Processing (continued)

A gradient in concentration causes a flow — diffusion.

The flow: \[ F = -D \frac{\partial C}{\partial x} \]

\[ \frac{\partial C}{\partial t} = - \frac{\partial F}{\partial x} \quad \Rightarrow \quad \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \]

If \( D \) is a constant.

Example:

\[ C(x,0) = Q S(x) \]

Total dose.

Solution:

\[ C(x,t) = \frac{Q}{2\sqrt{\pi D t}} e^{-\frac{x^2}{4Dt}} \]

—— Gaussian.

Start w/ a Gaussian; always Gaussian.

Recall that the implanted profile is Gaussian to the 1st order.
Figure 7-15 Arrhenius plot of the intrinsic diffusivity of the common dopants in silicon.

Figure 7-16 Temperature dependence of the intrinsic diffusion coefficient of common dopants in silicon.
Anomalous diffusion behaviors

B diffusion
under different
ambients

And, this seems to be an effect "over
distance"!

We must look into the microscopic mechanisms
to understand this anomaly.

In the solid state, dopants don't diffuse
by themselves — assisted by point defects.

Vacancy assisted

Interstitial assisted.
A clever experiment

oxidation
stress
interstitial injection (generation)

Figure 7-37 Generalized representation of point-defect generation (G), recombination (R), and diffusion processes in silicon. In this example, local oxidation (right side) generates interstitials which diffuse away from the Si/SiO₂ interface, locally enhancing the diffusion of dopants like B or P, while causing interstitial type stacking faults to grow.

Figure 7-38 TSUPREM IV [7.14] simulation of the interstitial supersaturation generation in wet and dry O₂ at various temperatures. The oxidation time is chosen to be at the transition between the linear and parabolic regimes.

This equation is a specific version of the more general forms given in (6.49). The interstitial supersaturation results from the balance between the rate of interstitials at the oxidizing interface and the recombination rate of interstitials at the oxidizing interface and excess above the equilibrium value (or supersaturation) depends on...
Some dopants are more interstitial-assisted, some more vacancy assisted.

B & P: 100% interstitial
As: 40% interstitial, 60% vacancy
Sb: almost 100% vacancy

For Sb: oxidation $\rightarrow$ interstitial injection $\rightarrow$ vacancy population decrease due to recombination $\rightarrow$ oxidation-retarded diffusion (ORD)

---

How many defects are there?

Under equilibrium,

$$C_{I_0} = 1 \times 10^{27} \text{ cm}^{-3} \cdot e^{-\frac{3.8 \text{ eV}}{kT}}$$

$$C_{V_0} = 9 \times 10^{23} \text{ cm}^{-3} \cdot e^{-\frac{2.6 \text{ eV}}{kT}}$$

*zero charge*

@ 1800°C, $C_{I_0} = 10^{12} \text{ cm}^{-3}$, $C_{V_0} = 5 \times 10^{13} \text{ cm}^{-3}$

Do you think these #s are big or small?
Another anomaly:

For high implant doses (e.g. used for S/D, > ~10^{14} \text{cm}^{-2}), diffusion is anomalously faster than usual in early stages of annealing.

**Transient-Enhanced Diffusion (TED)**

\[
\text{Implant} \rightarrow \text{defects} \\
\downarrow \\
\text{Most interstitials & vacancies recombine.} \\
\downarrow \\
\text{In} \sim 10^{-2} \text{ s, only interstitials are those kicked out by the dopants.} \\
\downarrow \\
\text{At high doses, the interstitials cluster up.} \\
\text{The clusters dissolve & release interstitials slowly} \Rightarrow C_I > \text{Equilibrium value} \\
\downarrow \\
\text{Enhanced diffusion.}
\]