http://www.fys.uio.no/studier/kurs/fys4310/LN_1_Solid_State.pdf

FYS 4310/9310

Semiconductor
materials science

introductions

Solid state physics
Crystal structure
Crystal defects

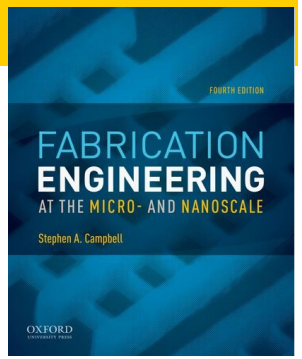
xx:
xx:

Lecture on
Solid State Physics
or Materials Science

Readings
* These notes
* S.A Campbel Chapter 1,2
* Electronic Materials Science:
for Integrated Circuits in Si and GaAs,
J. W. Mayer and S. S. Lau,
* Electronic Devices:
Streetman,
*

FYS 4310

Chapter-map



1 intro

1/2 cond mat. Solid st. Xtal struct

2 Defects

3 Si purification

Xtal growth

4

We are here :-)

Chapter 2 ½ cond substrates 1,2,3,4

Chapter 3 Impurity Diffusion

Chapter 4 Silicon Oxidation

Chapter 5 Ion Implant

Chapter 6 Rapid Thermal

Chapter 7 Optical Exposure

Chapter 8 Resist Materials

Chapter 9 X-ray and E-beam

Chapter 10 Vacuum Plasmas

Chapter 11 Etching and Patterning

Chapter 12 Physical Deposition

Chapter 13 Chemical Deposition

5

Chapter 14 Epitaxial Growth

Unit processes

Technologies

Chapter 15 Process Modules

Chapter 16 CMOS Technologies

Chapter 17 Other Transistors

Chapter 18 Opto-Electronics

Chapter 19 Microsystems

Chapter 20 IC Manufacturing

Figure 1.7 A roadmap for the course indicating the relationships between the chapters.

Semiconductors

Solids Xtals amorphous

Xtal structure

for describing the structure

We are mostly interested in a limited number of xtal structures - those of the most common semiconductors

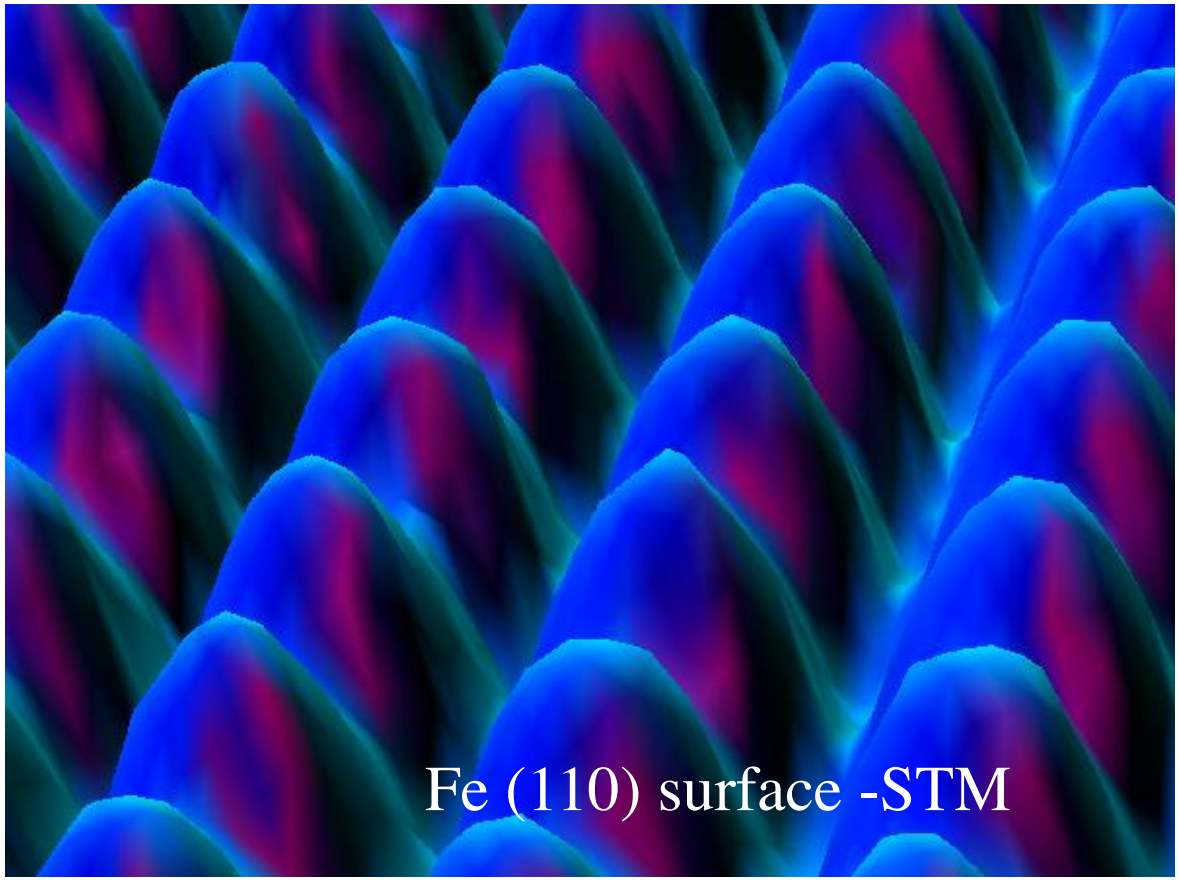
Si, Ge, SiGe, GaAs, GaAlAs, InP, InGaAs, HgCdTe, CdS, SiC, ZnO

Simple metals

Al, Pt, Au, Ti ..

The details of other structures, not here!

Xtal structure

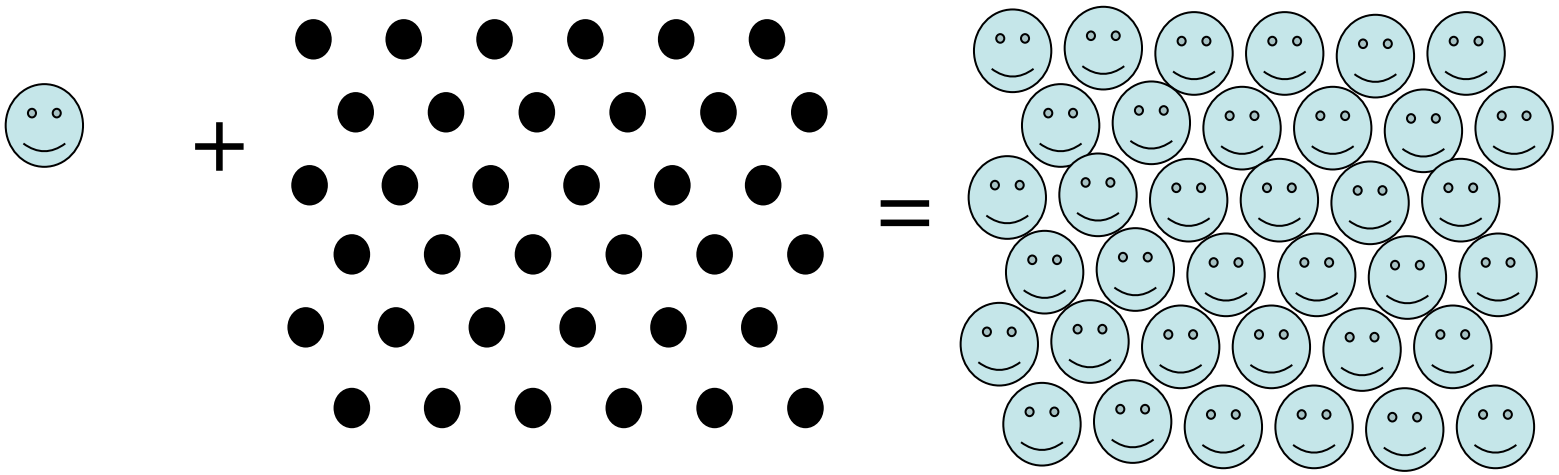


Different aggregation states:

- Liquid-state
  - (typically only) short range order
- Solid state
  - **Xtals - long range order**
  - Non Xtals - Cheese, pasta, rice, wood, ceramic chip holders, plastics

Description of Xtal structures I

- Association + Bravais lattice= xtal structure



operation + abstraction = the idealized real thing

Description of xtal structure I

Unit cells

Units which fill all space

when repeated in 3 dimensions

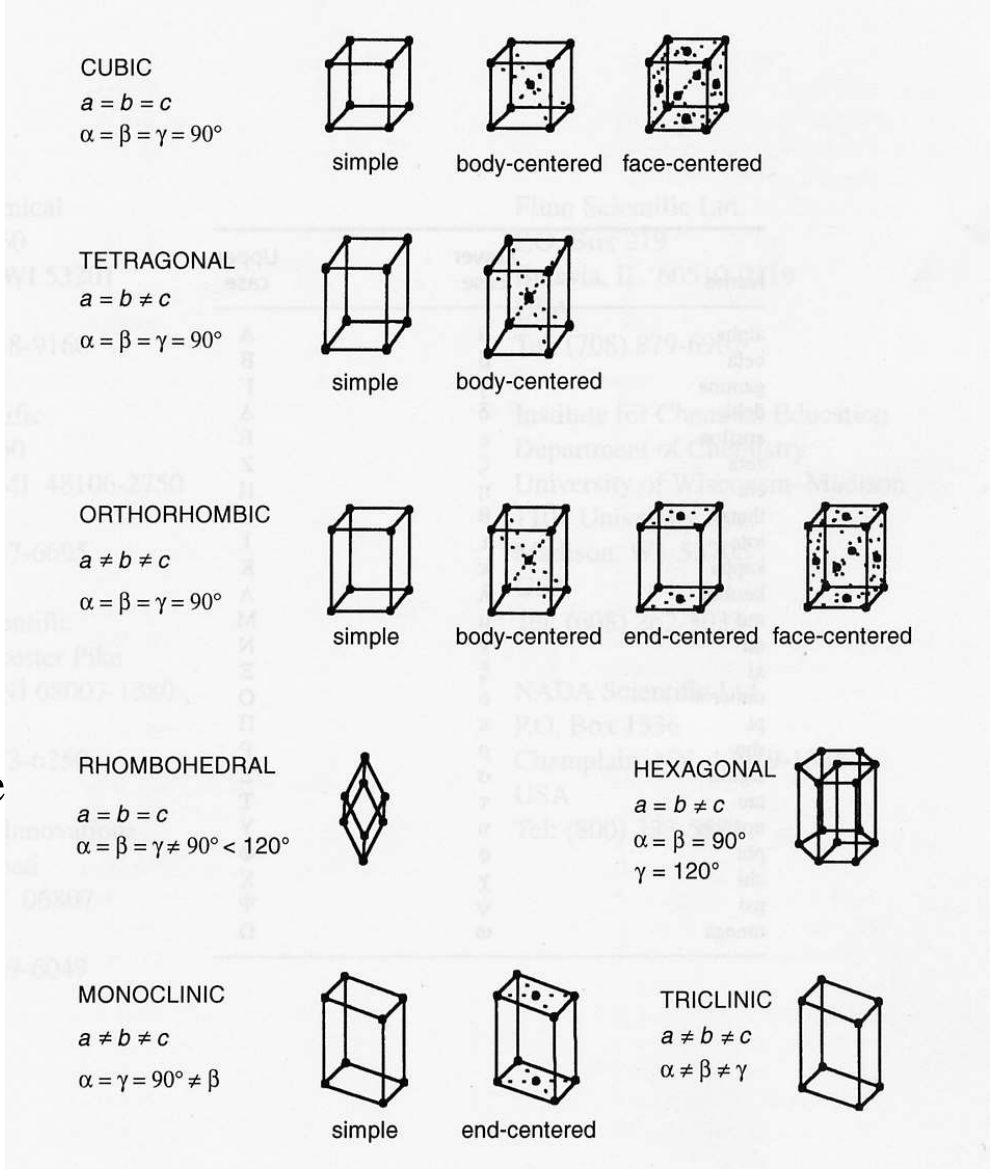
Primitive cell

The smallest unit cells

7 symmetries, with body centered, face centered and end centered extra positions;

Total 14 Bravais-lattices

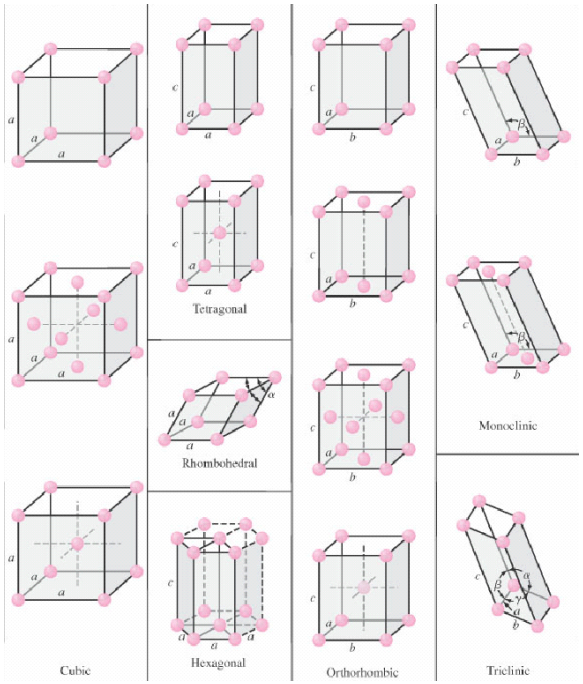
Can be filled with atoms in different ways, yields 230 space groups



Figur: M.A. White: Properties of Materials

Description of xtal structure II

- Bravais lattices
  - in 2D 5 distinct lattice types
  - in 3D there are 14 lattice types
    - (3 cubic, 1 hexagonal, 2 tetragonal, 1 rhombohedral, 4 ortorhombic, 1 triclinic, 2 monoclinic.)



Close packing

- Atoms as spheres,
- For simple metals, Al, Cu, Au
- also as basis for more complicated multi element structures.
- Dense packing of spheres
- Hexagonal dense packing: ABABAB or ABCABC

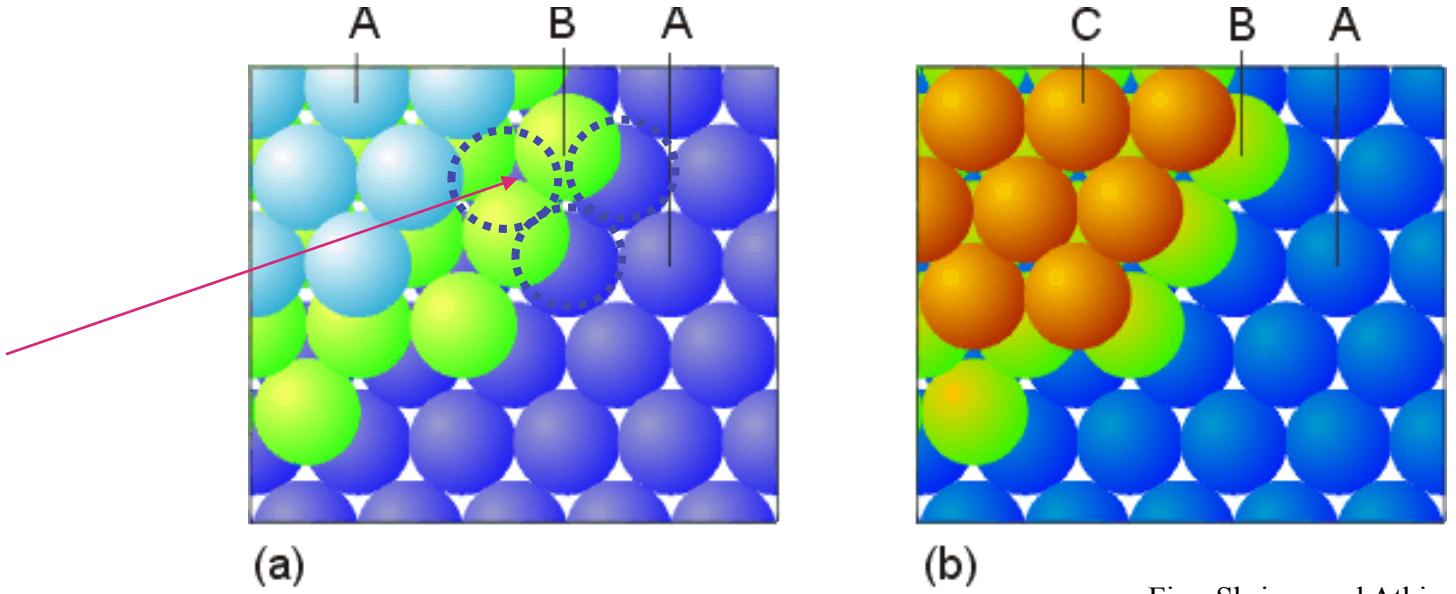
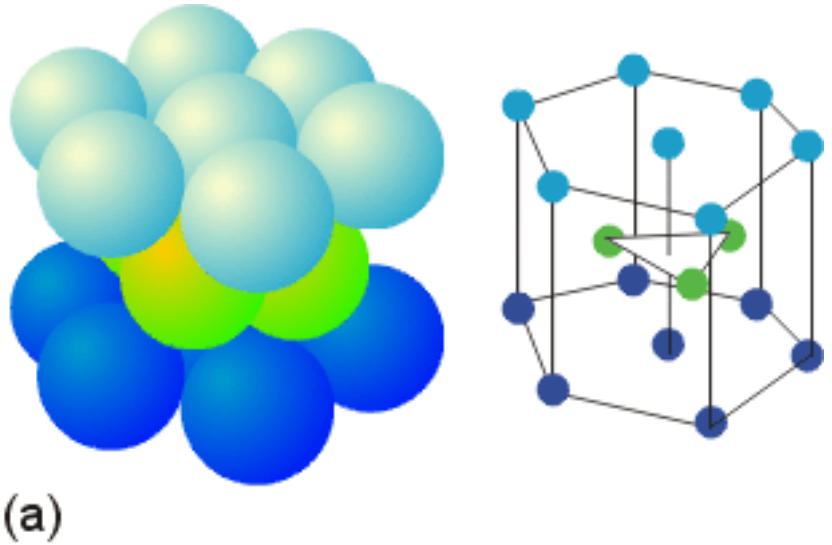


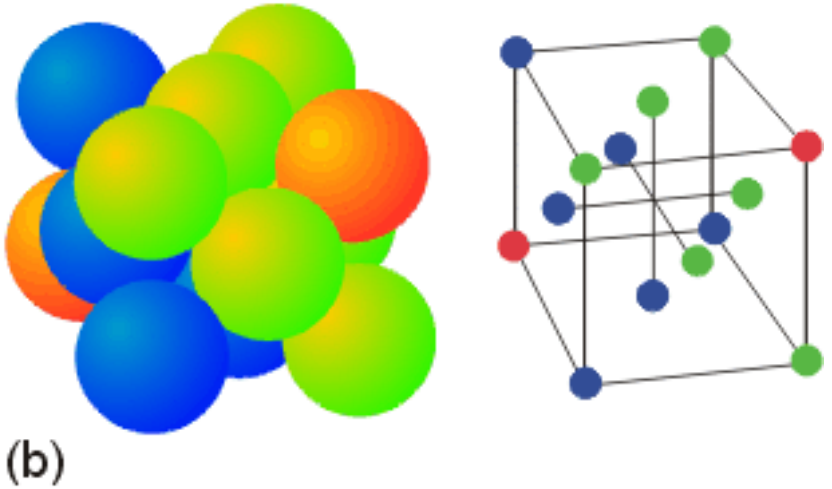
Fig.: Shriver and Atkins: Inorganic Chemistry

Close packed structures

- ABABAB
  - hexagonal close-packed (*hcp*)



- ABCABC
  - hexagonal origin
  - Rotate basis 45° gets:
  - face centered cubic (*fcc*)

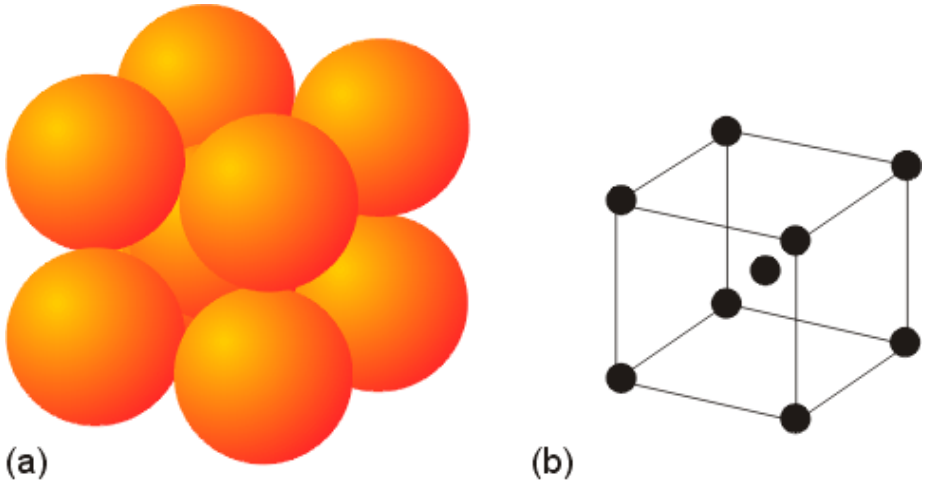


- hcp and fcc represents most dense packing possible of hard spheres.

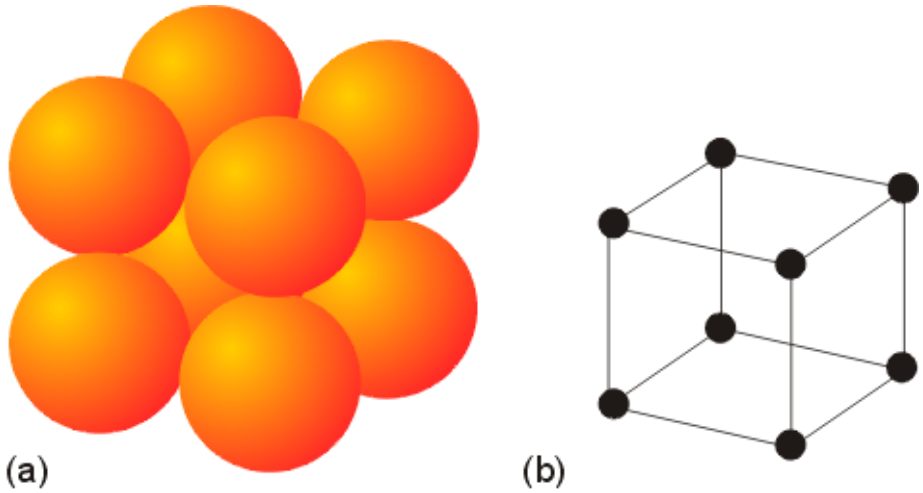
Figur: Shriver and Atkins: Inorganic Chemistry

Other , less dense packing of spheres

- Body centered cubic (bcc)



- Simple cubic (sc)



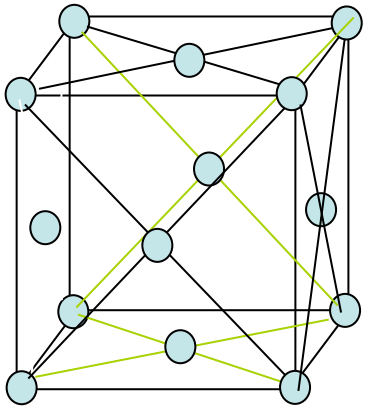
Figur: Shriver and Atkins: Inorganic Chemistry

Xtal structure Si (diamond)

Bravais lattice + association

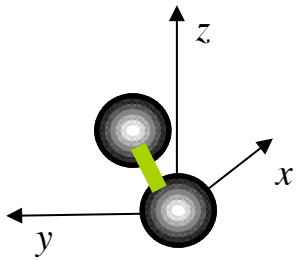
Bravais = fcc

assoc. = two at./pt., (0 0 0), and (1/4,1/4,1/4)



fcc

+



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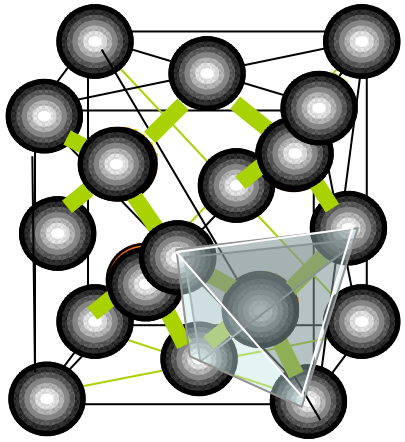


Xstal structure Diamond

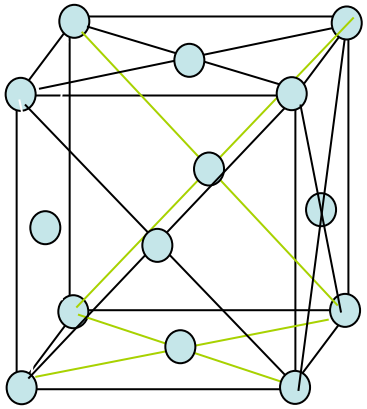
Note 4 next nearest neighbors

Xtal structure GaAs (ZinkBlende)

Bravais lattice + assoc.

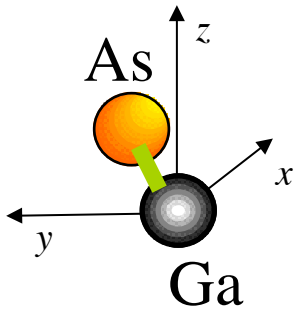
Bravais = fcc

assoc. = two at./pt, Ga(0 0 0), As (1/4,1/4,1/4)



fcc

+



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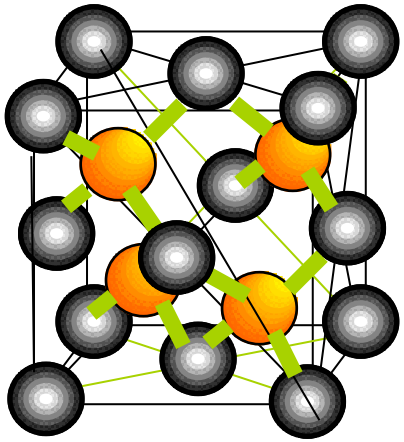


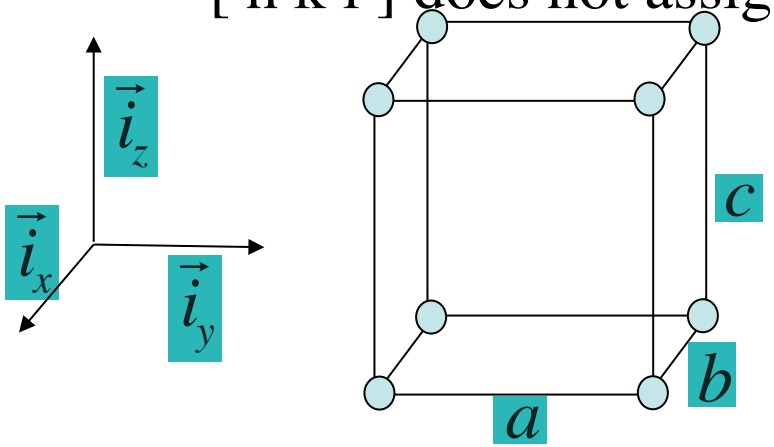
Xtal structure GaAs

Other Semicondoctors, III-V: AlAs, GaSb, InAs, InSb… II-VI: ZnS, ZnSe, CdS, CdTe..

IV-IV: SiC (3C)

Xtal structures

- Xtal directions ; Miller indices
  - 3 integers [h k l] $h \cdot a \cdot \vec{i}_x + k \cdot b \cdot \vec{i}_y + h \cdot c \cdot \vec{i}_z$
  - Direction
    - Along the vector=in the same direction as
    - [h k l] does not assign a line segment,



Example unit cell in Bravais lattice

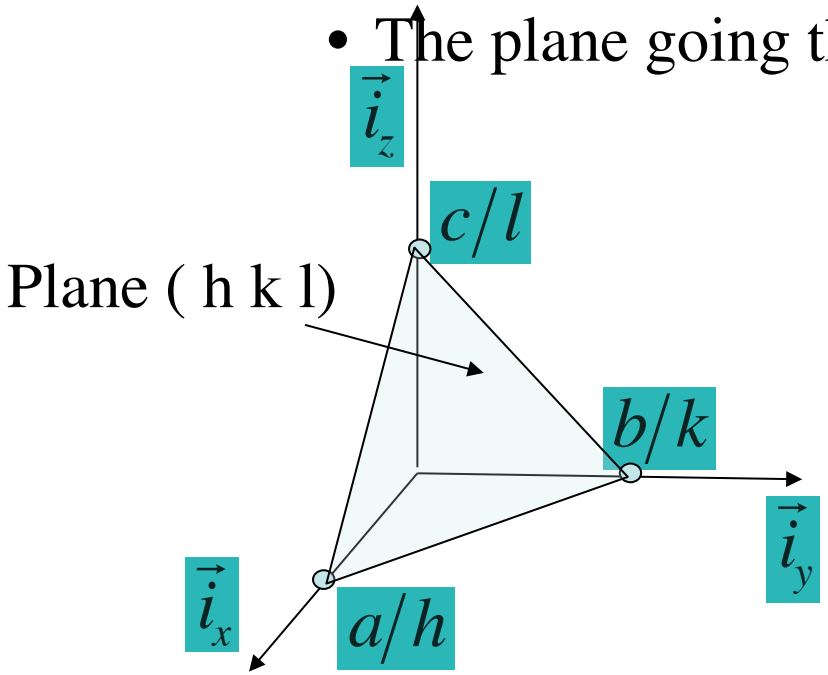
Family of directions

<h k l>, permutaions av h, k, l

In cubic Xtals these are equvalent in the Xtal structure, - depends upon symmetry

Xtal structures

- Xtal plane -Miller indices
  - 3 integers (h k l)
  - Recepy
    - Mark *a*/h, *b*/k , *c*/l along unit vectors in the Bravais lattice, (when *a*=*b*=*c*=1, 1/h, 1/k,1/l)
    - The plane going through the markings is (h k l) ,



Familiy of planes

{h k l}, permutations of h, k, l

Electron-structure -bands-gaps, Simplified

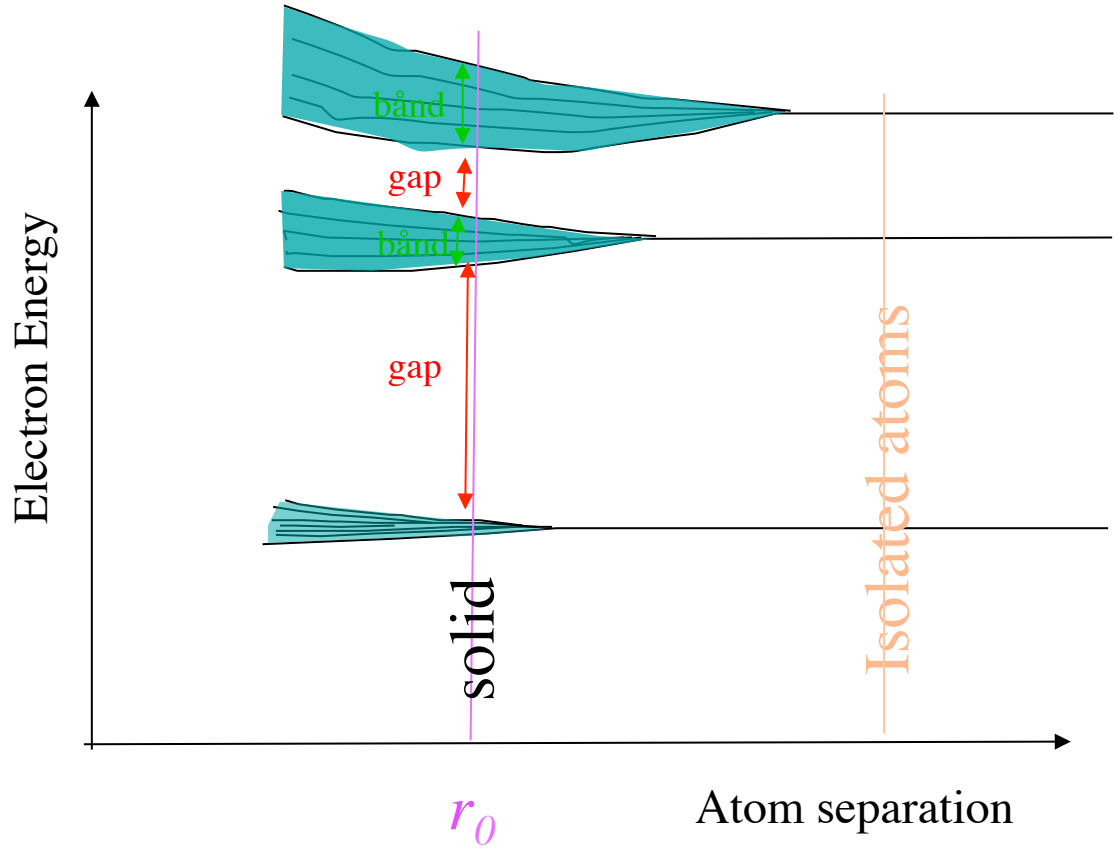
Energy levels in (xtaline) solids

Energy levels are discrete - quantization of states/levels analogous to atoms.

Energy levels split split when atoms kommer nærmere

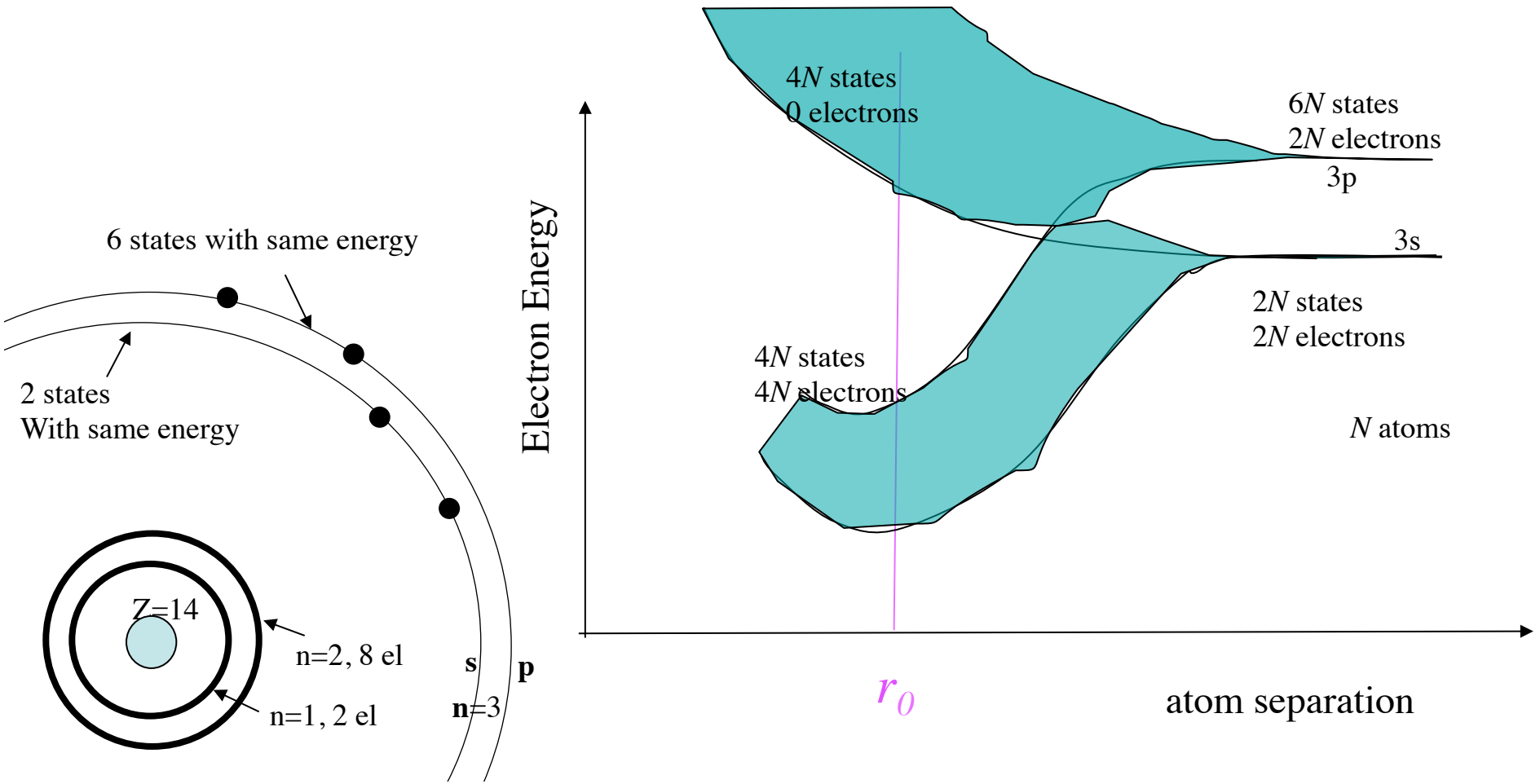
Each level splits as many times as there are atoms

Two electrons can not be in an identical quantum state



Electron-structure Si

Energy levels in Silicon



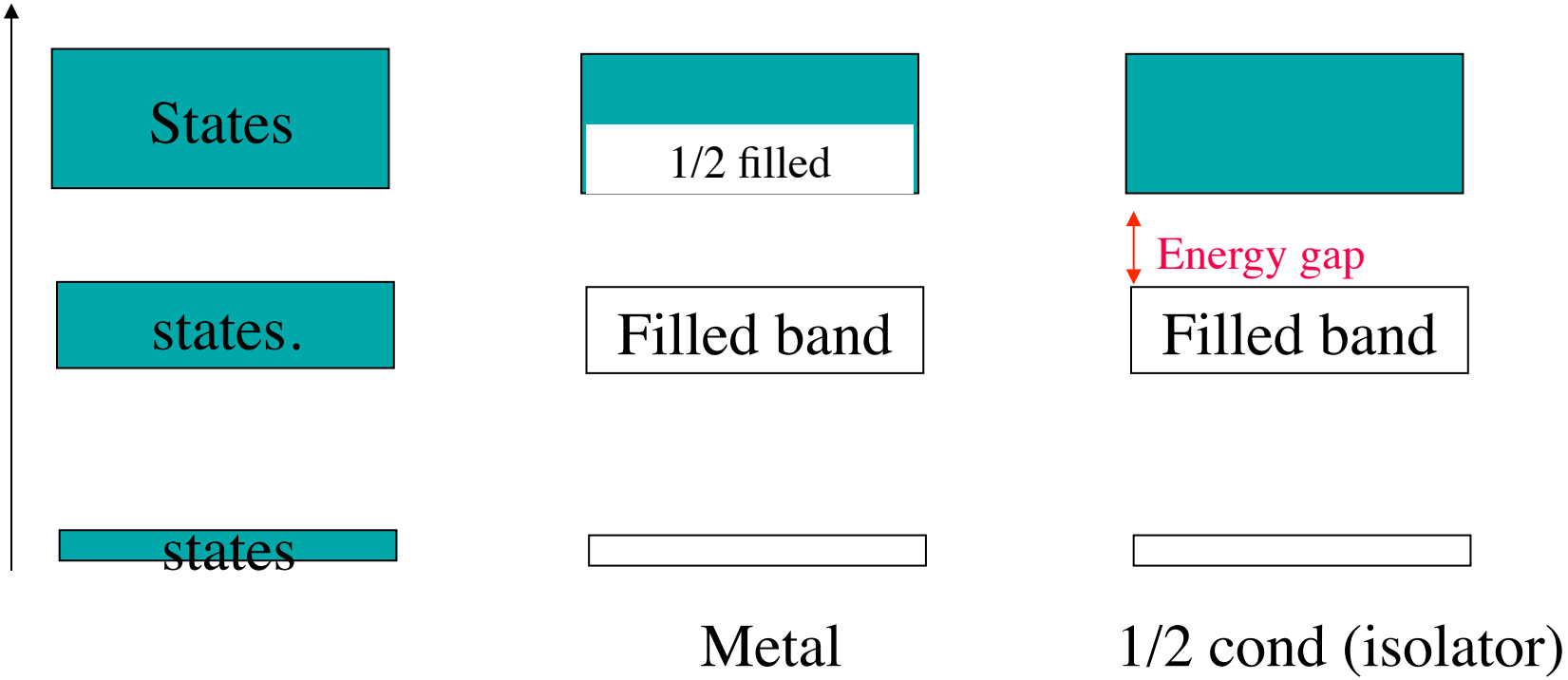
Electron-structure simplified

1/2 conductor vs. metal

Only one electron in each state

In zero magnetic field that means two electrons pr. energy level

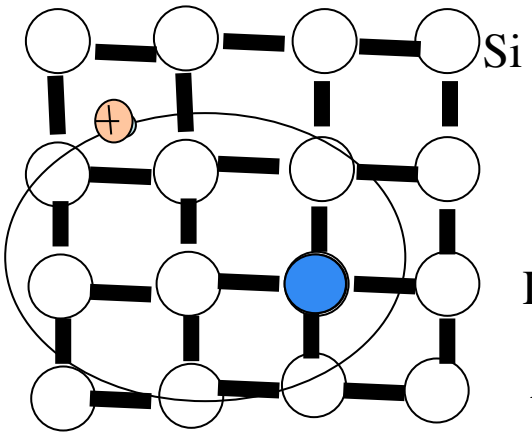
spin up/down s=1/2 og s=-1/2



Electronic structure-Doping of semiconductors, simplified

Doping av Si

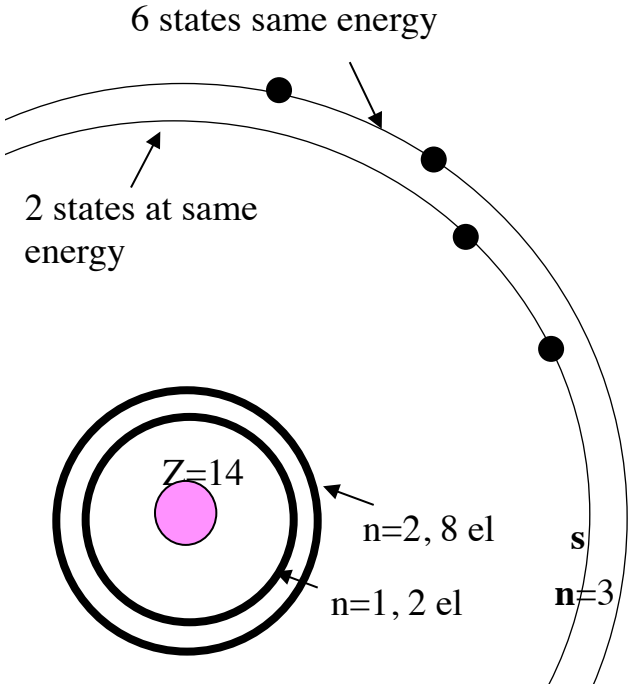
Si group IV
4 nearest neighbors

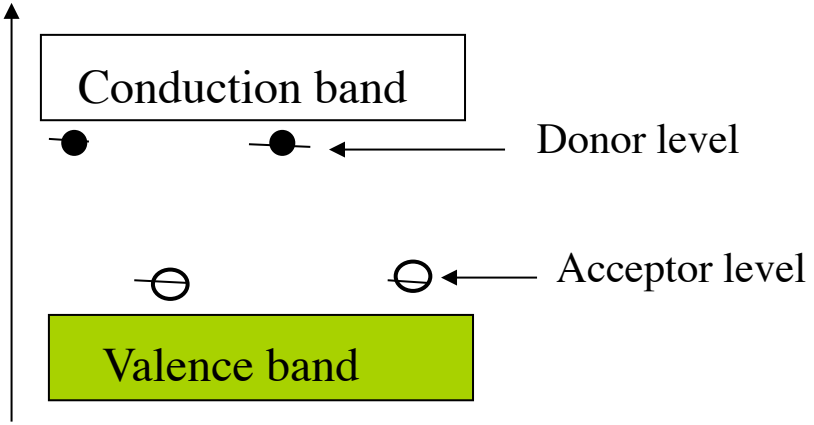


Covalent bonding

Donor- group V (P,As,Sb)

Acceptor: group III

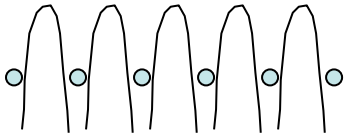




Electron-structure semiconductors

Energy bands and gaps

Xtal structure yields periodic potential



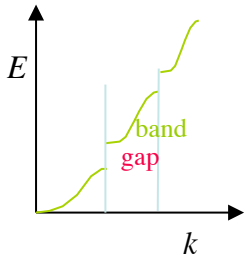
Periodic potential into Schrödinger equation gives energy levels

$$H\psi = E\psi \qquad H = \frac{\hat{p}^2}{2m} + V(r) \qquad V(\vec{r}) = V(\vec{r} + \vec{R})$$

Electrons wave nature, periodic potential - diffraction

(Bragg reflection - Zone boundaries)

Periodic potential yields energy bands and gaps



(superlattices , yields sub or miniature bands)

Semiconductor statistics

Student must learn

Fermi-Dirac distribution function $$f(E) = \frac{1}{\exp\left(\frac{E - E_F}{kT}\right) + 1}$$

Density of states - what is it, $D(E)$

Calculation of carrier concentration

Electrons $$n = \int_{E_c}^{\infty} f(E)D(E)dE \equiv N_c \exp\left(-\frac{E_c - E_F}{\mathrm{k}T}\right) \qquad \mathrm{k}T << E_c - E_F$$

Holes $$p = \int_{'0'}^{E_V} (1 - f(E))D_v(E)dE \equiv N_V \exp\left(-\frac{E_F - E_V}{\mathrm{k}T}\right)$$

$$np = n_i^{\,2}$$

Charge neutrality

$$p + N_D^{\,+} - n - N_A^{\,-} = 0$$

Calculation of Fermi level

DEFECTS

Atomic structural defects - Electronic defects

Point defects

Vacancies, Interstitials, Substitutional impurities, Clusters

Line defects

Dislocations

Edge dislocations, Screw dislocations, Loops, networks

Areal defects

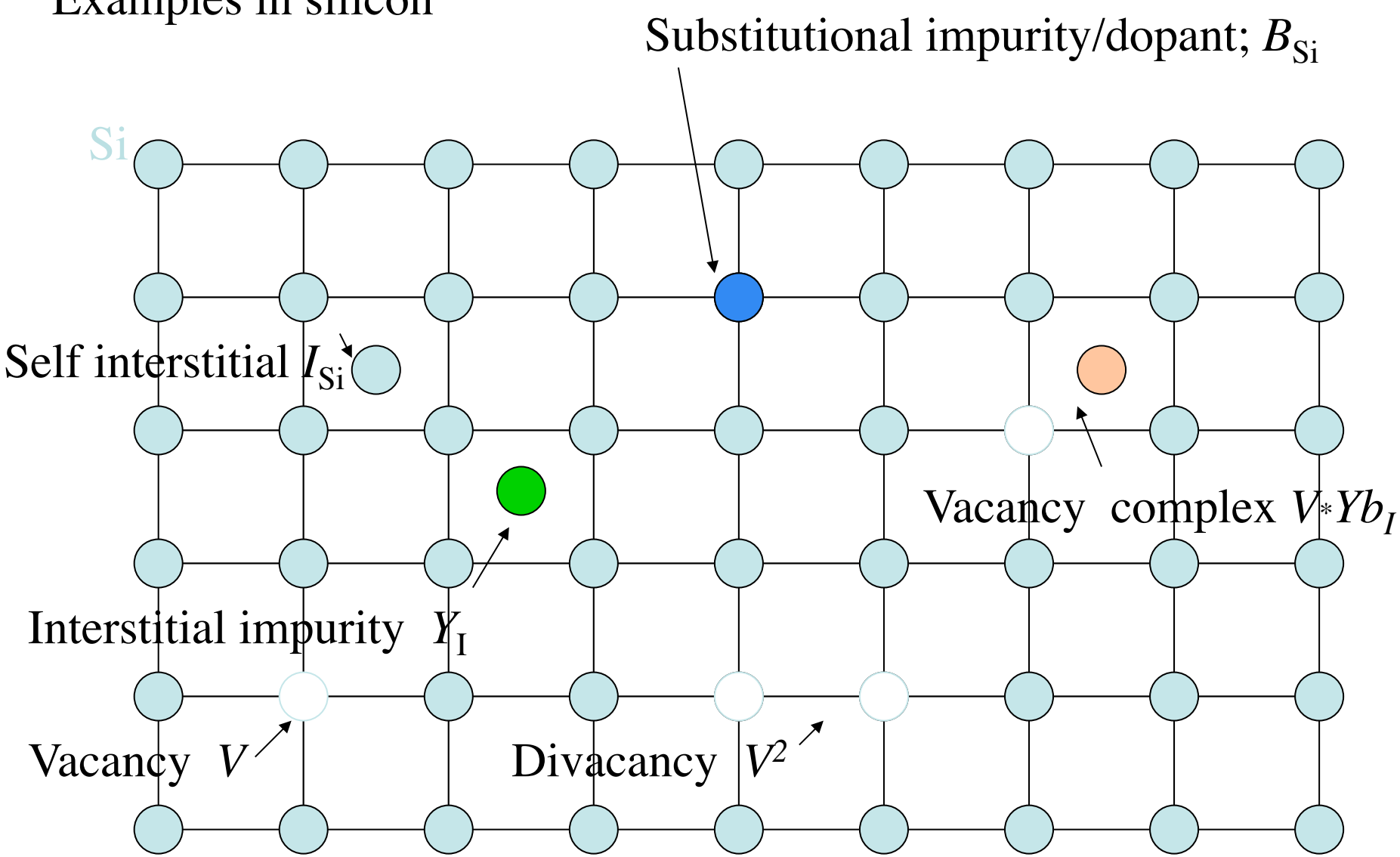
Stacking faults, Grain boundaries, Surfaces

Volume defects

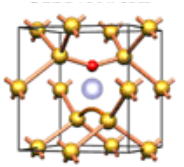
Precipitations

Point defects

Examples in silicon



Point defects:Vacancies:Concentration

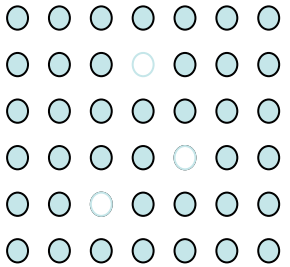


Is it possible to grow a Xtal with no defects?

Derivation

N_V # vac.

N # sites



$$\Delta G = N_v\,\Delta E - T\,(N_v\,\Delta S_v + k\ln(W_{mix}))$$

$$W_{mix} = \frac{N!}{N_v!(N-N_v)!}$$

ΔG Gibbs free energy =Helmholz ss

ΔS_V Entropy

$\ln(x!) = x*\ln x - x$ when $x>>1$

$$k\ln(W_{mix}) = k\left(N\ln N - N_v\ln N_v - (N-N_v)\ln(N-N_v)\right)$$

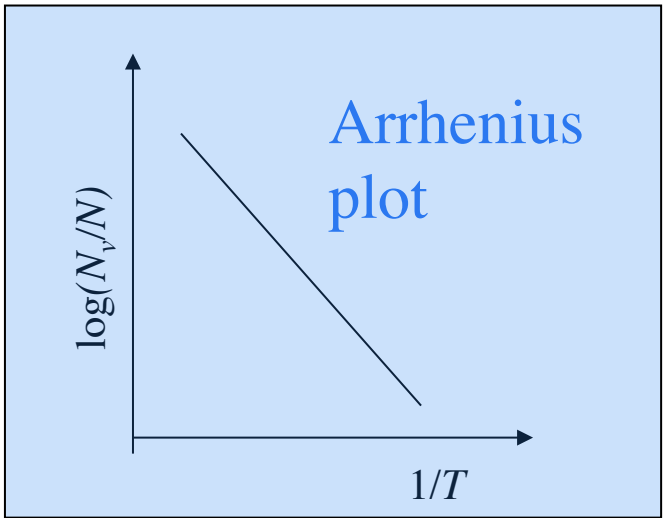
$$\Delta G = N_v\Delta E - N_v T\Delta S_v + kT(N\ln N - N_v\ln N_v - (N-N_v)\ln(N-N_v))$$

For equilibrium situation, ΔG is minimum,

Which N_v makes ΔG minimal?

$$\frac{\partial}{\partial N_V}\Delta G = 0 \qquad N_V << N$$

$$N_v = N\exp\left(\frac{\Delta S_v}{k}\right)\exp\left(-\frac{\Delta E_v}{kT}\right)$$



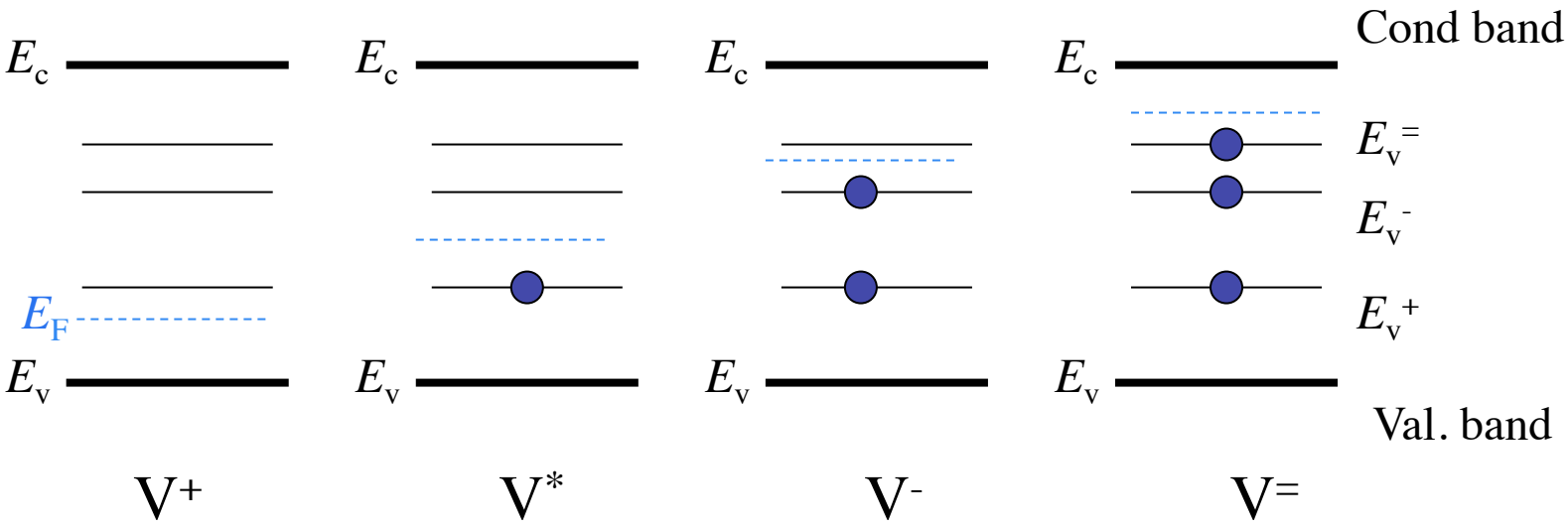
Point defects:Vacancies in Silicon

Periodic potential gives states in bands

- described as delocalized shared by the whole xtal

Breaking the periodicity by a vacancy yields localized states

- some can end up in the band gap
- can filled or empty dependent upon Fermi level i.e. doping



Point defects:Vacancies in Silicon

for your info, only

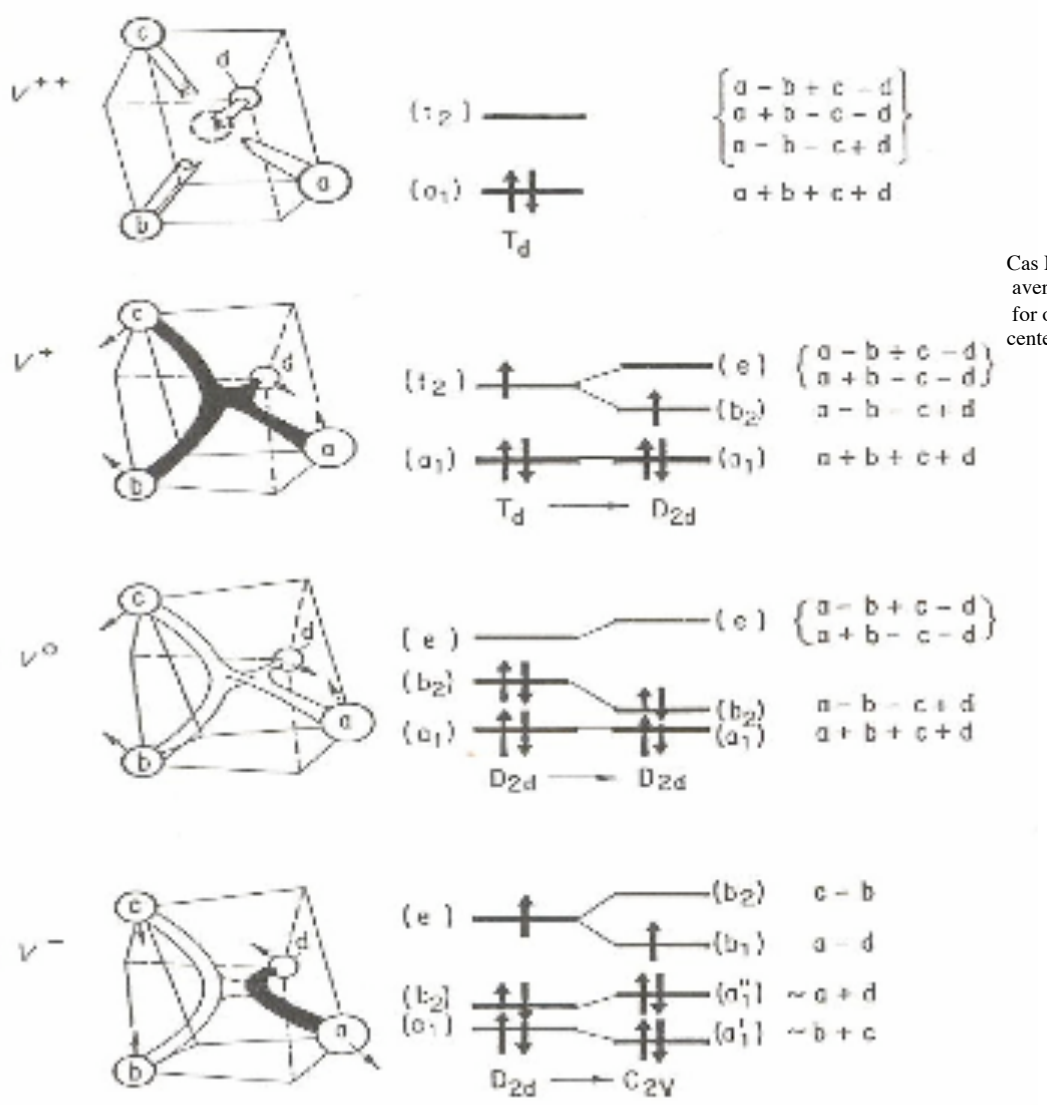
LCAO

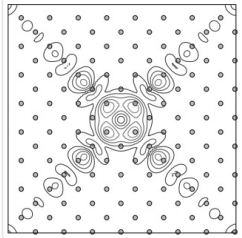
Linear Combination of Atomic Orbitals

a, b, c, d : Si ligands

Cubic point symmetry group ($\bar{4}3m$)

a_1:singlet, t_2:triplet





Cas Nsi=511, probability density averaged over the t_2 wave functions for on the (001) plane across a centered vacant site. *

* Ogawa et al
http://dx.doi.org/10.1016/j.ssc.2011.07.020

Point defects:Vacancies in Silicon

How are vacancies created?

How do vacancies disappear?

How long does it take to reach equilibrium?

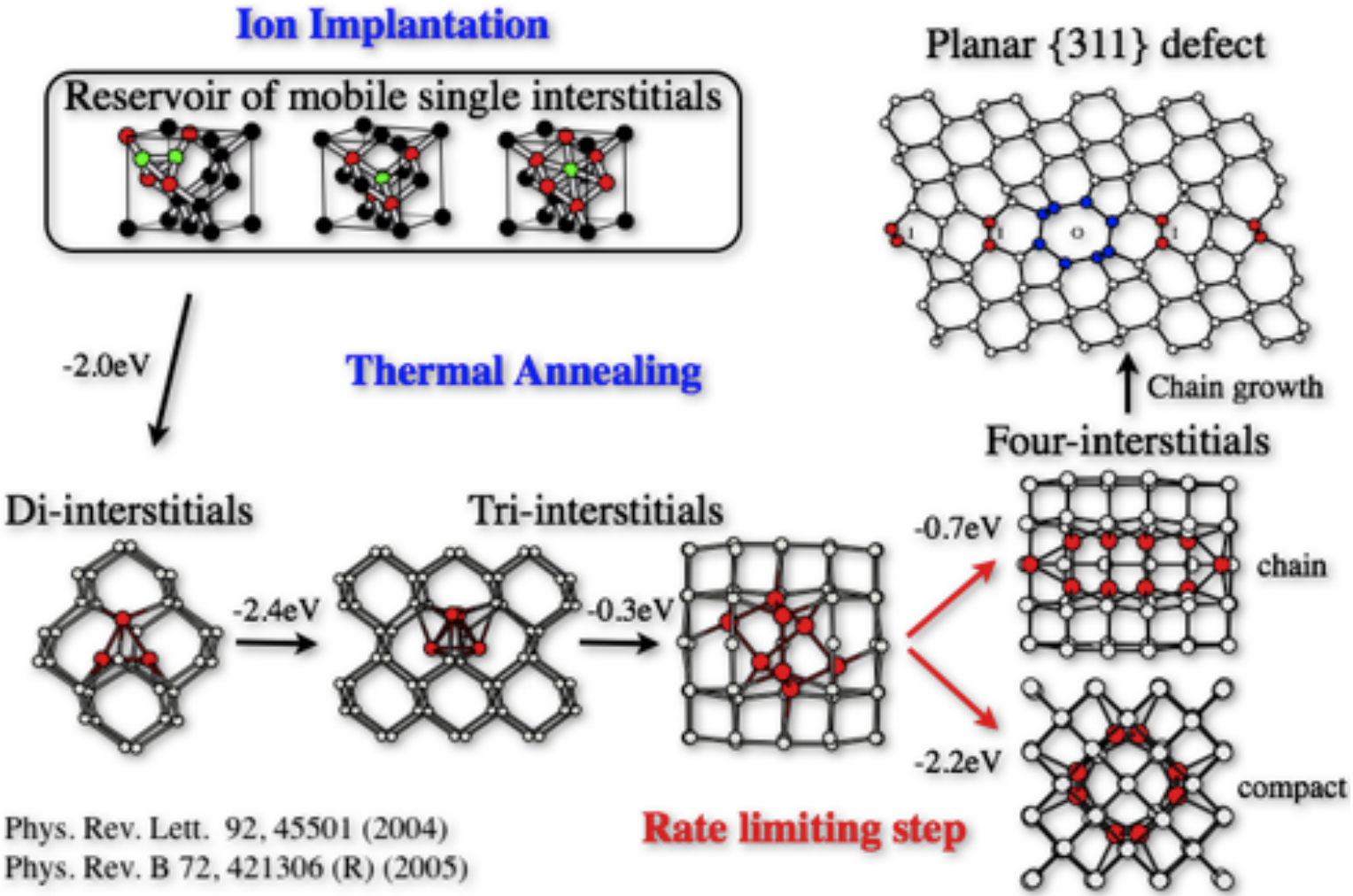
What are the benefits of vacancies?

What bad effects could vacancies have on a device?

What is the difference in formation energy for a neutral and single negative vacancy in Si?

Who will actually bother to read these questions?

Point defects: interstitials and complexes



Phys. Rev. Lett. 92, 45501 (2004)
Phys. Rev. B 72, 421306 (R) (2005)

Point defects: interstitials and complexes

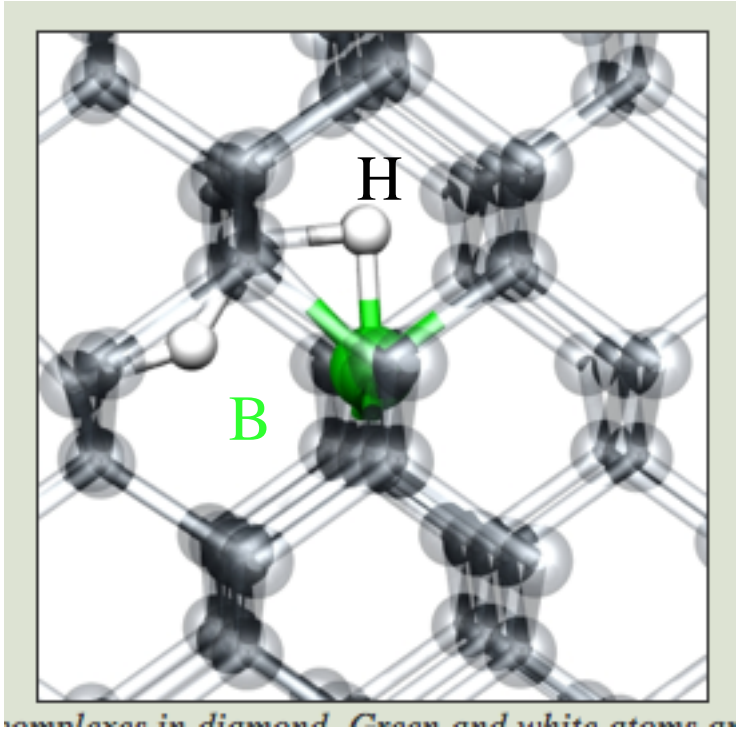
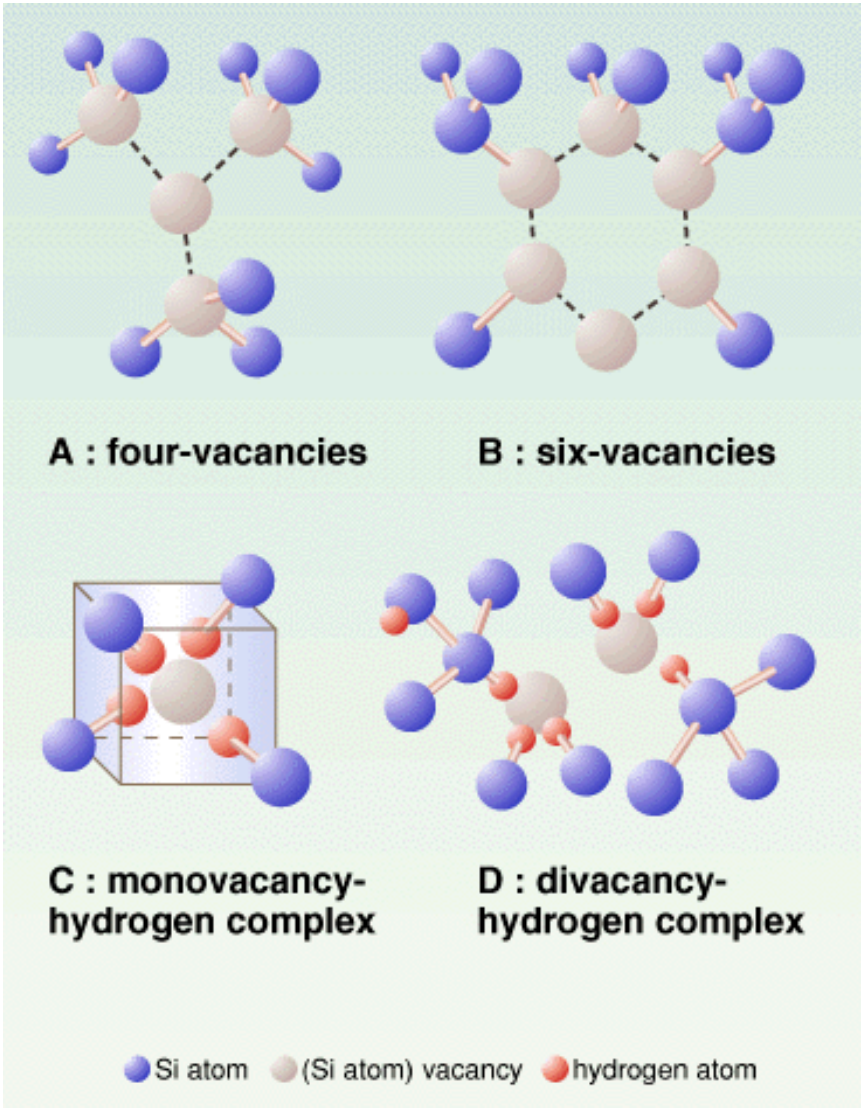
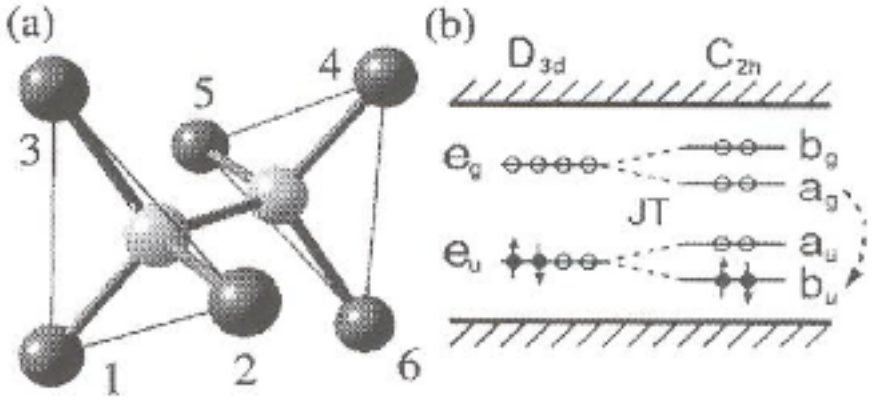


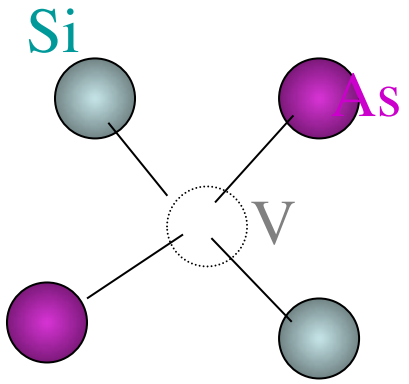
Figure 6: *Boron-hydrogen complexes in diamond. Green and white atoms are B and H, respectively. The structure can be viewed as a passive B-H complex adjacent to a hydrogen donor/acceptor (deep levels).*



Point defects: complexes, di vacancies, vacancy impurities



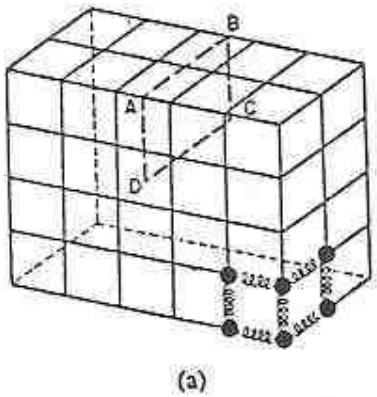
Di Vacancy



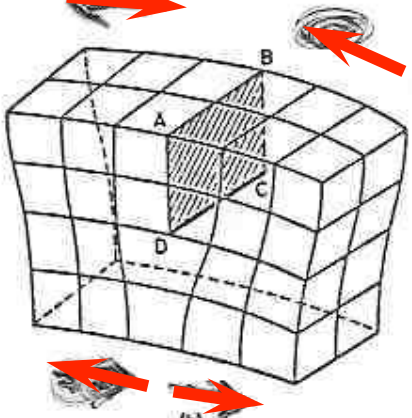
V-As_2

Line defects:dislocations

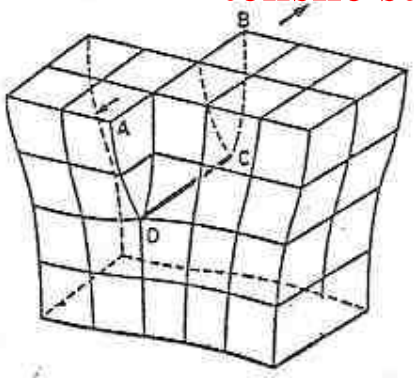
Edge dislocation



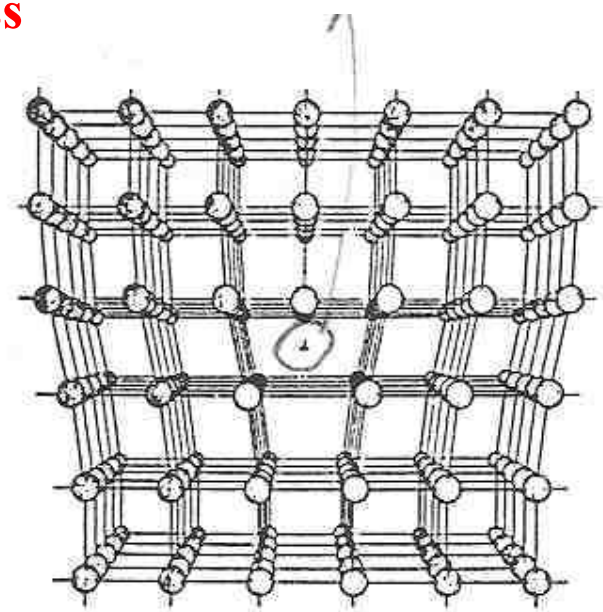
compressive stress



tensile stress

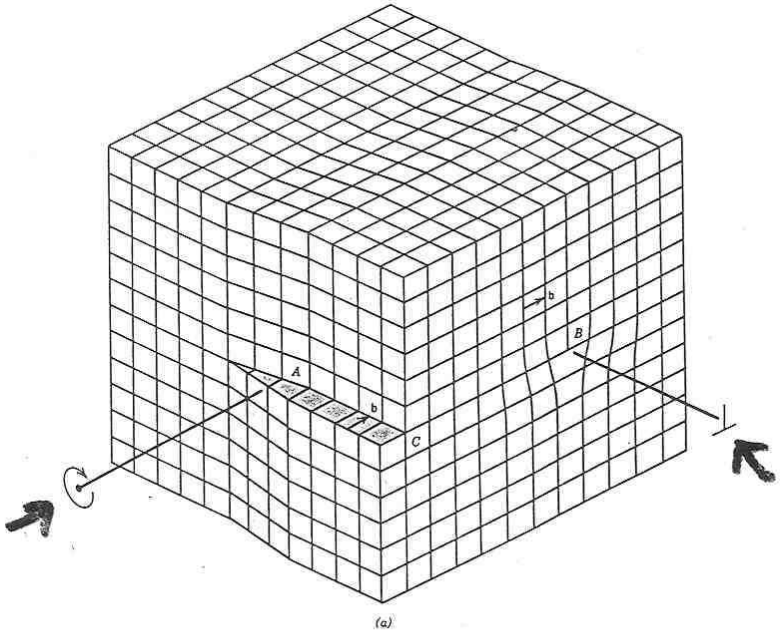


Screw dislocation



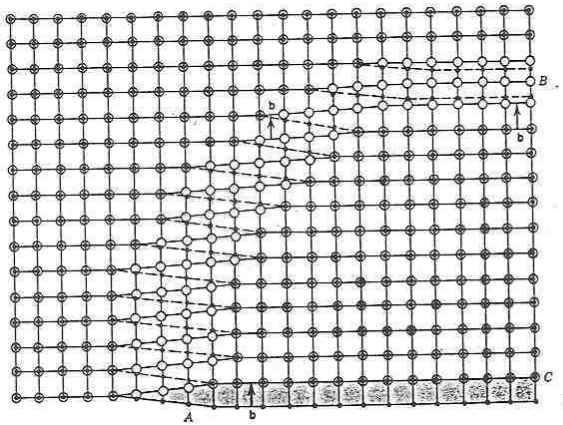
d) Picture of an edge dislocation

Line defects:dislocations



Screw dislocation

Edge dislocation



Top view

Line defects:dislocations:movement

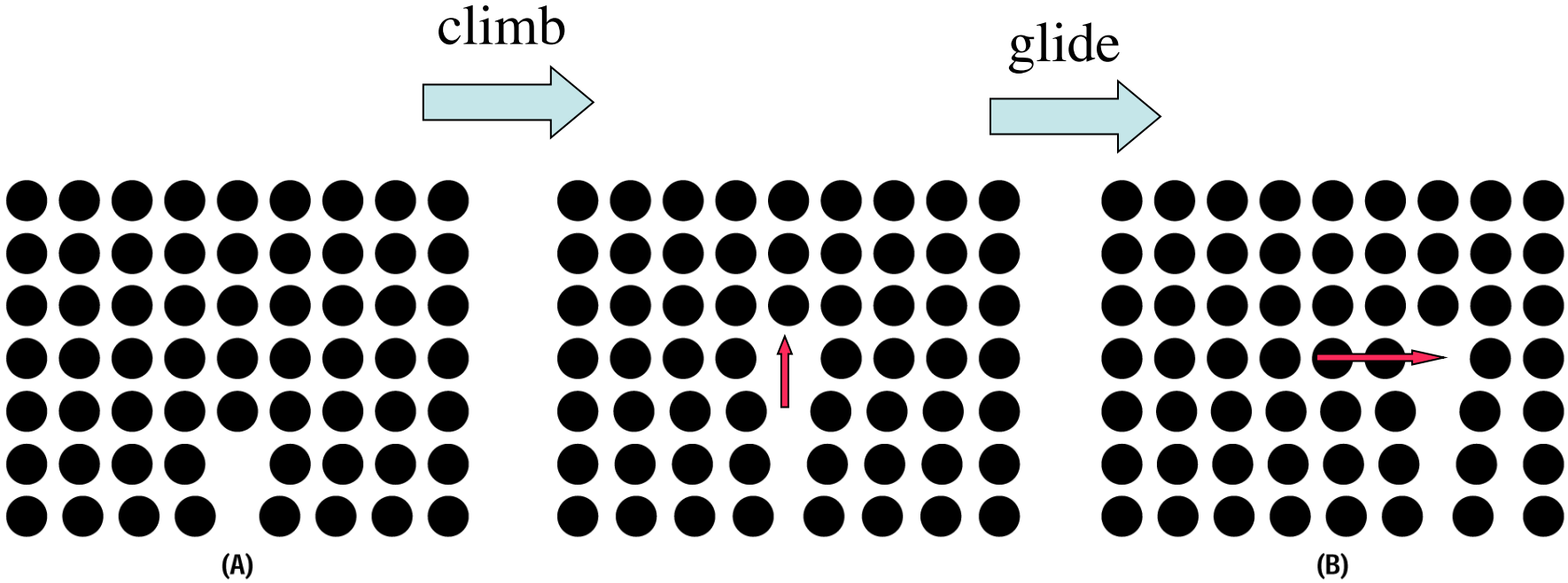
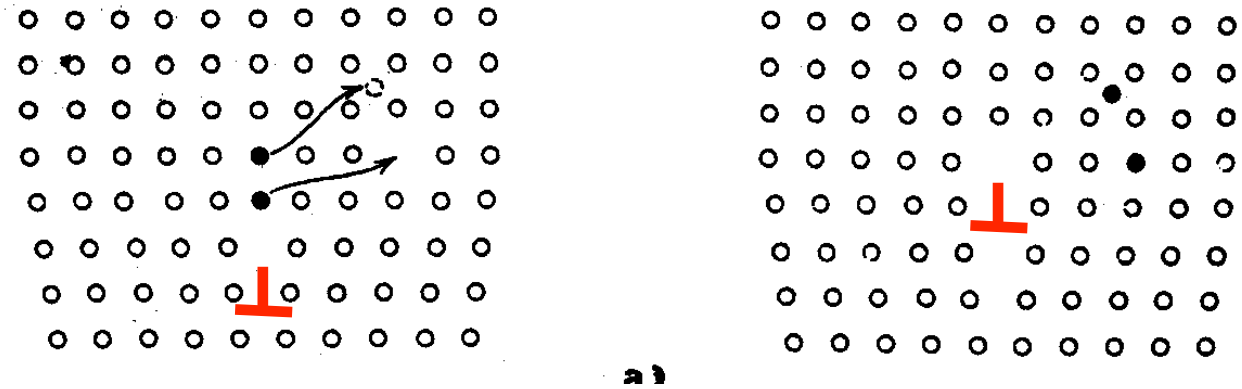


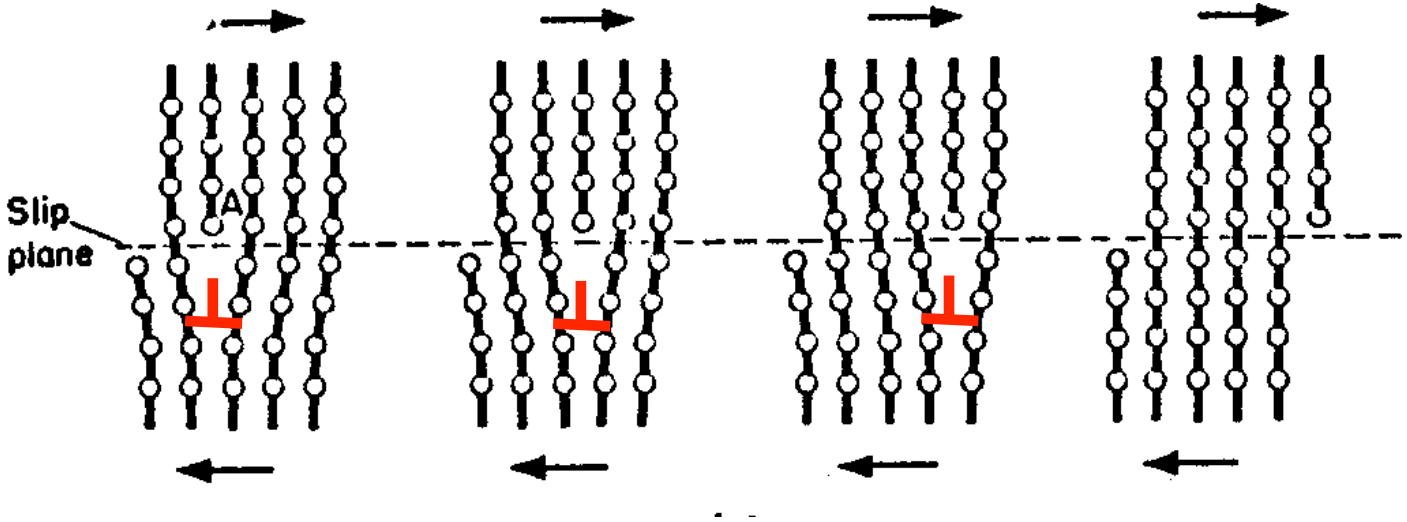
Figure 2.8 Movement of an edge dislocation (center figure) by (A) climb and (B) glide.

Line defects:dislocation:movement

Climb



Glide



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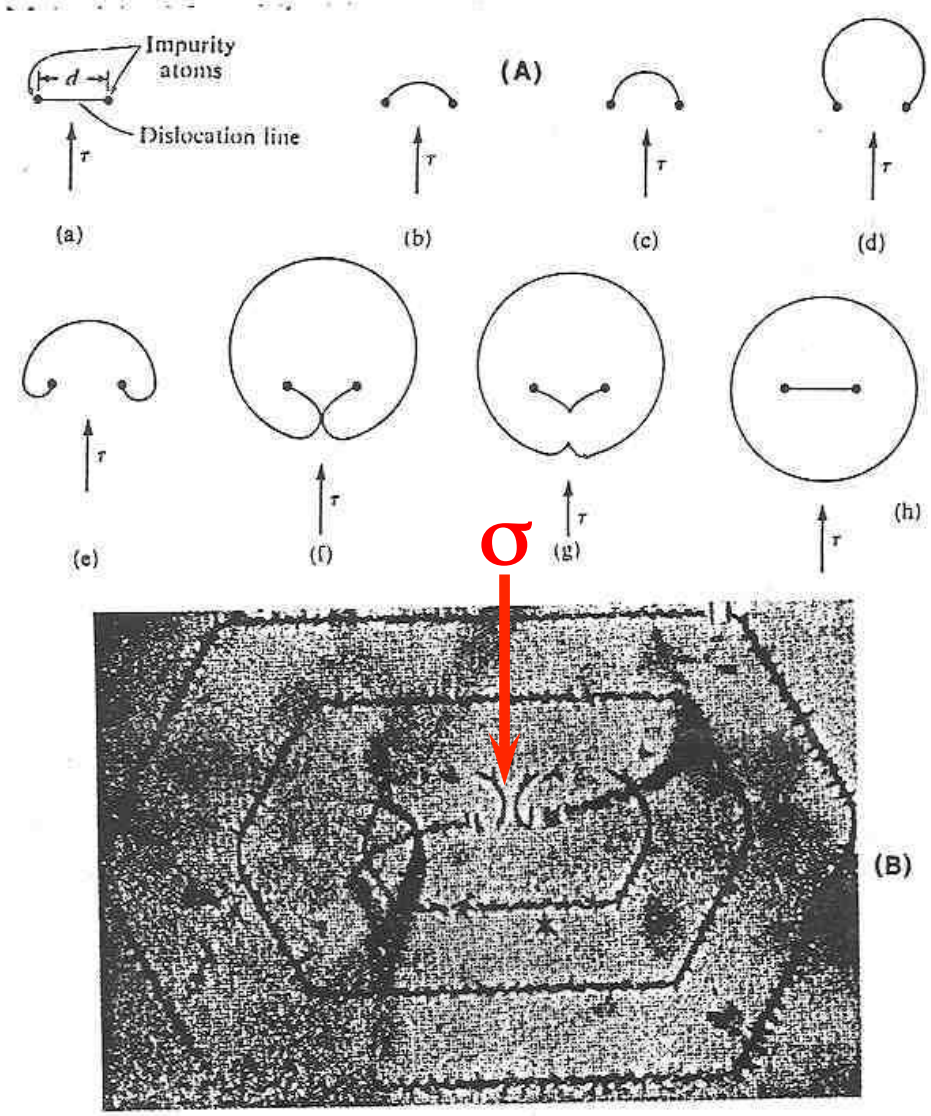
Line defects:dislocations:multiplication

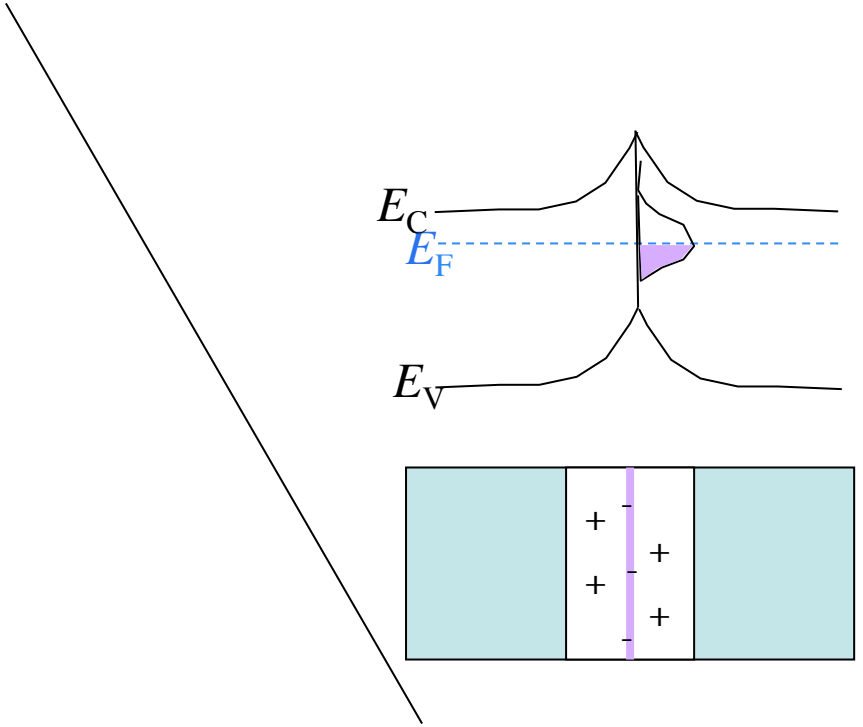


Mechanism

SEM picture

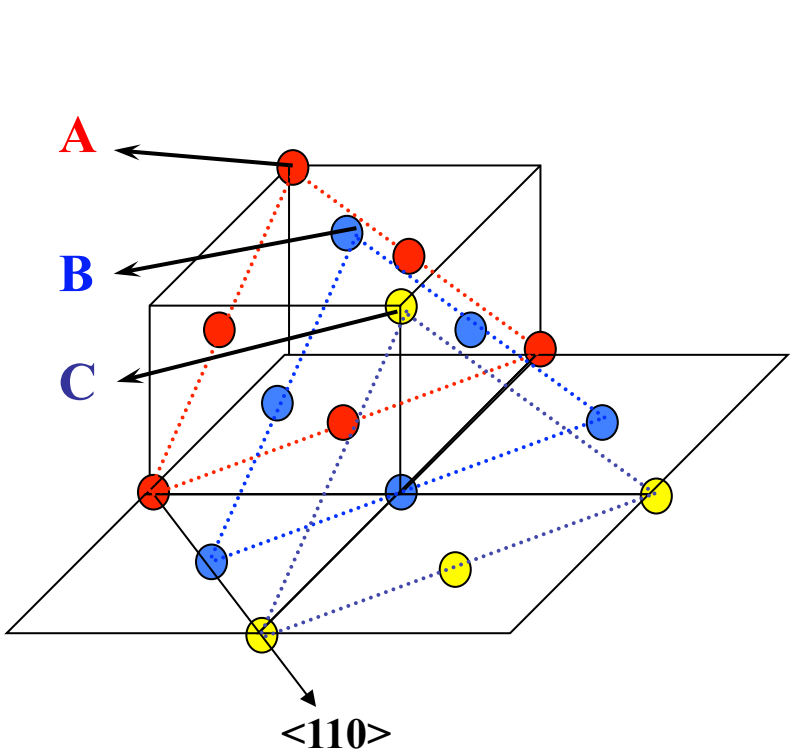
Line defects:dislocations:electrical effect

Localized electron states along the dislocation

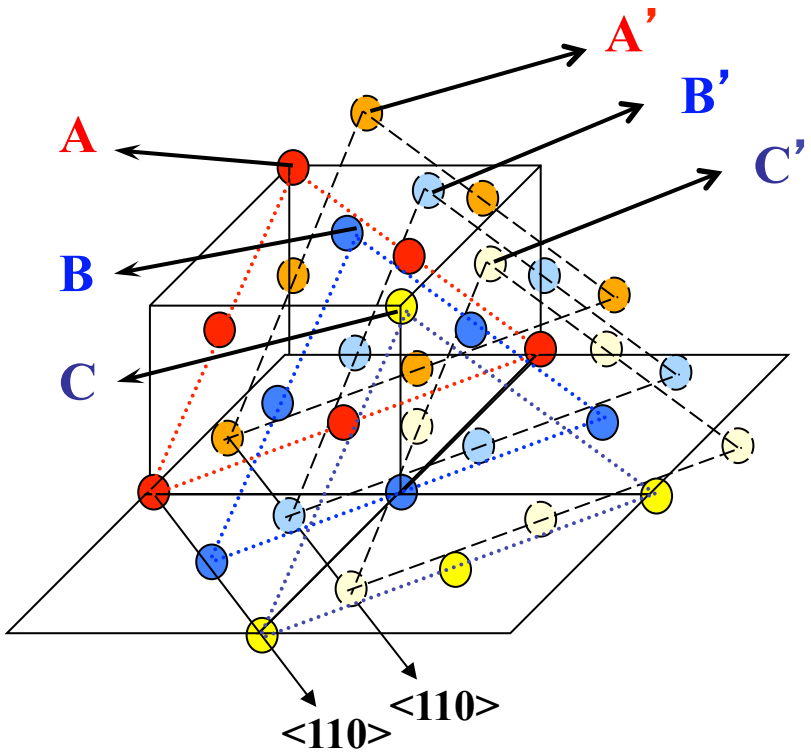


Areal defects:stacking faults

Stacking sequence for {111} planes



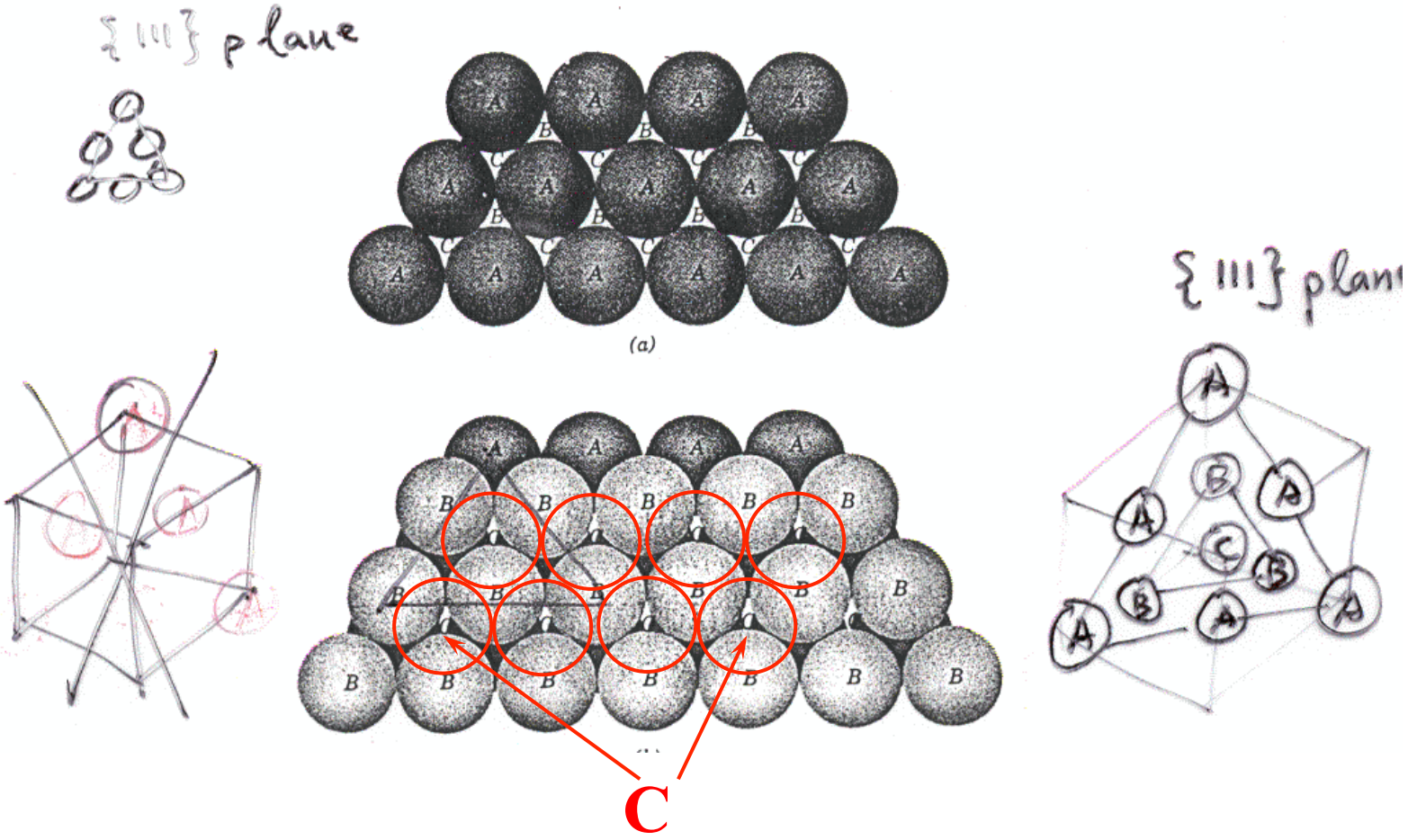
Face-centered cubic lattice



Diamond lattice

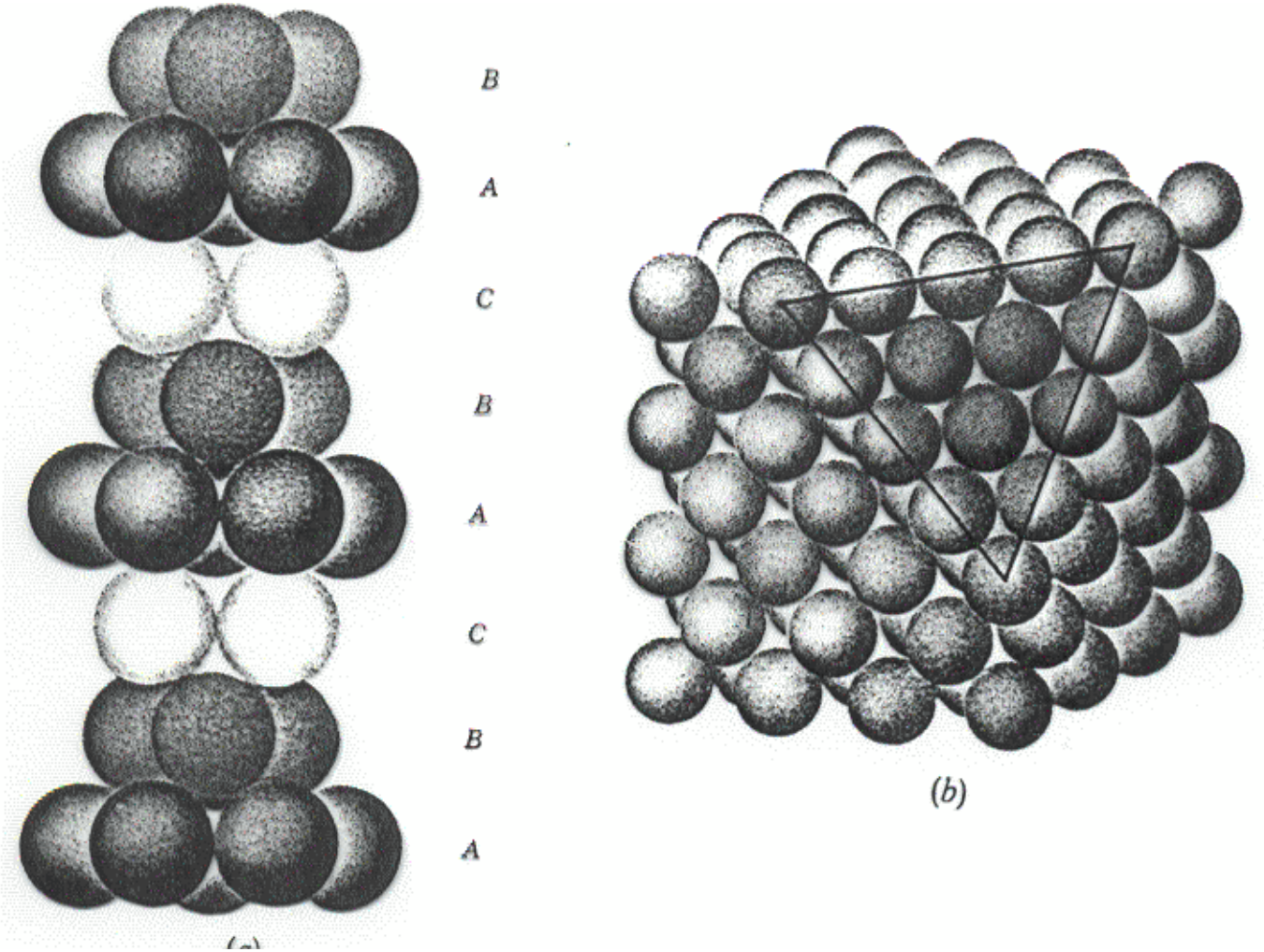
Areal defects:stacking faults

Stacking sequence for {111} planes fcc



Areal defects:stacking faults

Stacking sequence for {111} planes in fcc



Area defects:stacking faults

In Si

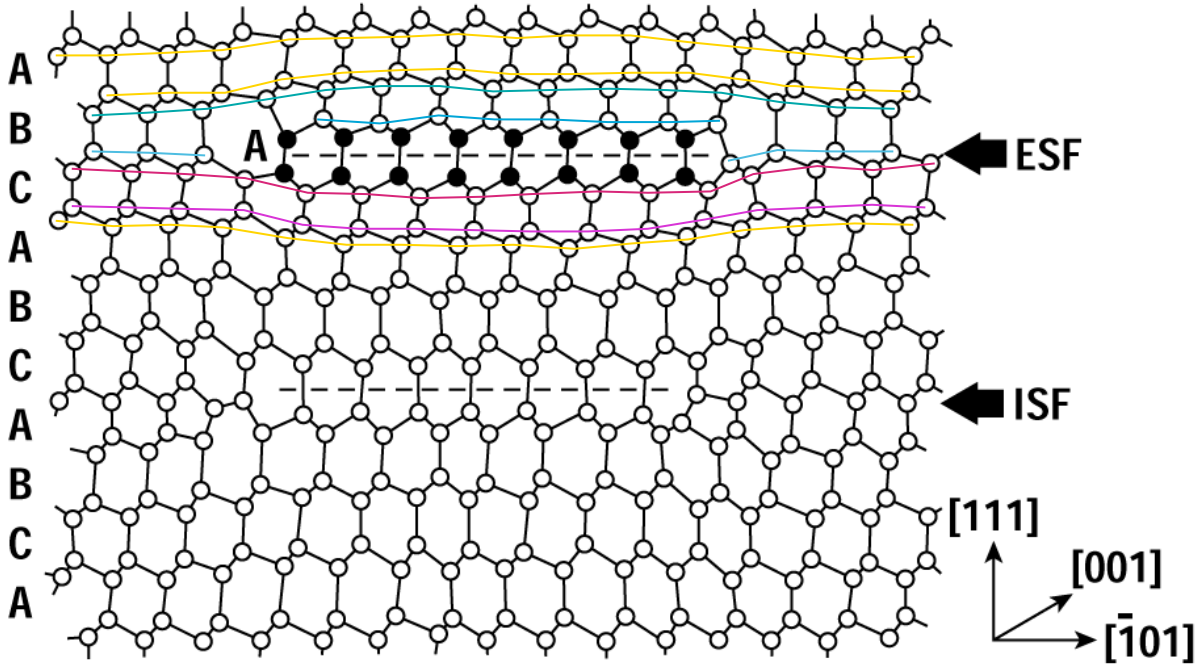


Figure 2.9 An intrinsic stacking fault is the removal of part of a plane of atoms in the {111} directions. An extrinsic stacking fault is the addition of a partial plane of atoms in the {111} directions. The labels A, B, and C correspond to the three different (111) planes in the diamond lattice *(after Shimura)*.

Area defects:stacking faults

In Si

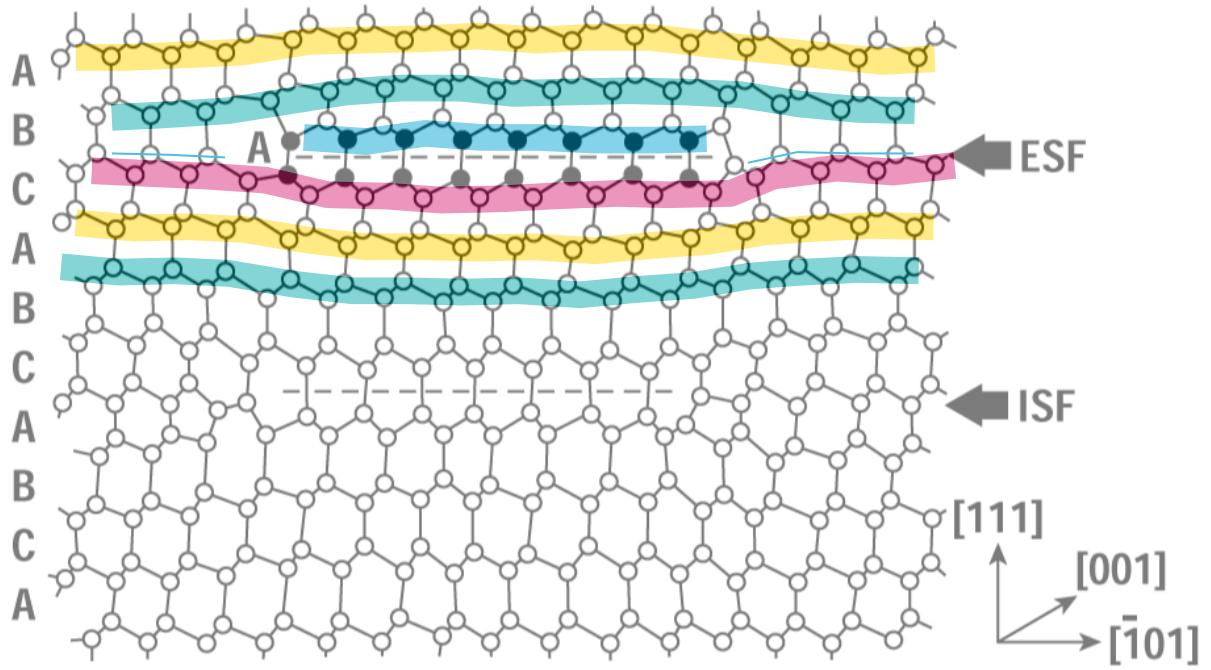


Figure 2.9 An intrinsic stacking fault is the removal of part of a plane of atoms in the {111} directions. An extrinsic stacking fault is the addition of a partial plane of atoms in the {111} directions. The labels A, B, and C correspond to the three different (111) planes in the diamond lattice *(after Shimura)*.

Area defects:stacking faults

How can stacking faults be created?

Are they good and/or bad?

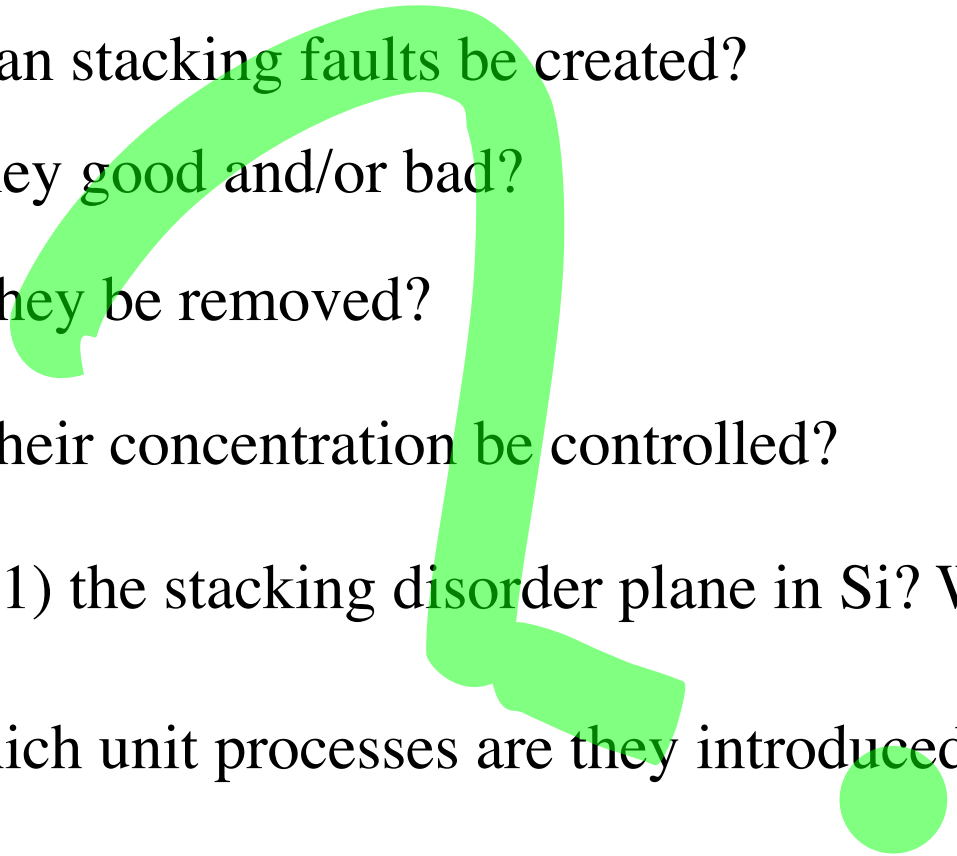
Can they be removed?

Can their concentration be controlled?

Is (111) the stacking disorder plane in Si? Why? Not?

In which unit processes are they introduced?

Do unit processes interact with respect to stacking faults?



Area defects:grain boundaries

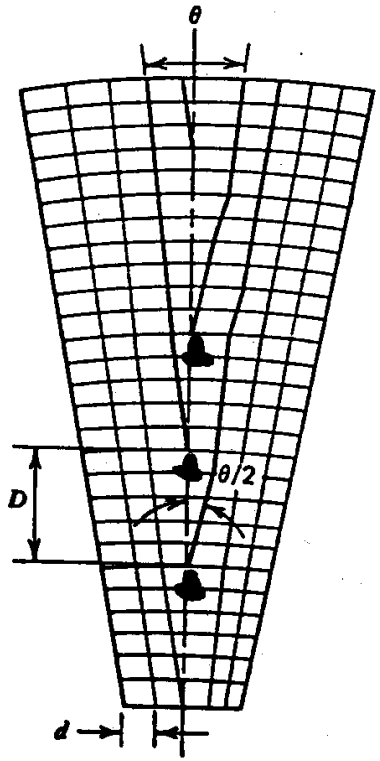


Fig. 1.27 Model for a low-angle grain boundary.

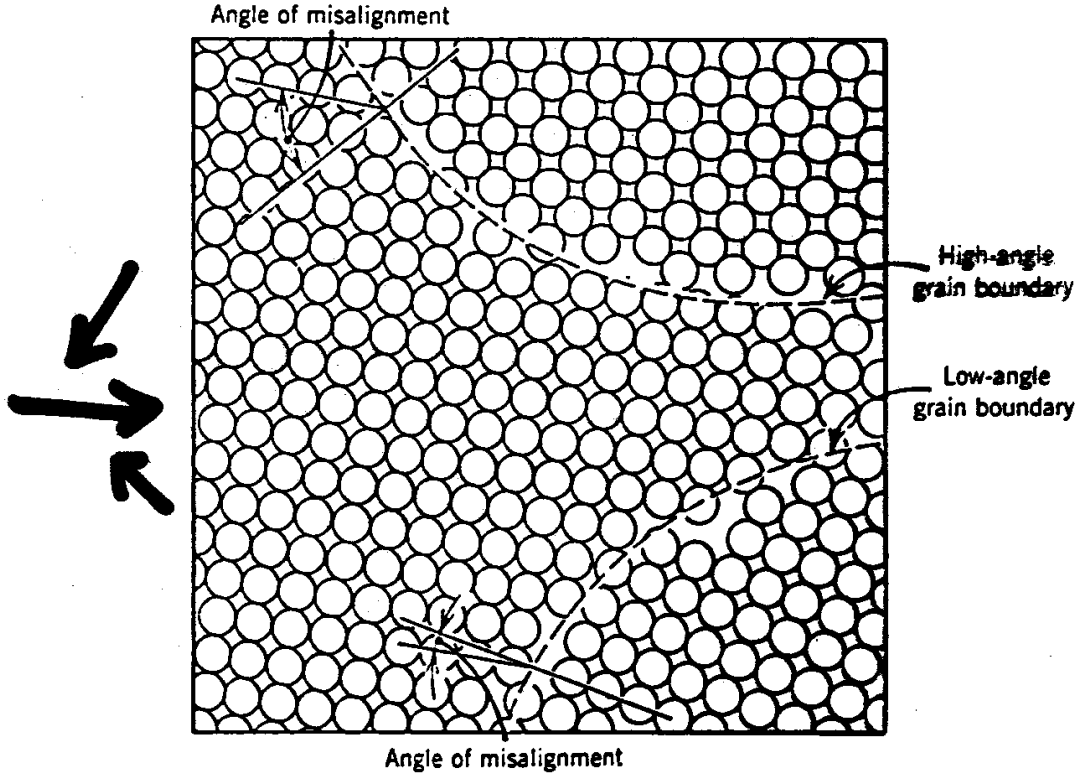


Figure 4.7 Schematic diagram showing low- and high-angle grain boundaries and the adjacent atom positions.

Area defects:antiphase domain boundaries

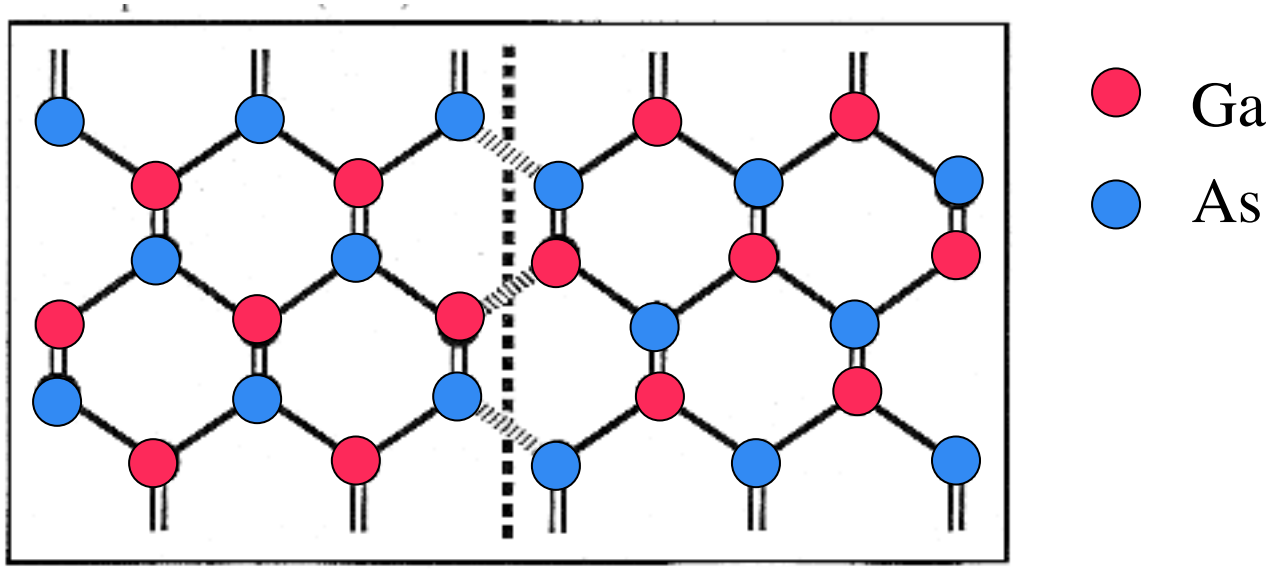


Fig 2 Antiphase boundary in GaAs.