1}^n)}{\Delta x^2} \right) \quad \text{=Crank-Nicholson method}$$



Diffusion equation w. Crank -Nicholsen



$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} D \frac{\partial C}{\partial x}$$

$$\left. \frac{\partial C}{\partial t} \right|_{n,j}^{1st} = \frac{1}{2} \left(\left. \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right) \right|_{2nd}^{n,j} + \left. \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right) \right|_{2nd}^{n+1,j} \right)$$

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} = \frac{1}{2} \frac{1}{\Delta x^2} \left(D_{j+\frac{1}{2}}^n (C_{j+1}^n - C_j^n) - D_{j-\frac{1}{2}}^n (C_j^n - C_{j-1}^n) \right)$$

$$+ \left[D_{j+\frac{1}{2}}^{n+1} (C_{j+1}^{n+1} - C_j^{n+1}) - D_{j-\frac{1}{2}}^{n+1} (C_j^{n+1} - C_{j-1}^{n+1}) \right]$$

collect C_j^{n+1} left and C_j^n right

$$-\alpha_+^{n+1} C_{j+1}^{n+1} + (1 + \alpha_+^{n+1} + \alpha_-^{n+1}) C_j^{n+1} - \alpha_-^{n+1} C_{j-1}^{n+1} = \alpha_+^n C_{j+1}^n + (1 - \alpha_+^{n+1} - \alpha_-^{n+1}) C_j^n + \alpha_-^n C_{j-1}^n$$

ie

$$\overleftrightarrow{A} \bullet \vec{C}^{n+1} = \overleftrightarrow{B} \bullet \vec{C}^n$$

$$\alpha_+^n \equiv \frac{\Delta t}{2(\Delta x)^2} D_{j+\frac{1}{2}}^n$$

$$\alpha_-^n \equiv \frac{\Delta t}{2(\Delta x)^2} D_{j-\frac{1}{2}}^n$$

Diffusion equation w Crank -Nicholsen



$$\vec{A} \bullet \vec{C}^{n+1} = \vec{B} \bullet \vec{C}^n$$

A and B tridiagonal i.e.

$$B : 0 \quad 0 \cdots \quad \alpha_-^n \quad 1 - \alpha_+^n - \alpha_-^n \quad \alpha_+^n \quad 0 \cdots$$

A diagram consisting of two parallel vertical black brackets. Inside each bracket is a thick grey line that slopes upwards from left to right. The number '0' is positioned at the top right end of the upper line and at the bottom left end of the lower line.

$$A : 0 \quad \dots \quad -\alpha_-^{n+1} \quad 1 + \alpha_+^{n+1} + \alpha_-^{n+1} \quad -\alpha_+^{n+1} \quad 0 \dots$$

Boundary cond , $j=1$ i.e. surface

$$\frac{C_1^{n+1} - C_1^n}{\Delta t} = \frac{1}{2\Delta x^2} \left(D_{1+\frac{1}{2}}^n (C_2^n - RC_1^n) \right) + \frac{1}{2\Delta x^2} \left(D_{1+\frac{1}{2}}^{n+1} (C_2^{n+1} - RC_1^{n+1}) \right) \quad \begin{array}{l} R=1 \text{ reflection} \\ R=0 \text{ trapping} \\ R=0.5 \text{ segregation coeff} \end{array}$$

$$\text{ie. } 0 + (1 + R\alpha_+^{n+1})C_j^{n+1} + (-\alpha_+^{n+1})C_{j+1}^{n+1} = 0 + (1 - R\alpha_+^n)C_j^n + \alpha_+^n C_{j+1}^n$$

j=2

$$\frac{C_2^{n+1} - C_2^n}{\Delta t} = \frac{1}{2\Delta x^2} \left(D_{2-\frac{1}{2}}^n (C_2^n - RC_1^n) + D_{2+\frac{1}{2}}^n (C_3^n - C_2^n) \right) + \\ \frac{1}{2\Delta x^2} \left(D_{2-\frac{1}{2}}^{n+1} (C_2^{n+1} - RC_1^{n+1}) + D_{2+\frac{1}{2}}^{n+1} (C_3^{n+1} - C_2^{n+1}) \right)$$

ie.

$$C_{j-1}^{n+1}(-R\alpha_-^{n+1}) + (1 + \alpha_+^{n+1} + \alpha_-^{n+1})C_j^{n+1} + (-\alpha_+^{n+1})C_{j+1}^{n+1} = C_{j-1}^n(R\alpha_-^n) + (1 - \alpha_+^n - \alpha_-^n)C_j^n + \alpha_+^n C_{j+1}^n$$

Diffusion equation w Crank -Nicholsen



$$\vec{A} \bullet \vec{C}^{n+1} = \vec{B} \bullet \vec{C}^n$$

unknown known

$$\begin{bmatrix} 1 + Ra_+^{n+1} & -\alpha_+^{n+1} & 0 \\ -Ra_-^{n+1} & 1 + \alpha_+^{n+1} + \alpha_-^{n+1} & -\alpha_-^{n+1} \\ 0 & -\alpha_-^{n+1} & 1 + \alpha_+^{n+1} + \alpha_-^{n+1} \\ \vdots & \ddots & -\alpha_-^{n+1} \\ 0 & \ddots & 1 + \alpha_-^{n+1} \end{bmatrix} \begin{bmatrix} C_1^{n+1} \\ C_2^{n+1} \\ \vdots \\ \vdots \\ C_N^{n+1} \end{bmatrix} =$$

$$\begin{bmatrix} 1 - Ra_+^n & \alpha_+^n & 0 \\ Ra_-^n & 1 - \alpha_+^n + \alpha_-^n & \alpha_+^n \\ 0 & \alpha_-^n & 1 - \alpha_+^n - \alpha_-^n \\ \vdots & \ddots & \alpha_+^n \\ 0 & \ddots & 1 - \alpha_-^n \end{bmatrix} \begin{bmatrix} C_1^n \\ C_2^n \\ \vdots \\ \vdots \\ C_N^n \end{bmatrix}$$

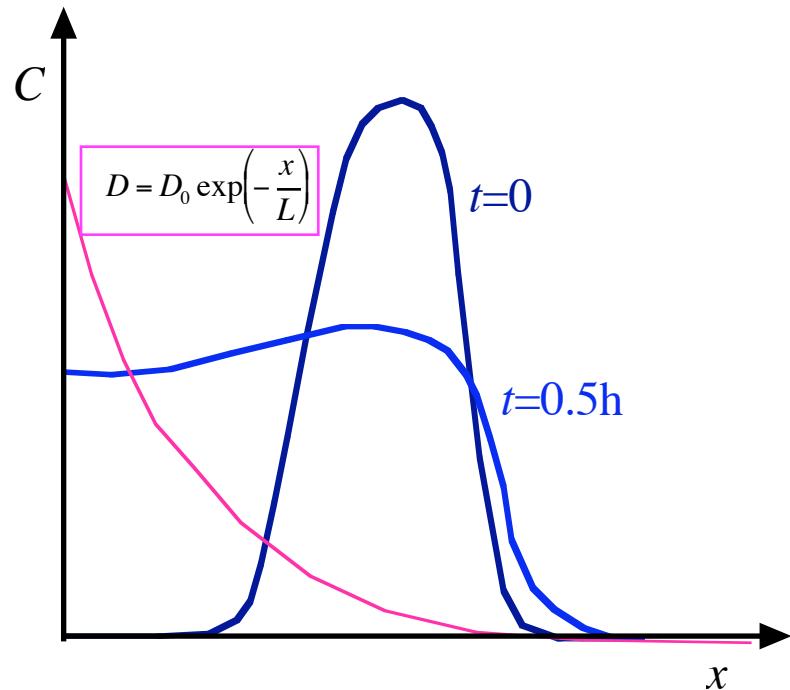
Can readily be solved when D only a function of x and t but not of C .

If $D=D(C)$ i.e. $\alpha^{n+1} = \alpha^{n+1}(C^{n+1})$ we have a nonlinear set of equations

Diffusion, numeric examples



schematic

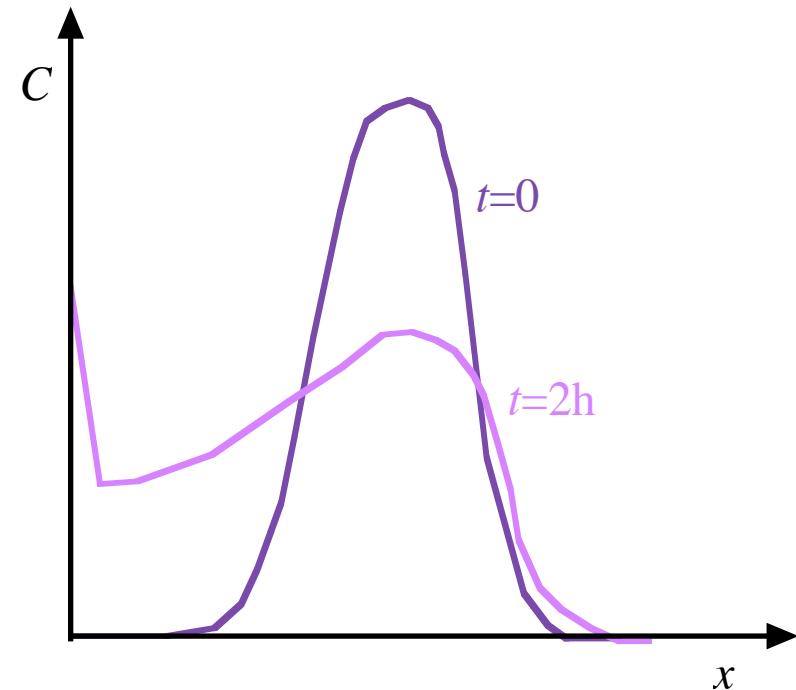


Implanted profile

Vacancy creation on surface

Vacancy annihilation in ion-damaged
region

Ge i Si



Implanted profile

Vacancy creation on surface

Vacancy annihilation in ion-damaged region

Surface segregation

$$\text{As i Si } D_{As} = (D^*(T) + D^-(T)C)(1 + \alpha \exp(-x/L))$$

Diffusion, numeric general



$$\begin{matrix} \vec{A} \bullet \vec{C}^{n+1} \\ \text{unknown} \end{matrix} = \begin{matrix} \vec{B} \bullet \vec{C}^n \\ \text{known} \end{matrix}$$

If $D=D(C)$ ie $\alpha^{n+1} = \alpha^{n+1}(C^{n+1})$

we have a nonlinear system of equations

But assume $\alpha^{n+1} \approx \alpha^{n+1}(C^n)$ as 1st approx. then calculate C^{n+1} , and put in A for next it.

$$C_j^{n+1} = C_j^n + B(C_j^{n+1}) \bullet C_j^{n+1} + S(C_1, C_2, \dots)$$

vector

matrix

Initial conditions

This equation is solved for example by Newton's method in the general case

Diffusion, numeric SOFTWARE PACKAGES



'curve-fitting' models / physical models

All processing stages/ all thermal/ just diffusion

Integrated, -masks, device, system-simulation (icecream silvaco)

1D, 2D,



SUPREM III (1D), SUPREM IV(2D) [Stanford]
TSUPREM4, SSUPREM4[Silvaco],
ATHENA[Silvaco]
ICECREAM, DIOS, STORM
Floops, Foods, ACES,

Diffusion, Measurements of diffusion profiles, $D(C)$

In many situations we have $C=C(x)$,

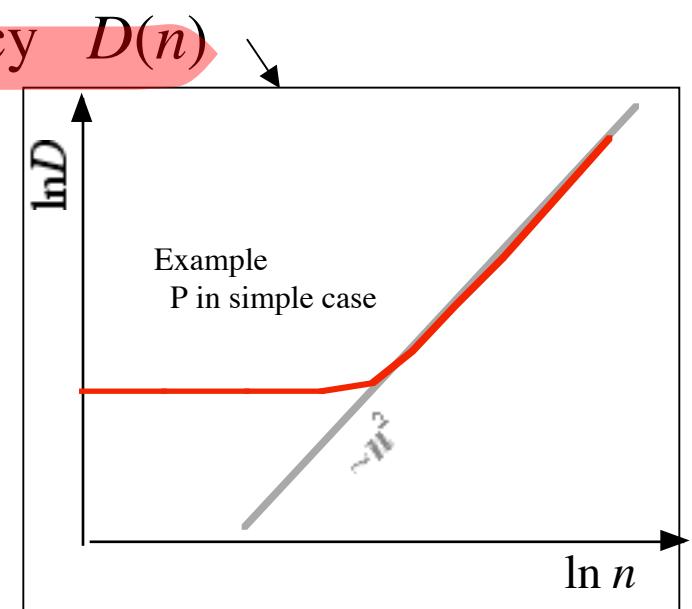
We can find $D(C)$ by measuring $C(x)$ at different T

Can find $D^*, D^+, D^-, D^=$ from the dependency $D(n)$

So measurement of C , and n el. P is needed

Methods for C
SIMS, TOFSIMS
Neutron activation
RBS, ESCA, EDAX
IR abs.

Methods for n
Spreading Resistance
Differential Hall
i.e., +strip
Capacitance, C-V
+ strip
SCM, SRM



Diffusion, Measurement of diffusion, process surveillance

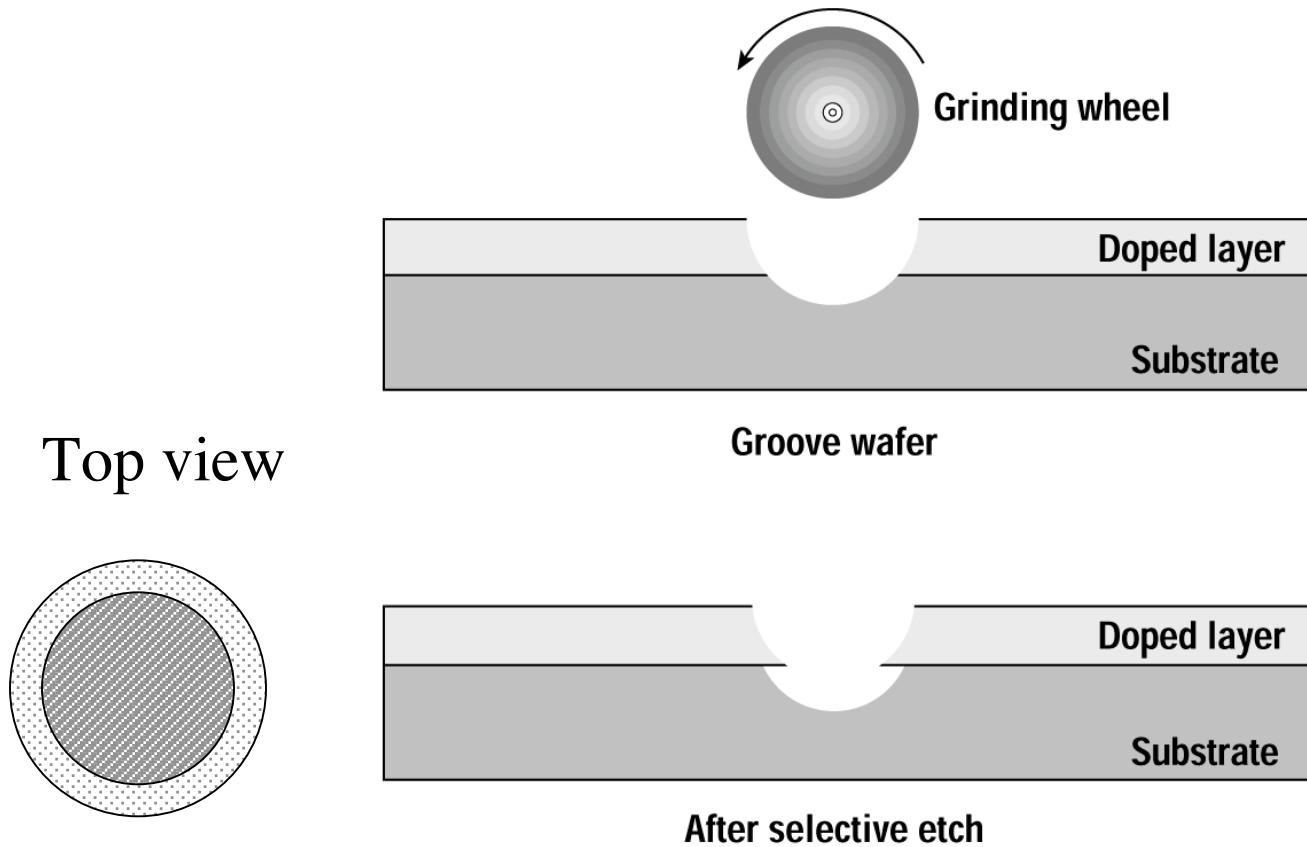
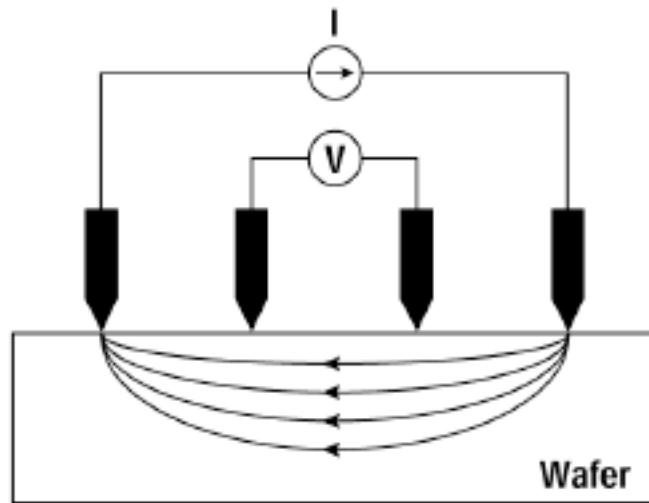


Figure 3.15 In junction staining, a cylinder is used to groove the wafer. A doping sensitive etch then removes part of the top layer. The junction depth can be found from the known diameter of the sphere and the measured width of the lower abraded groove.

Diffusion, Measurement of diffusion, process surveillance

'Four-point probe'

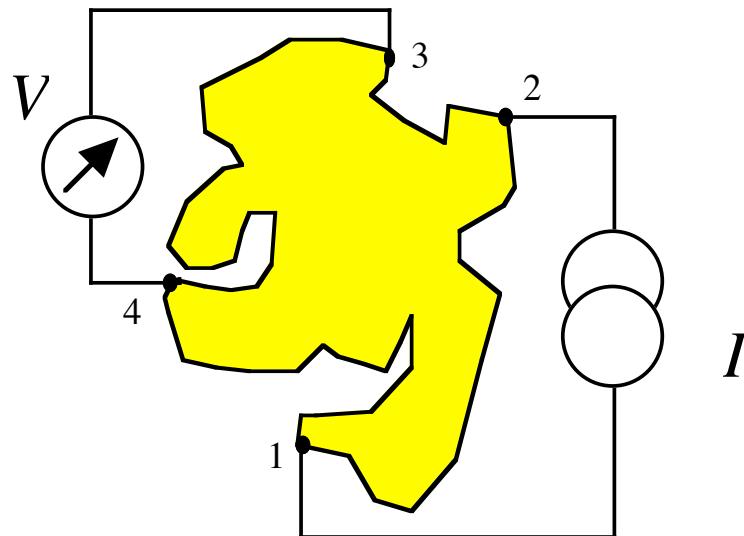


Measures so-called sheet resistance

Can find resistivity if the depth distribution of n and μ is found

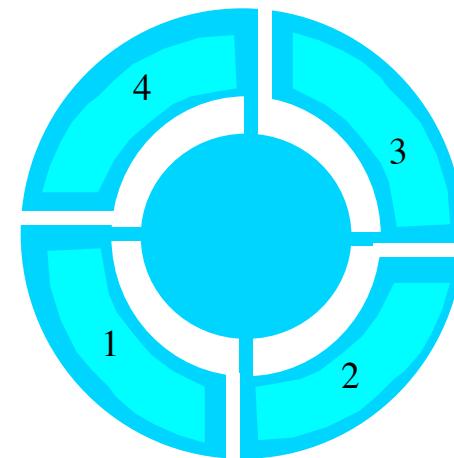
Mostly for process surveillance-reproducibility tests

Diffusion, Measurements of diffusion profiles



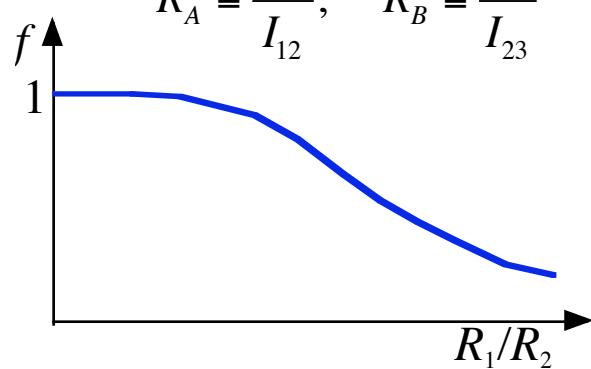
van der Peuw method

More common geometry



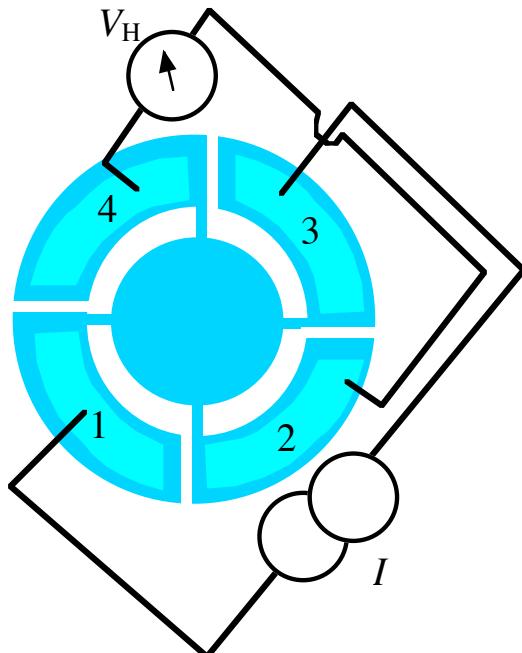
$$\rho_s = \frac{\pi}{2 \ln 2} (R_A + R_B) \cdot f(R_A / R_B)$$

$$R_A \equiv \frac{V_{34}}{I_{12}}, \quad R_B \equiv \frac{V_{41}}{I_{23}}$$



Diffusion, Measurement of electric profile

Hall measurements



$$R_{HS} = \frac{\int_0^d n(x)\mu^2(x)dx}{q\left(\int_0^d n(x)\mu(x)dx\right)^2}$$

$$\mu_H = \frac{R_{HS}}{\rho_s} = \frac{\int_0^d n(x)\mu^2(x)dx}{\int_0^d n(x)\mu(x)dx}$$

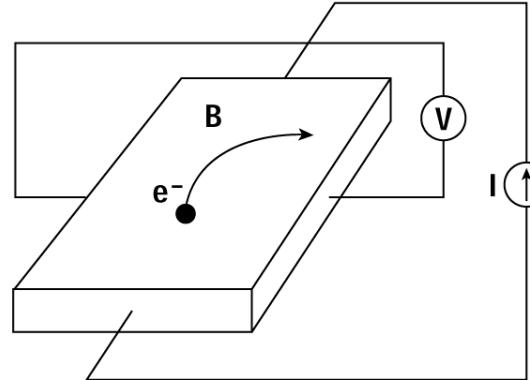
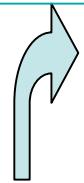


Figure 3.16 The Hall effect is able to simultaneously measure the carrier type, mobility, and sheet concentration.

Measurement-procedure



Measure ρ_s, R_{HS} gives μ_H
Strip a layer
Repeat to d

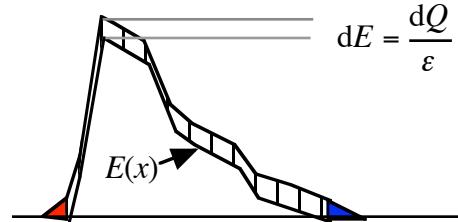
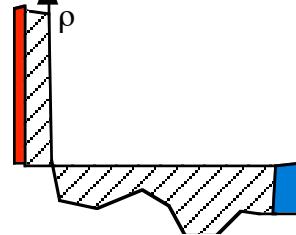
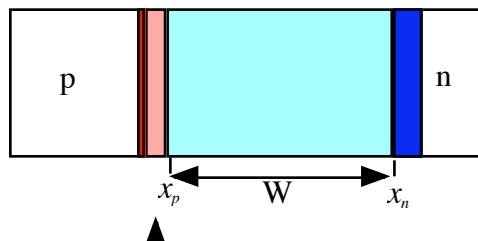
$$R_{HS} = \frac{V_H}{I} \frac{10^8}{B}$$

$$\rho_s = \frac{\pi}{2\ln 2} (R_A + R_B) \cdot f$$

Calc individual n and μ

$$\mu_i = \frac{\Delta(R_{HS}/\rho_s^2)_i}{\Delta(1/\rho_s)_i} \quad n_i = \frac{\Delta(1/R_s)_i}{qd_i\mu_i}$$

Diffusion, Measurement of electric profile



$$dV_{tot} = \int_{-x_p}^{x_n} \left(E(x) + \frac{dQ}{\epsilon} \right) dx - \int_{-x_p}^{x_n} E(x) dx + \delta$$

$$dV_{tot} = W \frac{dQ}{\epsilon} + \delta \quad W \frac{dQ}{\epsilon} \gg \delta$$

$$dV_{tot} \approx W \frac{dQ}{\epsilon}$$

$$C = \frac{dQ}{dV} = \frac{\epsilon}{W}$$

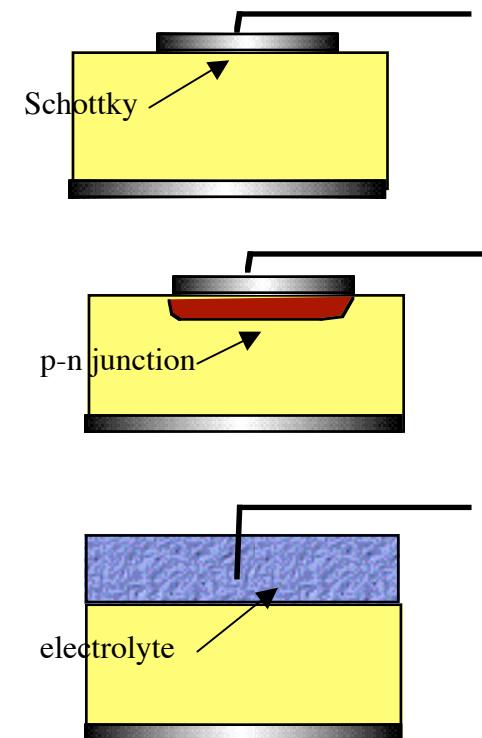
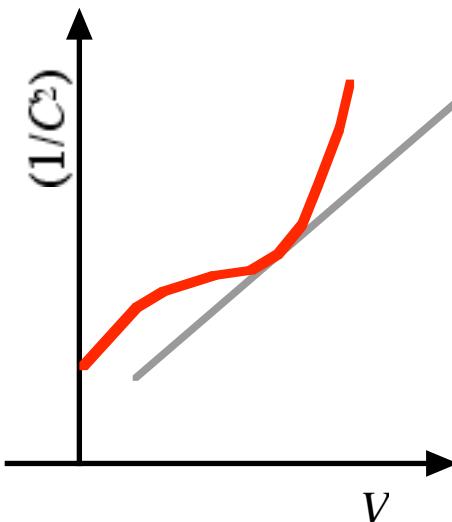
Capacitance voltage characteristic method

$$dQ = qN(W)dW$$

$$dV = dE \cdot W = \frac{dQ}{\epsilon} W = \frac{qN(W)WdW}{\epsilon} = \frac{qN(W)d(W^2)}{2\epsilon}$$

$$C = \frac{\epsilon}{W} \quad W^2 = \frac{\epsilon^2}{C^2} \quad d(W^2) = d(1/C^2)\epsilon^2$$

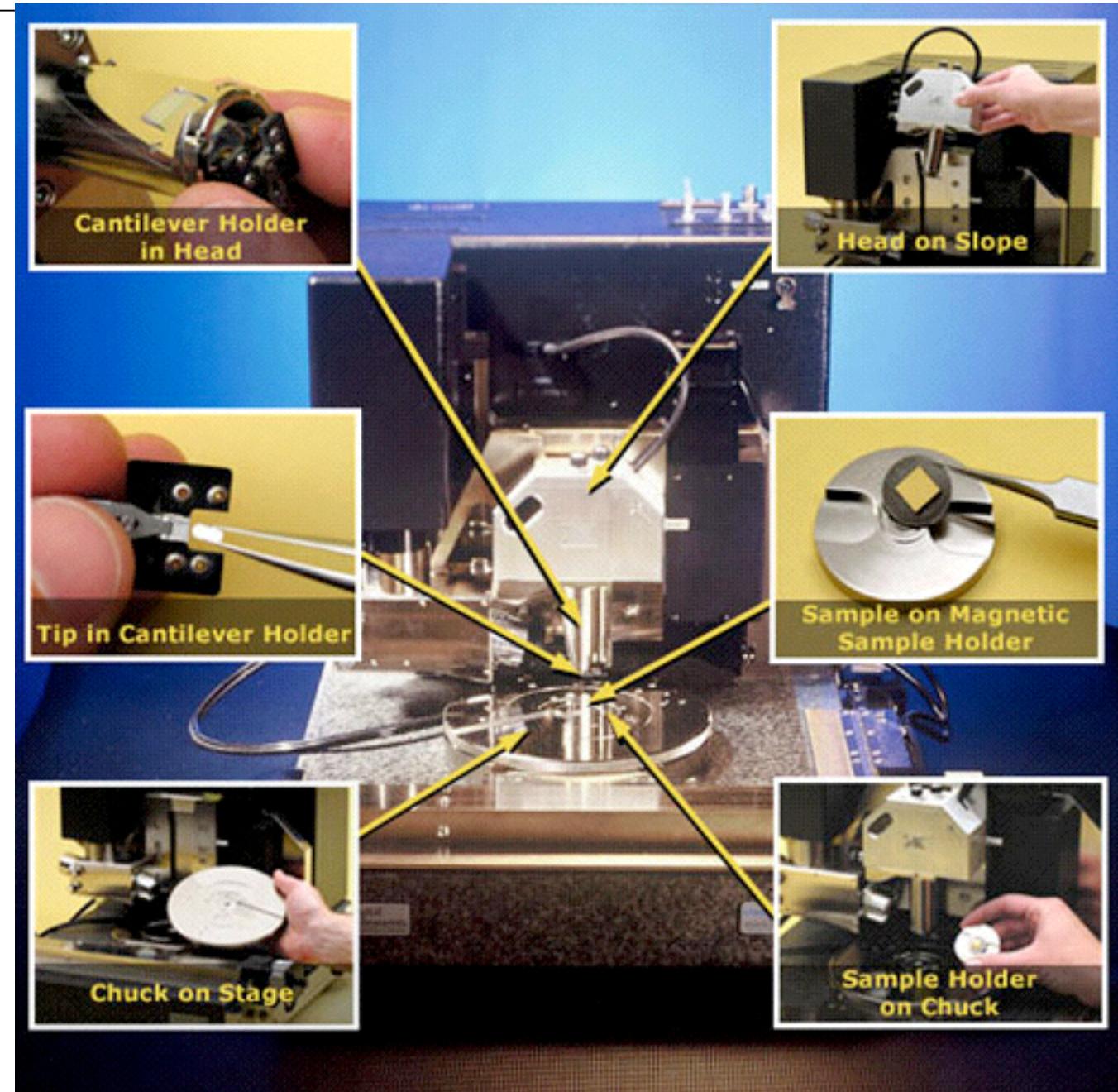
$$N(W) = \frac{2}{q\epsilon} \frac{dV}{d(1/C^2)} = \frac{2}{q\epsilon} \left(\frac{d(1/C^2)}{dV} \right)^{-1}$$



Diffusion, Measurement of diffusion profile

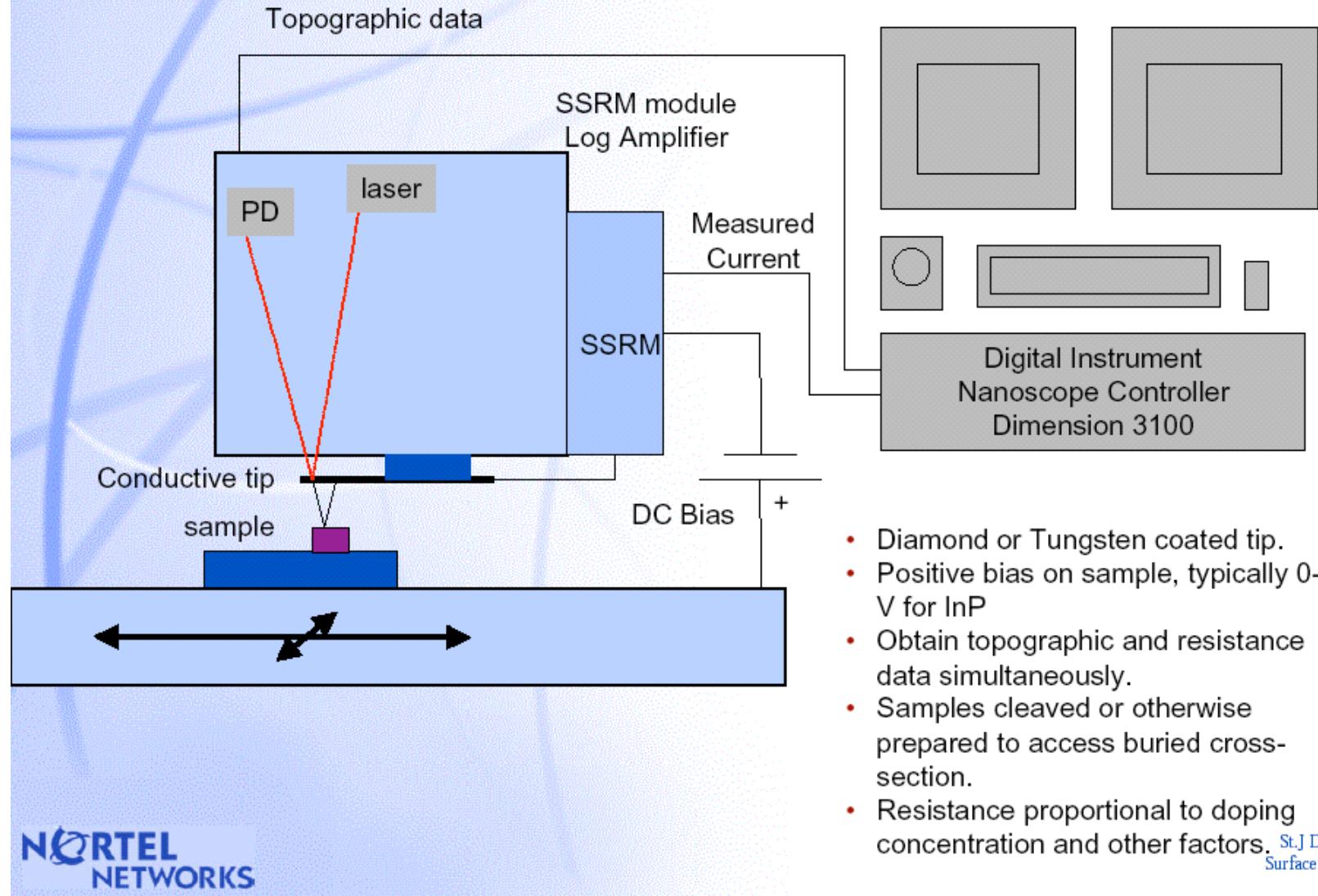
Scanning
Probe
Microscopy

SSRM
SCM



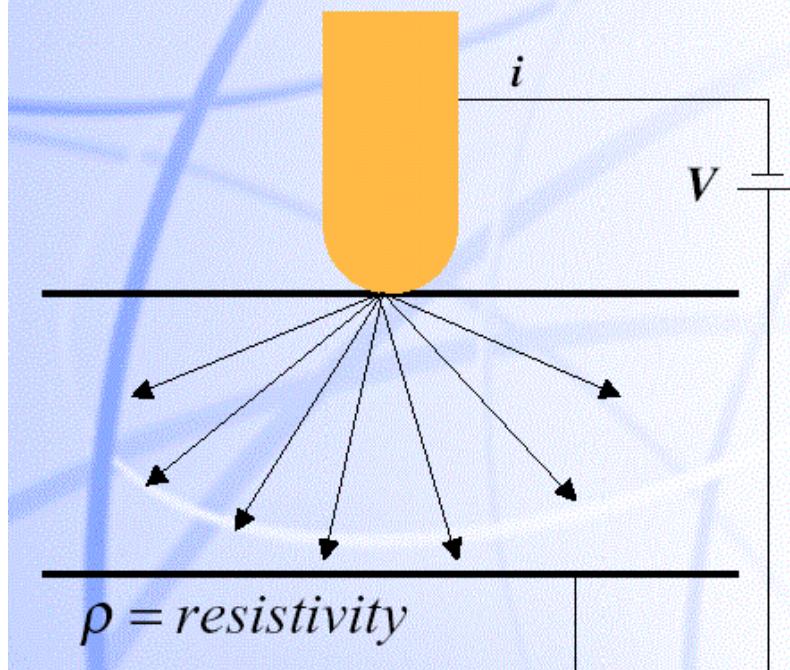
Diffusion, Measurement of diffusion profile

Scanning Spreading Resistance Microscopy



Diffusion, Measurement of diffusion profile

Simple SSRM Theory



$n = \text{carrier concentration}$

$\mu = \text{carrier mobility}$

- The resistance is proportional to thickness and inversely proportional to the cross-sectional area.

$$R \propto \frac{\rho l}{A}$$

- In SSRM the total resistance is dominated by the resistivity near the point contact.
- For an ideal semi-infinite uniformly doped sample the spreading resistance R of a non-penetrating ohmic contact of radius a is given by,

$$R = \frac{\rho}{4a} = \frac{1}{4\sigma a}$$

- Given that,

$$\sigma = ne\mu$$

- Hence assuming Ohm's Law,

$$i = \frac{V}{R} = 4V\sigma a = 4Vne\mu a \propto n\mu$$

- and the measured current is proportion to the *carrier concentration* and the *mobility*.
- But...real samples are not this simple. Require 3D finite element simulation to fully analyze.

Diffusion, Measurement of diffusion profile

Spreading resistance
measurements

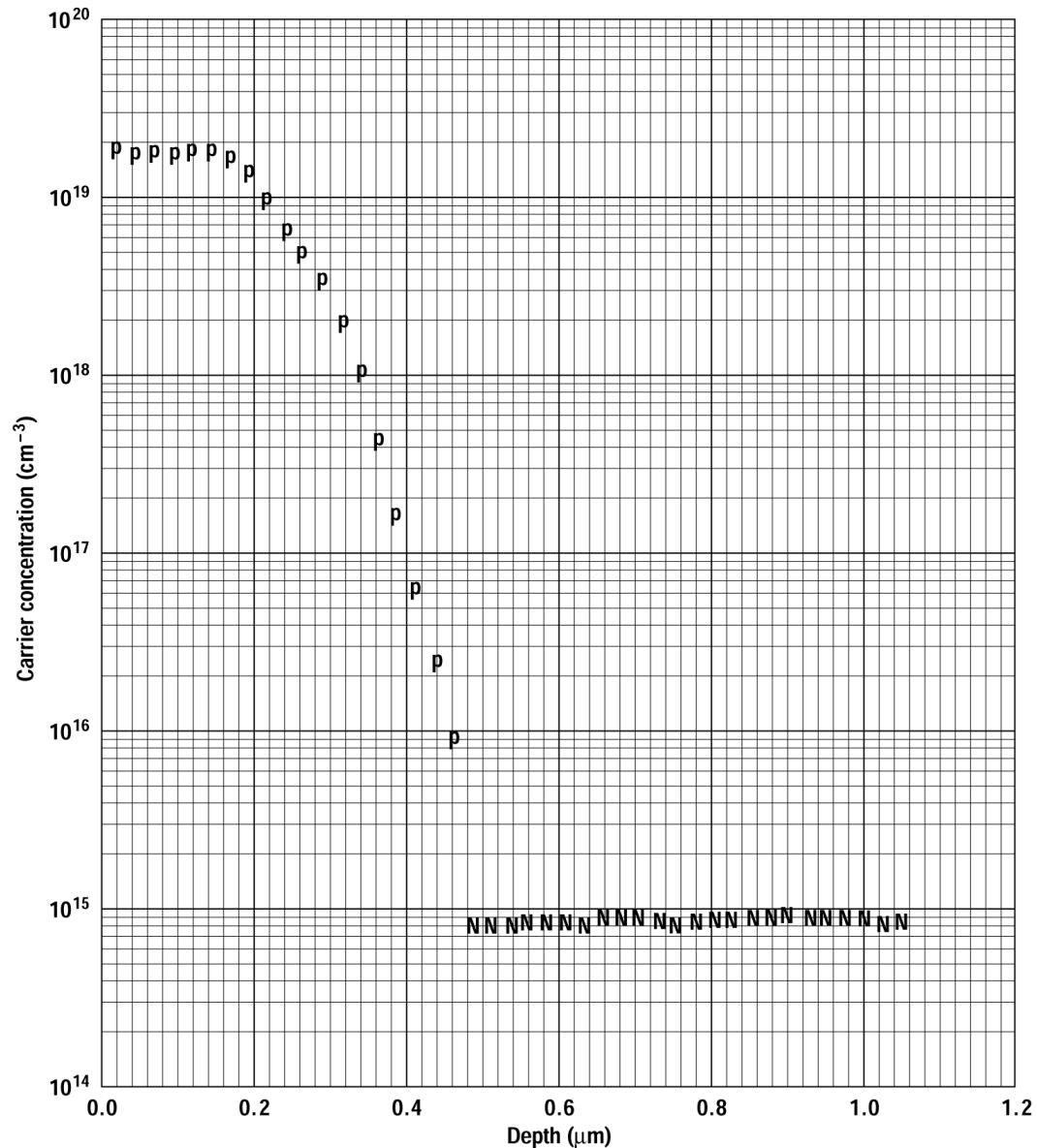
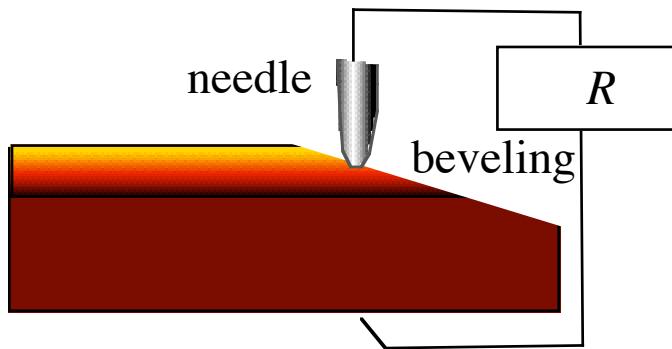
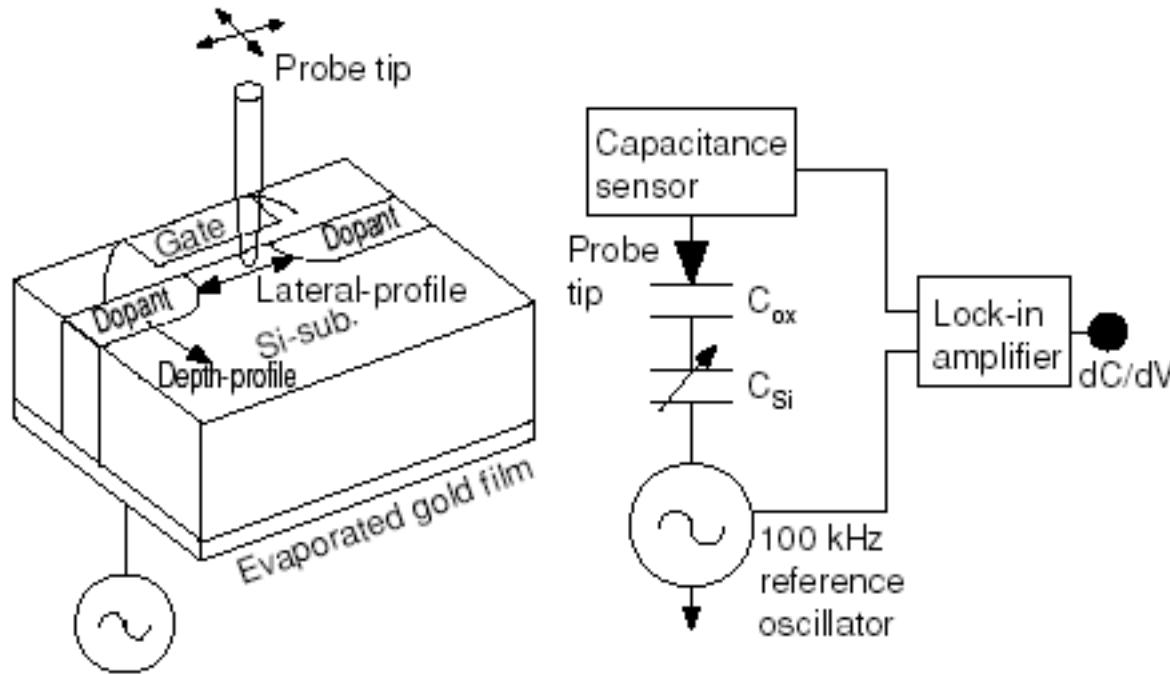


Figure 3.17 Typical spreading resistance profile showing measured carrier concentration as a function of depth (used with permission, Solecon Labs).

Diffusion, Measurement of diffusion profile

Scanning capacitance microscopy

Electric

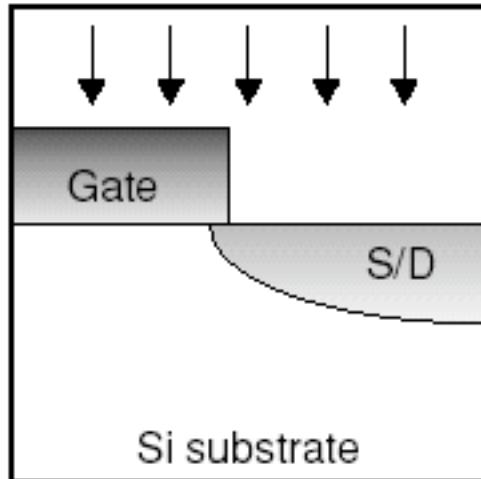


(a) Schematic model of SCM measurement

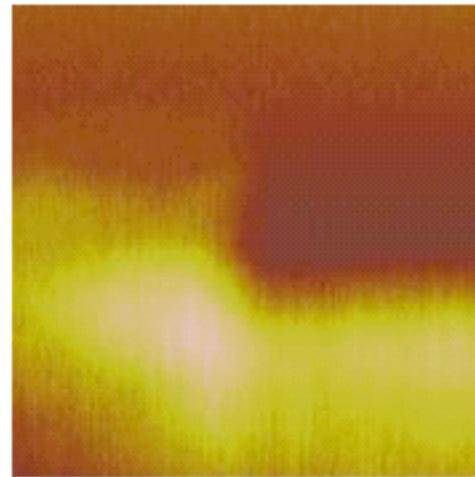
(b) Block diagram of SCM measurement

Diffusion, Measurement of diffusion profile

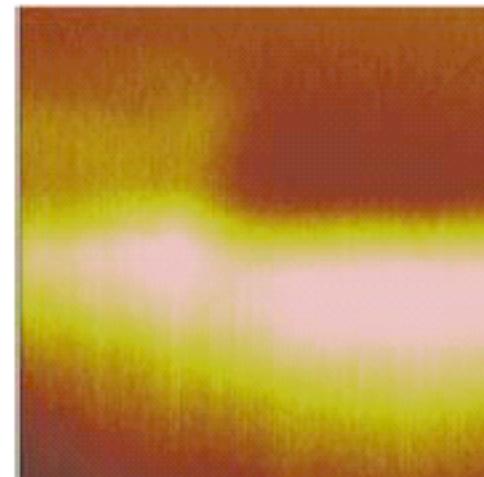
Scanning capacitance microscopy



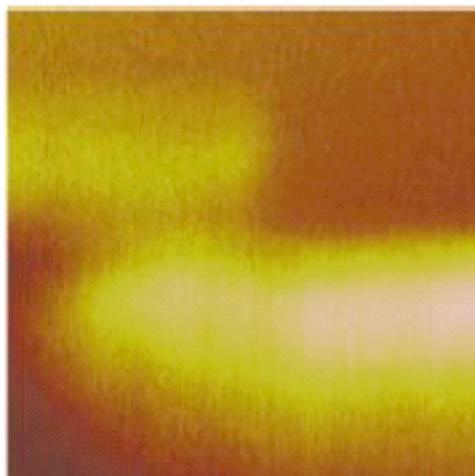
(a) Schematic model



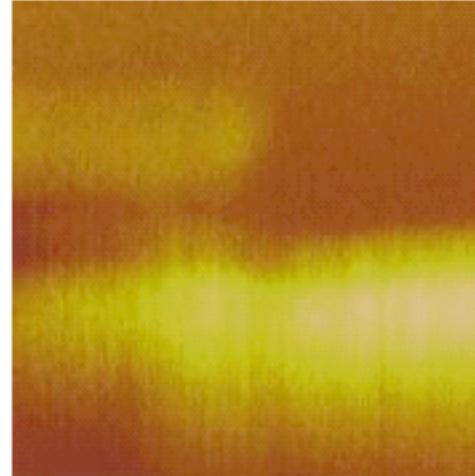
(b) DC = -1.0 V



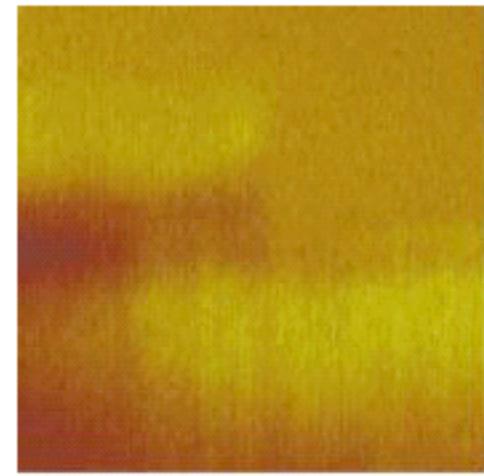
(c) DC = -0.5 V



(d) DC = 0 V



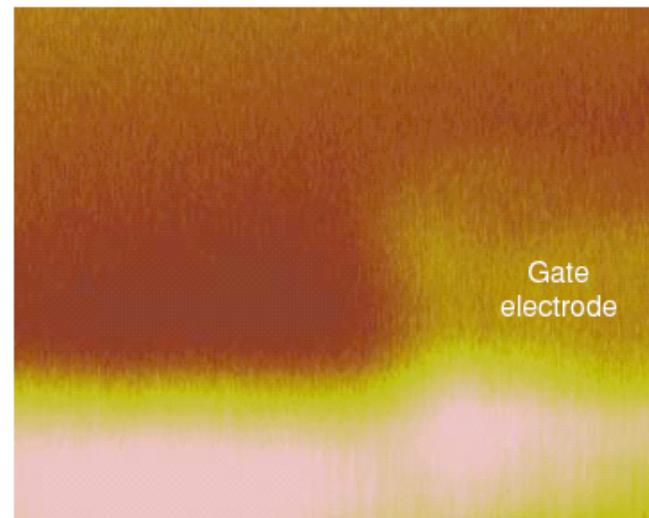
(e) DC = 0.5 V



(f) DC = 1.0 V

$\overline{0.1 \mu\text{m}}$

Diffusion, Measurement of diffusion profile



(a) SCM image

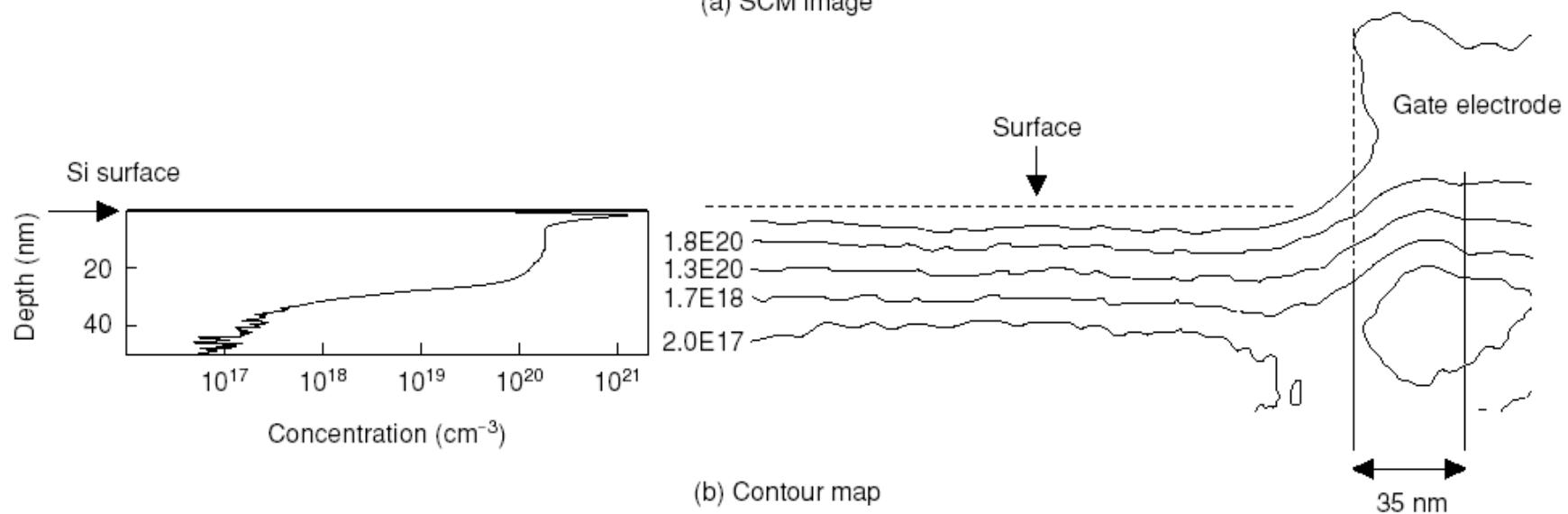


Figure 5

Quantitative two-dimensional dopant profile. (a) cross-sectional SCM image of an n-MOS transistor. Brighter areas correspond to the n-type regions, while the darker areas correspond to insulating materials. (b) The contours show the concentrations in the vicinity of the gate electrode. The positions of the gate edge and silicon surface were determined

Diffusion, Measurement of diffusion profile

SIMS,

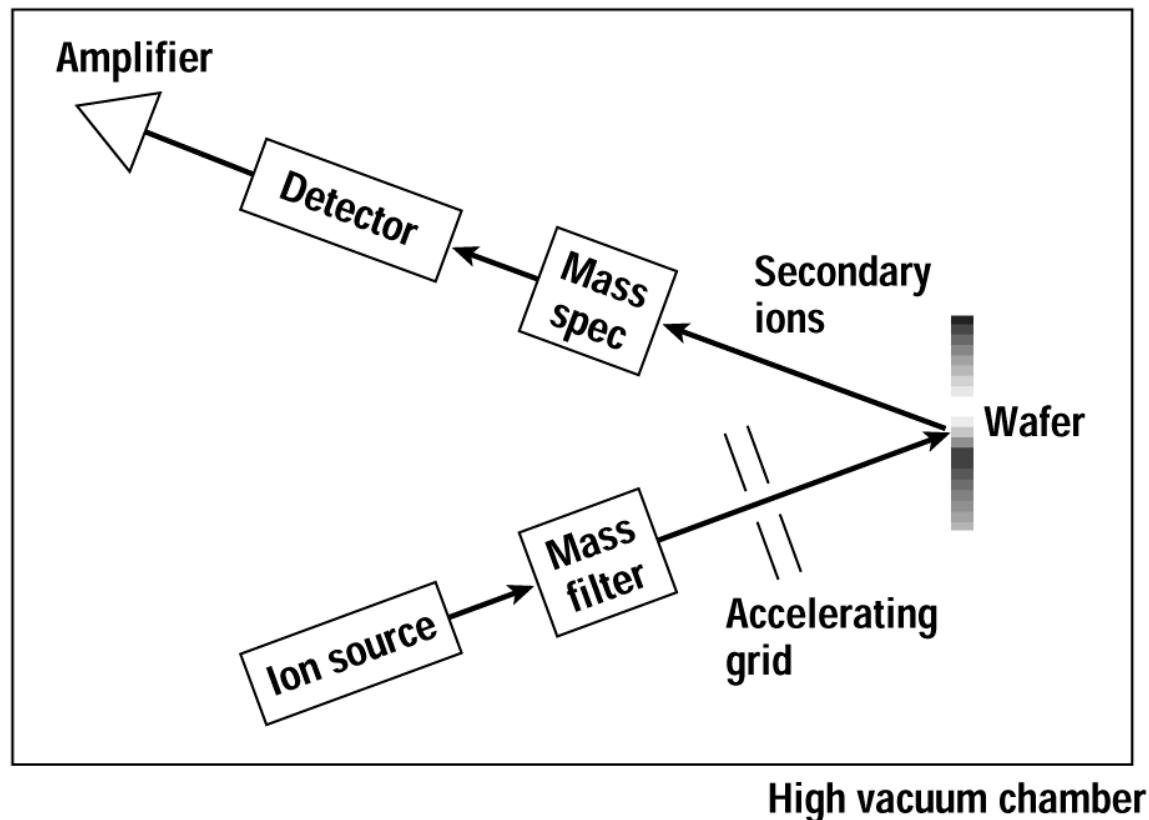


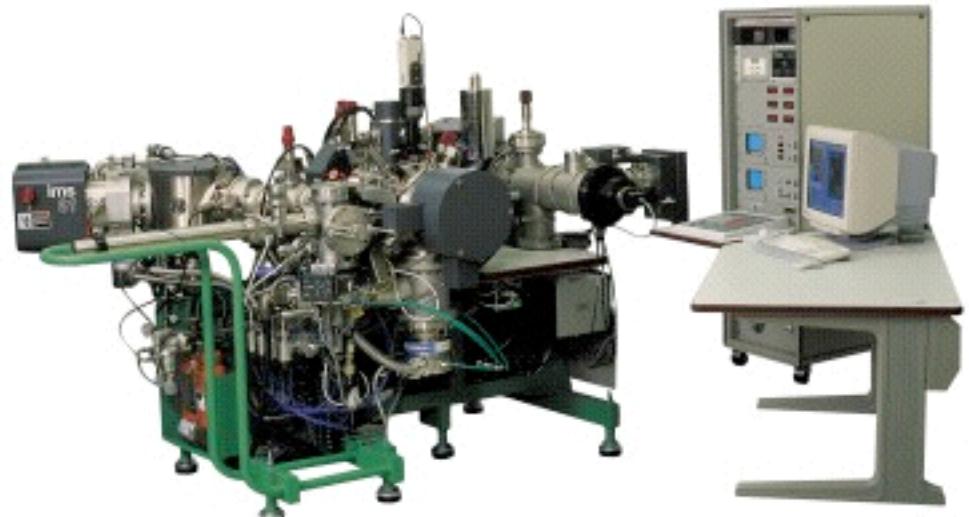
Figure 3.18 A typical SIMS arrangement. The sample is bombarded by high-energy ions. The sputtered material is mass analyzed to determine the composition of the substrate.



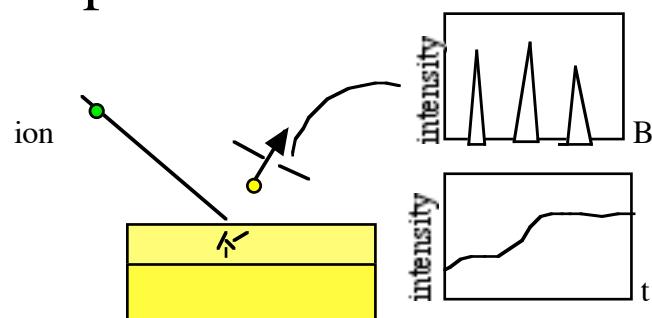
Equipment at MRL-Uo:

SIMS Cameca 6F

Installed April-Aug. 2004



principle



Characteristics of SIMS:

Well suited for measurements of diffusion profiles in high tech 1/2 conductors:

Sensitivity:

All elements can be detected

Sensitivity depends on element. in Si: B, P 10^{14}cm^{-3}

Accuracy:

Through standards (not absolute spectro-scopy/-metry)

Good reproducibility

Matrix-effects:

Ionization coeff. depends on surface,

oxidation, sputter w. oxygen yields good reproducibility

Interface-effects

Depth resolution:

Limited by sputter process, 2 nm - 50 nm

ion mixing, segregation, run away erosion

Diffusion, Measurement of diffusion profile

RBS

Absolute measurement

Depth resolution 10-30 nm

Sensitivity:

Matrix effects.

Heavy in light matrix 10^{18} cm^{-3}

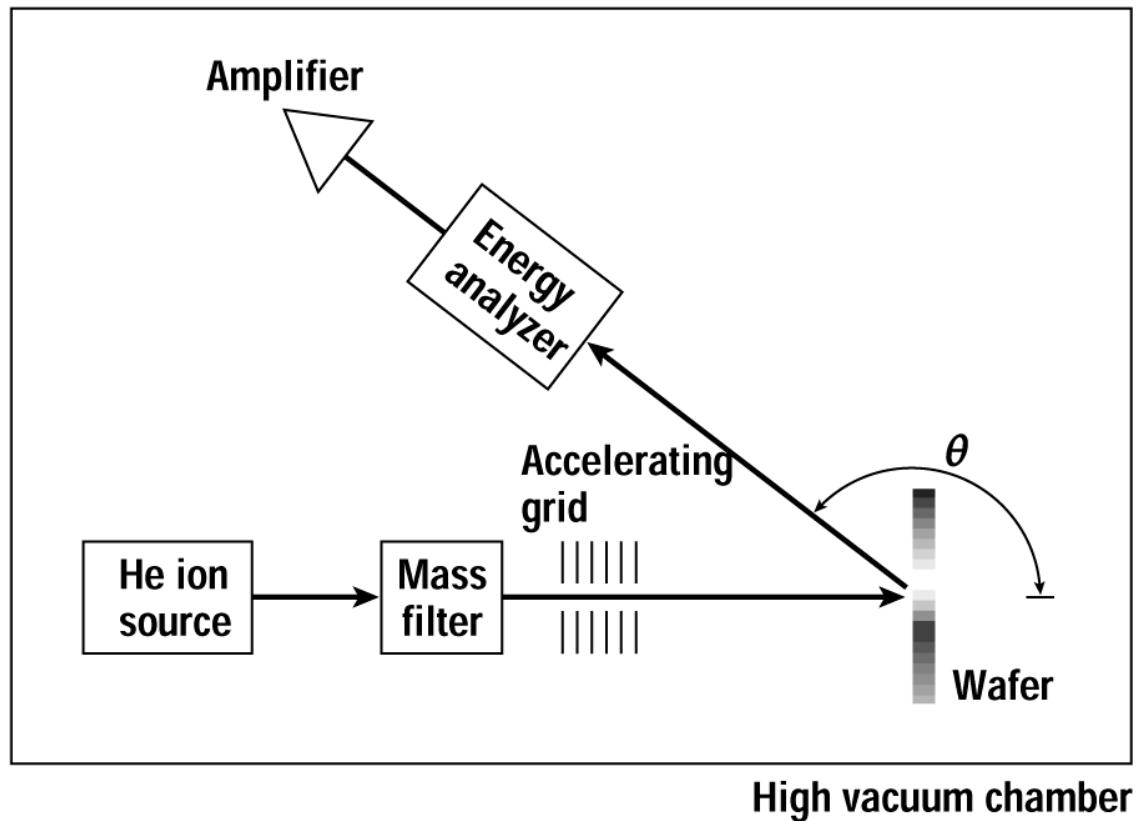
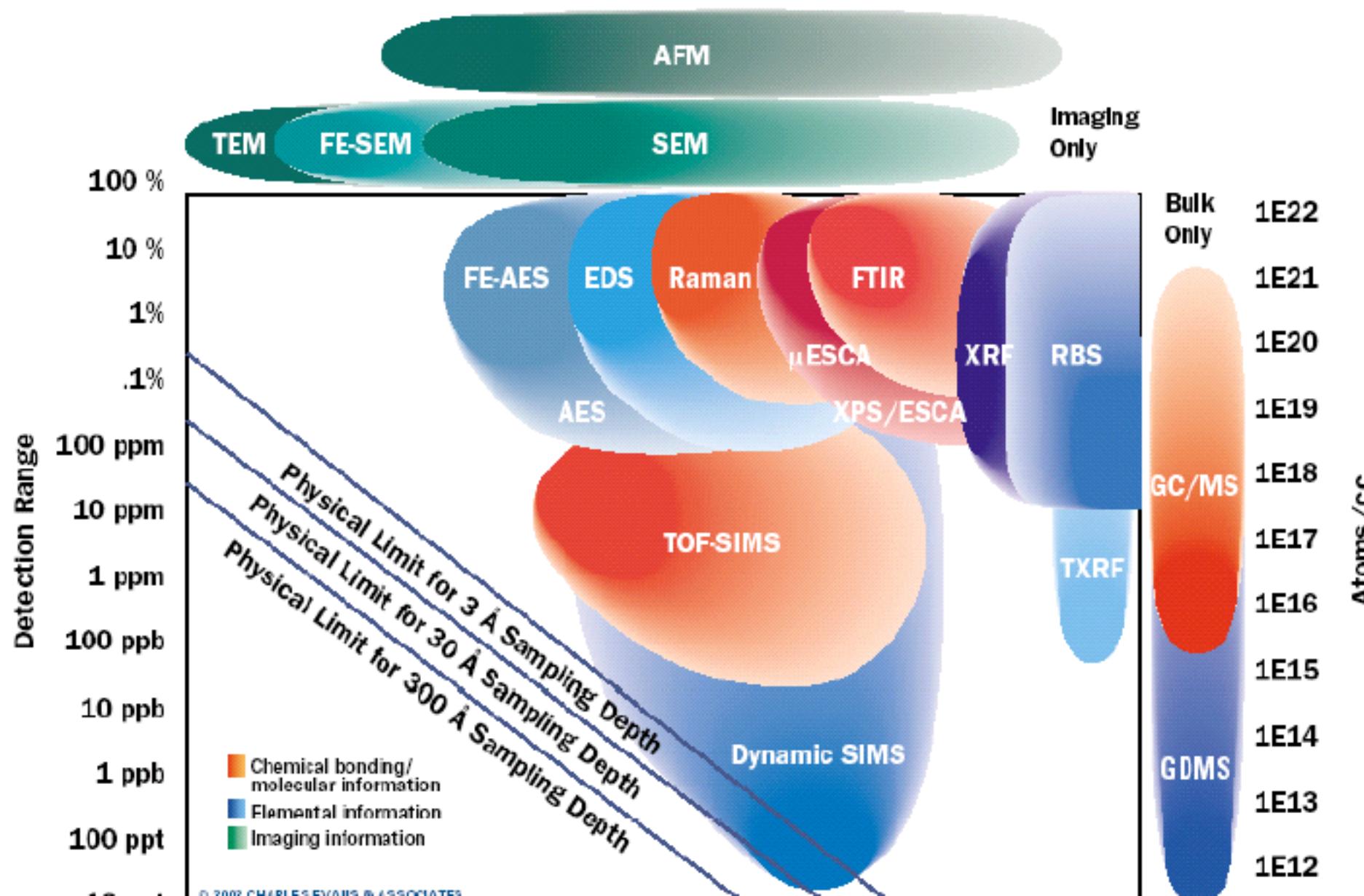
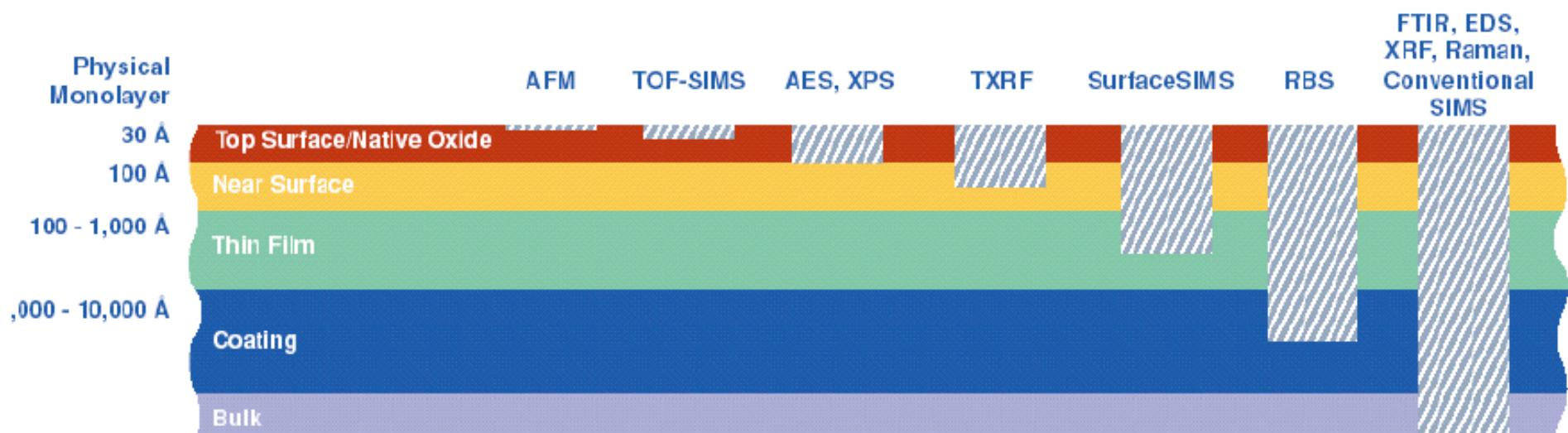


Figure 3.19 In Rutherford backscattering, the energy of the backscattered helium ions can be used to determine the depth profile of the chemical composition of the wafer.

Analytical Resolution versus Detection Limit



Typical Analysis Depths for Techniques



Diffusion, doping sources

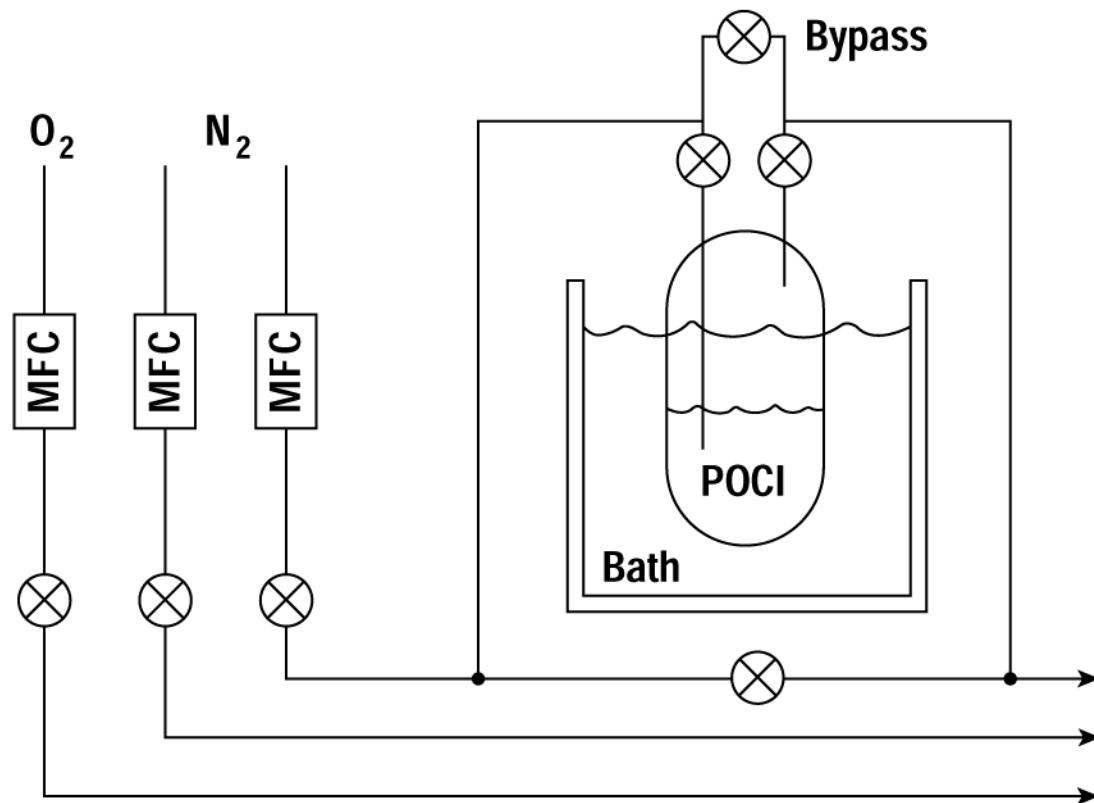
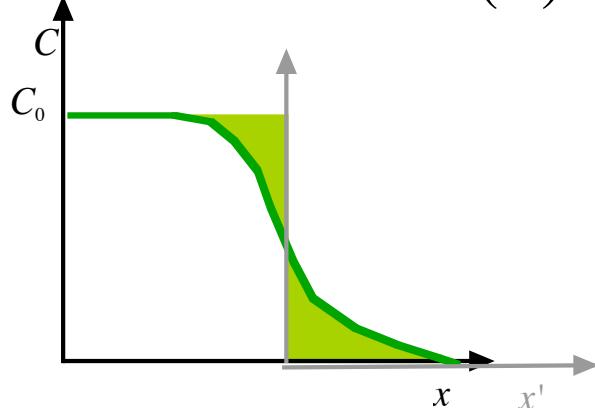


Figure 3.20 A typical bubbler arrangement for doping a silicon wafer using a $POCl$ source. The gas flow is set using mass flow controllers (MFC).

Bolzman Matano method

Point: Extract $D(C)$ from $C(x)$



Introduce a new coordinate system x' by

$$\int_{C(x'=0)}^{C_0} x' dC = - \int_0^{C(x'=0)} x' dC$$

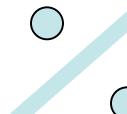
$C=C(x',t)$ is a function only of $\lambda = \frac{x'}{\sqrt{t}}$ i.e. $C=C(\lambda)$

We may write Ficks 2 law by λ

$$\text{LHS } \frac{\partial C}{\partial t} = \frac{\partial C}{\partial \lambda} \frac{\partial \lambda}{\partial t} = \frac{\partial C}{\partial \lambda} \left(-\frac{x'}{2} t^{-\frac{3}{2}} \right)$$

$$\text{RHS } \frac{\partial}{\partial x'} \left(D \frac{\partial C}{\partial x'} \right) = \frac{\partial}{\partial \lambda} \left(D \frac{\partial C}{\partial x'} \right) \frac{\partial \lambda}{\partial x'} = \frac{\partial}{\partial \lambda} \left(D \frac{\partial C}{\partial \lambda} \frac{\partial \lambda}{\partial x'} \right) t^{-\frac{1}{2}} = \frac{1}{t} \frac{\partial}{\partial \lambda} \left(D \frac{\partial C}{\partial \lambda} \right)$$

Setting LHS=RHS

$$-\frac{x'}{2} t^{-\frac{1}{2}} \frac{\partial C}{\partial \lambda} = \frac{\partial}{\partial \lambda} \left(D \frac{\partial C}{\partial \lambda} \right) \Rightarrow -\frac{\lambda}{2} \frac{\partial C}{\partial \lambda} = \frac{\partial}{\partial \lambda} \left(D \frac{\partial C}{\partial \lambda} \right)$$


Bolzman Matano method

$$-\frac{\lambda}{2} \frac{\partial C}{\partial \lambda} = \frac{\partial}{\partial \lambda} \left(D \frac{\partial C}{\partial \lambda} \right)$$

Here we have the same differential on both sides, so we integrate $\left[-\frac{\lambda}{2} dC = d\left(D \frac{\partial C}{\partial \lambda}\right) \right]$

Integration between $C=0$ and $C=C_1$ and assume $\left. \frac{\partial C}{\partial \lambda} \right|_{C=0} = 0$

$$-\int_{C=0}^{C_1} \frac{\lambda}{2} dC = D_{C=C_1} \frac{\partial C}{\partial \lambda}$$

C_1 is one particular conc. we wish to investigate

$$D_{C=C_1} = -\frac{1}{2} \frac{\partial \lambda}{\partial C} \int_{C=0}^{C_1} \lambda dC \quad [I]$$

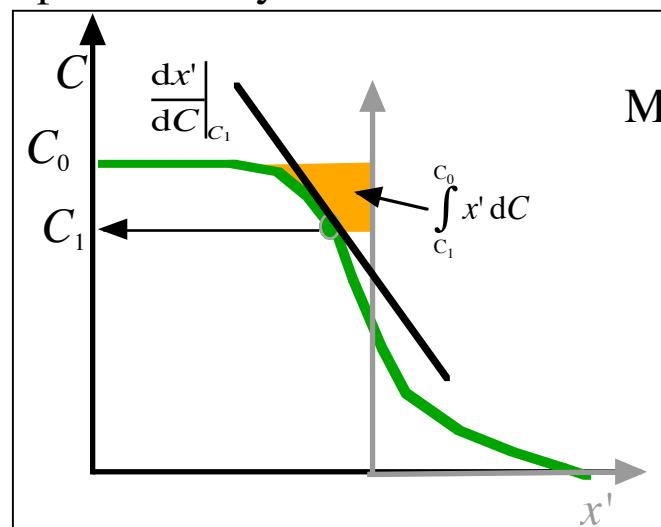
Slight rewriting:

$$-\int_{C=0}^{C_1} \lambda dC = 0 + -\int_{C=0}^{C_1} \lambda dC = \int_{C=0}^{C_0} \lambda dC - \int_{C=0}^{C_1} \lambda dC = \int_{C=0}^{C_1} \lambda dC + \int_{C_1}^{C_0} \lambda dC - \int_{C=0}^{C_1} \lambda dC = \int_{C_1}^{C_0} \lambda dC$$

Put in to [I] and choose a particular experimentally measured time for diffusion t_1 :

A $D_{C=C_1} = -\frac{1}{2t_1} \left(\frac{dx'}{dC} \right)_{C=C_1} \int_{C=C_1}^{C=C_0} x' dC$

B $\int_{C=C_1}^{C=C_0} x' dC = 0$



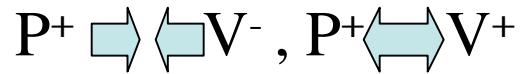
Method

1. x' origo from B
2. dC/dx' from curve
3. $\text{Int}(x', C=C_1..C_0)$

1+2+3 gives D from A

Diffusjon, example P

P donor, P^+

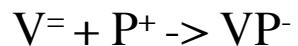


$$D_P = \left(D^* + D^- \frac{n}{n_i} + D^= \frac{n^2}{n_i^2} \right) \cdot h$$

Fair -Tsai model

Vacancies are created at the surface

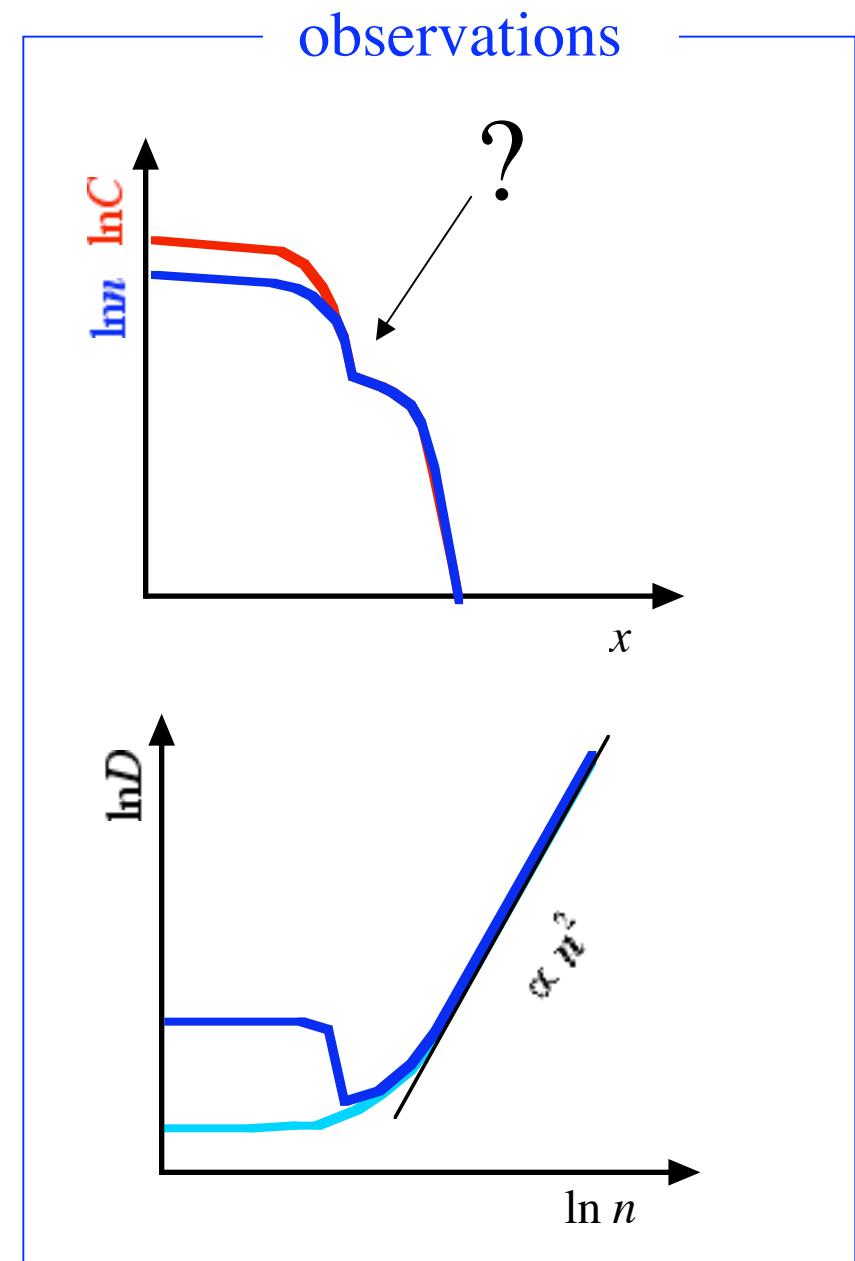
Conc of vac depends on n at surface



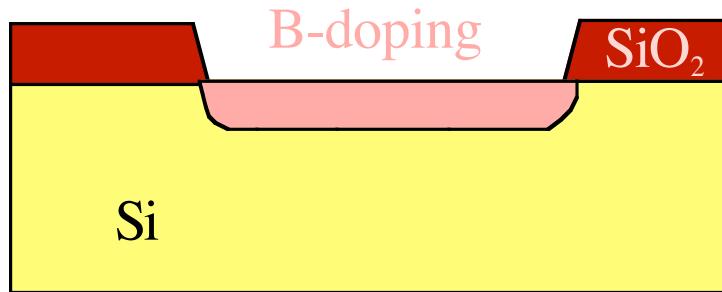
$E_C - E_F$ depends on depth when $dC/dx < 0$

VP^- breaks up \rightarrow excess vac'

Conc. of vacancy controlled by surface and
not by local doping

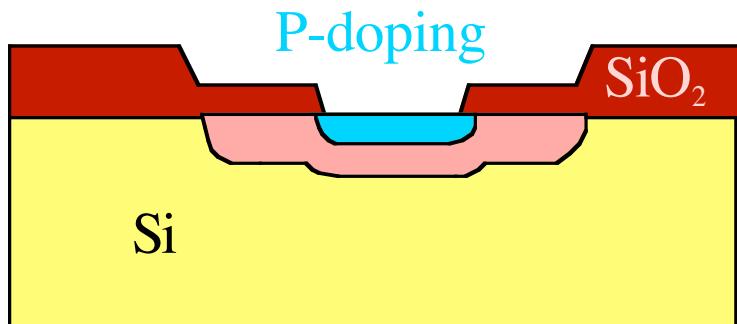


Diffusion, "Emitter-push"



Many models

Fair-Tsai diff. Model for P
+
Band gap narrowing

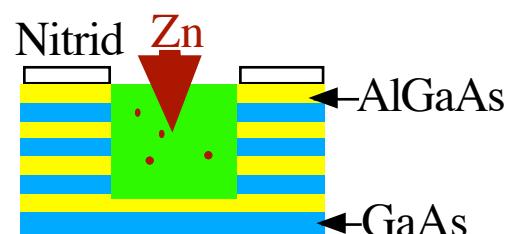
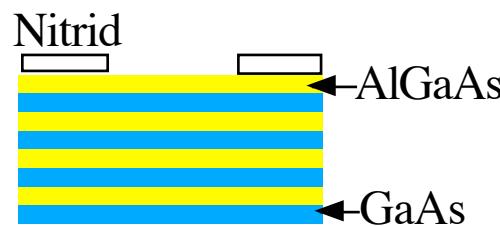
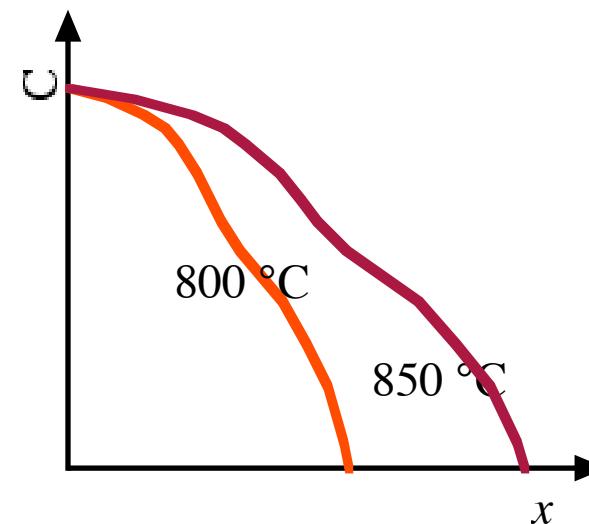
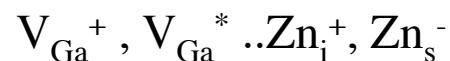
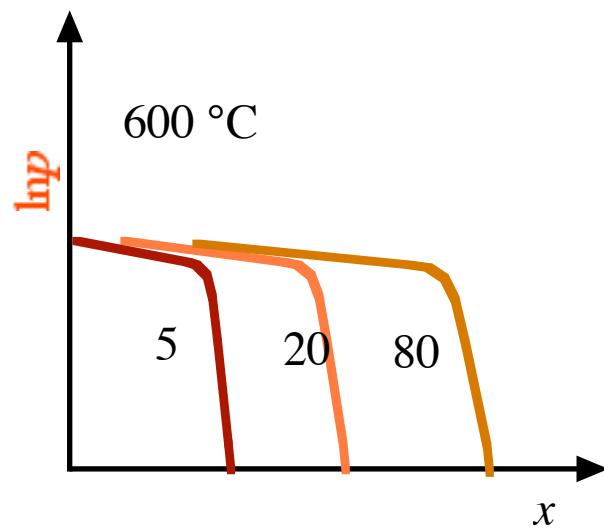


Describes results adequately

Diffusion, Example: Zn i GaAs

Zn acceptor in GaAs , Substitutes for Ga

$$D_{Zn} \approx AC_s^2$$



Confinement of waveguides, etc..