Defects and "Damage"

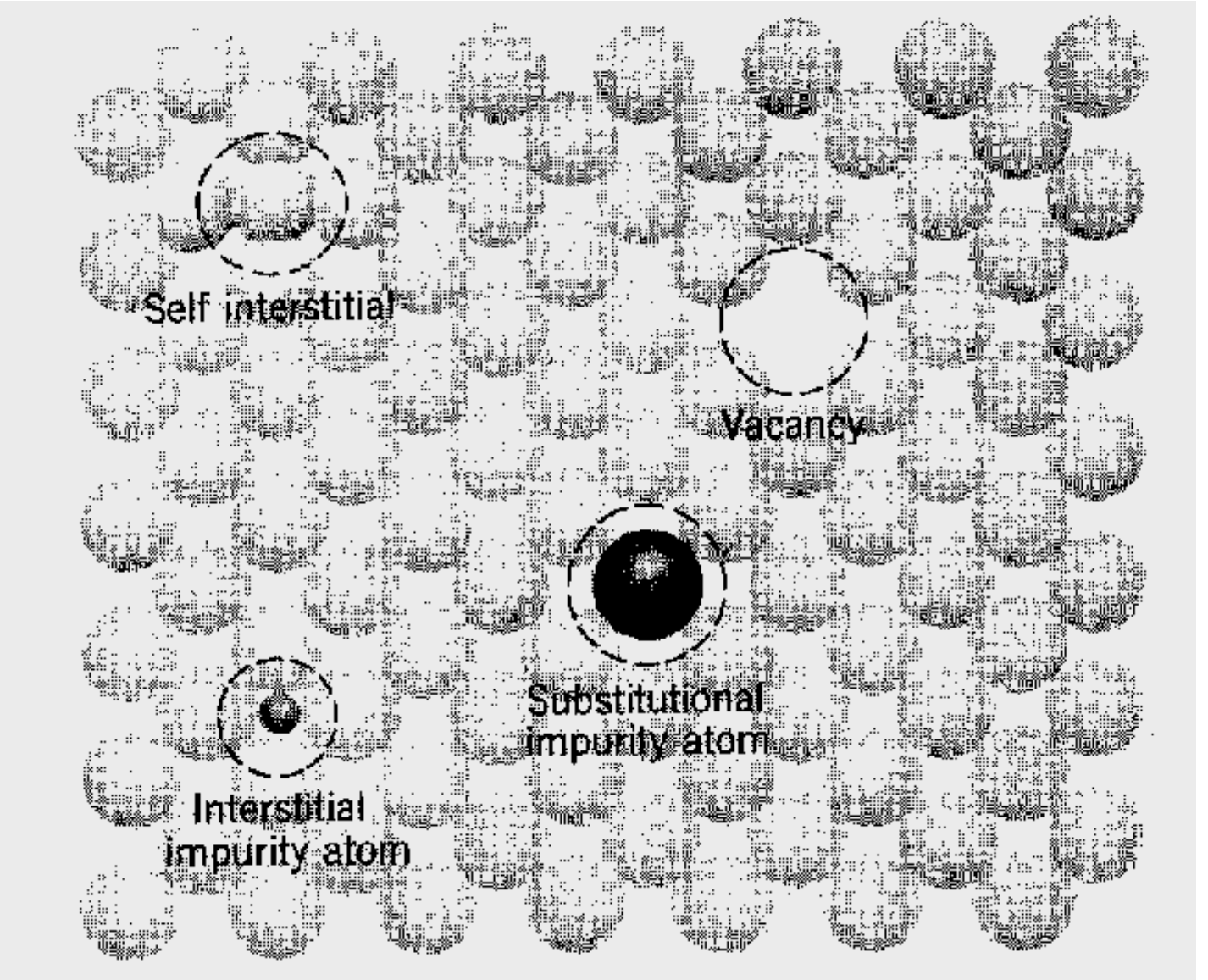
- **Point Defects, Point Defects clusters. Line Defects, Extended Defects**

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

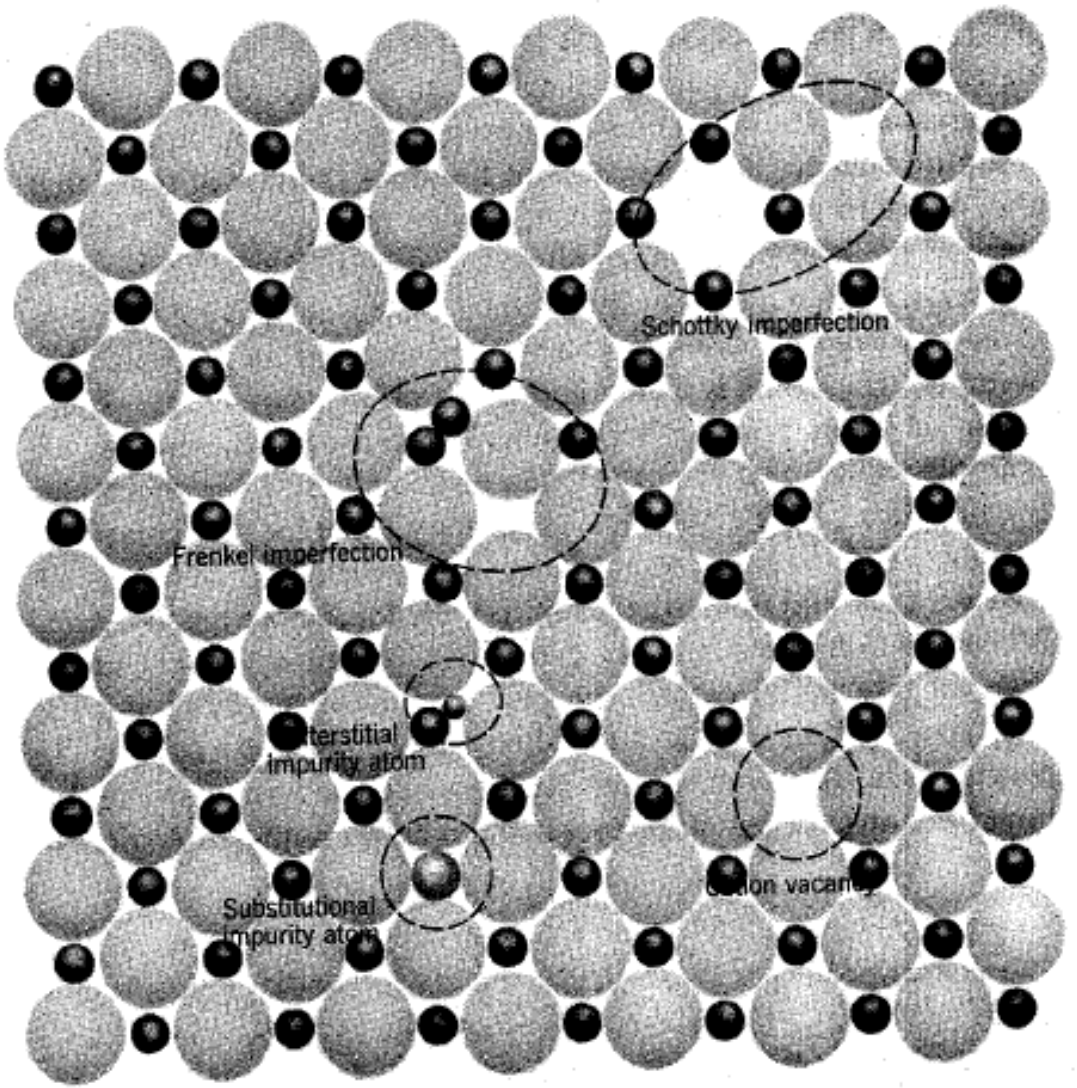
- **Effect of defects on**

  -Electrical resistivity
  -PN junction leakage current
  -Diffusion
  -Mechanical stress

Simple Point Defects (Elemental crystal)

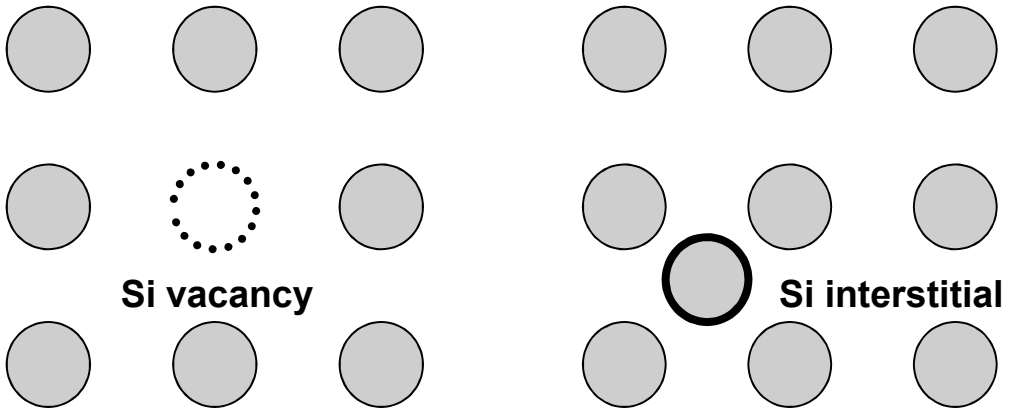


More complicated Point Defects (AB compound)



For reference only

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)

$$C_{I^0}^* \cong 1 \times 10^{27} \exp\left(\frac{-3.8\ \text{eV}}{kT}\right)$$

$$C_{V^0}^* \cong 9 \times 10^{23} \exp\left(\frac{-2.6\ \text{eV}}{kT}\right)$$

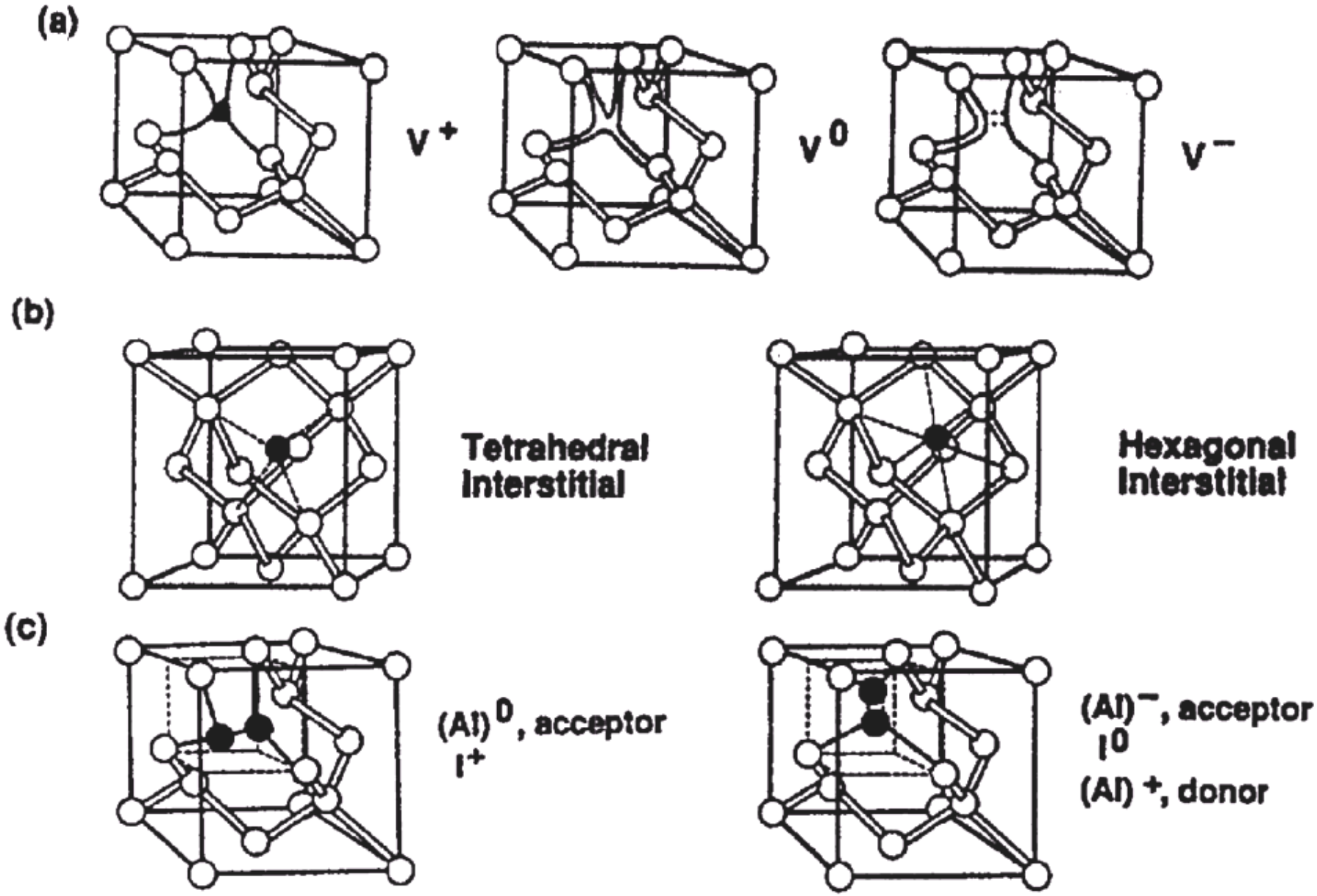
At 1000°C, $C_{Io}^* \sim 10^{12}$ /cm3
$C_{Vo}^* \sim 10^{13}$ /cm3

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

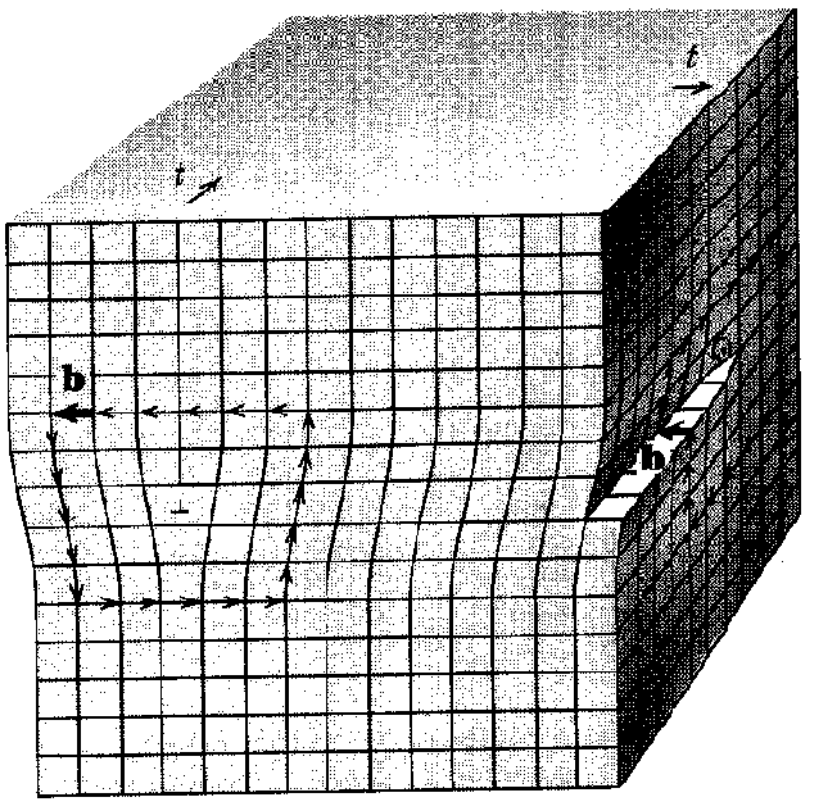
$$d_I = 1.58 \times 10^{-1} \exp\left(-\frac{1.37}{kT}\right) \text{cm}^2\ \text{sec}^{-1}$$

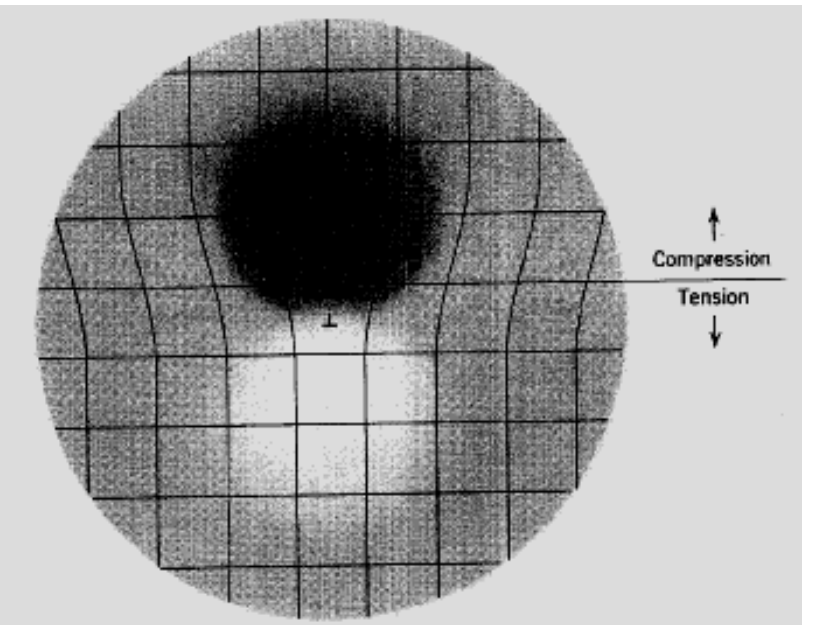
$$d_V = 1.18 \times 10^{-4} \exp\left(-\frac{0.1}{kT}\right) \text{cm}^2\ \text{sec}^{-1}$$

Neutral and Charged Point Defects



Line Defects (dislocations)

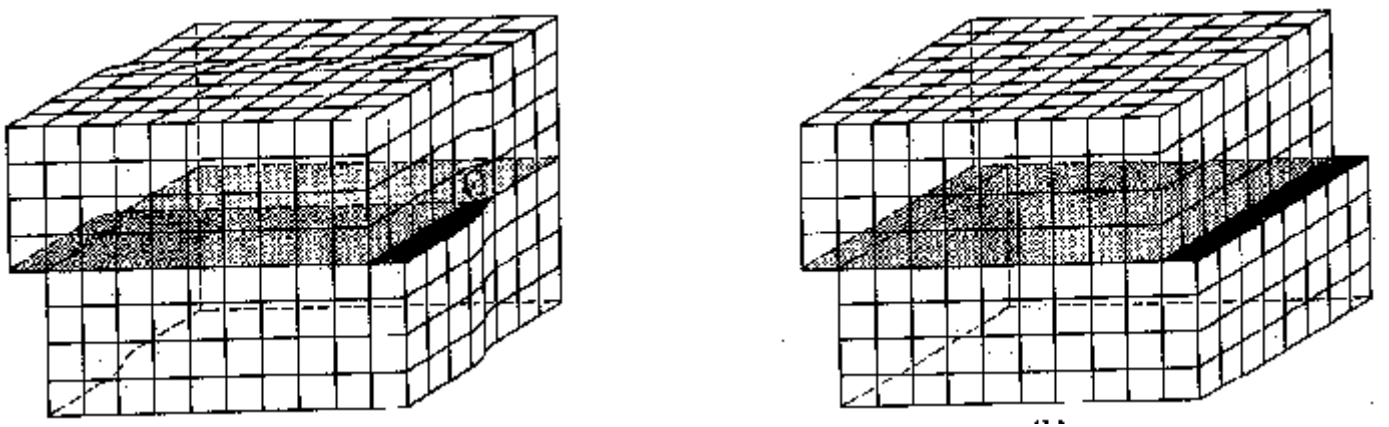




A dislocation line can:

- Create mechanical stress
- Getter Impurities

Movement of Dislocation can create slippage



Misfit Dislocation of Epitxial layers

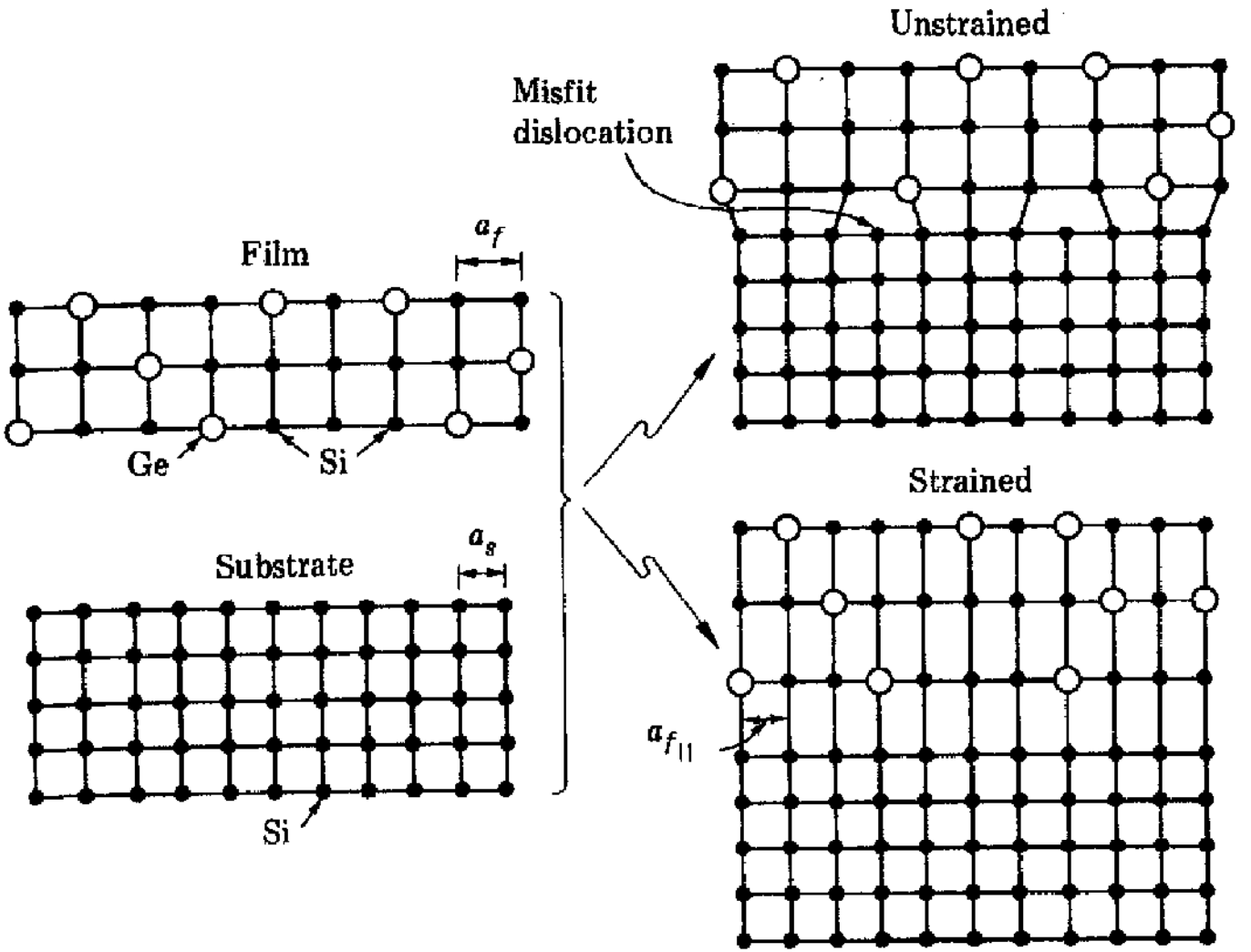
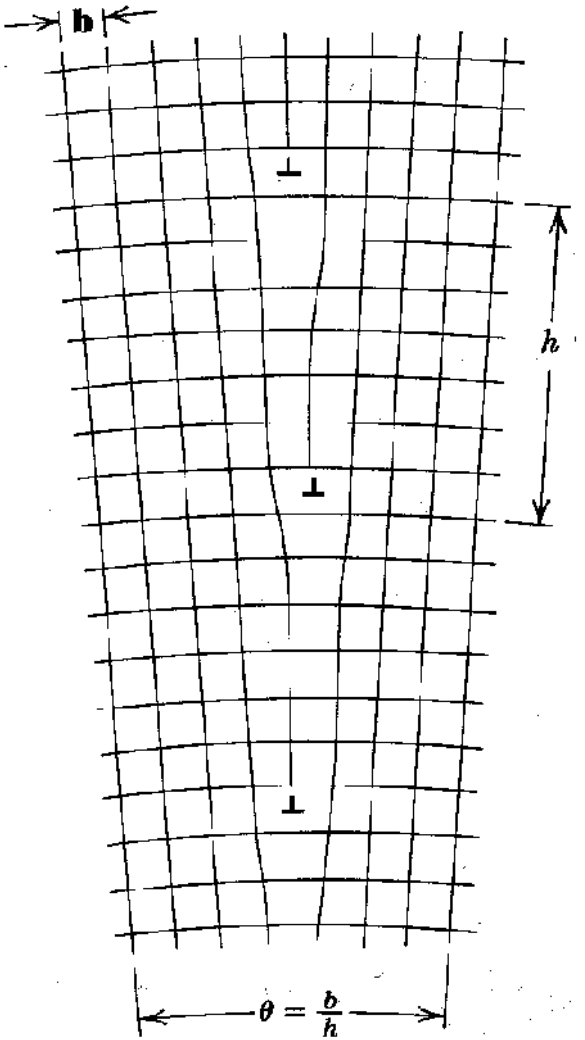
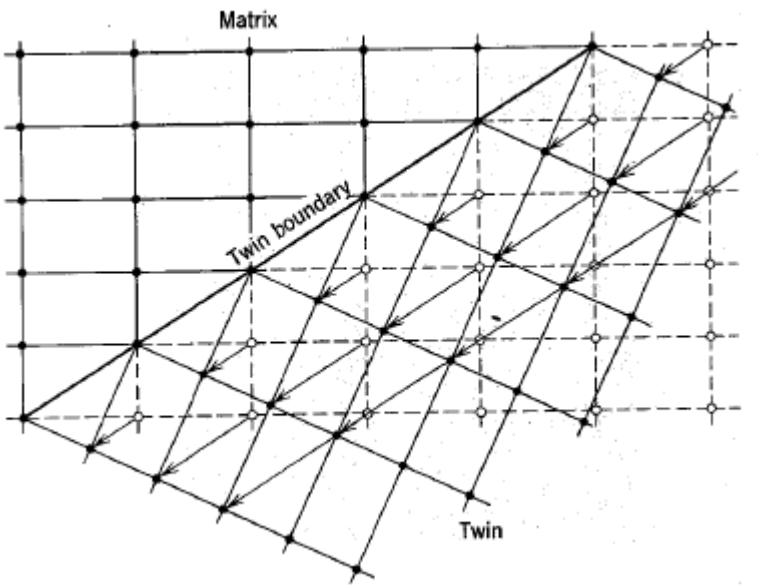


FIGURE 7.4 A Ge_xSi_{1-x} film and a Si single-crystal substrate are joined to form a lattice-mismatched heterostructure that is either strained or unstrained with misfit dislocations.

Two-Dimensional Defects

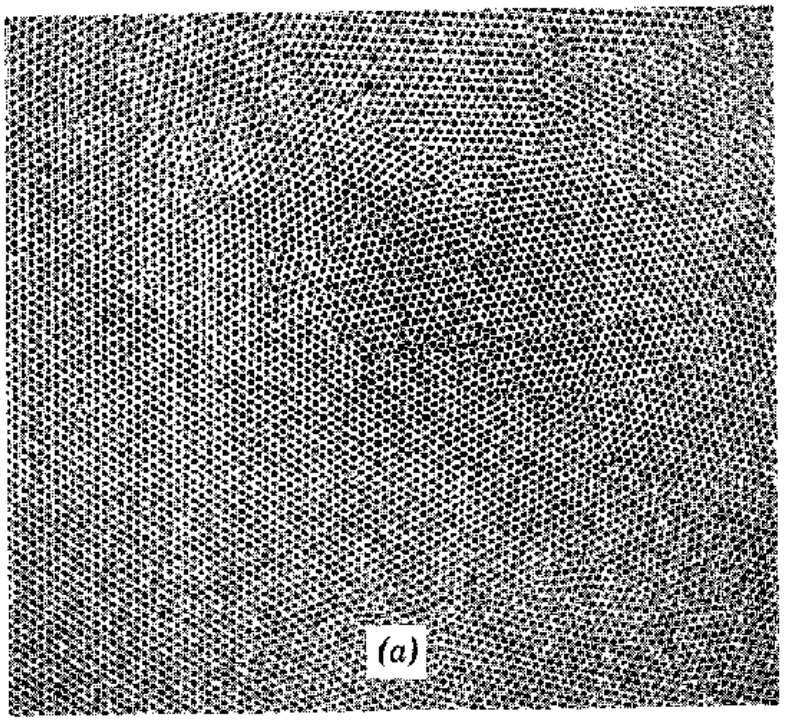


Grain Boundary

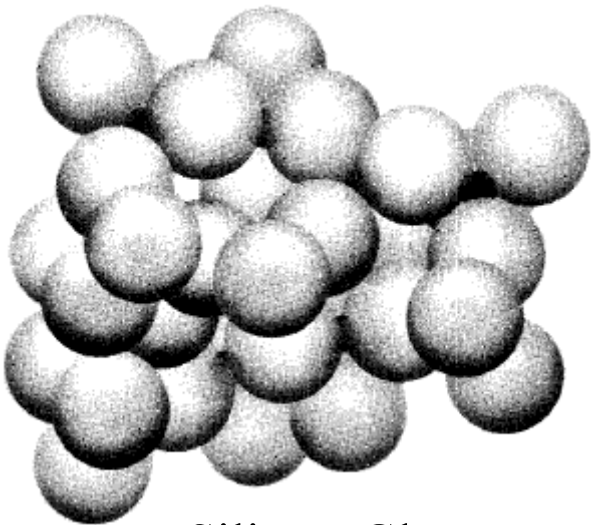


Twins Boundary

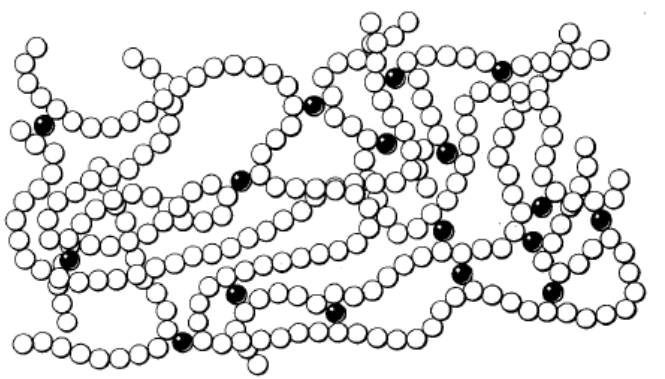
Polycrystalline Solids



Amorphous Solids

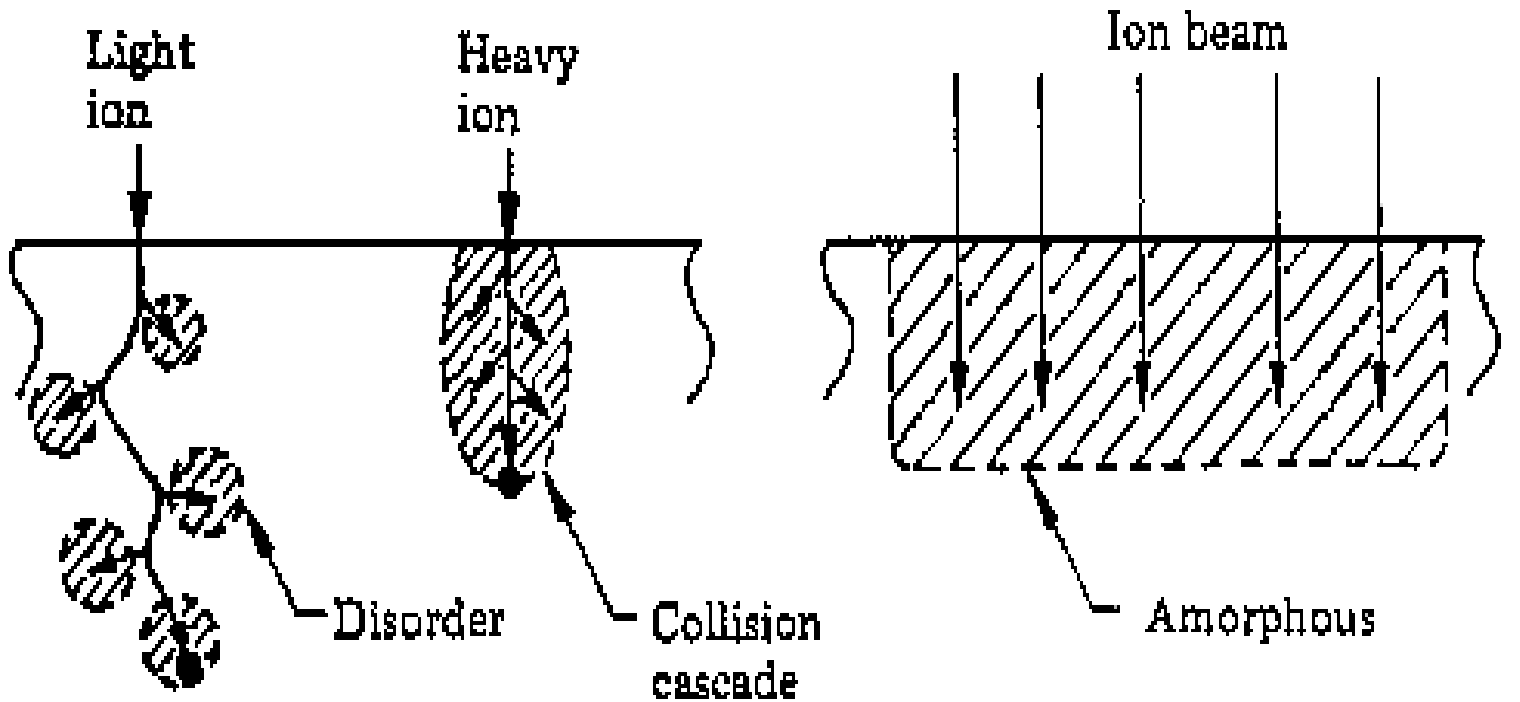


Silicate Glass



Polymers

Implantation "Damage"



Schematic of the disorder produced along the individual paths of light and heavy ions and the formation of an amorphous region.

Substrate Interstitials and Vacancies are created by momentum transfer collision process

End-of-Range "EOR" Dislocation Loops

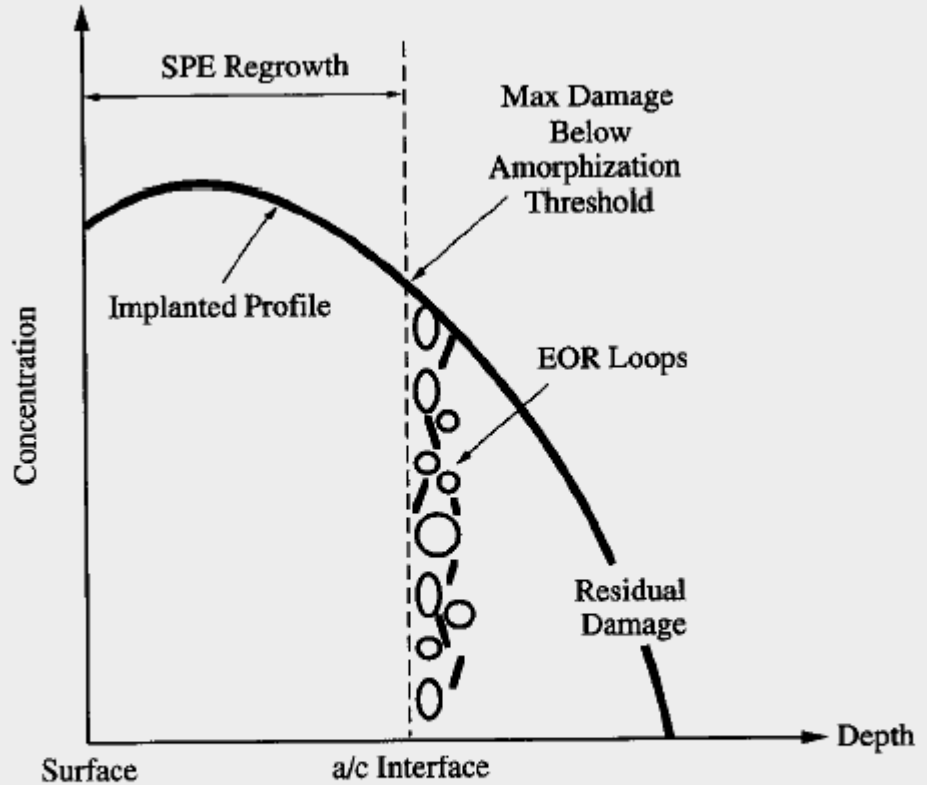
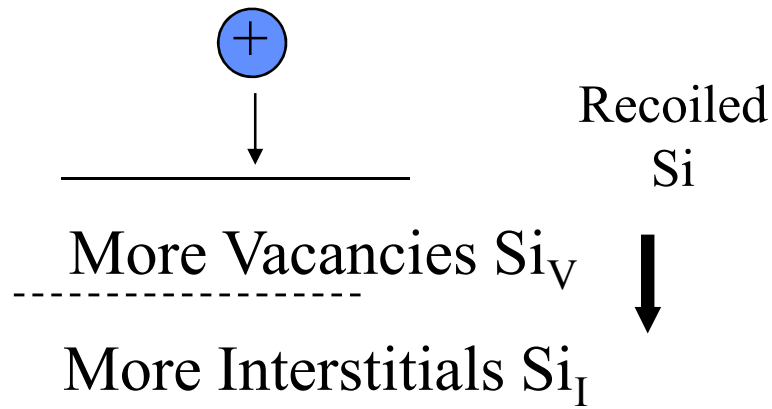
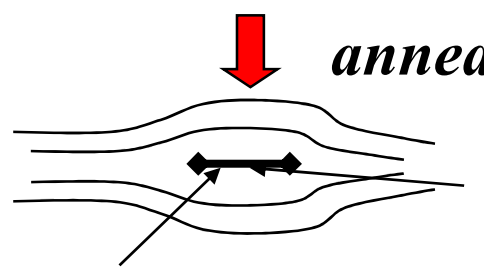


Figure 8–25 Schematic of the stable End-Of-Range (EOR) dislocation loops that form at the amorphous/crystalline (a/c) interface after solid-phase epitaxial regrowth.

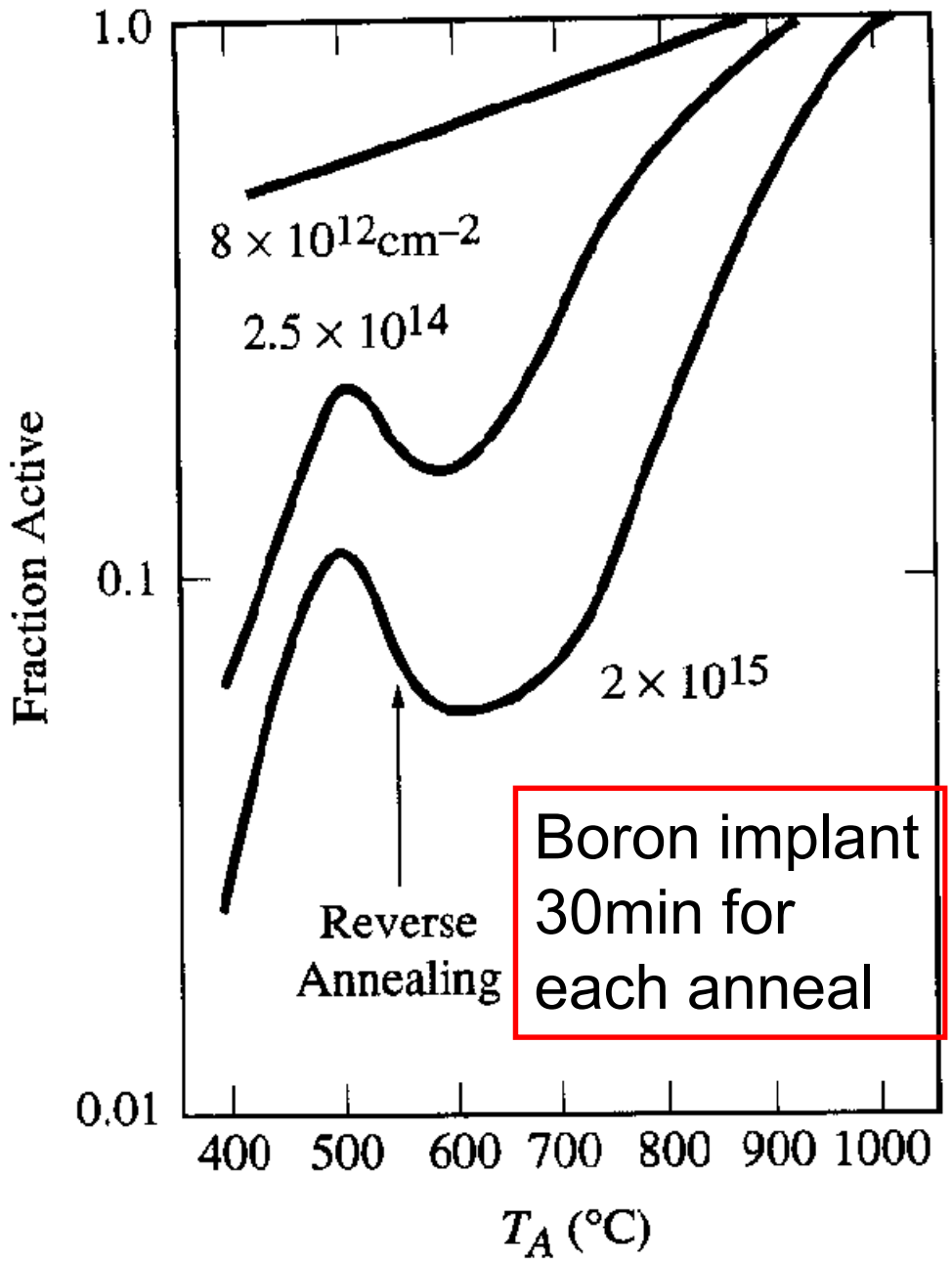




"Extrinsic" dislocation loops

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

Plummer et al , *Si VLSI Technology*

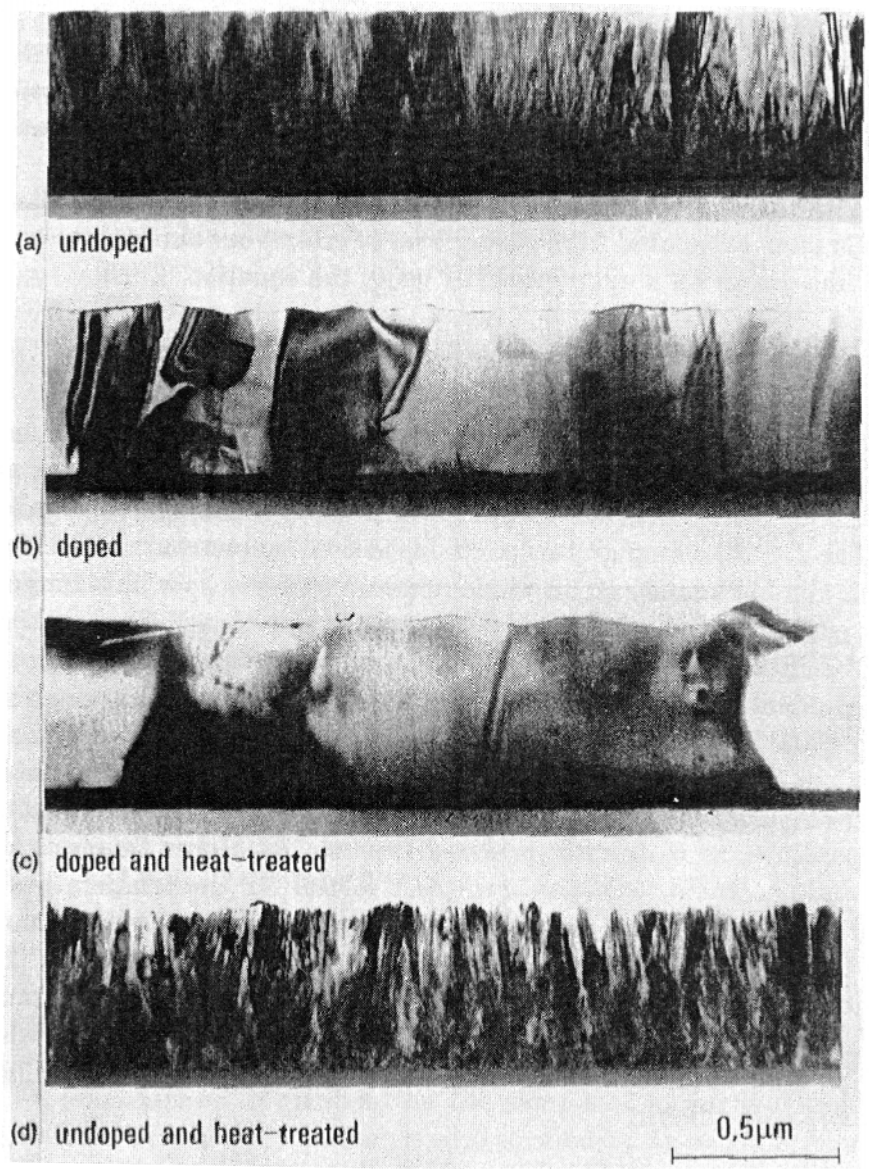


Boron implant 30min for each anneal

Dopant Activation

From 450 to 550C,
Si interstital compete with B for Si substuitional sites
or
Si interstials pairs with B to form inactive complex

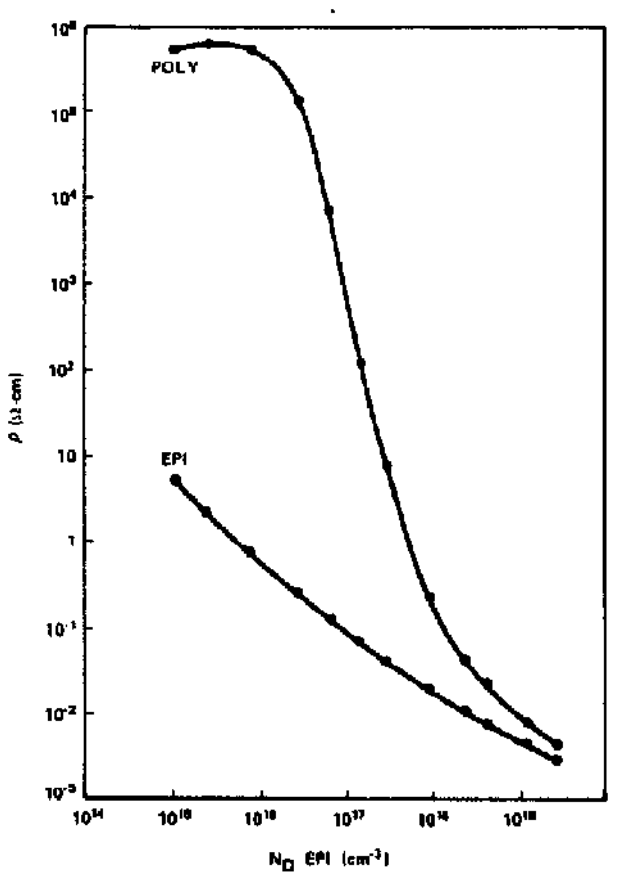
Example : Poly-Si

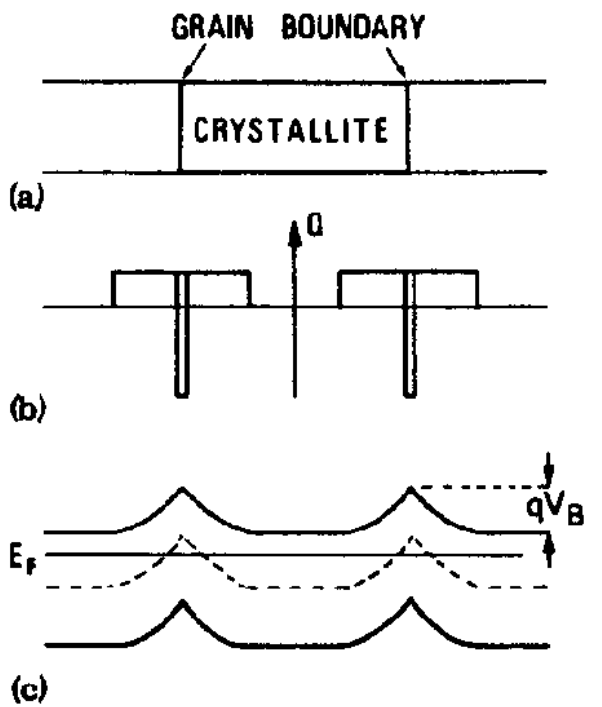


- Average grain size depends on deposition, doping conc & annealing conditions !

Electrical Resistivity of Polycrystalline Materials

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

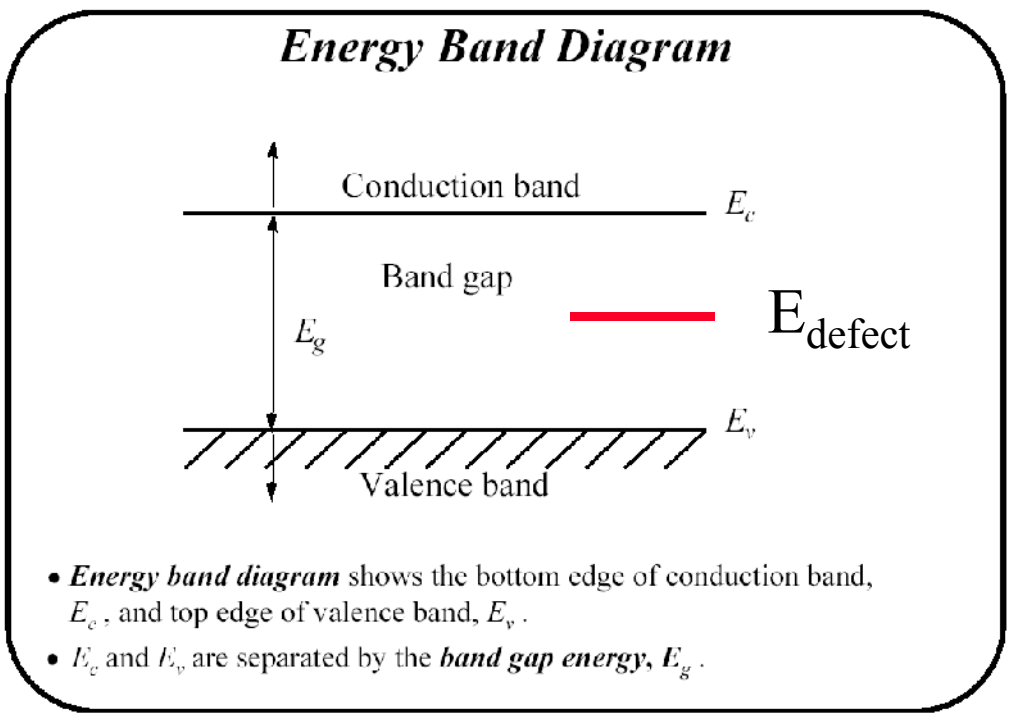


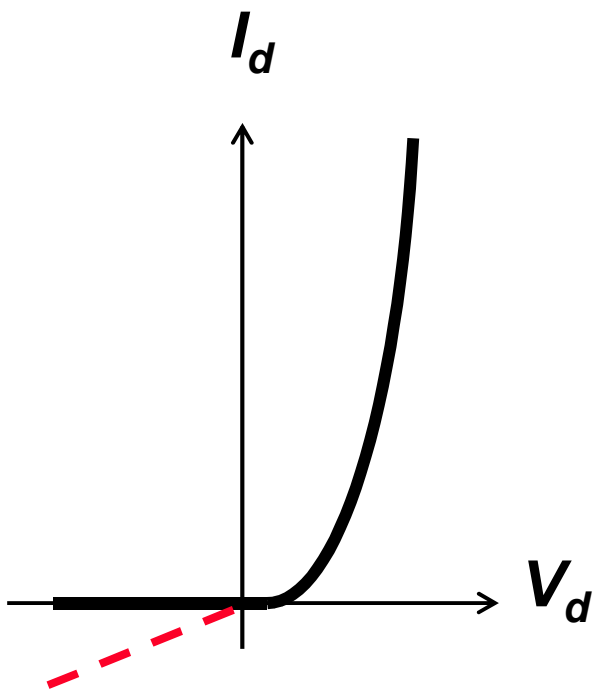


Trapped charges at GB create energy barriers for mobile carriers

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





Excessive leakage current

How processing steps affect point defect concentrations

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

At 1000°C, $C_{Io}^* \sim 10^{12}$ /cm^3

$C_{Vo}^* \sim 10^{13}$ /cm^3

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

I^+, I^o, I^-

V^+, V^o, V^-, $V^=$

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

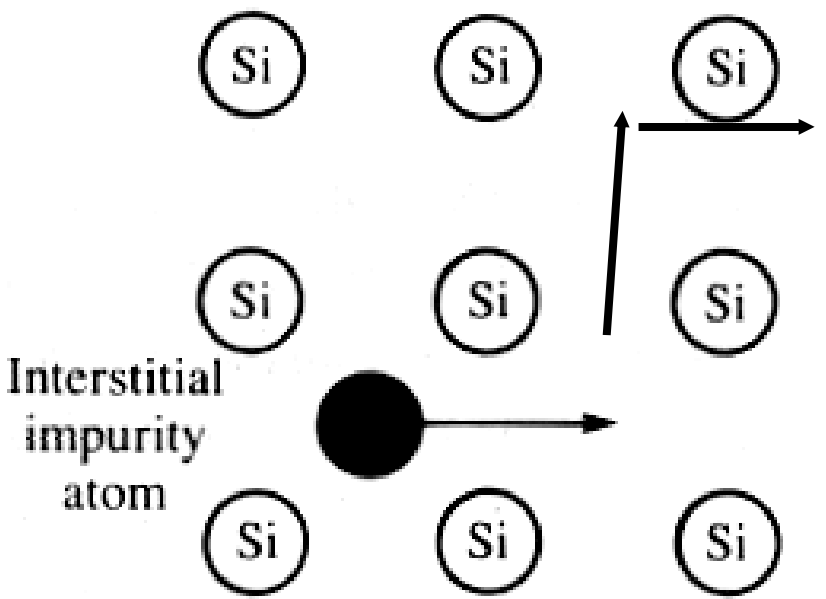
• **Implantation collisions** (total point defect concentration enhanced by ~ 1000X)

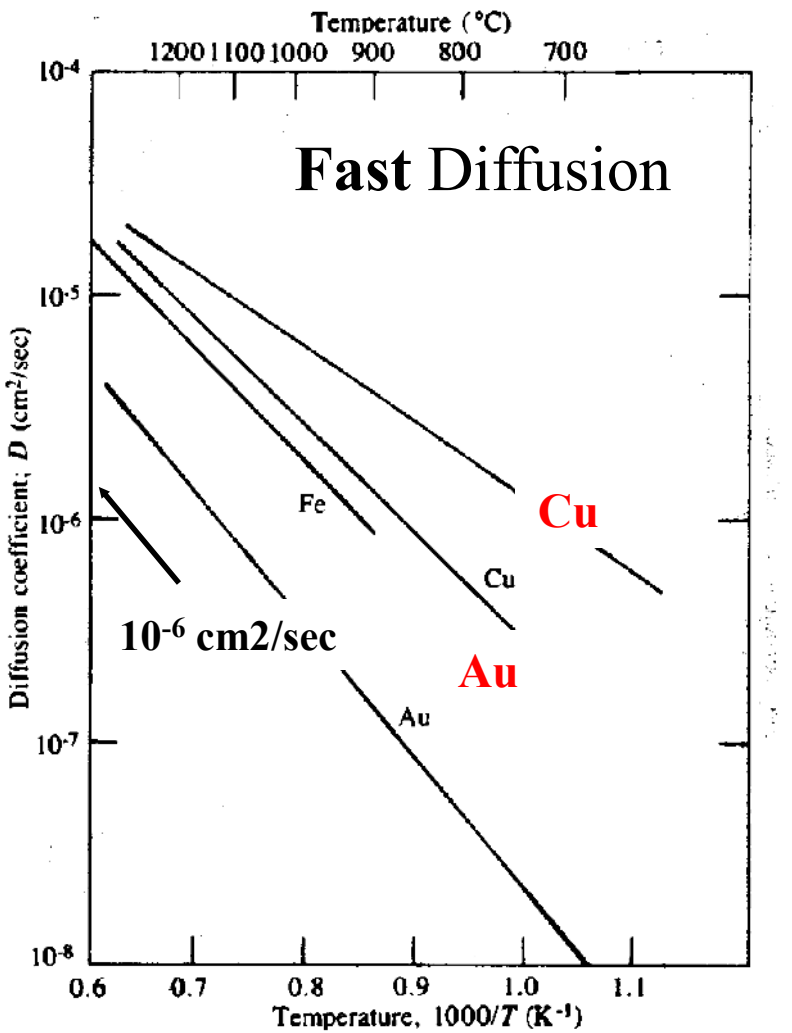
Diffusion Mechanisms in Si

(A) No Si Native Point Defect Required

Example: Cu, Fe, Li, H

(a) Interstitial Diffusion



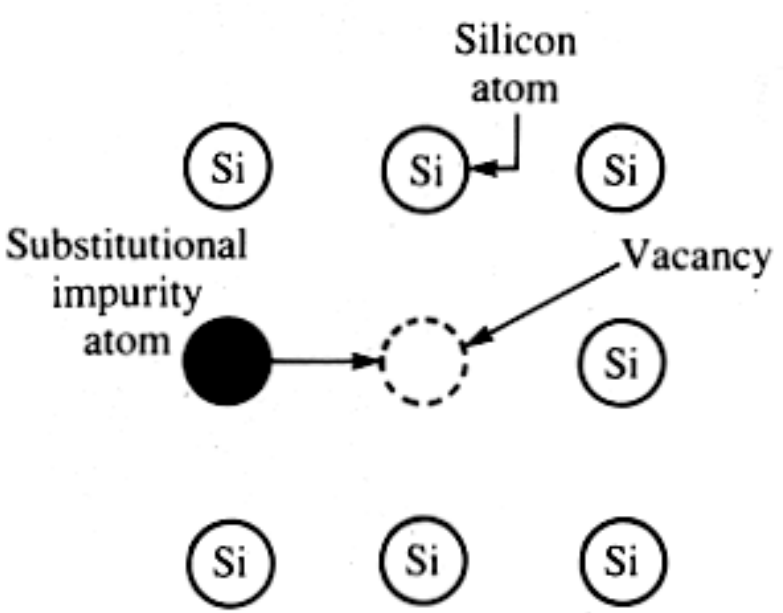


Diffusion Mechanisms in Si

(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

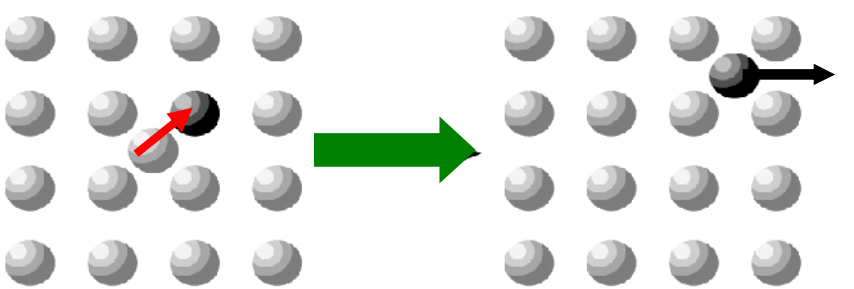


Figure 3.5 In interstitialcy diffusion an interstitial silicon atom displaces a substitutional impurity, driving it to an interstitial site where it diffuses some distance before it returns to a substitutional site.

Diffusivity Comparison:
Dopants, Si interstitial, and interstitial diffusers

For reference only

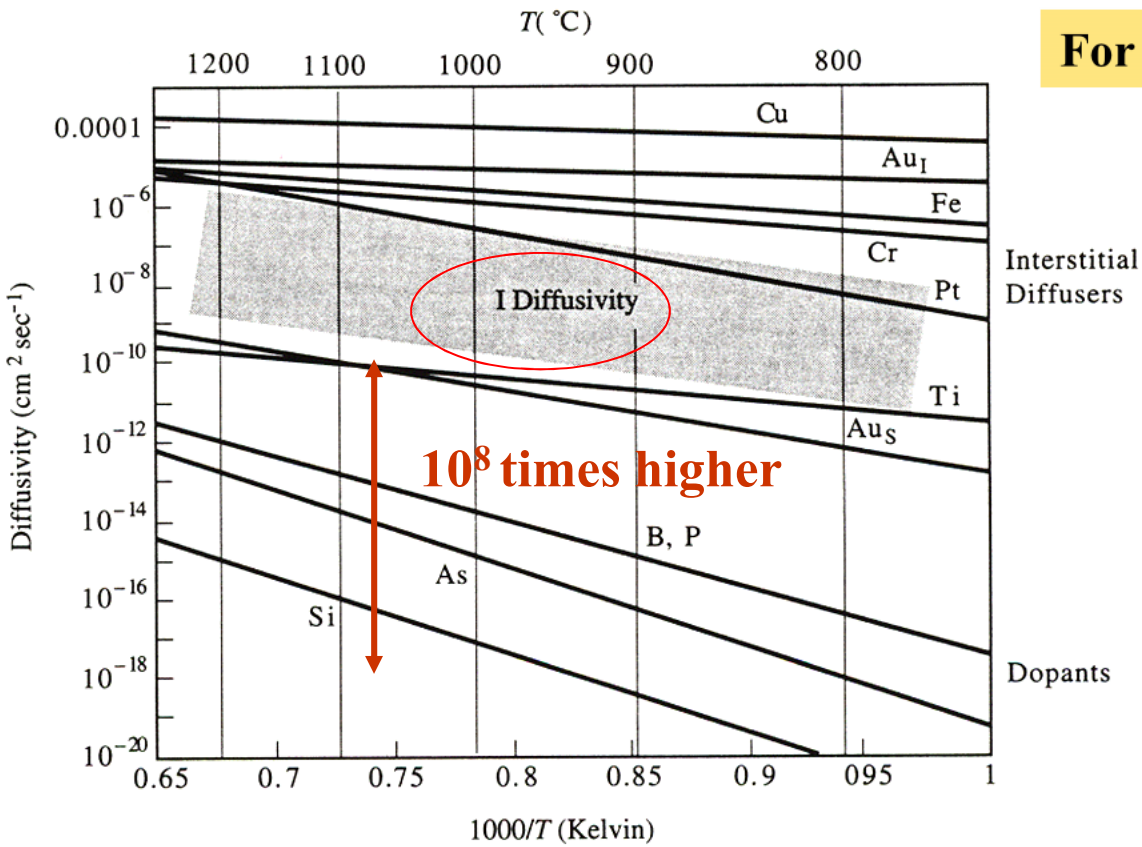
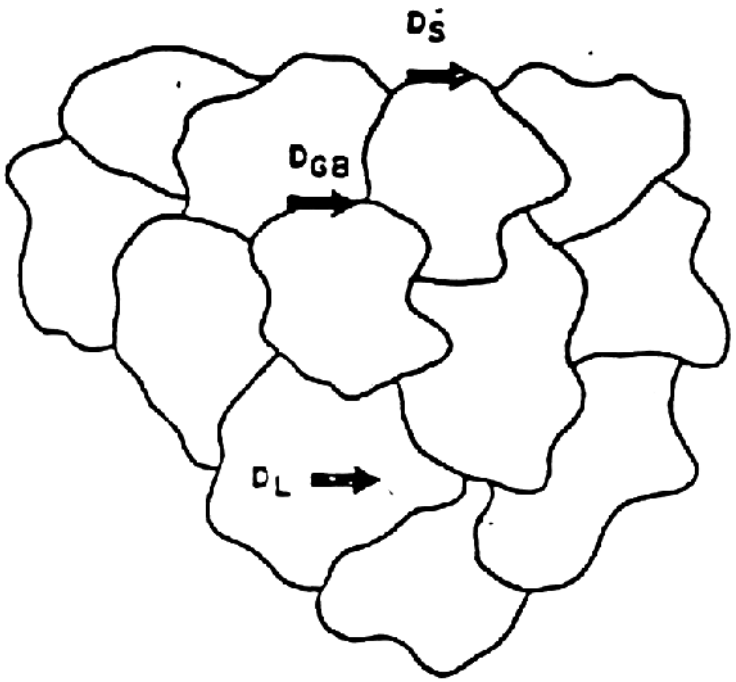
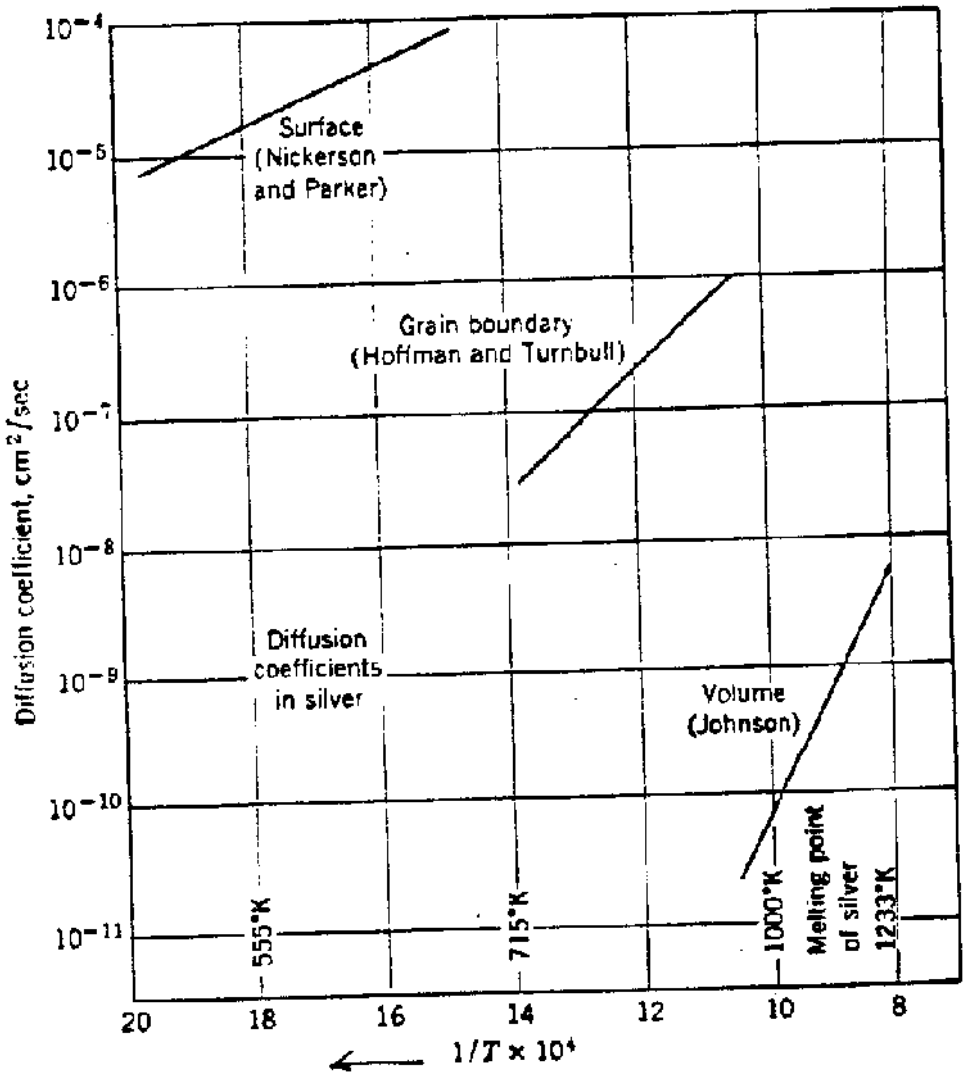


Figure 4–8 Diffusivities of various species in silicon. Au_S refers to gold in substitutional form (on a lattice site); Au_I to gold in an interstitial site. The silicon interstitial (I) diffusivity is also shown and will be discussed later. The gray area representing the I diffusivity indicates the uncertainty in this parameter. (After [4.10, 4.11].)

Diffusivity along defect paths



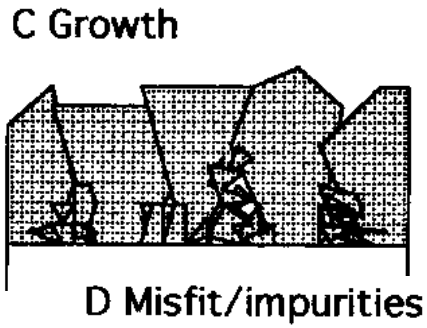
Surface diffusion
> GB diffusion
> Bulk diffusion



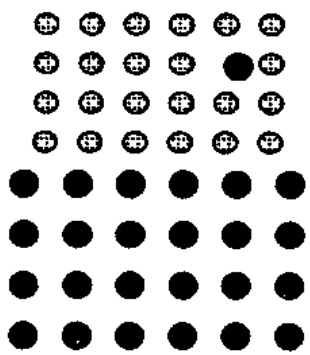
Self Diffusion coefficients in silver.

Defects and Thin-film Stress

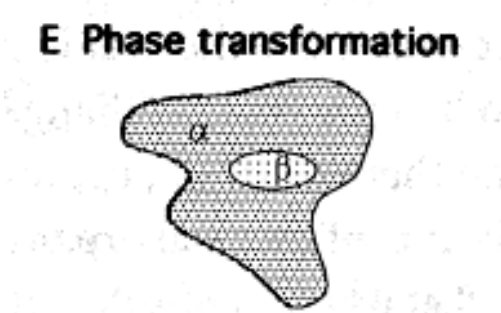
– Growth morphology



– 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, 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, 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