Kinds of Impurities

- **Interstitial Impurities**
  - Impurity is not a part of the crystal lattice (thus, is not acting as a dopant)
  - Can diffuse very quickly
  - Examples: transition elements (Cu, Fe, Au, Ni)
- **Substitutional Impurities**
  - Atom occupies a lattice position in place of Si
  - Diffusion is slow – bonds must be broken

Mechanisms for Diffusion

- **Direct Exchange**
  - Impurity swaps position with a neighboring silicon
  - 6 or 7 bonds must be broken

- **Vacancy Exchange**
  - Impurity moves into an adjacent vacancy
  - Only 3 bonds must be broken
  - Lower energy = more likely = faster
  - Vacancies are often charged, which affects rate of exchange since dopant is ionized

Other Mechanisms

- **Transient Enhanced Diffusion**
  - At the beginning of the anneal step, the implant-damaged silicon is amorphous
  - Dopants can diffuse quickly through the amorphous material
  - Thus, at the very beginning of the anneal step, diffusion is rapid (TED)

- **Interstitialcy Mechanism**
  - Silicon self-interstitials move around then displace a lattice atom
  - If a lattice atom is a dopant, it becomes an interstitial and can rapidly diffuse before displacing a different lattice atom
Other Mechanisms (2)

- Oxidation during diffusion
  - Often oxidation accompanies diffusion (whether desired or not)
  - Boron is more soluble in oxide than silicon, but all the n-type dopants are less soluble in oxide
  - The result is a redistribution of dopant in the silicon just below the oxide interface

\[
\text{segregation coefficient } m = \frac{\text{Conc. in Si}}{\text{Conc. in SiO}_2}
\]

For Boron, \( m = 0.2 - 0.7 \); for n-type dopants, \( m = 10 \)

Electric Field Enhancement

- Charge carriers diffuse faster than dopants, creating a built-in voltage (especially near the junction)
- This results in an electric field that pushes the ionized dopants, enhancing their diffusion
- Approximate result (for a single impurity):

\[
D_{\text{enhanced}} = D (1 + \eta)
\]

\[
\eta = \frac{C(x) \sqrt[4]{C^2(x) + 4n^2}}{n^2}
\]

Impact of Non-constant Diffusivity

- In general, analytical solutions are only available for constant diffusivity and simple boundary conditions
- For other cases, numerical solutions are required
- A popular simulator is Supreme (Stanford University Process Modeling), and its commercial variants
- 2D oxidation and diffusion simulation

Solving Diffusion Problems

- Solving Diffusion Problems

Multiple Diffusion Steps

- Wafer processing involves many high temperature steps
  - For each step, there is more diffusion
- Recall the analytical solution of a Gaussian dopant distribution that diffuses
  - The final variance equals the original variance plus the diffusion length squared
- The total effect of all high temperature steps is approximately

\[
D_{\text{eff}} = D_1 + D_2 + D_3 + \ldots
\]

- In general, the highest temperature process dominates
- It is critical to control the entire thermal budget of the process

Characterizing Diffused Dopants

- C-V curves
- Sheet resistance measurements

\[
R = \rho \frac{L}{A} = \left( \frac{L}{W} \right) \rho L
\]

- Cross-section, decorate/stain, measure in SEM
- Secondary Ion Mass Spectroscopy (SIMS)
Lecture 15: What have we learned?

- How does charge in a vacancy affect diffusivity?
- What is the main cause of the concentration dependence of the diffusivity of dopants in silicon?
- Define `transient-enhanced diffusion`.
- What is electric field enhancement of diffusivity?
- Explain how the overall thermal budget for dopant diffusion is accounted for.