

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  $\text{SiO}_2$  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  $\frac{\partial C}{\partial t} = D\nabla^2 C \stackrel{1D}{=} D \frac{\partial^2 C(x,t)}{\partial x^2}$

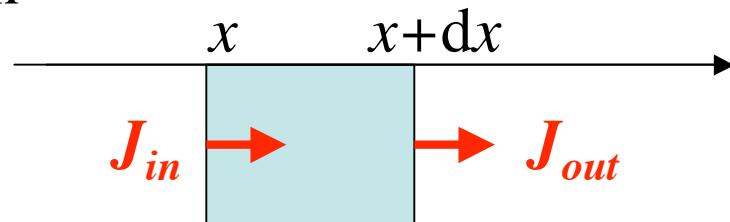
# Continuity equation should be well known

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

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

$J$ : flux  
 $C$ : concentration  
 $t$ : time

Derivation



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

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

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

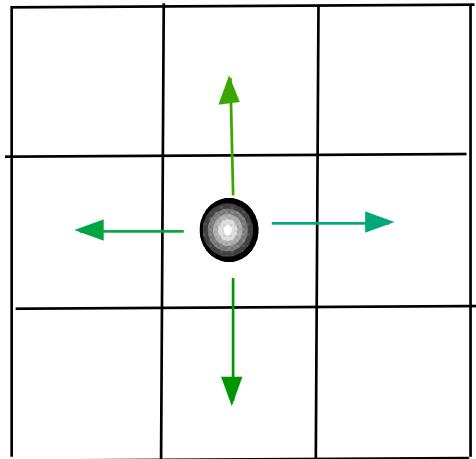
$$\Rightarrow -\frac{(J(x + dx) - J(x))}{dx} \underset{dx \rightarrow 0}{=} \boxed{\frac{\partial J}{\partial x} = \frac{\partial C}{\partial t}}$$

qed

# Diffusion in general microscopically

Random walk  
Brownian motion

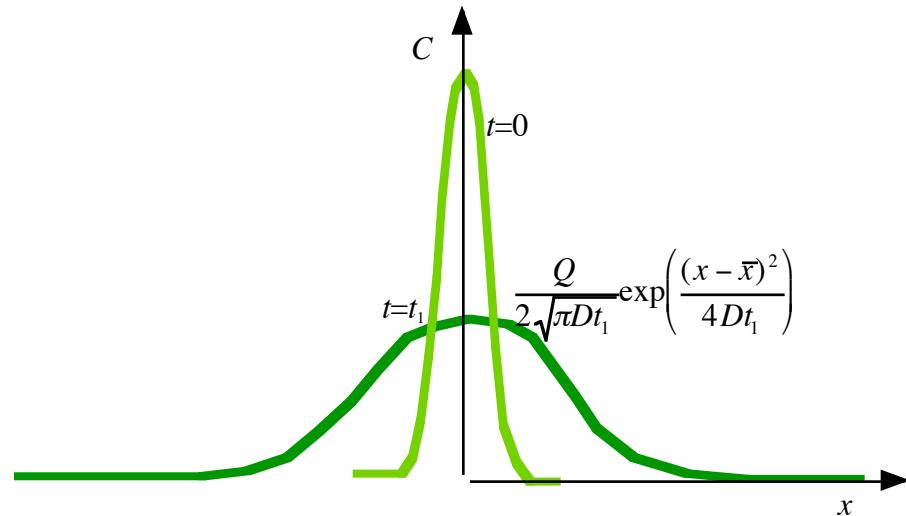
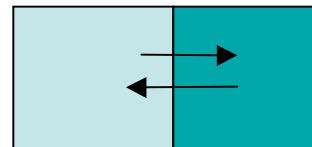
Microscopic lattice modelling



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

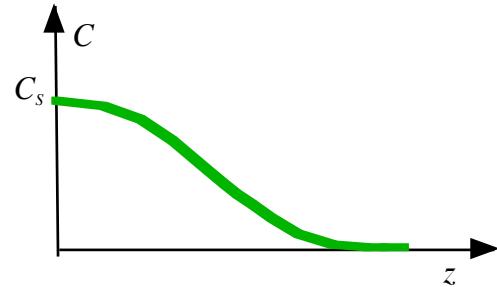
$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial z^2}$$

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

$$C(z,0) = 0$$

$$C(0,t) = C_s$$

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



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"

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

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

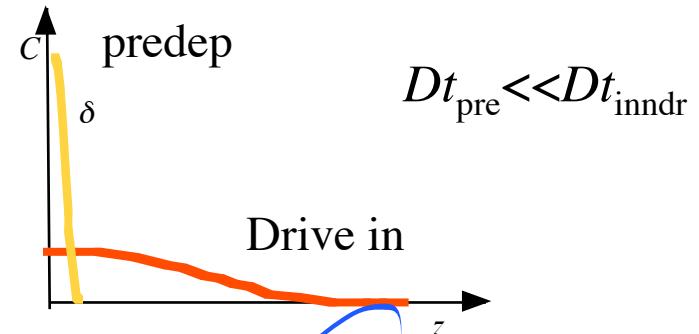
$$C(\infty, t) = 0$$

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

Solution

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

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

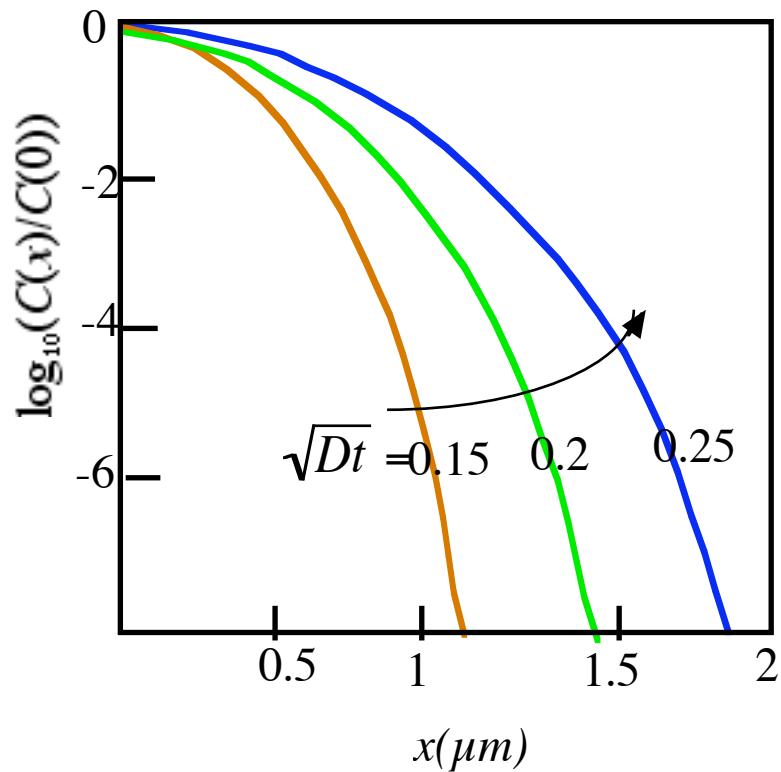


Gaussian  
fun

# Curve shape for idealized case

INTRINSIC Diffusion

Pre deposition



Drive in

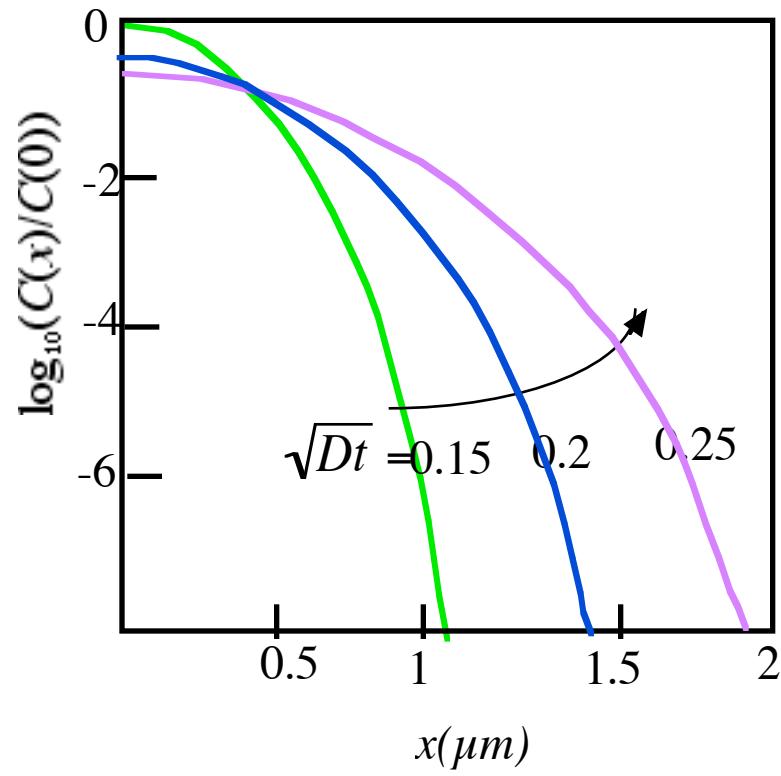
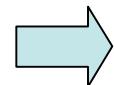


Fig. 3-7 a b, Cambell

# Electric field assisted diffusion - doping

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



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

Elec field

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

$$\eta = 0..1$$

$$C \approx n$$

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

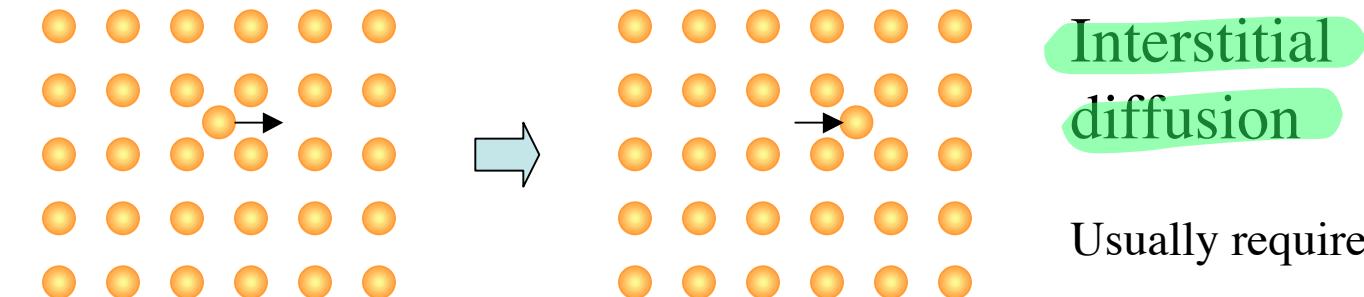
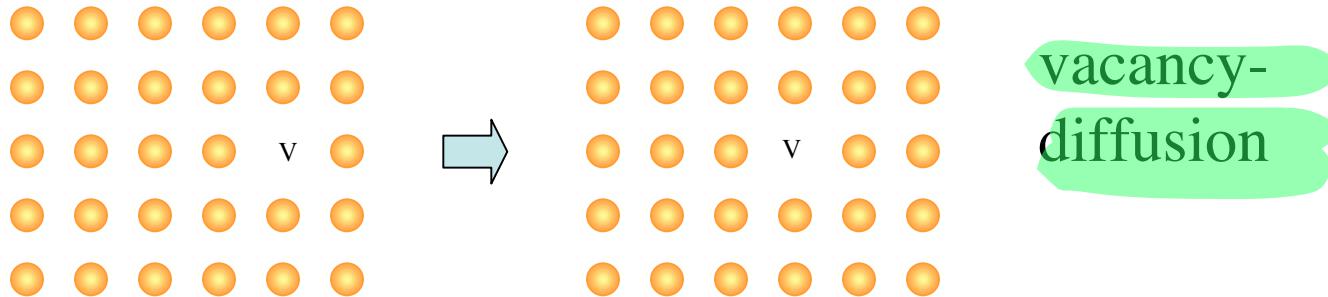
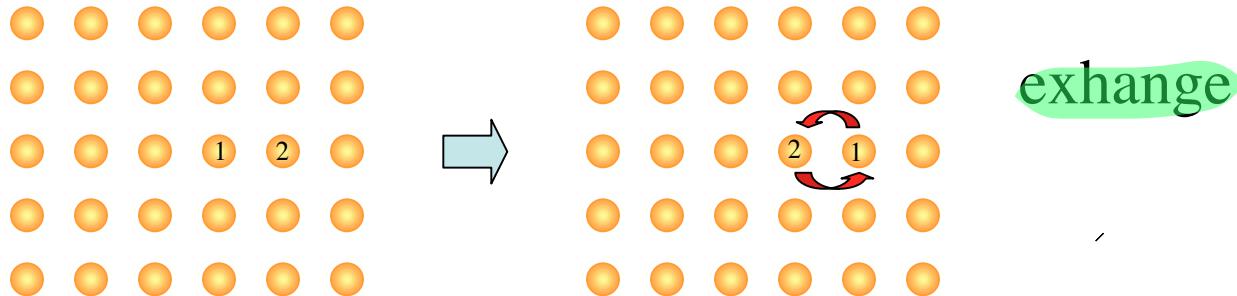
$$\frac{dE_F}{dz} = 0 !!$$



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

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

# Atomic diffusion -self diffusion



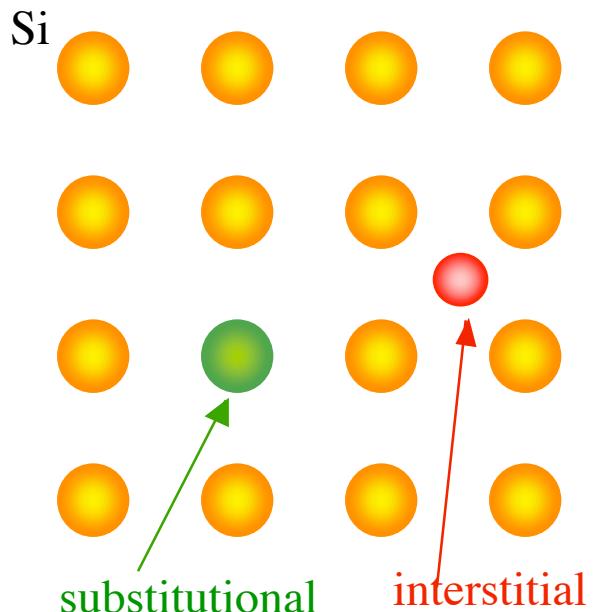
Usually requires little energy

Interstitials can knock  
out regular atoms -  
interstitialcy

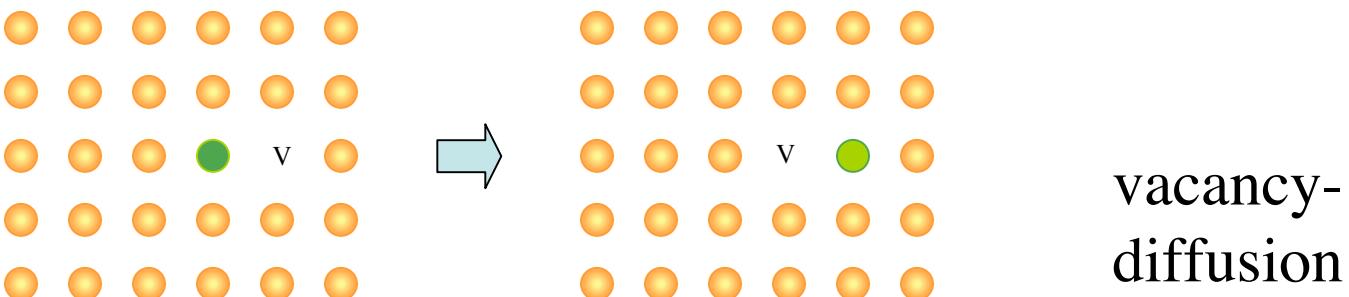
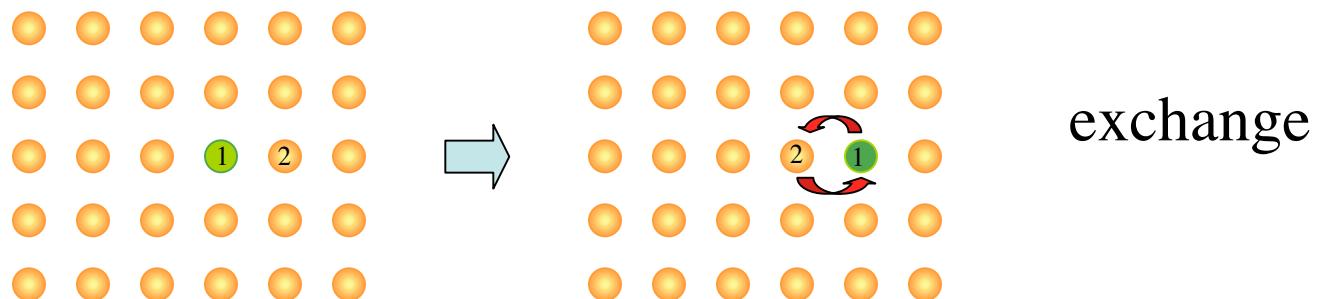
# Atomic diffusion

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



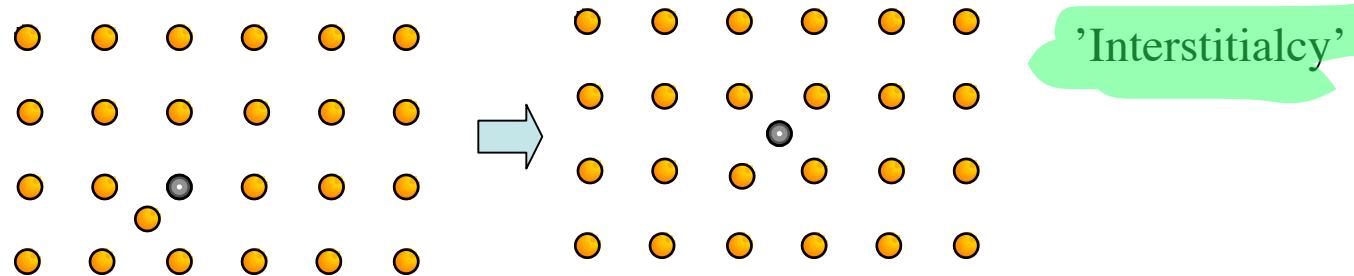
**Substitutionals may move in various ways**



# Atomic diffusion

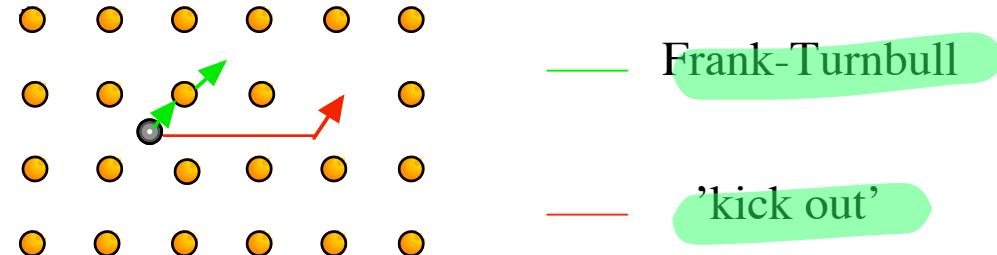
Various diffusion mechanisms for doping atoms

Fig 3.5



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

Fig 3.6

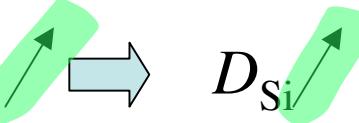


# Atomic diffusion

**Si self diffusion** - guess vacancy diffusion

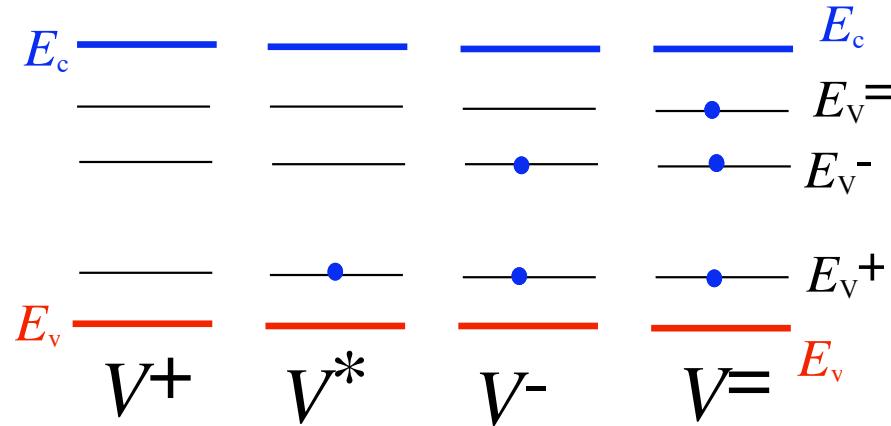
Can be measured by labeling the Si atoms by radioactive Si\*

Assume  $D_{\text{Si}}$  can be  
measured  
Finds:

P conc.   $D_{\text{Si}}$   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

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# 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

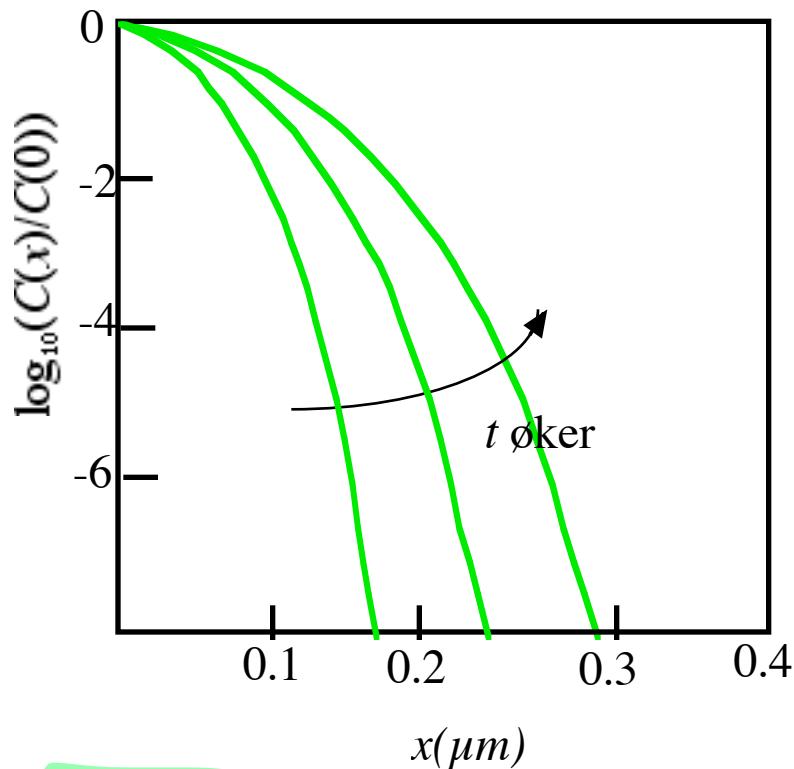
$$D^y = D_0^y \exp\left(-\frac{E_a^y}{kT}\right) \quad y: \text{charge state } *, -, +, =$$

Measured

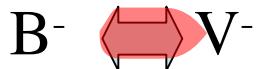
Atom	Do+	Ea+	Do*	Ea*	Do-	Ea-	Do=	Ea=
As			7e-3	3.44	12	4.05		
P			3.9	3.66	4.4	4	44	4.4
B	0.41	3.46	4e-2	3.46				

# Diffusion, typical profiles

Fig 3.8 B high conc.

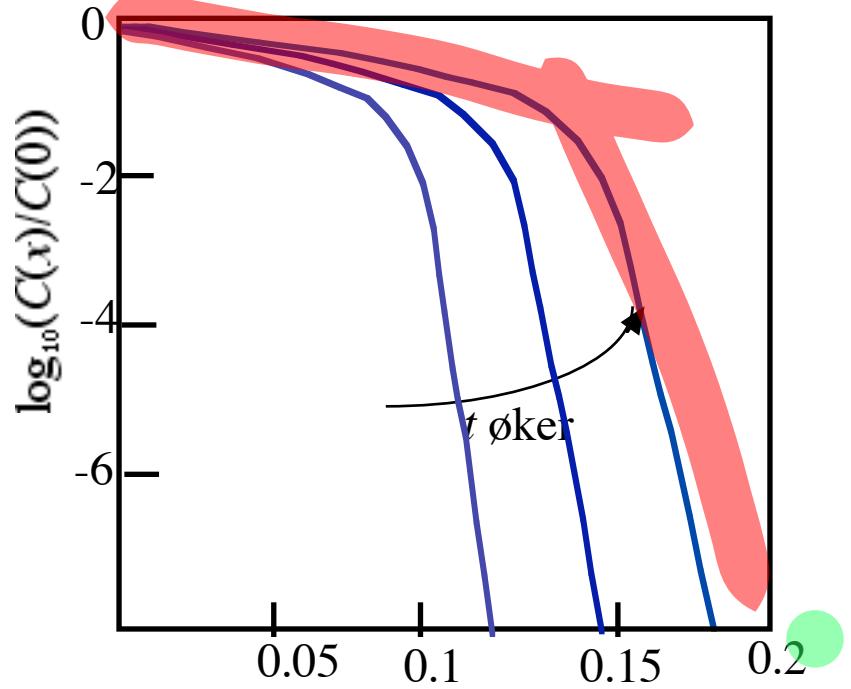


B acceptor

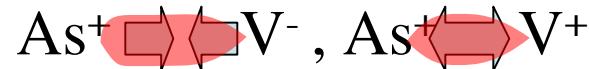


$$D_B = \left( D^* + D^+ \frac{p}{n_i} \right) \cdot h$$

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

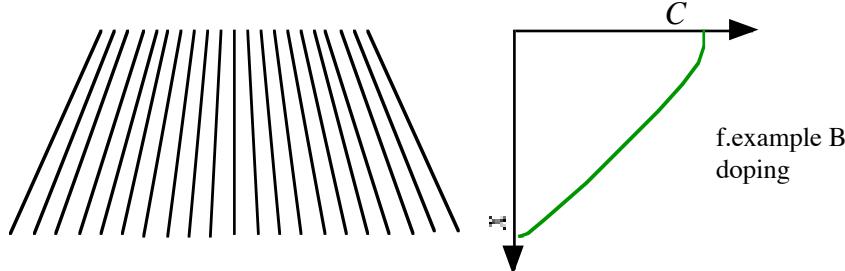
Cluster formation

Segregation

# Diffusion, High doping effects

Dislocations

Stress-no disloc.



f.example B  
doping

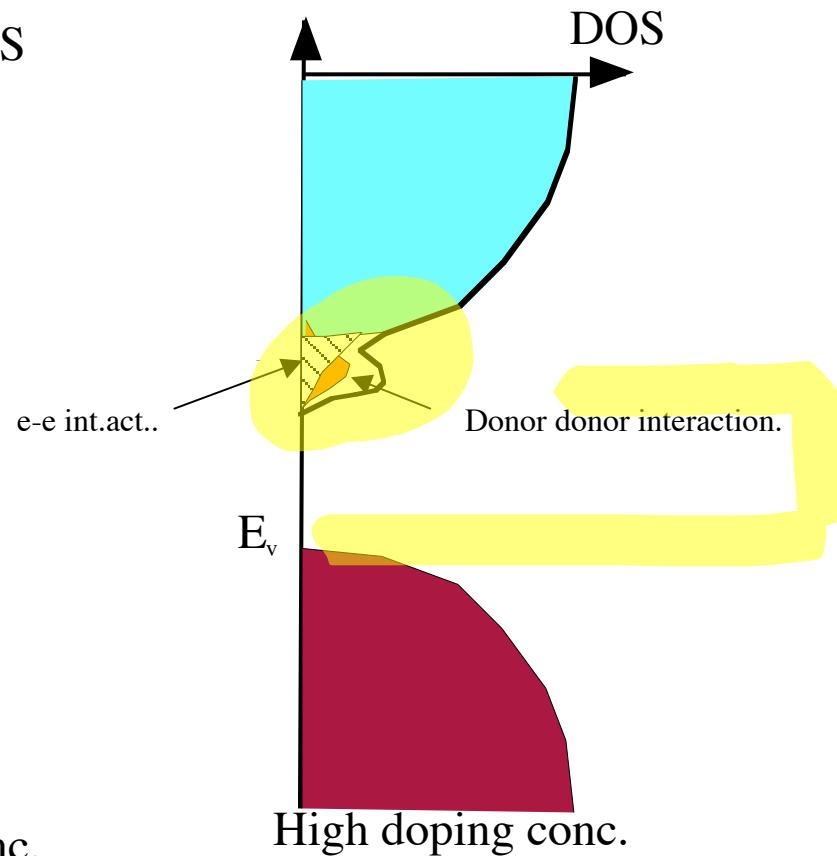
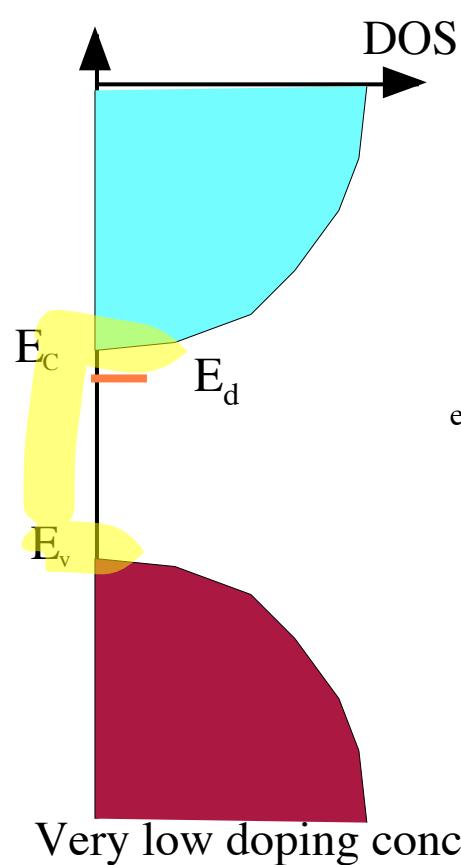
Disadvantage for stress in membranes for MEMS, ie for pressure sensors

Elastic energy released by creating a dislocation

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

# Diffusion, High doping effects

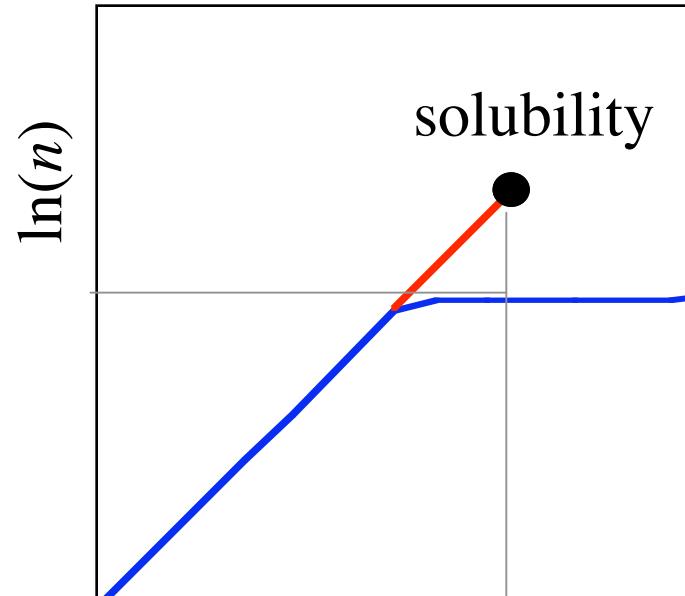
Band-gap narrowing



$E_g$  varies  
 $n_i$  varies  
[V] varies.

# Diffusion, High doping effects

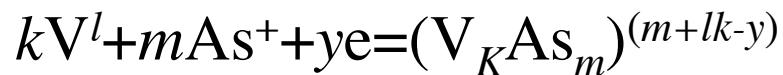
Cluster formation



Complexes/clusters

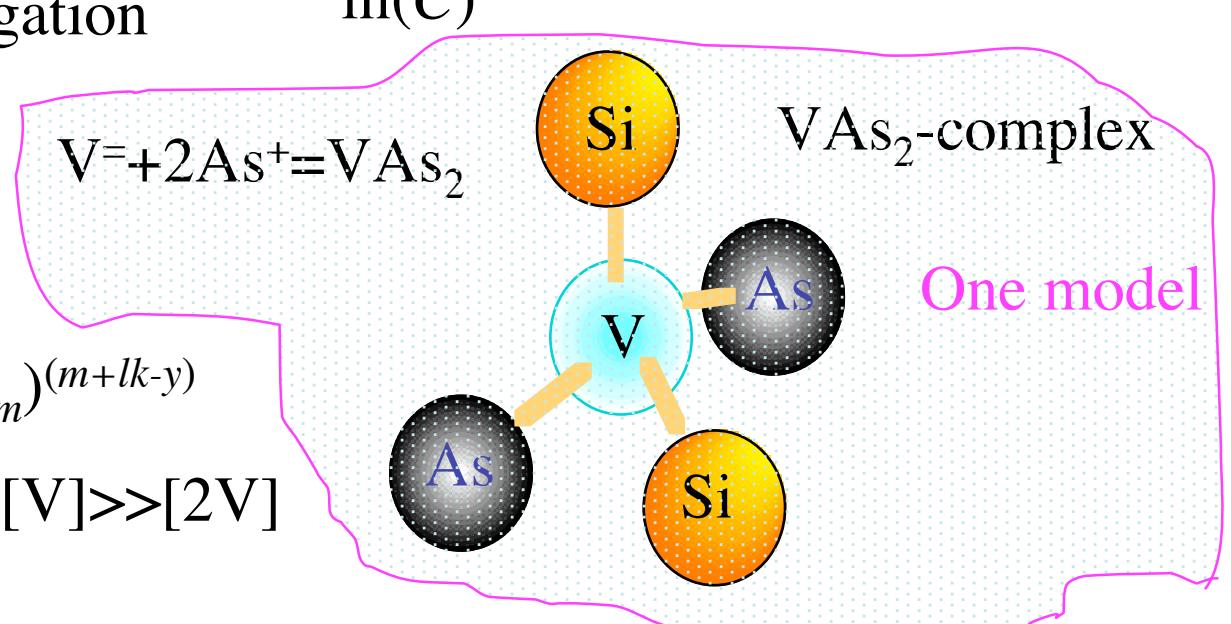
Maybe precursor to segregation

Various reactions



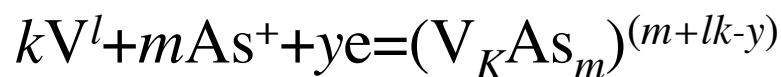
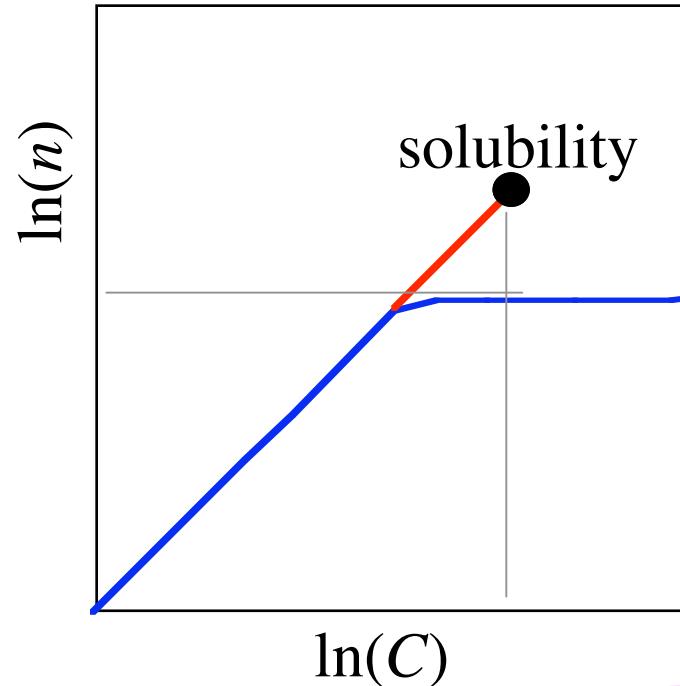
Complex neutral, el.neg,  $[V] \gg [2V]$

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

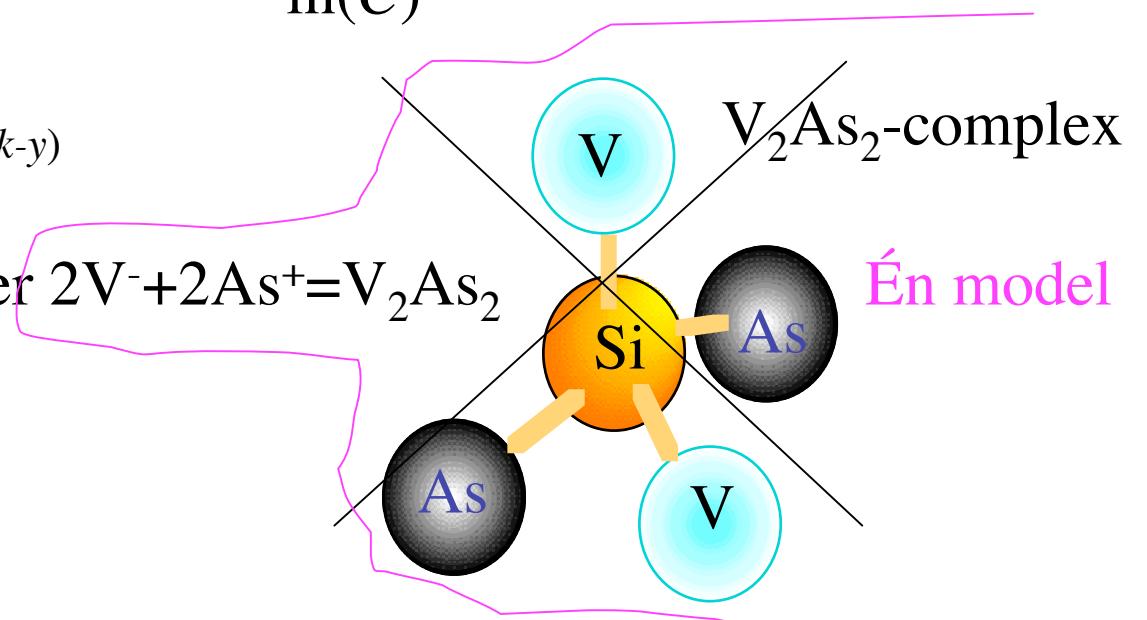


# Diffusion, High doping effects

Cluster formation



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

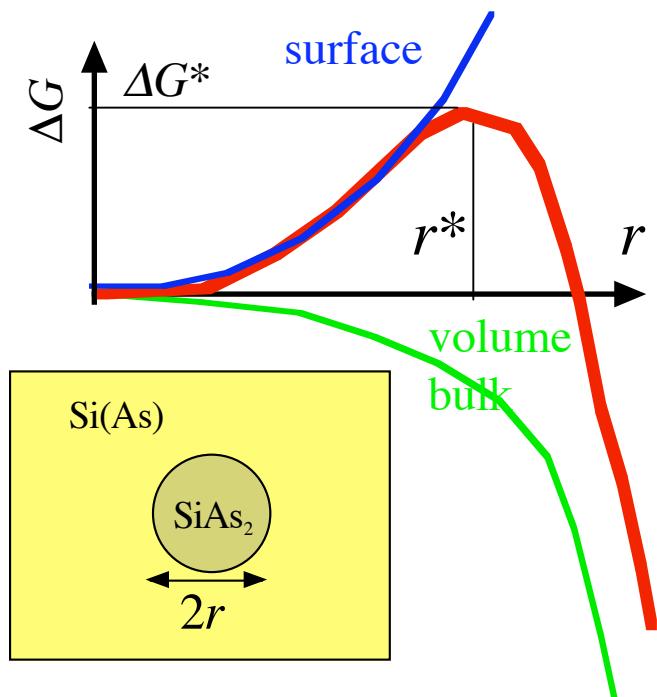


# Diffusion, High doping effects

## 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)

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General methods

→ Finite differencing

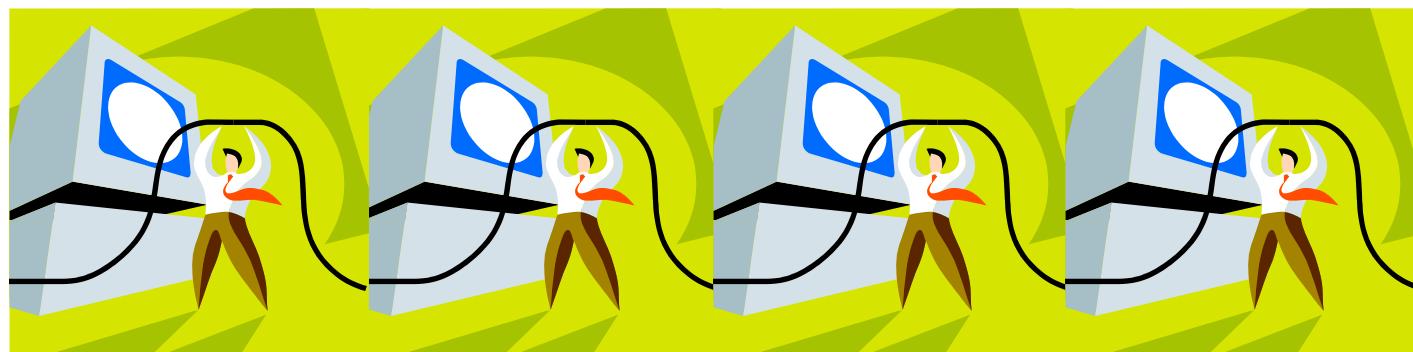
Finite element

Monte Carlo

Spectral

Variational

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# 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  $\Delta t$



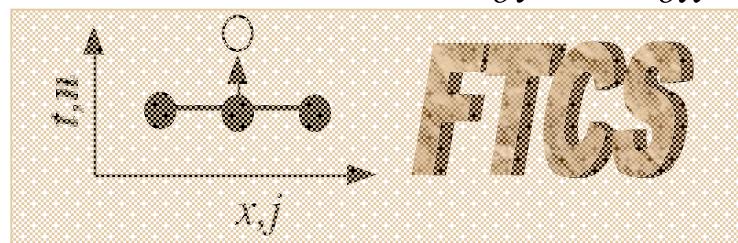
$$\frac{\partial u}{\partial x} \Big|_{j,n} = \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} + O(\Delta x^2)$$

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'

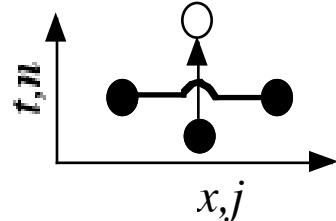


$$\frac{\partial C}{\partial t} = -\frac{\partial F(C)}{\partial x}$$

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  $\Delta t$

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:

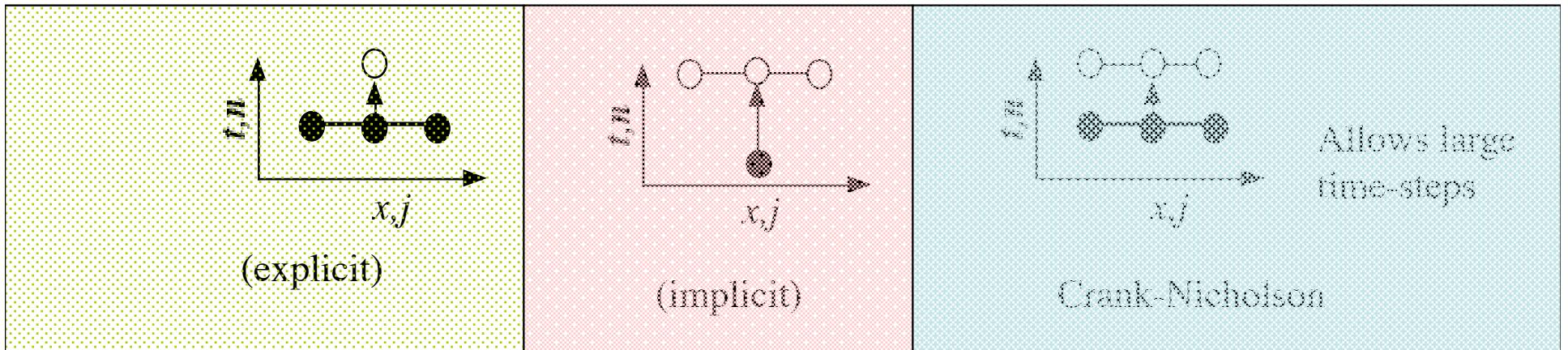
$$\frac{C_j^{n+1} - C_j^n}{\Delta t} = D \left( \frac{C_{j+1}^n - 2C_j^n + C_{j-1}^n}{\Delta x^2} \right)$$

(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. Between the brackets, the number '0' is written vertically in a large, bold, black font.

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

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

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

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

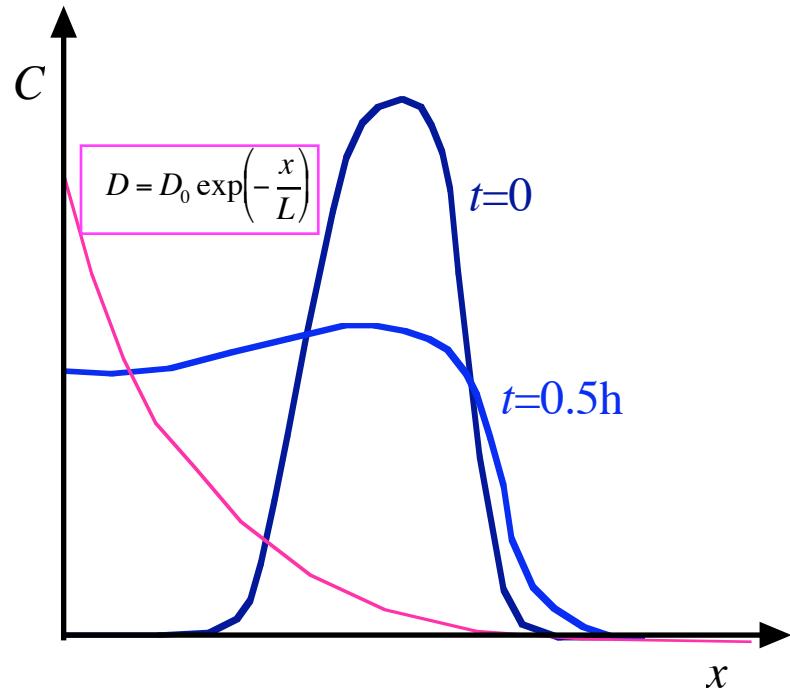
Can readily be solved when  $D$  only a function of  $x$  and  $t$  but not of  $C$ .

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

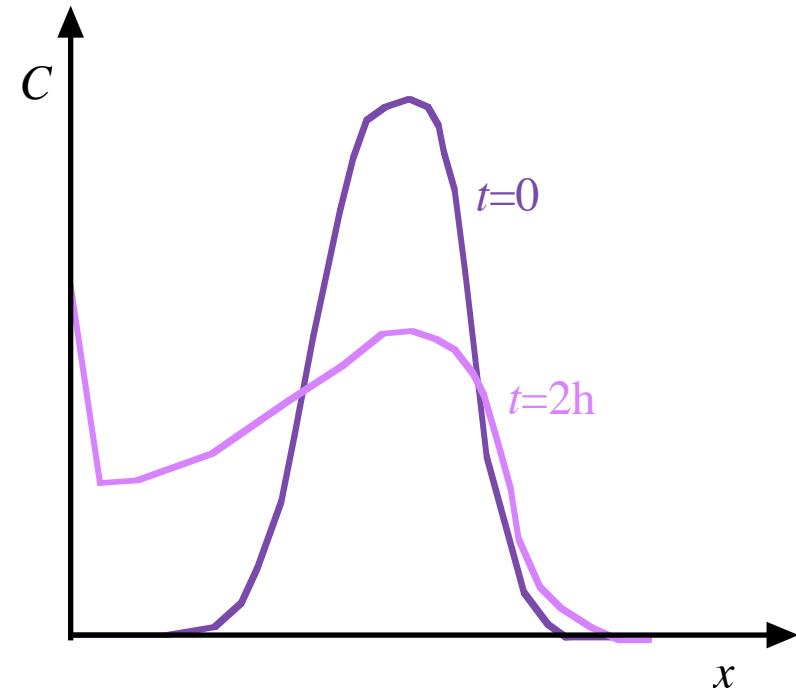


Implanted profile

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  $C=C(x)$ ,

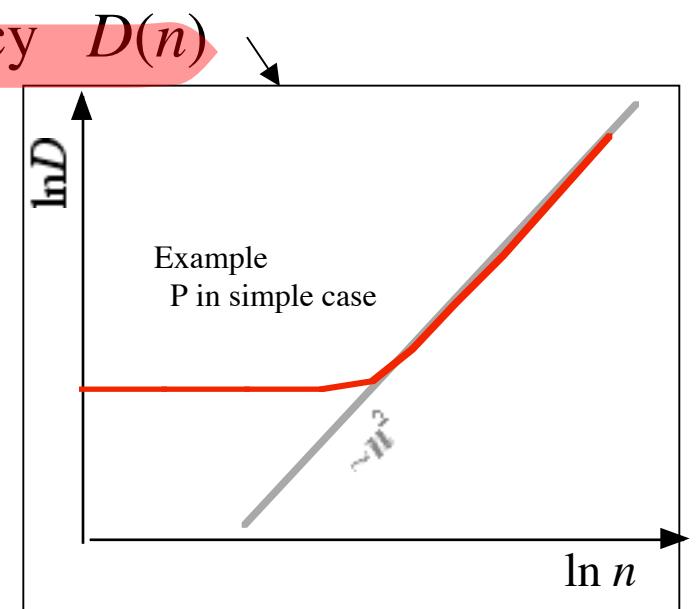
We can find  $D(C)$  by measuring  $C(x)$  at different  $T$

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

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

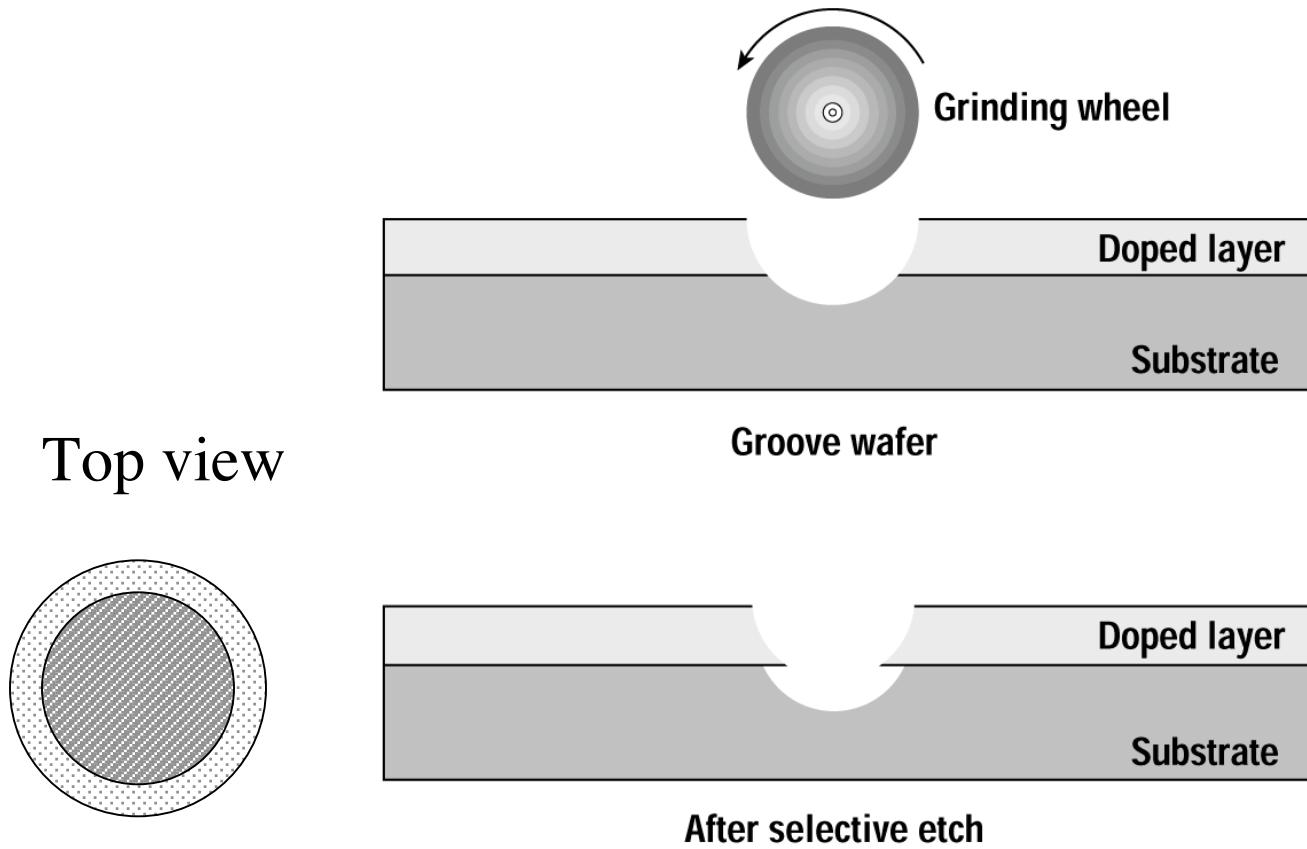
Methods for $C$
SIMS, TOFSIMS
Neutron activation
RBS, ESCA, EDAX
IR abs.

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



# Diffusion, Measurement of diffusion, process surveillance

---

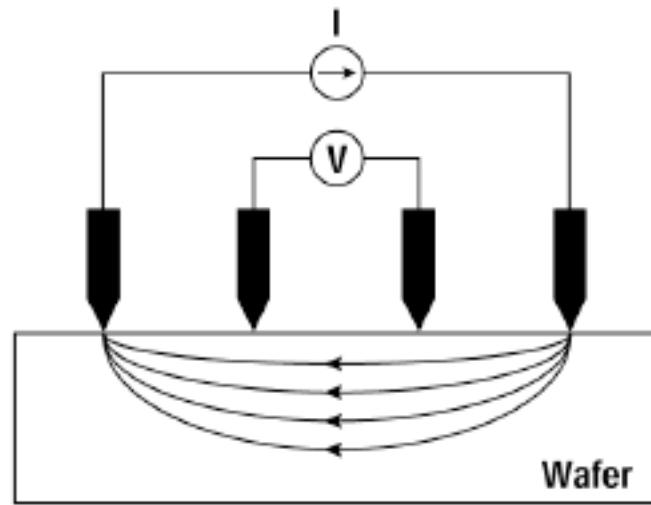


**Figure 3.15** In junction staining, a cylinder is used to groove the wafer. A doping sensitive etch then removes part of the top layer. The junction depth can be found from the known diameter of the sphere and the measured width of the lower abraded groove.

# Diffusion, Measurement of diffusion, process surveillance

---

'Four-point probe'

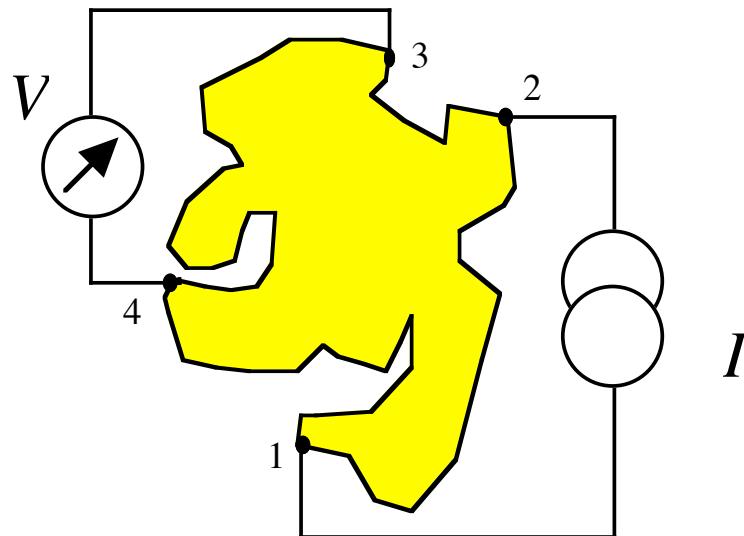


Measures so-called sheet resistance

Can find resistivity if the depth distribution of  $n$  and  $\mu$  is found

Mostly for process surveillance-reproducibility tests

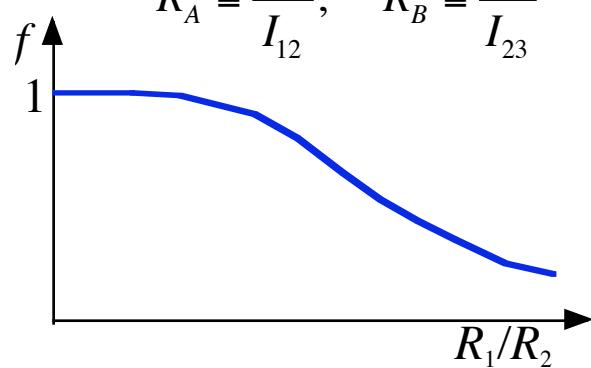
# Diffusion, Measurements of diffusion profiles



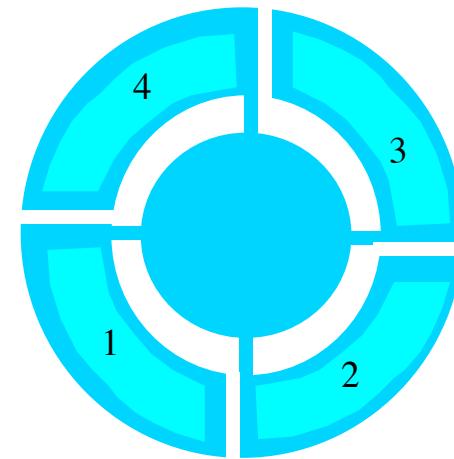
van der Peuw method

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

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

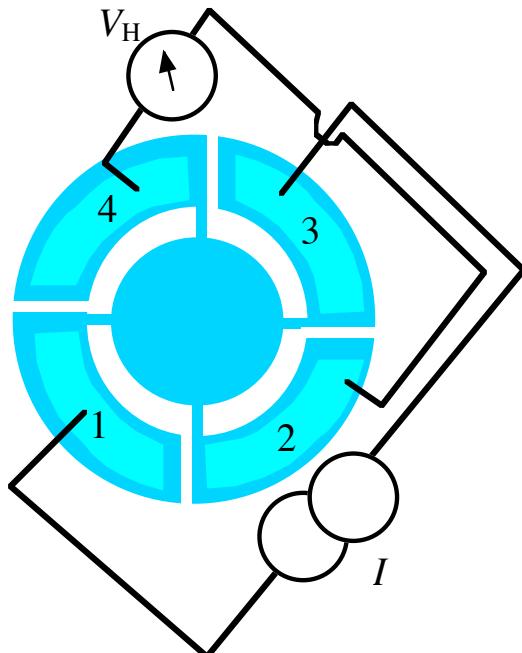


More common geometry



# Diffusion, Measurement of electric profile

## Hall measurements



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

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

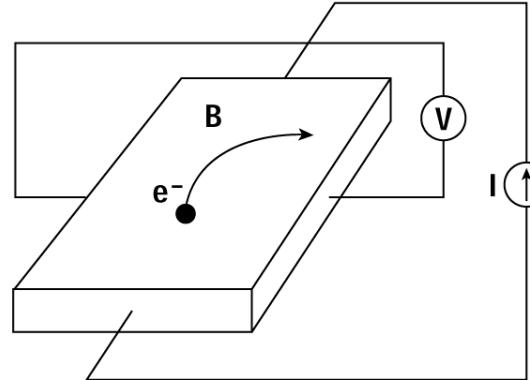
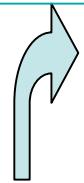


Figure 3.16 The Hall effect is able to simultaneously measure the carrier type, mobility, and sheet concentration.

### Measurement-procedure



Measure  $\rho_s, R_{HS}$  gives  $\mu_H$   
Strip a layer  
Repeat to  $d$

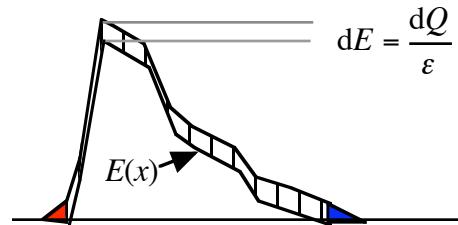
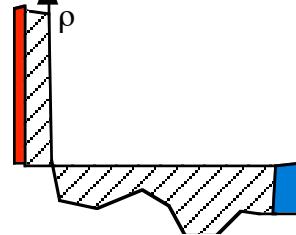
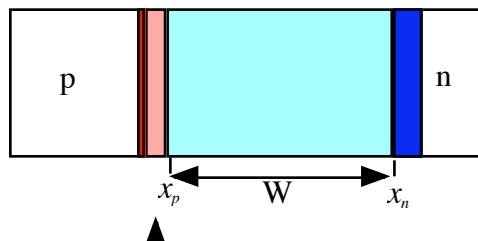
$$R_{HS} = \frac{V_H}{I} \frac{10^8}{B}$$

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

Calc individual  $n$  and  $\mu$

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

# Diffusion, Measurement of electric profile



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

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

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

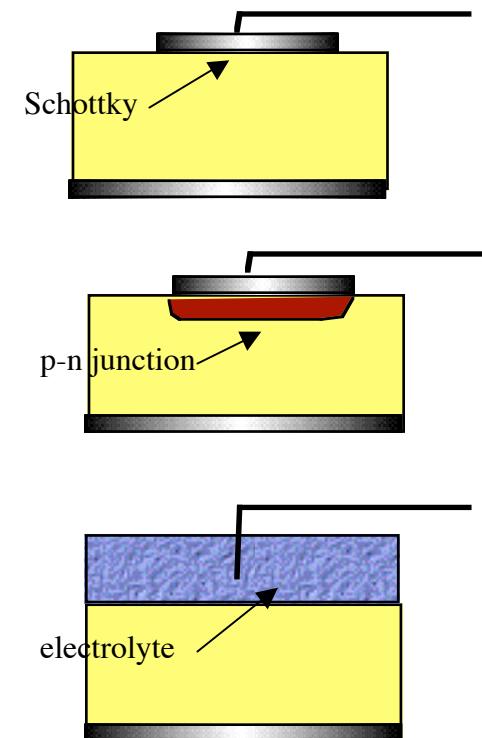
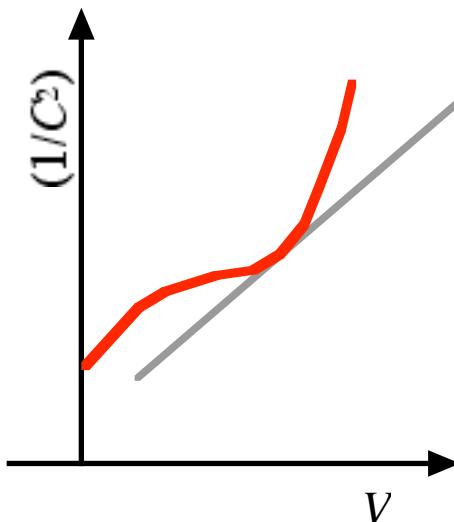
$$C \equiv \frac{dQ}{dV} = \frac{\epsilon}{W}$$

$$dQ = qN(W)dW$$

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

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

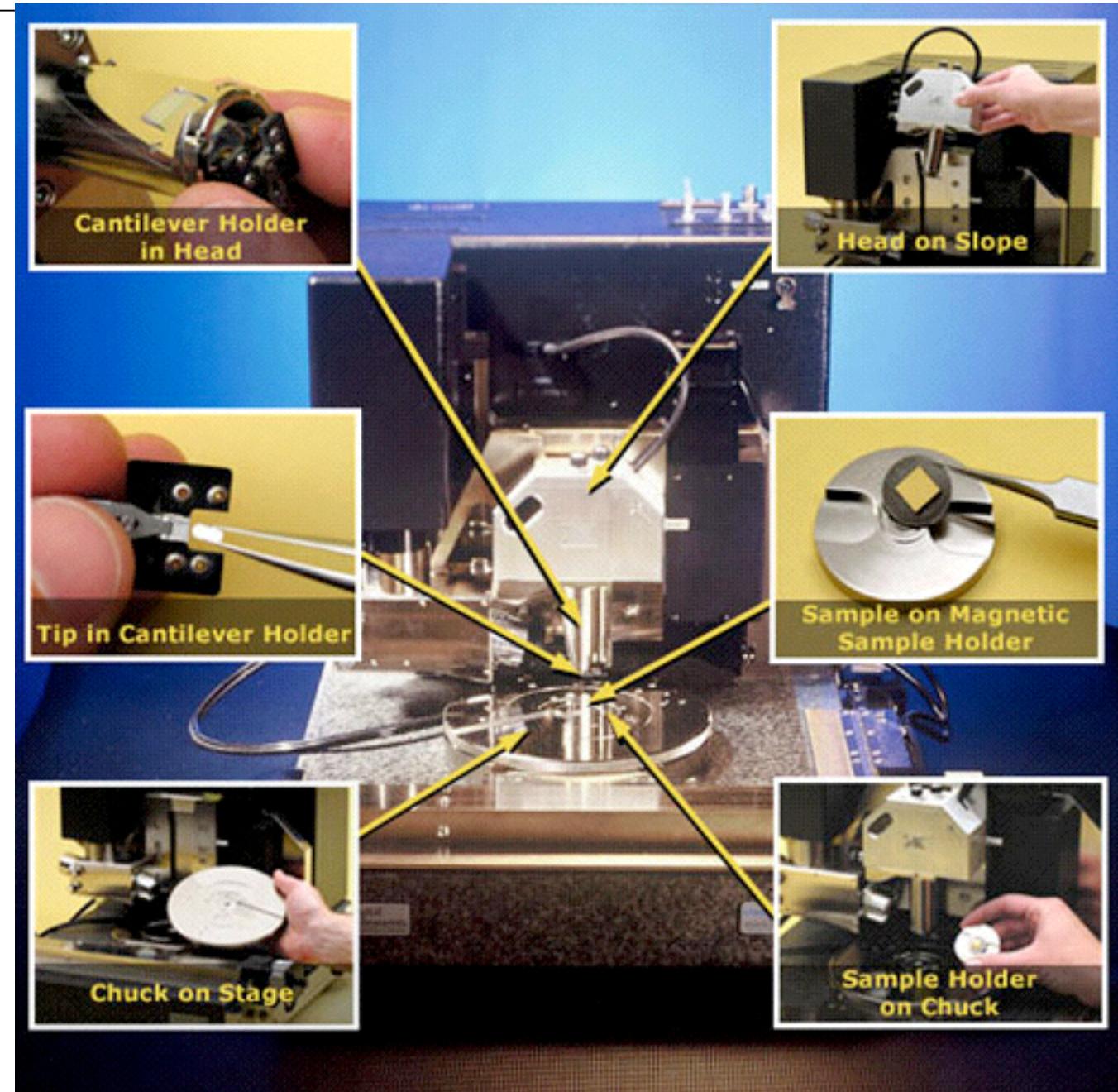
$$N(W) = \frac{2}{q\epsilon} \frac{dV}{d(1/C^2)} = \frac{2}{q\epsilon} \left( \frac{d(1/C^2)}{dV} \right)^{-1}$$



# Diffusion, Measurement of diffusion profile

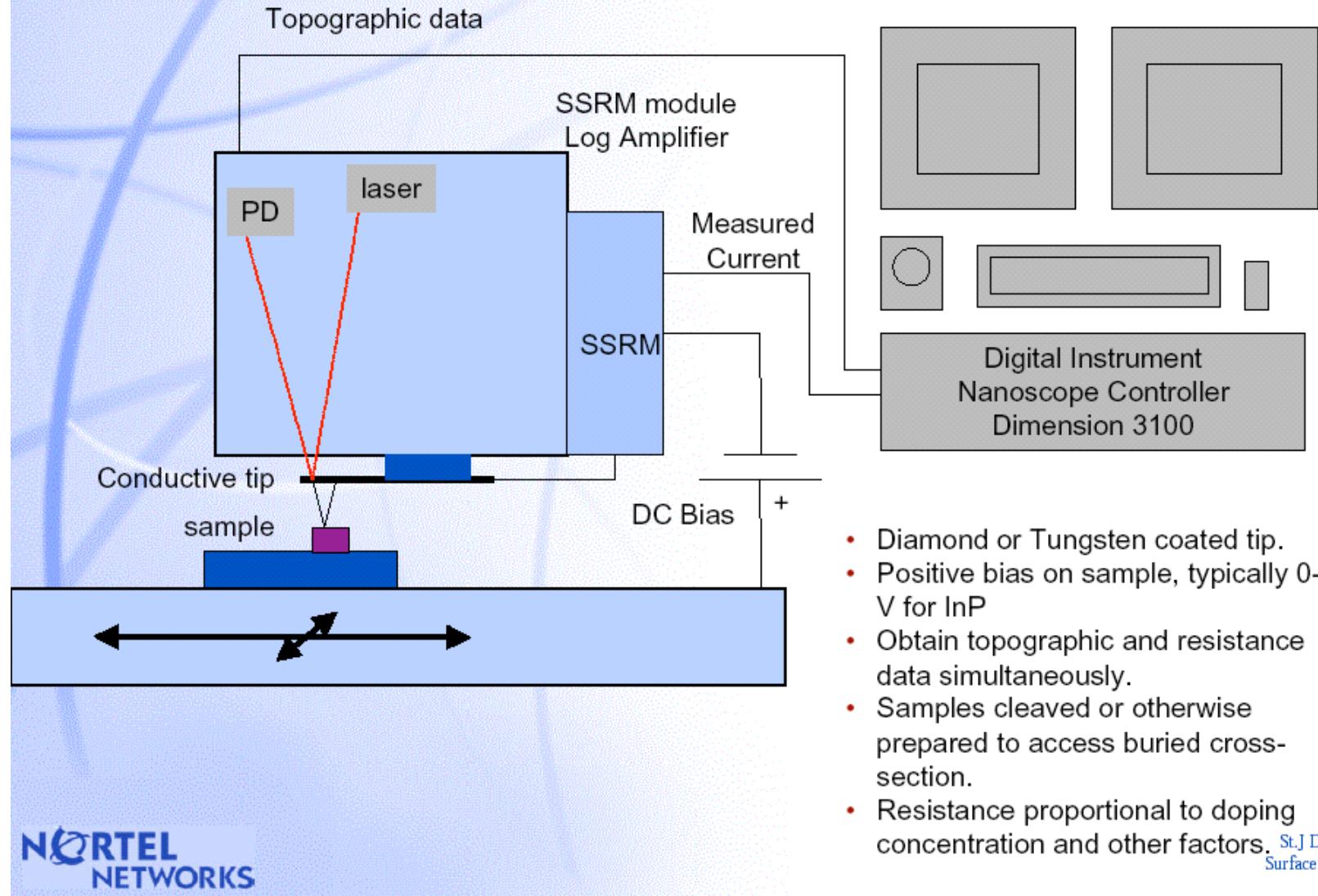
Scanning  
Probe  
Microscopy

SSRM  
SCM



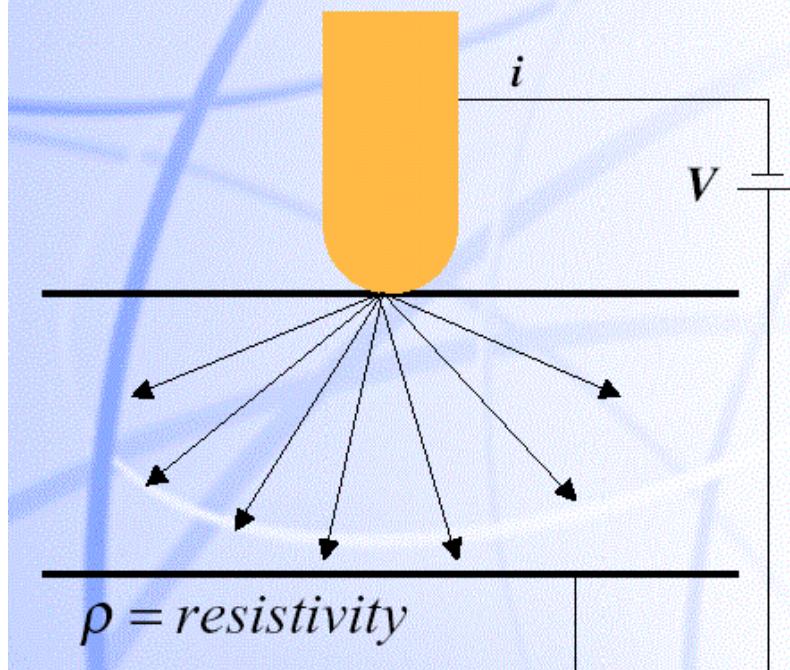
# Diffusion, Measurement of diffusion profile

## Scanning Spreading Resistance Microscopy



# Diffusion, Measurement of diffusion profile

## Simple SSRM Theory



$\rho = \text{resistivity}$

$\sigma = \text{conductivity}$

$n = \text{carrier concentration}$

$\mu = \text{carrier mobility}$

- 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

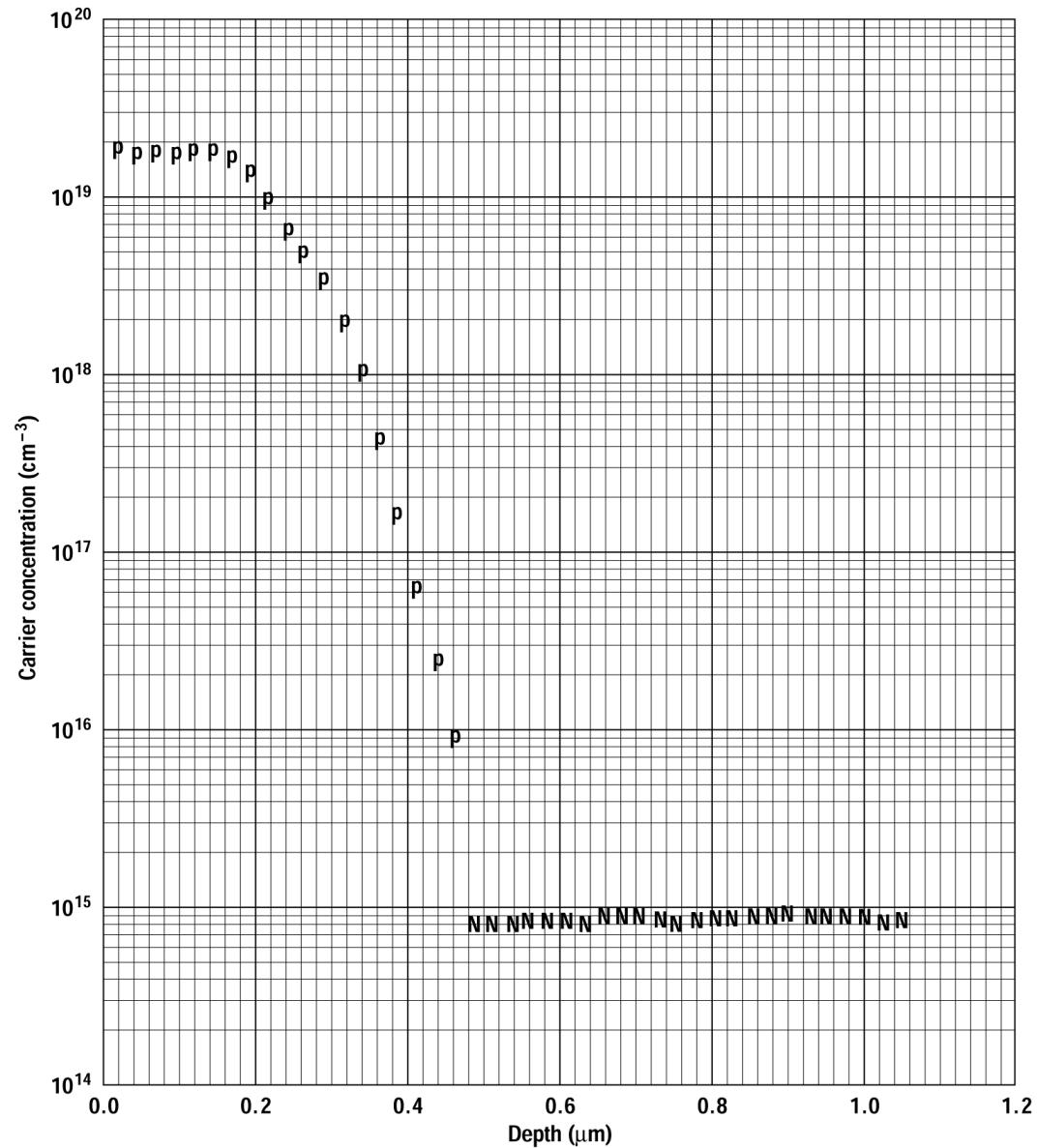
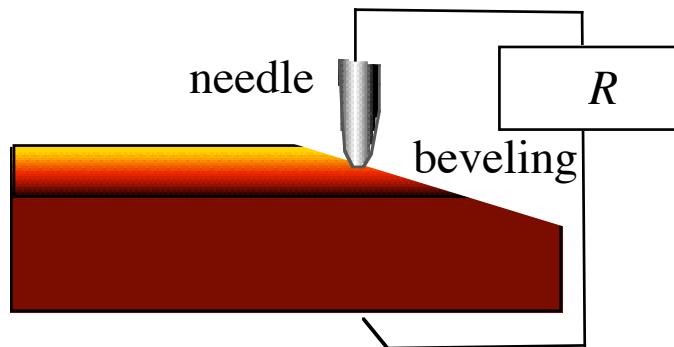
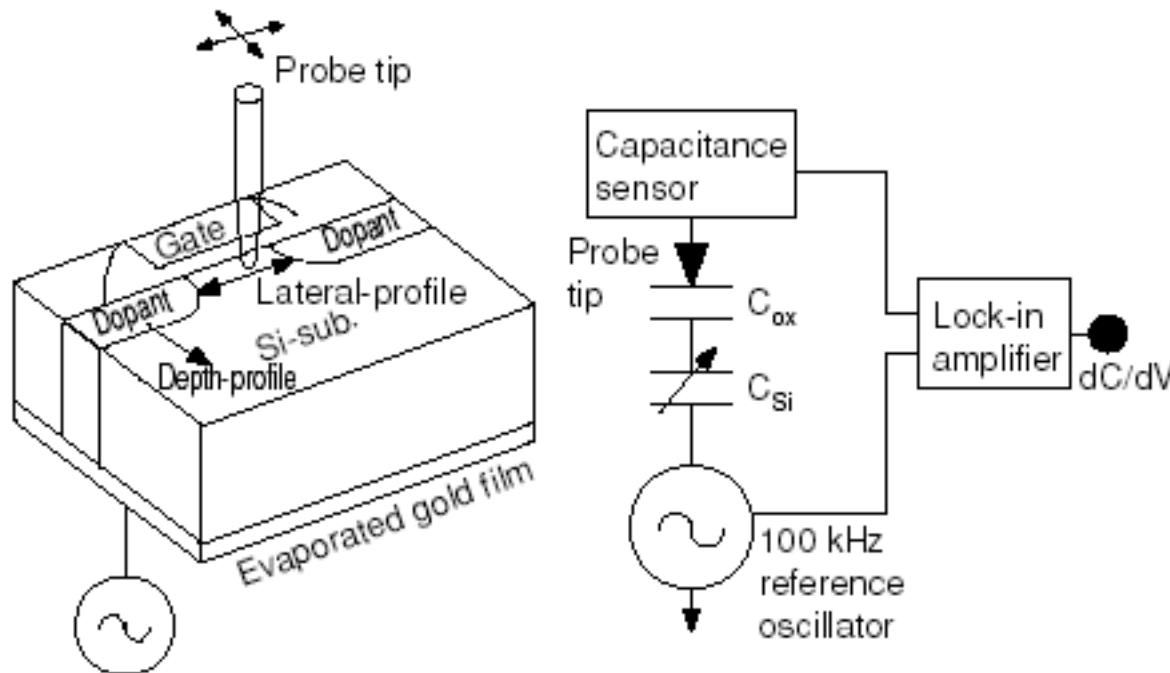


Figure 3.17 Typical spreading resistance profile showing measured carrier concentration as a function of depth (used with permission, Solecon Labs).

# Diffusion, Measurement of diffusion profile

## Scanning capacitance microscopy

Electric

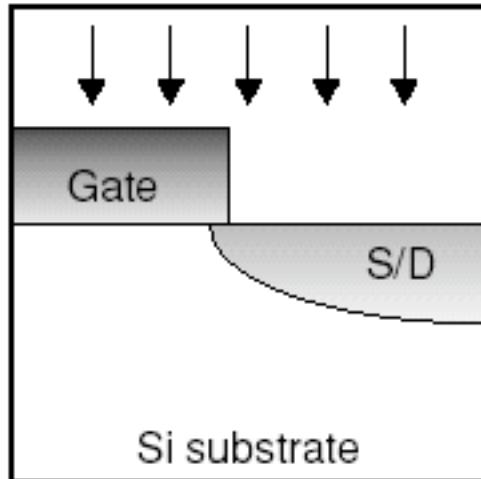


(a) Schematic model of SCM measurement

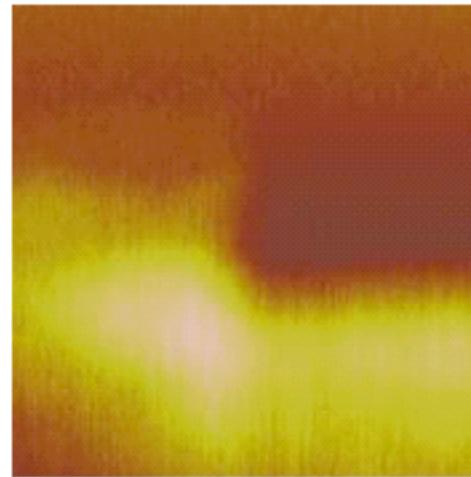
(b) Block diagram of SCM measurement

# Diffusion, Measurement of diffusion profile

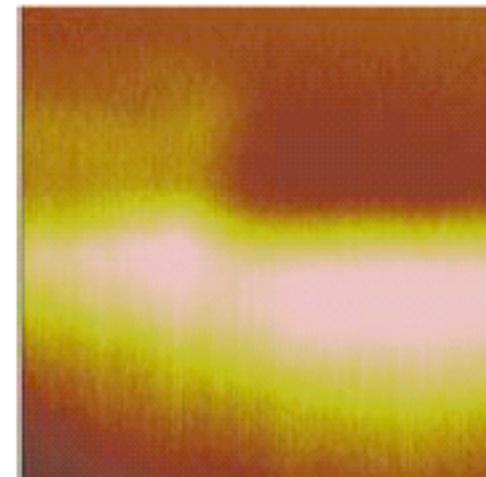
Scanning capacitance microscopy



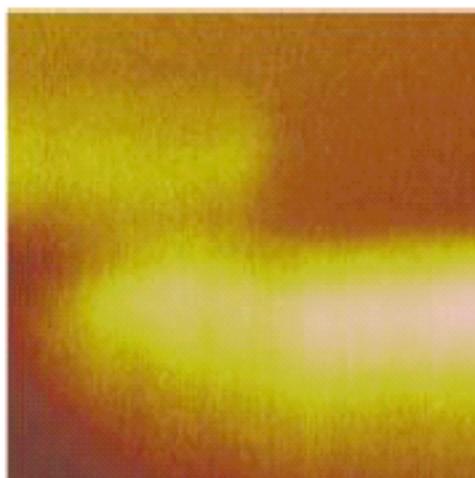
(a) Schematic model



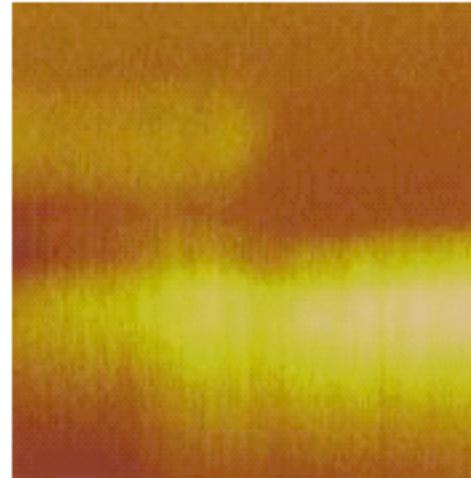
(b) DC = -1.0 V



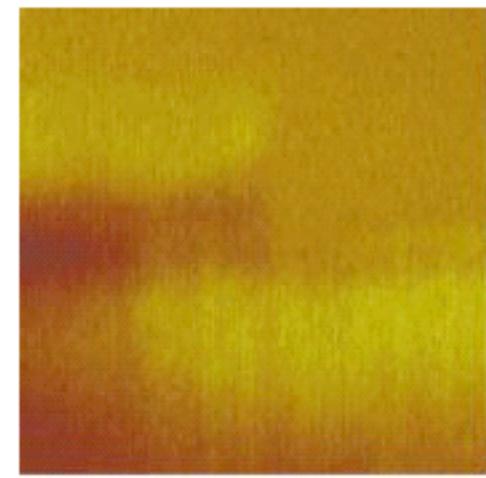
(c) DC = -0.5 V



(d) DC = 0 V



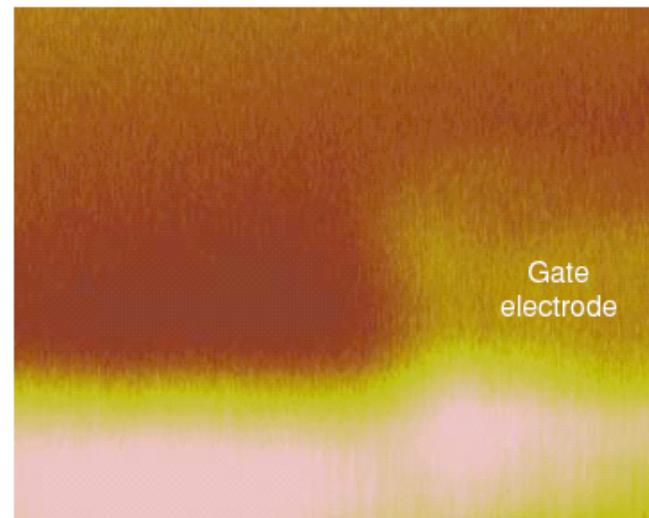
(e) DC = 0.5 V



(f) DC = 1.0 V

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

# Diffusion, Measurement of diffusion profile



(a) SCM image

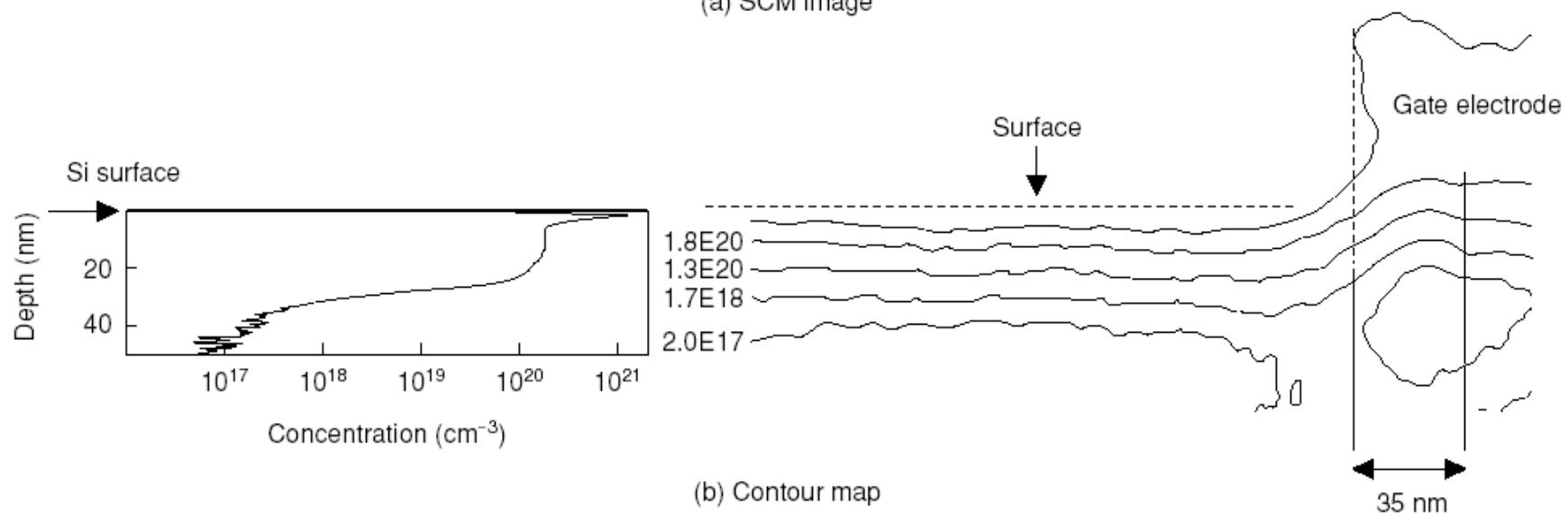
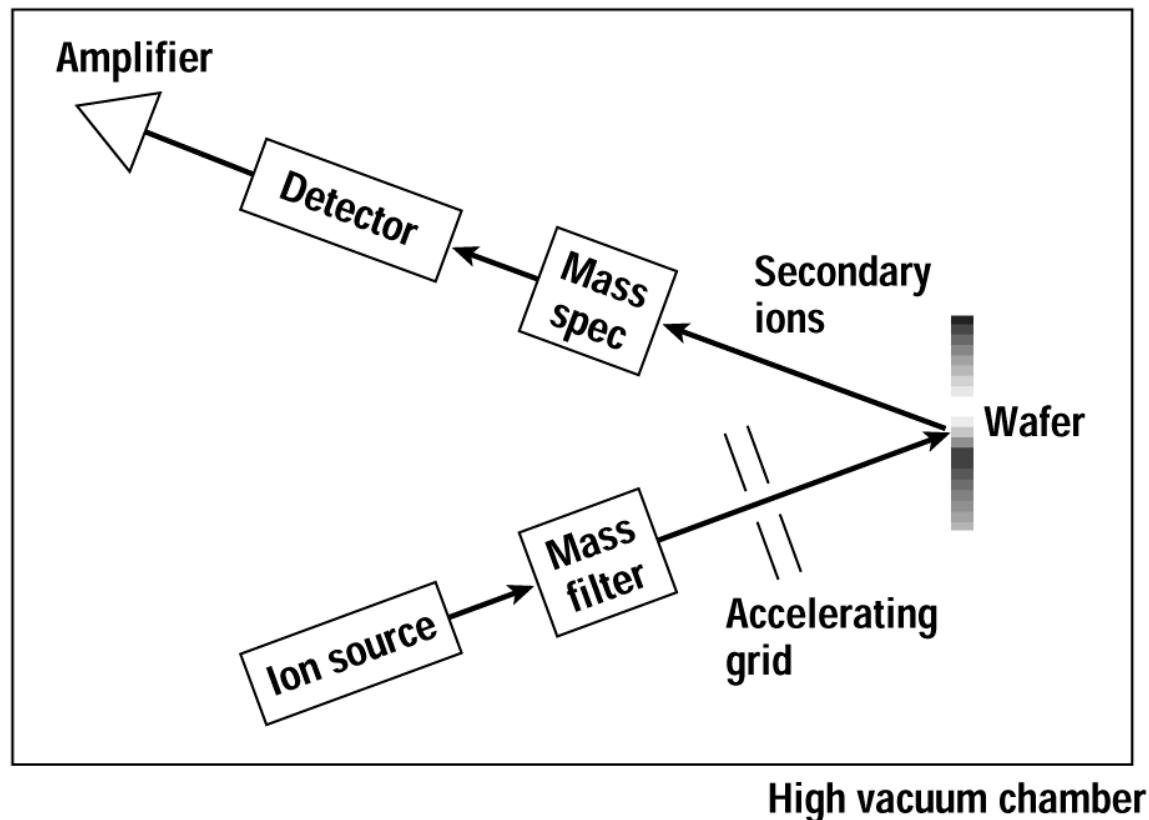


Figure 5

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,



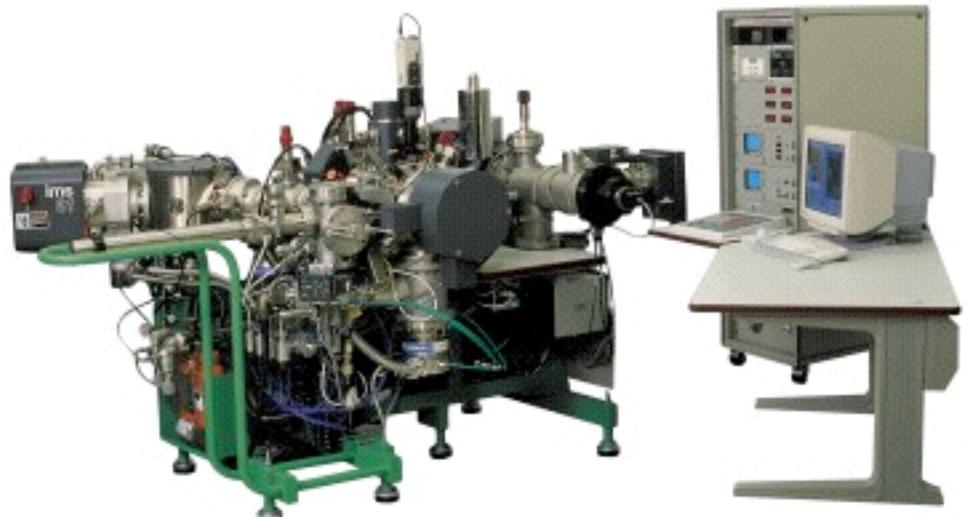
**Figure 3.18** A typical SIMS arrangement. The sample is bombarded by high-energy ions. The sputtered material is mass analyzed to determine the composition of the substrate.



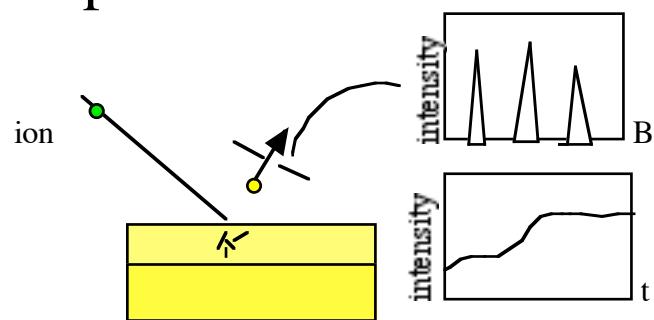
Equipment at MRL-Uo:

## 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  $10^{14}\text{cm}^{-3}$

### 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

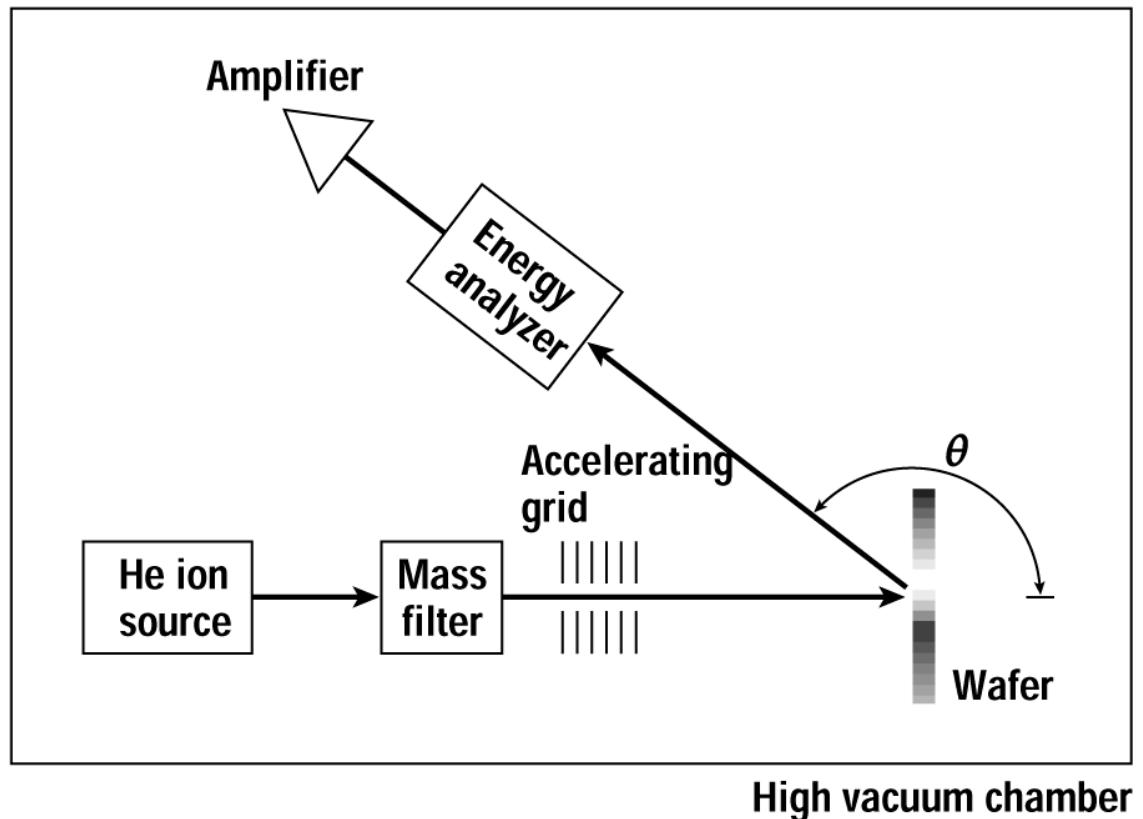
Absolute measurement

Depth resolution 10-30 nm

Sensitivity:

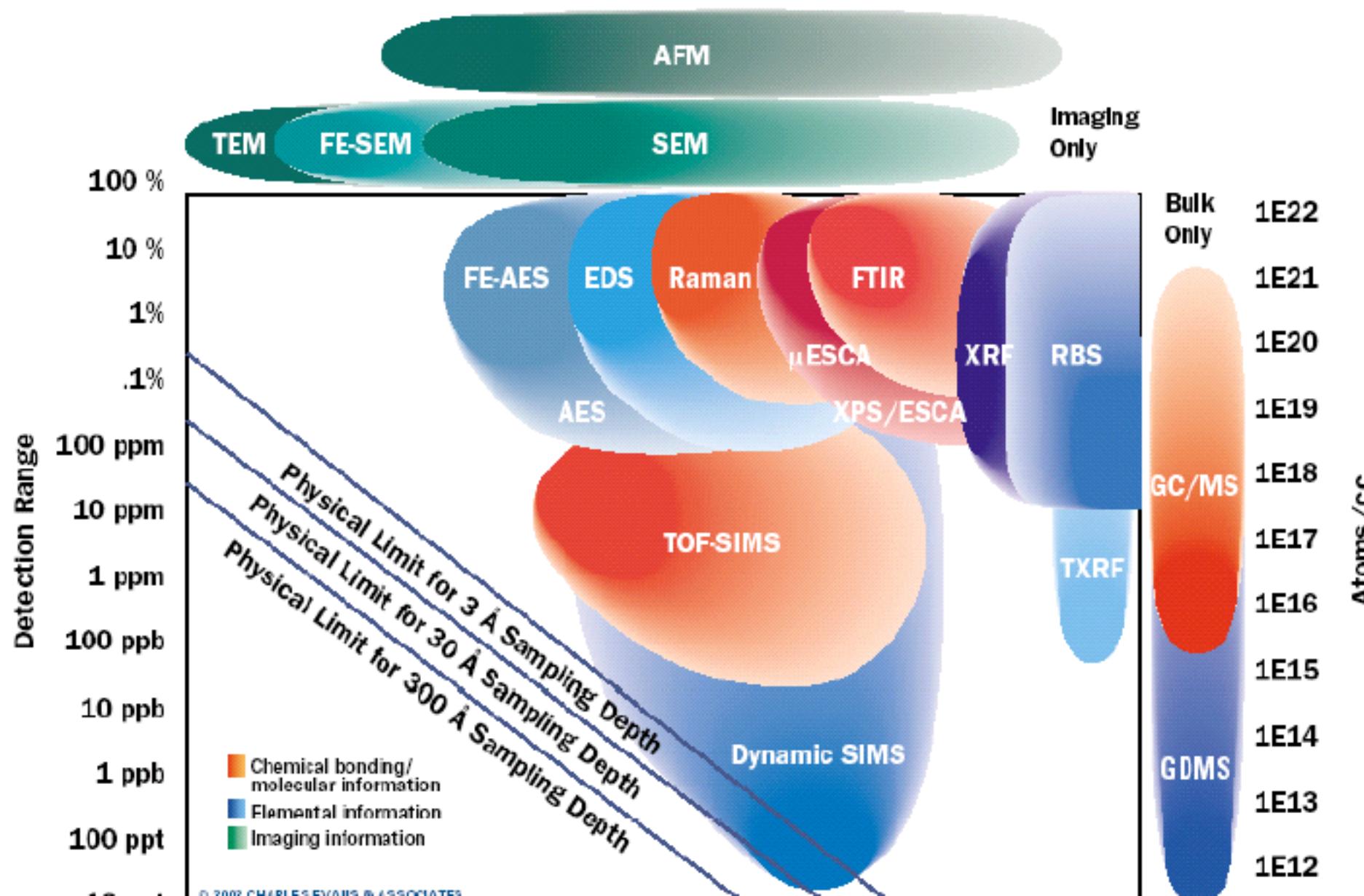
Matrix effects.

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

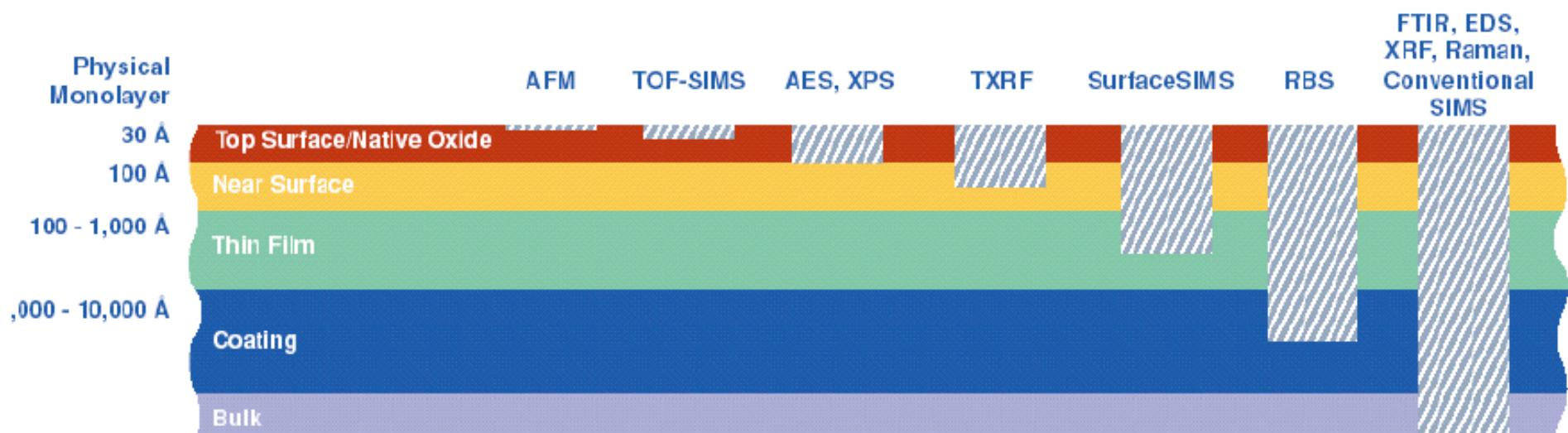


**Figure 3.19** In Rutherford backscattering, the energy of the backscattered helium ions can be used to determine the depth profile of the chemical composition of the wafer.

# Analytical Resolution versus Detection Limit

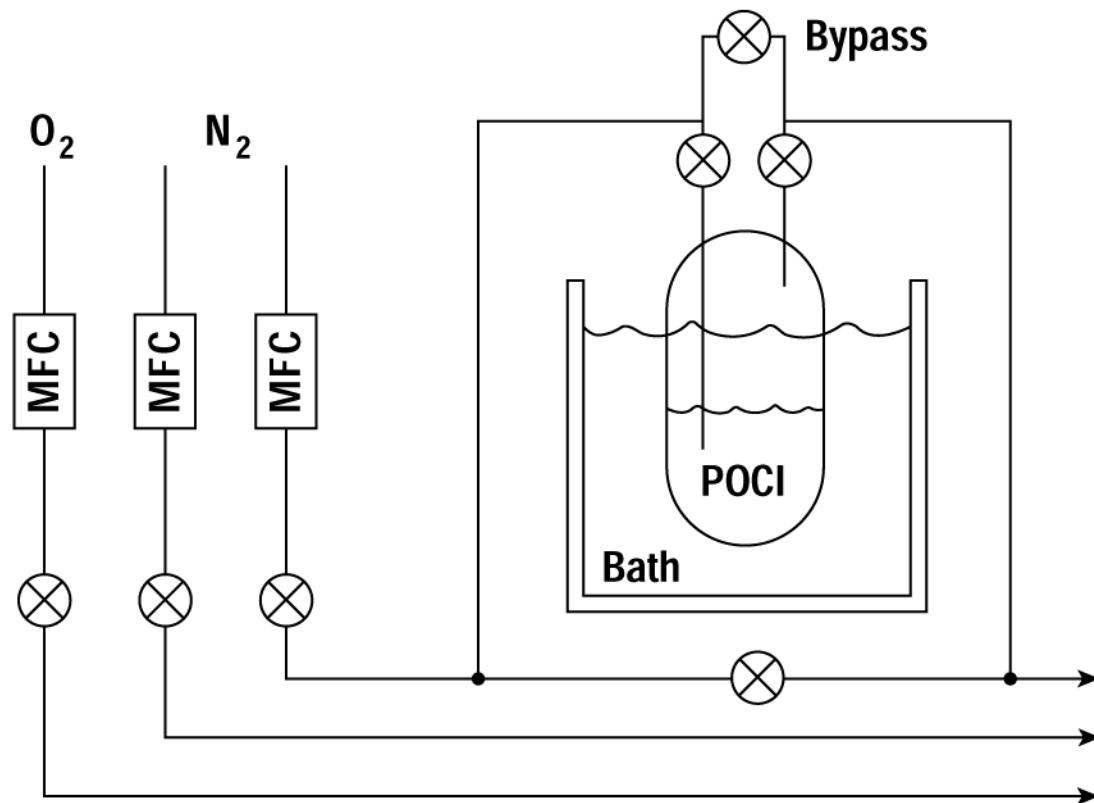


## Typical Analysis Depths for Techniques



# Diffusion, doping sources

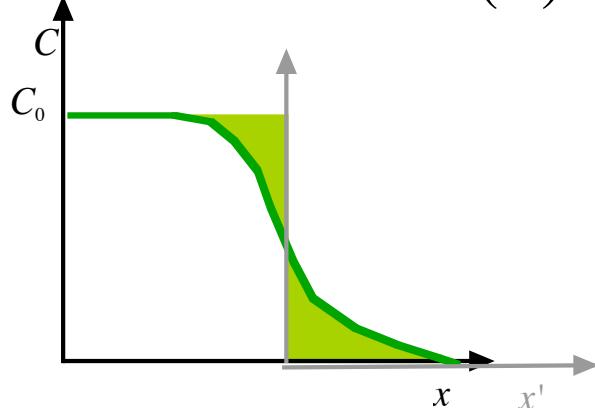
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**Figure 3.20** A typical bubbler arrangement for doping a silicon wafer using a  $POCl$  source. The gas flow is set using mass flow controllers (MFC).

## 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  $\lambda$

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

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

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

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

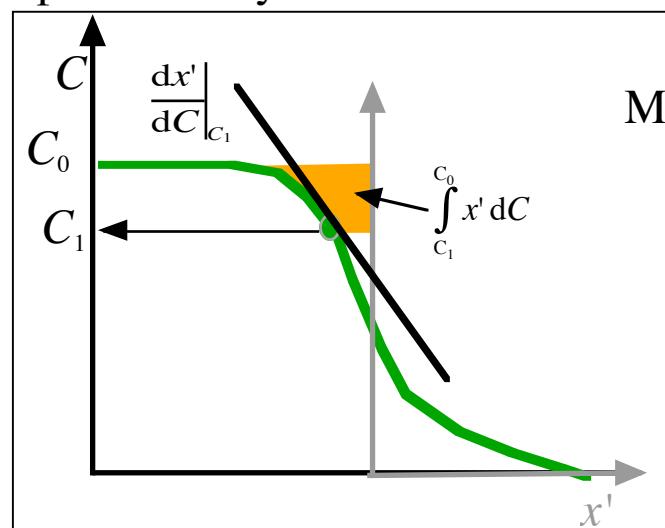
Slight rewriting:

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

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



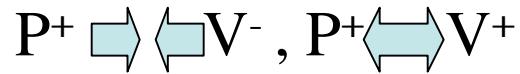
Method

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,  $P^+$

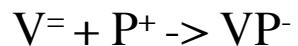


$$D_P = \left( D^* + D^- \frac{n}{n_i} + D^= \frac{n^2}{n_i^2} \right) \cdot h$$

Fair -Tsai model

Vacancies are created at the surface

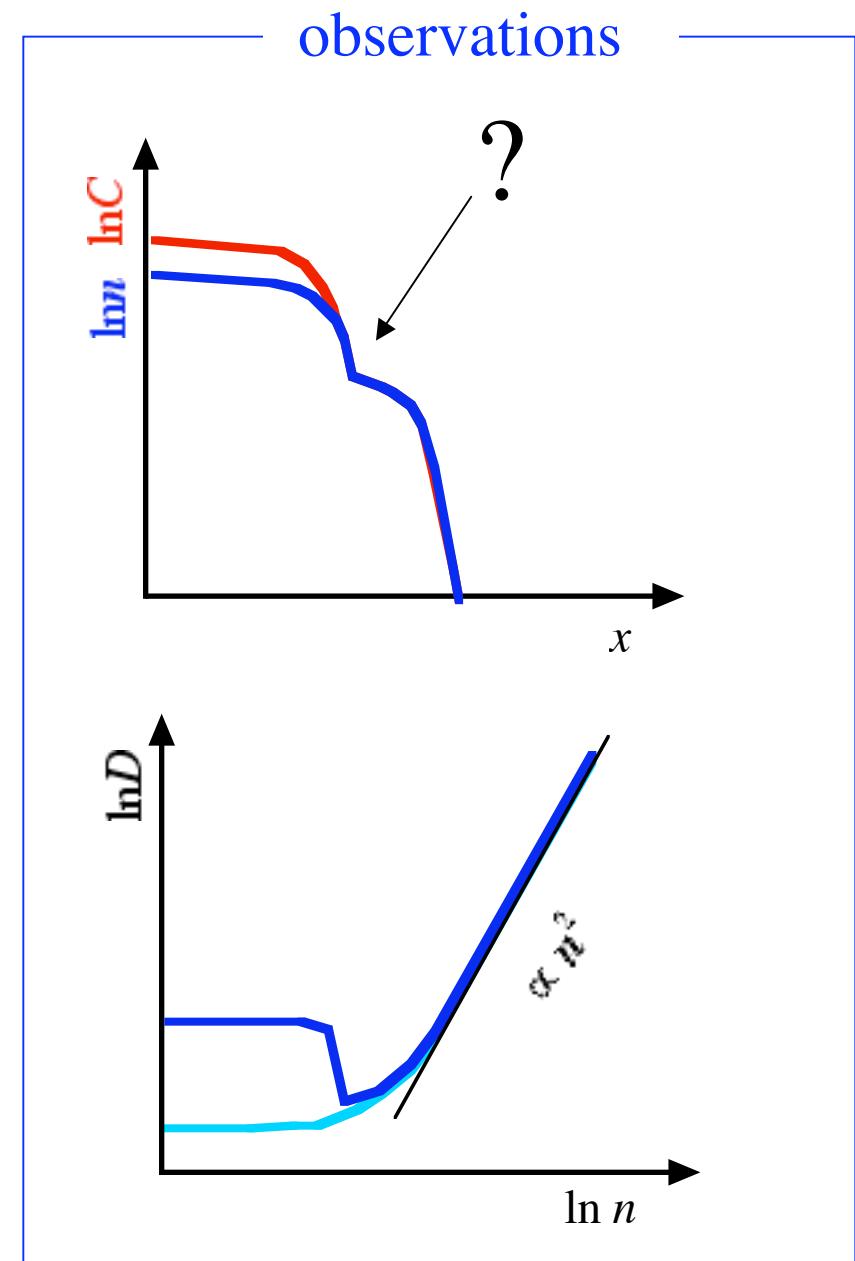
Conc of vac depends on  $n$  at surface



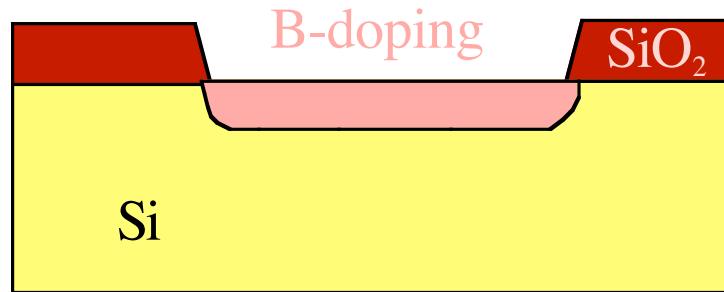
$E_C - E_F$  depends on depth when  $dC/dx < 0$

$VP^-$  breaks up  $\rightarrow$  excess vac'

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

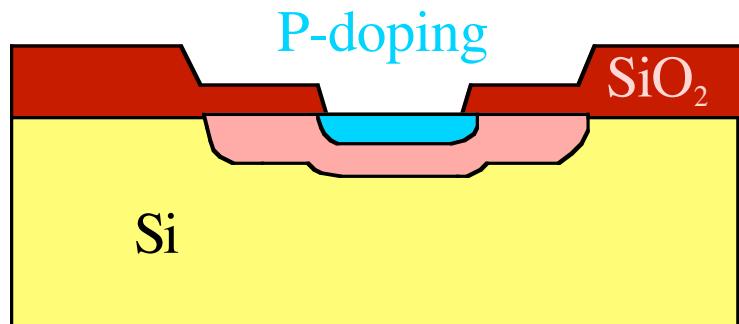


# Diffusion, "Emitter-push"



Many models

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

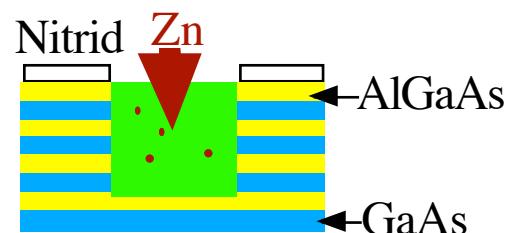
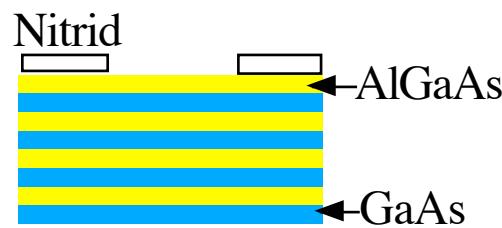
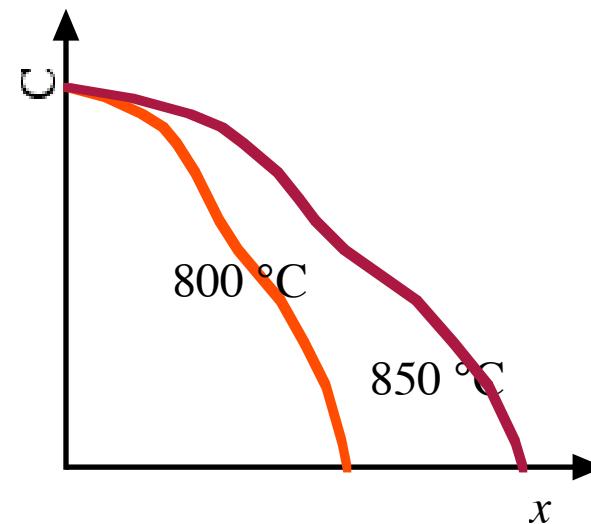
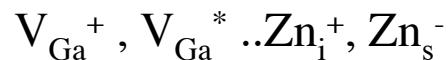
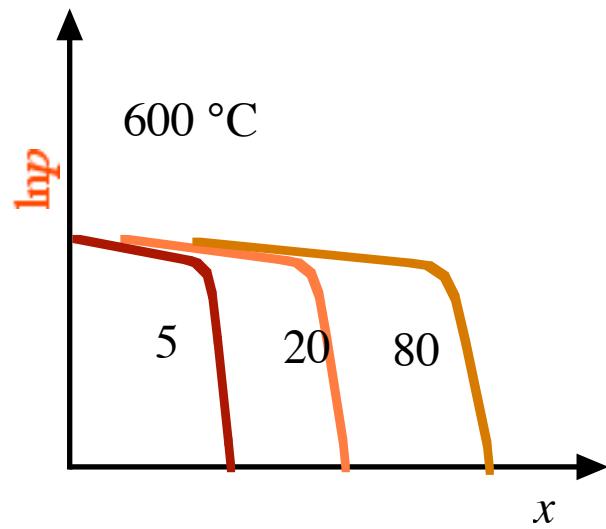


Describes results adequately

# Diffusion, Example: Zn i GaAs

Zn acceptor in GaAs , Substitutes for Ga

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



Confinement of waveguides, etc..