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 \textit{neutral} interstitials and vacancies at diffusion temperatures

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

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

At 1000\degree C,

\[ C_{Io}^* \sim 10^{12} \text{ /cm}^3 \]

\[ C_{Vo}^* \sim 10^{13} \text{ /cm}^3 \]

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) $v^+$, $v^0$, $v^-$

(b) Tetrahedral Interstitial
Hexagonal Interstitial

(c) $(Al)^0$, acceptor $I^+$
$(Al)^-$, acceptor $I^0$
$(Al)^+$, donor
A dislocation line can:
• Create mechanical stress
• Getter Impurities
Movement of Dislocation can create slippage
Misfit Dislocation of Epitaxial layers

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

*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 interstitial 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 Juncion 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.

\[ I_d \]

\[ V_d \]

Excessive leakage current

*Energy band diagram* shows the bottom edge of conduction band, \( E_c \), and top edge of valence band, \( E_v \).

\( E_c \) and \( E_v \) are separated by the band gap energy, \( E_g \).
How processing steps affect point defect concentrations

• **Neutral** interstitial and vacancy point defects present at thermal equilibrium
  
  \[
  At \ 1000^\circ C, \ C_{I_0}^* \sim 10^{12} \text{ /cm}^3 \\
  C_{V_0}^* \sim 10^{13} \text{ /cm}^3
  \]

• **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

\[ \text{Diffusion Mechanism in Si} \]

\[ \text{Example: Cu, Fe, Li, H} \]

\[ \text{(a) Interstitial Diffusion} \]

\[ \text{Fast Diffusion} \]
(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

For reference only

Figure 4–8  Diffusivities of various species in silicon. Au₅ refers to gold in substitutional form (on a lattice site); Auₓ 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 typically polycrystalline or amorphous. One can obtain single-crystal film only with special Epitaxial Growth conditions (monocrystalline substrate, ultras-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).

• 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 trap) will give excess leakage current in active device regions (e.g. pn junctions).

• Defects alter the mechanical properties of thin films.