CHE323/CHE384
Chemical Processes for Micro- and Nanofabrication
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Lecture 15
Diffusion, part 3

Chris A. Mack
Adjunct Associate Professor

Reading:
Chapter 3, *Fabrication Engineering at the Micro- and Nanoscale*, 4th edition, Campbell

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

(substitutional impurities)

- 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

Mechanisms for Diffusion

- Example: N-type, ionized donor atom (+ charge)
- Let D^- be the diffusivity into a negatively charged vacancy

$$\text{overall diffusivity} \propto D^- \times \text{Probability the vacancy is negatively charged} = D^- \left(\frac{n}{n_i}\right)$$

- Add neutral and doubly negative vacancy diffusion

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

Mechanisms for Diffusion

- For n-type material, $n \approx N_D$
- Therefore, diffusivity is concentration dependent, $D(N_D)$, increasing with higher doping levels
- The same is true for positively charged vacancies and p-type material
- Near the junction, $n \approx p \approx n_i$, so both positively and negatively charged vacancies may affect diffusion

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

$$segration\ coefficient\ m = \frac{Conc.\ in\ Si}{Conc.\ in\ SiO_2}$$

For Boron, m ≈ 0.2 – 0.7; for n-type dopants, m ≈ 10

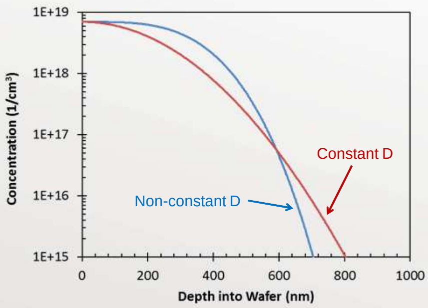
Electric Field Enhancement

- 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):

$$D_{enhanced} = D(1+\eta)$$

$$\eta \approx \frac{C(z)}{\sqrt{C^2(z) + 4n_i{}^2}}$$

Impact of Non-constant Diffusivity



Solving Diffusion Problems

- 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

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

$$Dt_{eff} = Dt_1 + Dt_2 + Dt_3 + \ldots$$

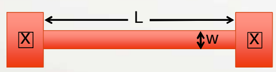
- In general, the highest temperature process dominates
- It is critical to control the entire thermal budget of the process

Characterizing Diffused Dopants

- C-V curves
- Sheet resistance measurements

$$R = \rho\frac{L}{A} = \left(\frac{\rho}{t}\right)\left(\frac{L}{W}\right)$$

R_s



- 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