Defects and “Damage”

- Point Defects, Point Defects clusters. Line Defects, Extended Defects

- Ion Implantation Defects
  Amorphization
  Secondary Defects (end-of-range loops)

- Effect of defects on
  - Electrical resistivity
  - PN junction leakage current
  - Diffusion
  - Mechanical stress
Simple Point Defects (Elemental crystal)
More complicated Point Defects (AB compound)
Si Native Point Defects

1) Thermal-equilibrium values of Si neutral interstitials and vacancies at diffusion temperatures << doping concentration of interest (10^{15} – 10^{20} /cm^3)

\[ C^*_I \approx 1 \times 10^{27} \exp\left(-\frac{3.8 \text{ eV}}{kT}\right) \]

\[ C^*_V \approx 9 \times 10^{23} \exp\left(-\frac{2.6 \text{ eV}}{kT}\right) \]

At 1000^oC, \( C_{I_0}^* \sim 10^{12} /\text{cm}^3 \)
\( C_{V_0}^* \sim 10^{13} /\text{cm}^3 \)

2) Diffusivity of Si interstitials and Si vacancies >> diffusivity of dopants

\[ d_I = 1.58 \times 10^{-1} \exp\left(-\frac{1.37}{kT}\right) \text{cm}^2 \text{sec}^{-1} \]

\[ d_V = 1.18 \times 10^{-4} \exp\left(-\frac{0.1}{kT}\right) \text{cm}^2 \text{sec}^{-1} \]
Neutral and Charged Point Defects

(a) 

$v^+$  

$b^0$  

$v^-$

(b) 

Tetrahedral Interstitial 

Hexagonal Interstitial

(c) 

$(Al)^0$, acceptor $I^+$  

$(Al)^-$, acceptor $I^0$  

$(Al)^+$, donor
Line Defects (dislocations)

A dislocation line can:
• Create mechanical stress
• Getter Impurities
Movement of Dislocation can create slippage
FIGURE 7.4 A Ge$_x$Si$_{1-x}$ film and a Si single-crystal substrate are joined to form a lattice-mismatched heterostructure that is either strained or unstrained with misfit dislocations.
Two-Dimensional Defects

Grain Boundary

Twins Boundary
Polycrystalline Solids

Amorphous Solids

Silicate Glass

Polymers
Implantation “Damage”

Substrate Interstitials and Vacancies are created by momentum transfer collision process
**End-of-Range “EOR” Dislocation Loops**

- **Recoiled Si**
- More Vacancies $\text{Si}_V$
- More Interstitials $\text{Si}_I$
- **annealing**
  - extra plane of Si atoms
  - “Extrinsic” dislocation loops

*This is called “secondary” defect because it is caused by the primary point defects created by ion implantation.*

Plummer et al, *Si VLSI Technology*
Dopant Activation

From 450 to 550°C, Si interstitials compete with B for Si substitutional sites or Si interstitials pairs with B to form inactive complex.
Example: Poly-Si

- Average grain size depends on deposition, doping conc & annealing conditions!
Electrical Resistivity of Polycrystalline Materials

• For metals, GB has negligible effect
• For doped semiconductors, poly material has higher resistivity than single-crystal material

Trapped charges at GB create energy barriers for mobile carriers
Defects and PN Junction Leakage current

Native Si points defects, or some special impurities trapped by point/line/extended defects can create additional electronic states inside the energy gap. The inter-gap states will increase reverse biased current of a pn junction.

Excessive leakage current
How processing steps affect point defect concentrations

• **Neutral** interstitial and vacancy point defects present at thermal equilibrium

  At 1000°C, \( C_{\text{lo}}^* \sim 10^{12} / \text{cm}^3 \)
  \( C_{\text{Vo}}^* \sim 10^{13} / \text{cm}^3 \)

• **Charged** Point Defects enhanced by heavy doping; total point defect concentrations enhanced by ~10x

  \( I^+, I^0, I^- \)
  \( V^+, V^0, V^-, V^- \)

• Point defects Injected by interfaces during oxidation
  (total point concentrations enhanced by ~10x)

• **Implantation collisions** (total point defect concentration enhanced by ~ 1000X)
Diffusion Mechanisms in Si

(A) No Si Native Point Defect Required

Example: Cu, Fe, Li, H

(a) Interstitial Diffusion
Diffusion Mechanisms in Si

(B) Si Native Point Defects Required (Si vacancy and Si interstitials)

Example: Dopants in Si (e.g. B, P, As, Sb)

(a) Substitutional Diffusion

(b) Interstitialcy Diffusion

Figure 3.5 In interstitialcy diffusion an interstitial silicon atom displaces a substitutional impurity, driving it to an interstitial site where it diffuses some distance before it returns to a substitutional site.
Diffusivity Comparison:
Dopants, Si interstitial, and interstitial diffusers

\[ \text{Diffusivity (cm}^2\text{ sec}^{-1}) \]

\[ T(\ ^\circ\text{C}) \]

1200 1100 1000 900 800

\[ \text{Cu, Au}_I, \text{Fe, Cr, Pt, Ti, Au}_S, \text{Si, As, B, P} \]

Interstitial Diffusers

Dopants

\[ 10^8 \text{ times higher} \]

For reference only

Figure 4–8 Diffusivities of various species in silicon. \(	ext{Au}_S\) refers to gold in substitutional form (on a lattice site); \(	ext{Au}_I\) to gold in an interstitial site. The silicon interstitial (I) diffusivity is also shown and will be discussed later. The gray area representing the I diffusivity indicates the uncertainty in this parameter. (After [4.10, 4.11].)
Diffusivity along defect paths

Surface diffusion
> GB diffusion
> Bulk diffusion
Defects and Thin-film Stress

– Growth morphology

– Lattice misfit†

– Phase transformation

Defects can create intrinsic thin-film stress which is of big concern for MEMS fabrication and small-feature IC devices
Relevance of Defects to Microfabrication

• Deposited thin films are usually polycrystalline or amorphous. One can obtain single-crystal film only with special Epitaxial Growth conditions (i.e., monocrystalline substrate, ultra-clean surface, and high deposition temperature)

• Monocrystalline semiconductor is needed for active regions of high-performance devices such as integrated circuits. If polycrystalline or amorphous semiconductors is used, performance will be compromised (e.g. Poly-Si thin-film transistors, amorphous Si solar cells)

• Heavily doped Poly-Si can be used as a metallic conductor (e.g, the gate material of a MOSFET which is not part of the active device region)

• Point defect concentration and their distribution controls the diffusivity of dopants

• Defects (and the impurities they can trap) will give excess leakage current in active device regions (e.g. pn junctions)

• Defects alter the mechanical properties (build-in stress, fracture strength, etc) of thin films