CERN, TA1/SSD coffee-meeting 11.6.2004

Defects in silicon crystals

- Some very basic remarks -

Michael Moll

CERN - Geneva - Switzerland

People are like crystals. It is the defects in them that make them interesting. Sir F.Charles Frank

Perfection has one grave defect : it is apt to be dull

William Somerset Maugham

- **Defects give silicon crystals new properties**
- **These properties can be useful (e.g. doping, defect engineering) or not (e.g. radiation damage, metal contaminations)**

CERN, TA1/SSD coffee meeting 11.6.2004

Outline

- **Silicon and Silicon crystal structure**
- **Defect types in silicon crystals**
- **Silicon doping (Dopants = Defects)**

} **Easy level**

- **Radiation induced defects**
- **What are defects doing to detectors?**
- **How to measure defects?**

} **More difficult level**

- **Coffee**

} **Relax level**

Silicon

Atomic number = 14 **Atomic mass 28.0855 amu**

- **Most abundant solid element on earth 50% O, 26% Si, 8% Al, 5% Fe, 3% Ca, ...**
- **90% of earth's crust is composed of silica (SiO_2) and silicate !**

Very pure sand or quartz → ? → **Silicon**

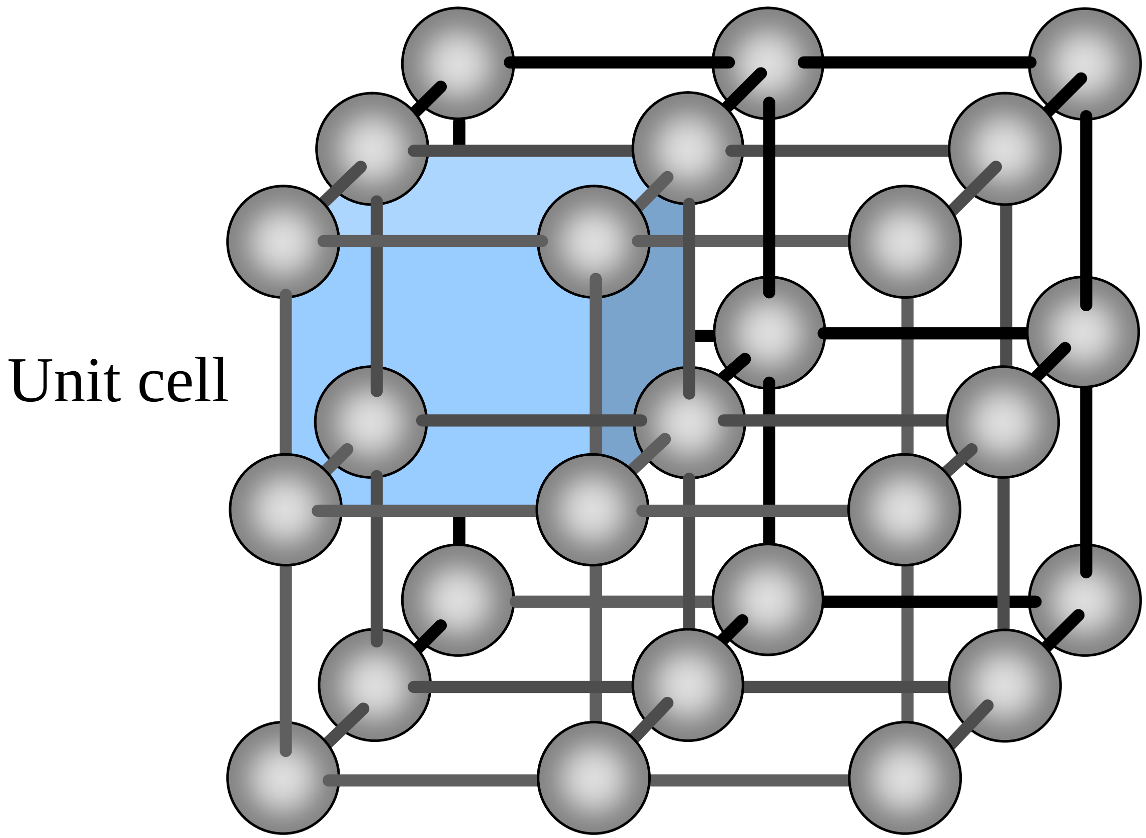
(e.g. from Australia or Nova Scotia in Canada)

≈ 99% **SiO_2**

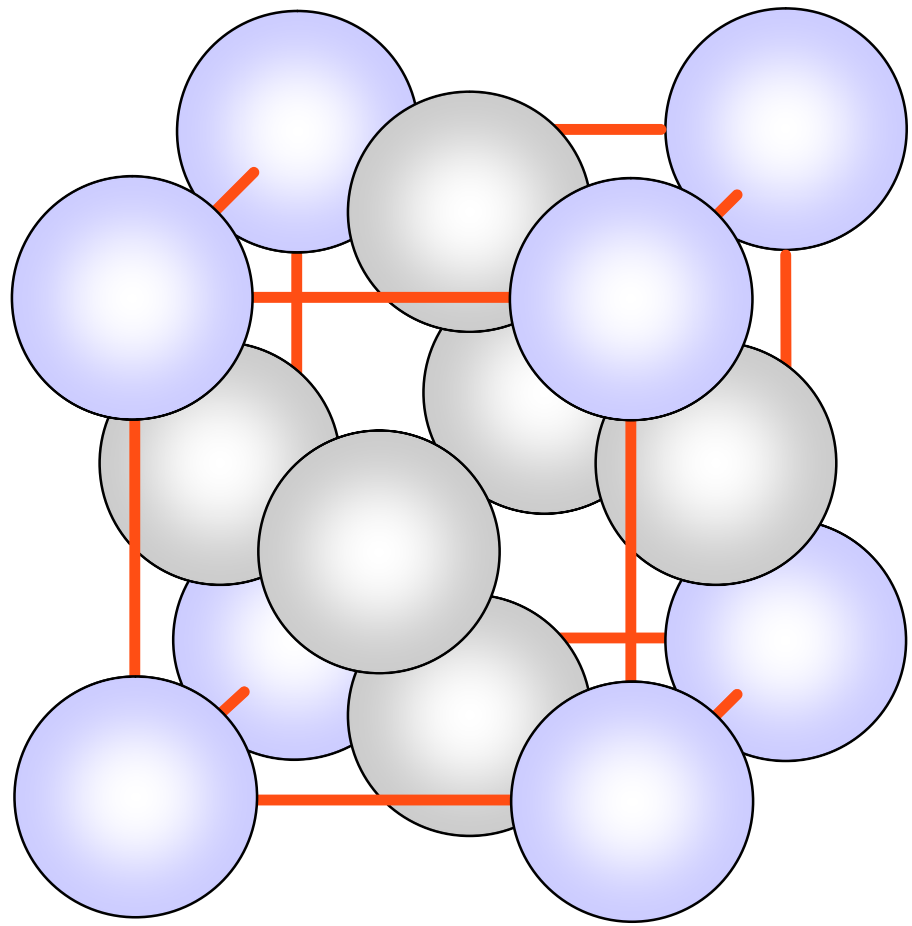
≈ 1% Al_2O_3, Fe_2O_3, TiO_2 (CaO,MgO)

Another coffee meeting ?

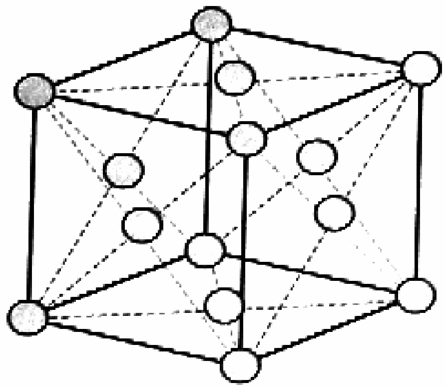
Unit Cell in 3-D Structure



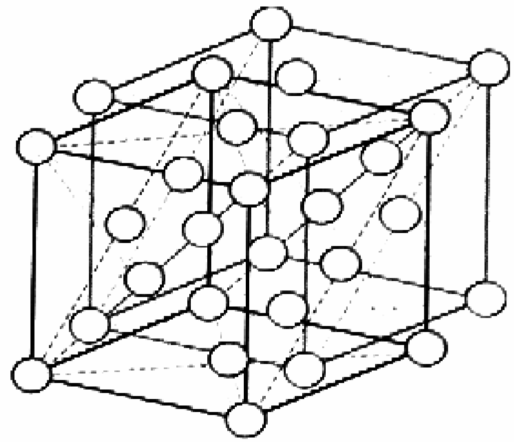
Faced-centered Cubic (FCC) Unit Cell



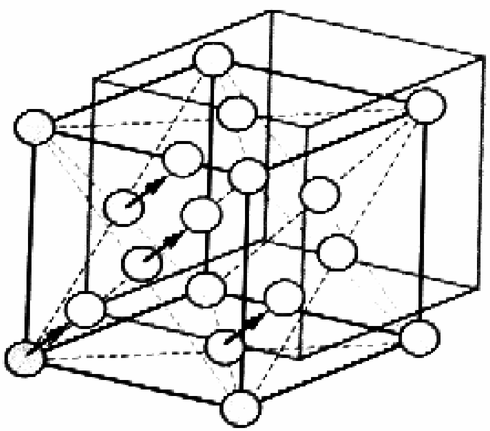
Silicon Crystal Structure



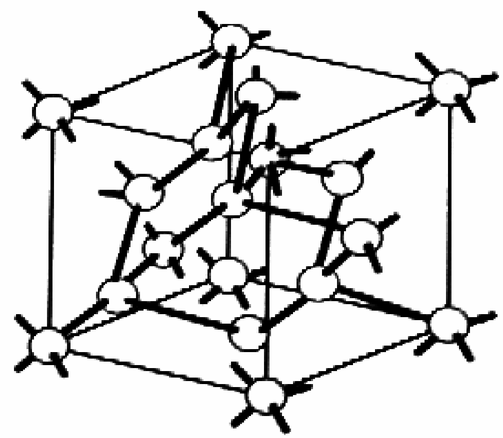
Basic FCC Cell



Merged FCC Cells



Omitting atoms outside Cell



Bonding of Atoms

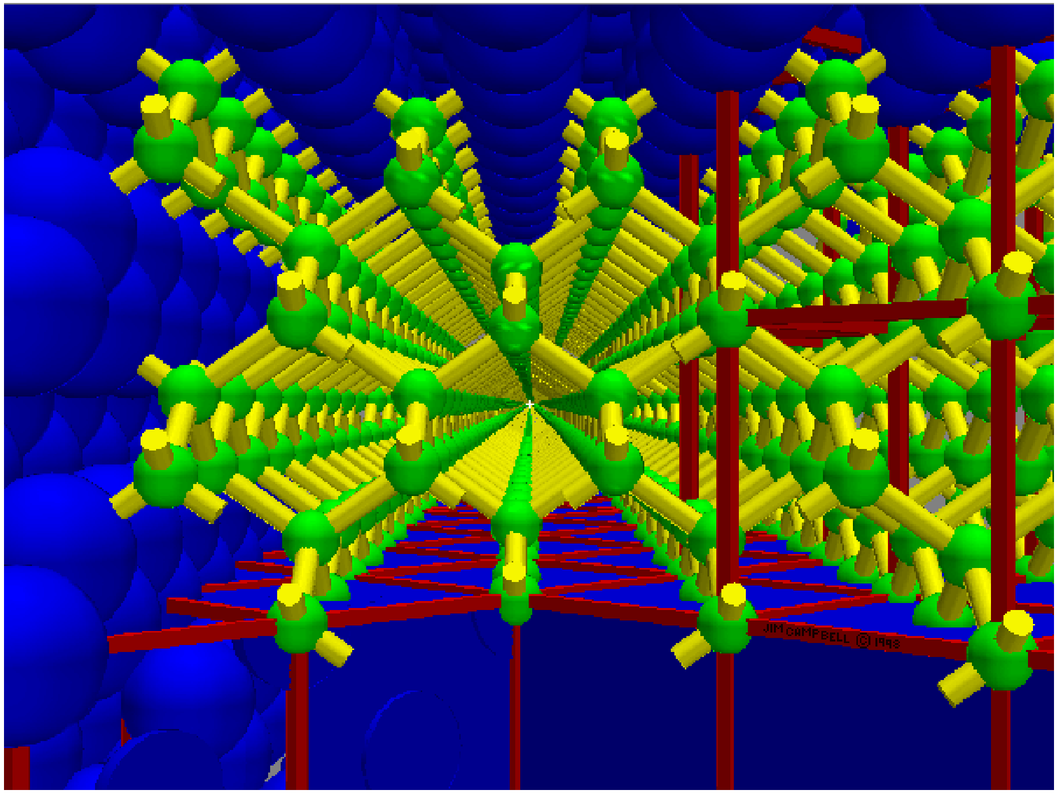
Silicon has the basic diamond crystal structure: two merged FCC cells offset by a/4 in x, y and z

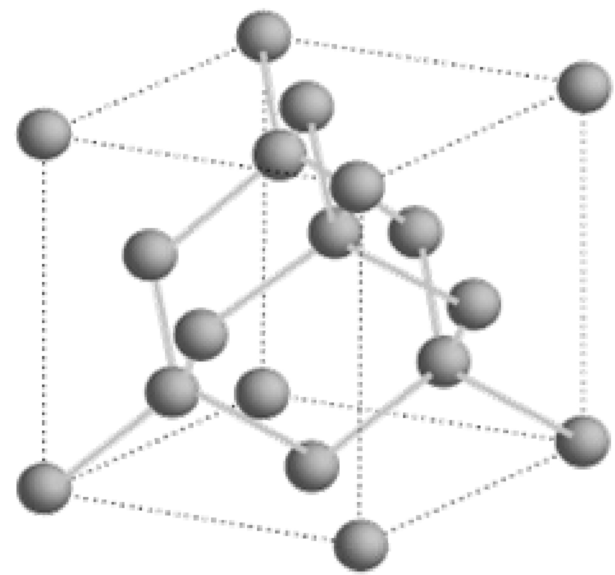
Silicon Crystal Structure

Link: BC8 Structure of Silicon

Link: Silicon lattice (wrl)

Link: Silicon lattice with bonds (wrl)





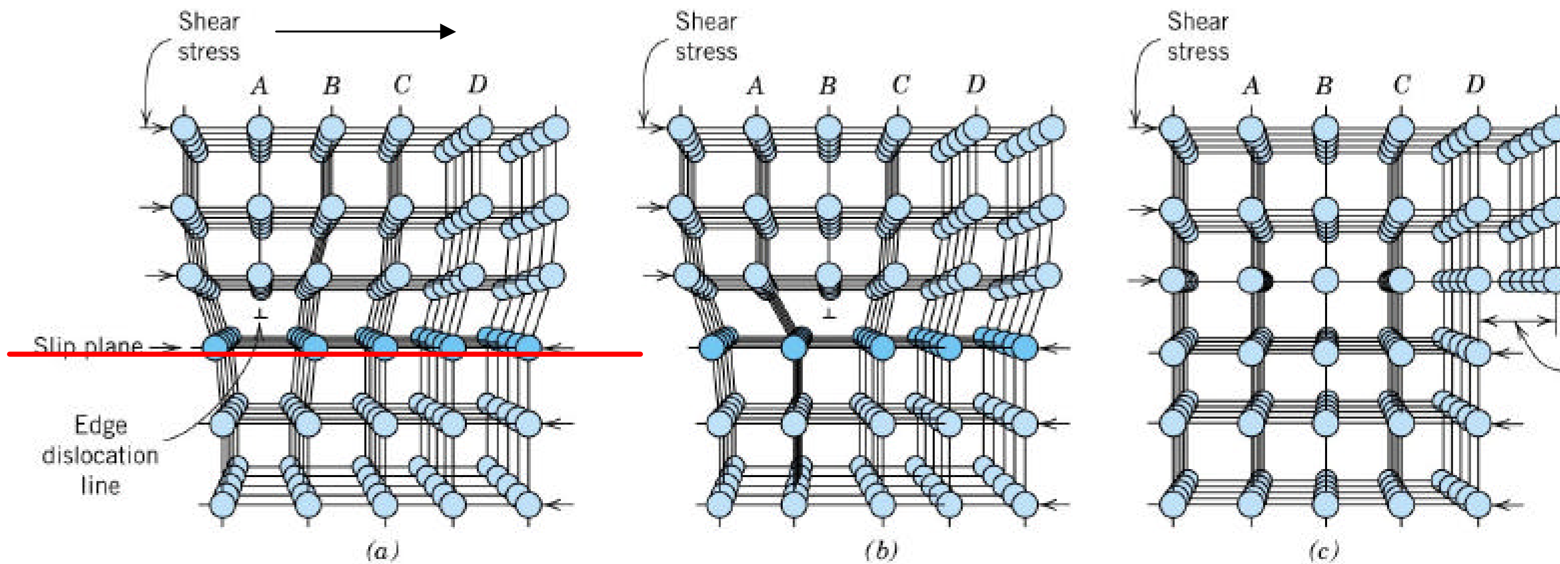
Silicon crystallizes in the same pattern as **Diamond**, in a structure called "two interpenetrating face-centered cubic" primitive lattices. The lines between silicon atoms in the lattice illustration indicate nearest-neighbor bonds. The cube side for silicon is 0.543 nm.

Outline

- Silicon and Silicon crystal structure
- Defect types in silicon crystals
    - Lattice defects (Dislocations)
    - Point defects (e.g. Impurities)
    - Cluster defects and Precipitates

- Silicon doping (Dopants = Defects)
- Radiation induced defects
- What are defects doing to detectors?
- How to measure defects?
- Coffee

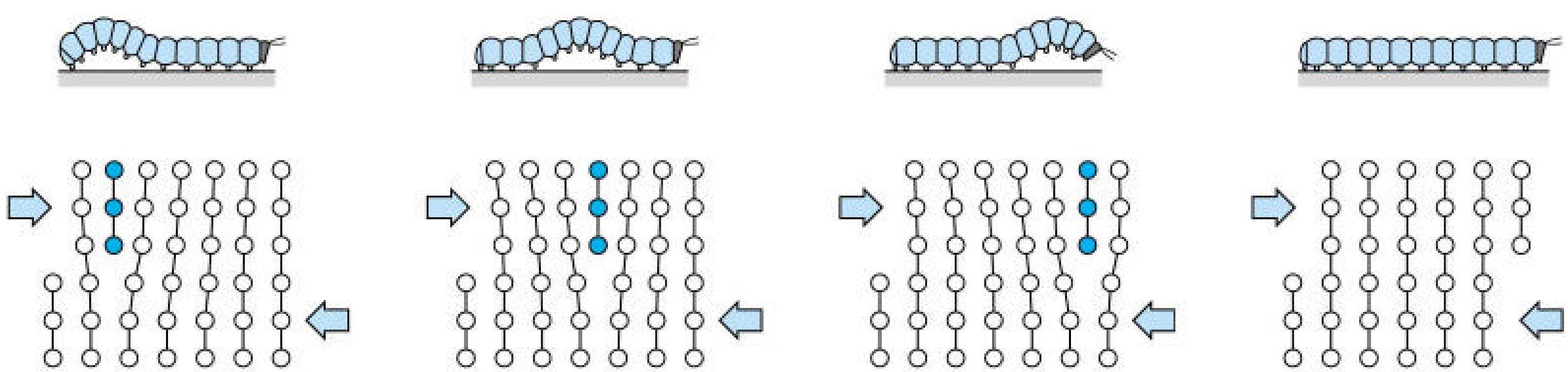
Dislocations



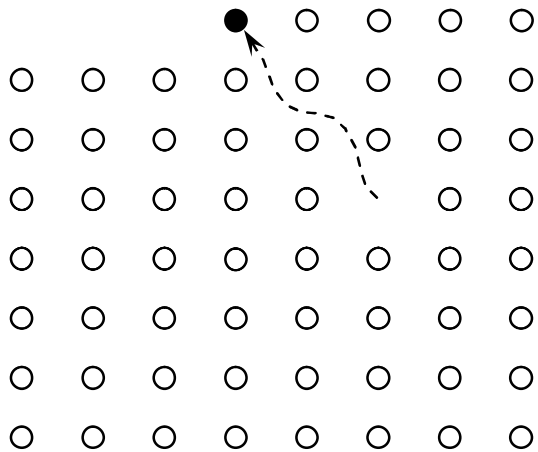
Burger's
Vector = b

Shear stress

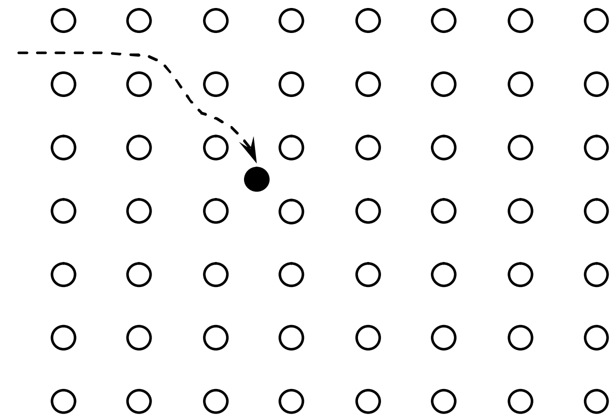
The caterpillar or rug-moving analogy



Point Defects

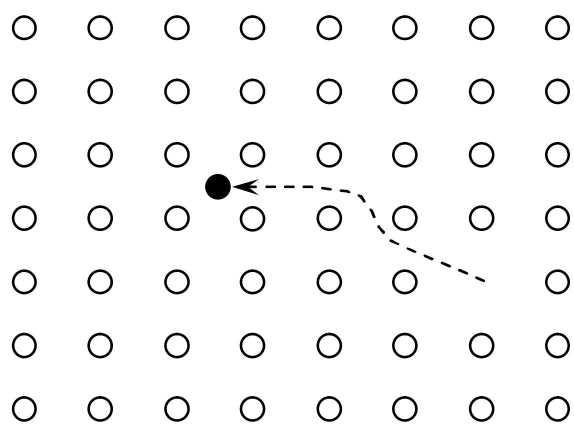


Vacancy defect



Interstitial defect

Link: Split-interstititial (wrl)



Frenkel defect

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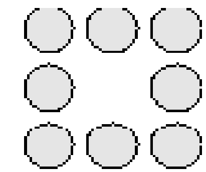
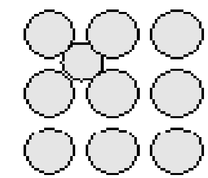
Point Defects

- **Intrinsic defects:**

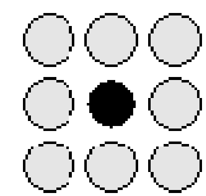


  - **The Vacancy (denoted V): an atom is removed.**

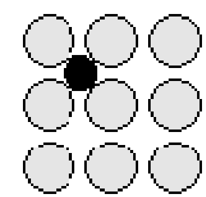


  - **The Self-interstitial (denoted I): a host atom sits in a normally unoccupied site or** interstice **(various sites: bond centres, tetrahedral sites, interstitial + displaced regular atom).**

- **Extrinsic defects: due to an impurity.**
  These can be:

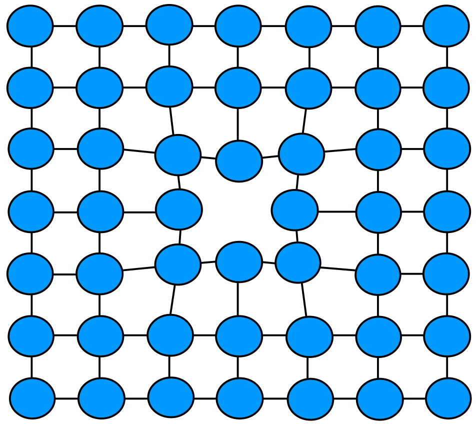


  - **Substitutional, such as carbon substitutional (denoted C_s)**



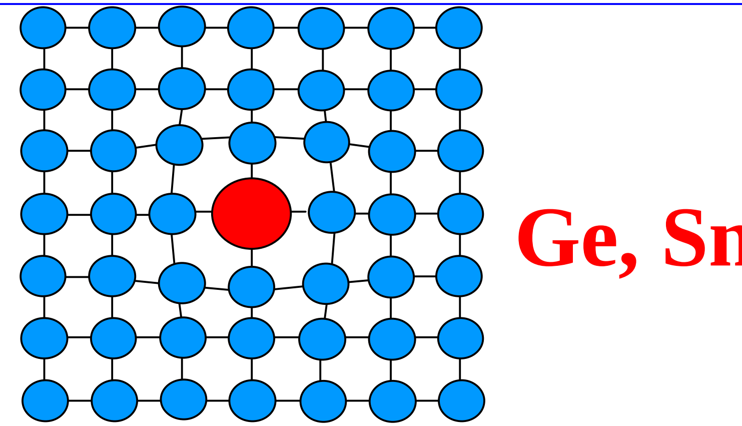
  - **Interstitial (such as the carbon interstitial (denoted C_i).**

Point Defects - Lattice strain

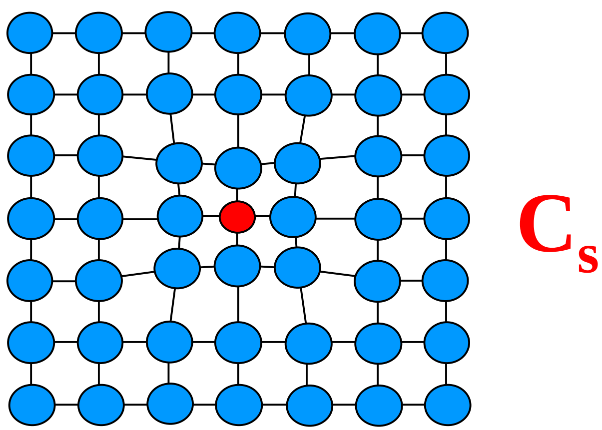


(a) A vacancy in the crystal.

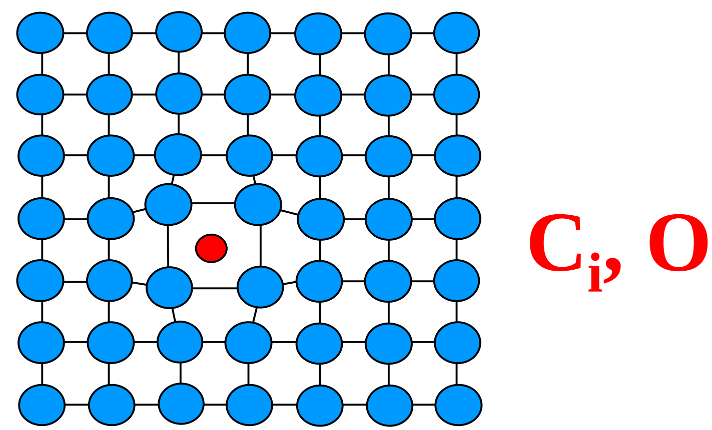
Link: Vacancy - Hydrogen Defect



(b) A substitutional impurity in the crystal. The impurity atom is larger than the host atom.



(c) A substitutional impurity in the crystal. The impurity atom is smaller than the host atom.

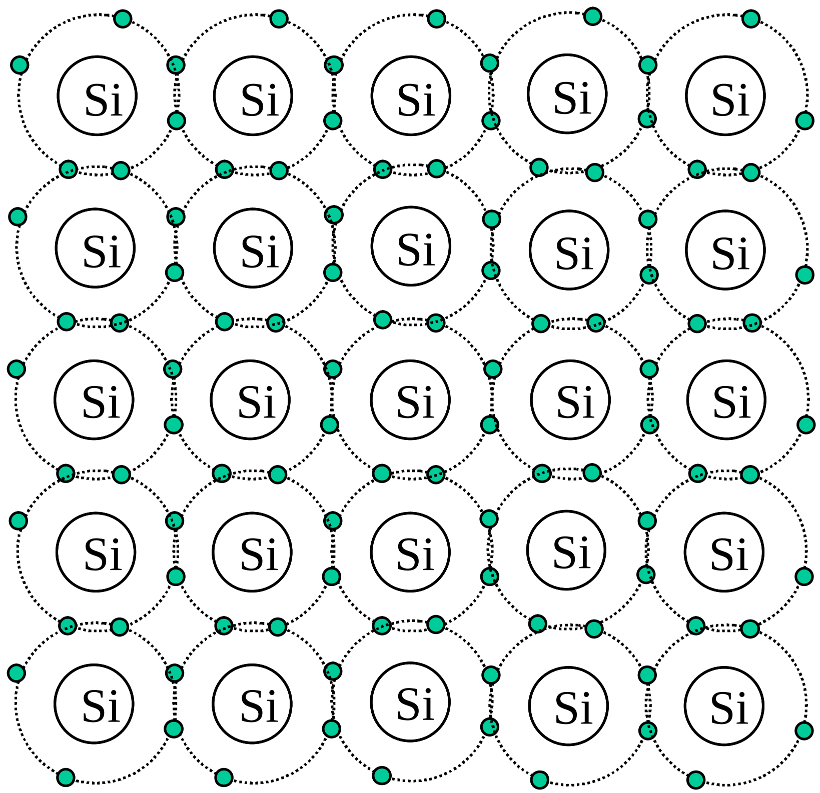


(d) An interstitial impurity in the crystal. It occupies an empty space between host atoms.

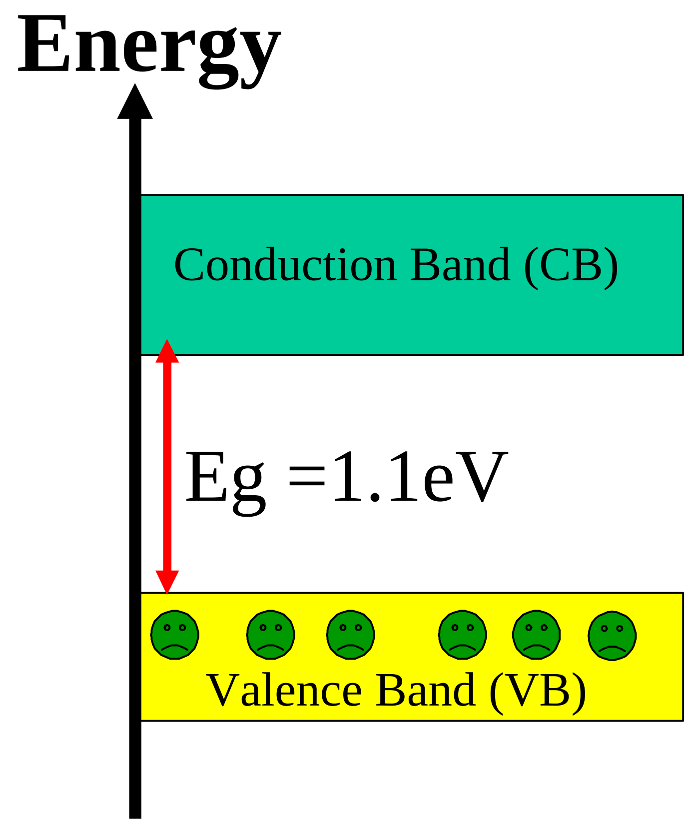
Outline

- Silicon and Silicon crystal structure
- Defect types in silicon crystals
- Silicon doping (Dopants = Defects)
    - Intrinsic silicon
    - n-type silicon
    - p-type silicon
- Radiation induced defects
- What are defects doing to detectors?
- How to measure defects?
- Coffee

Covalent Bonding of Pure Silicon

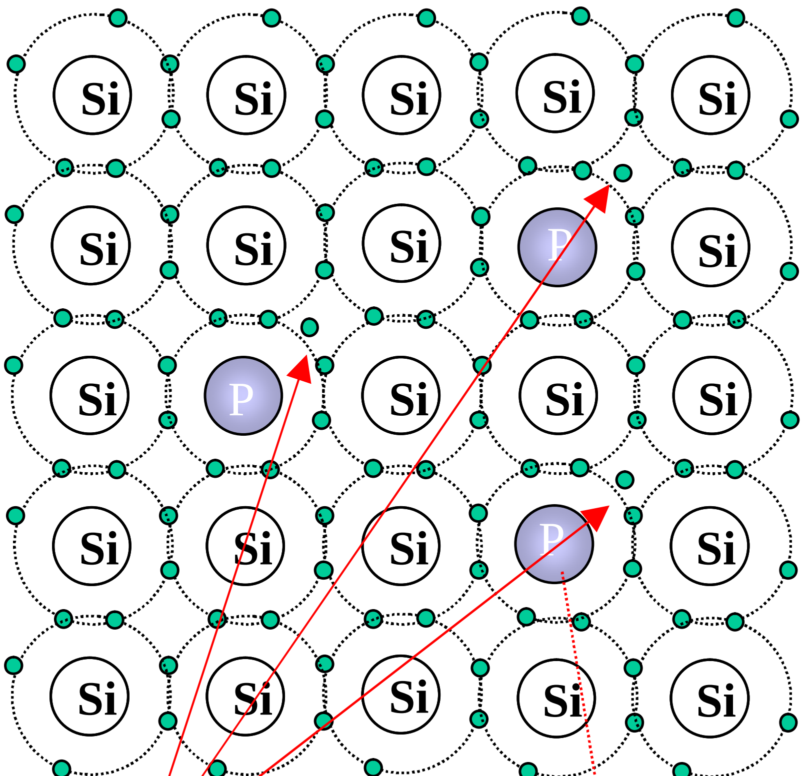


Silicon atoms share valence electrons
to form insulator-like bonds.



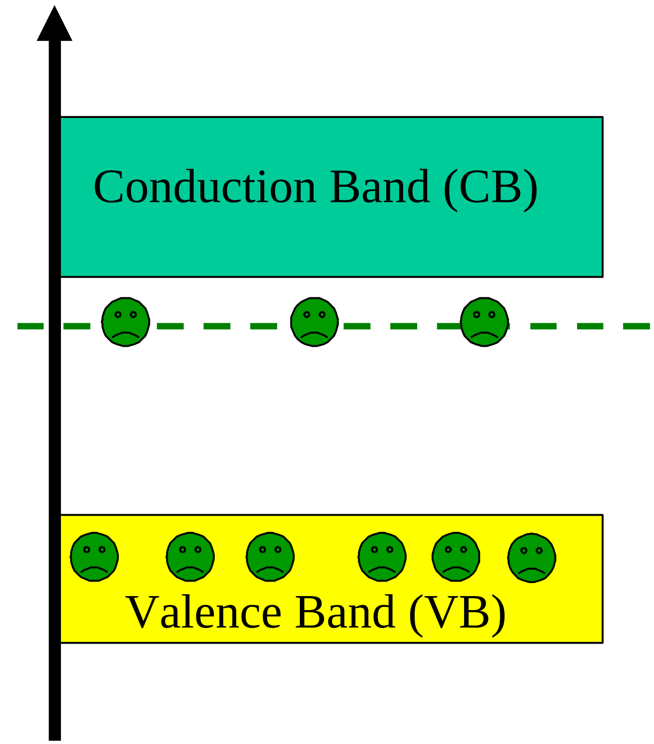
Electrons in N-Type Silicon with Phosphorus Dopant

Donor atoms provide excess electrons to form n-type silicon.



Excess electron (-)

Phosphorus atom serves as n-type dopant



Conduction in n-Type Silicon

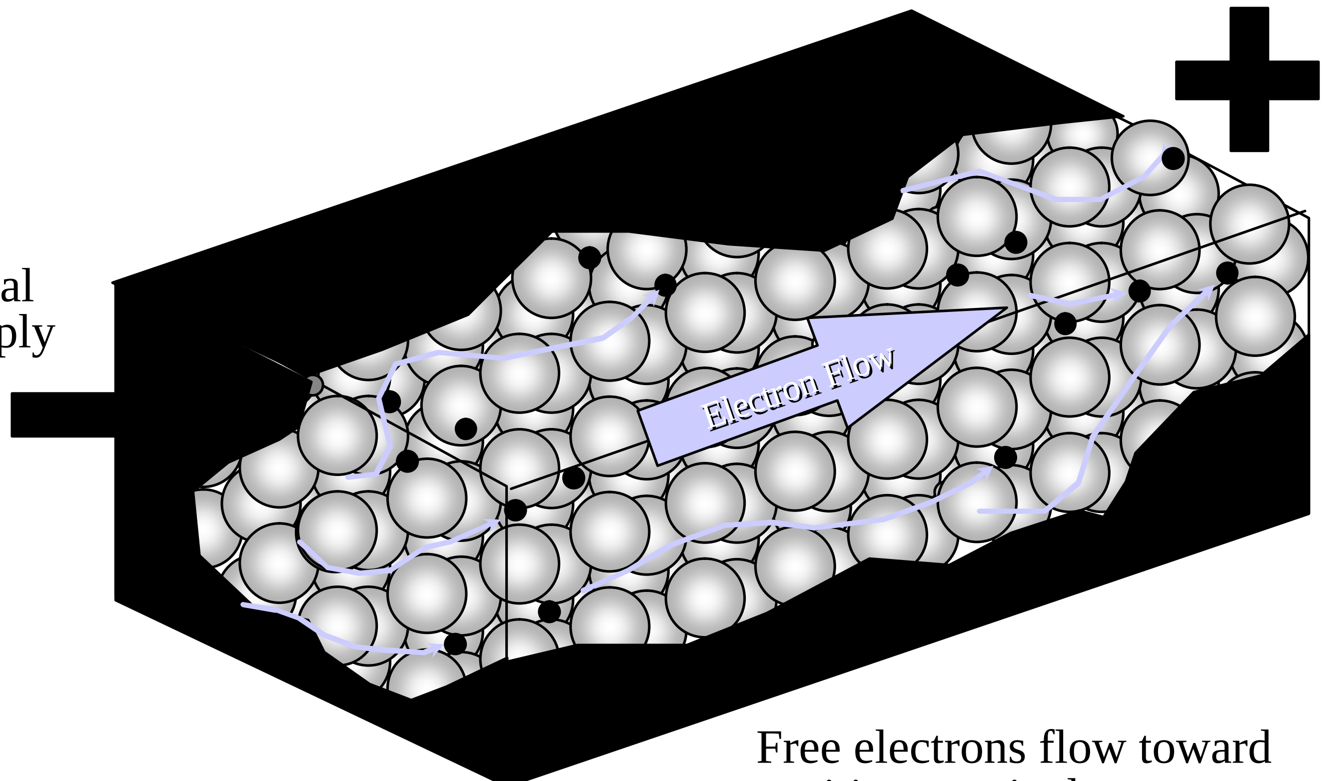
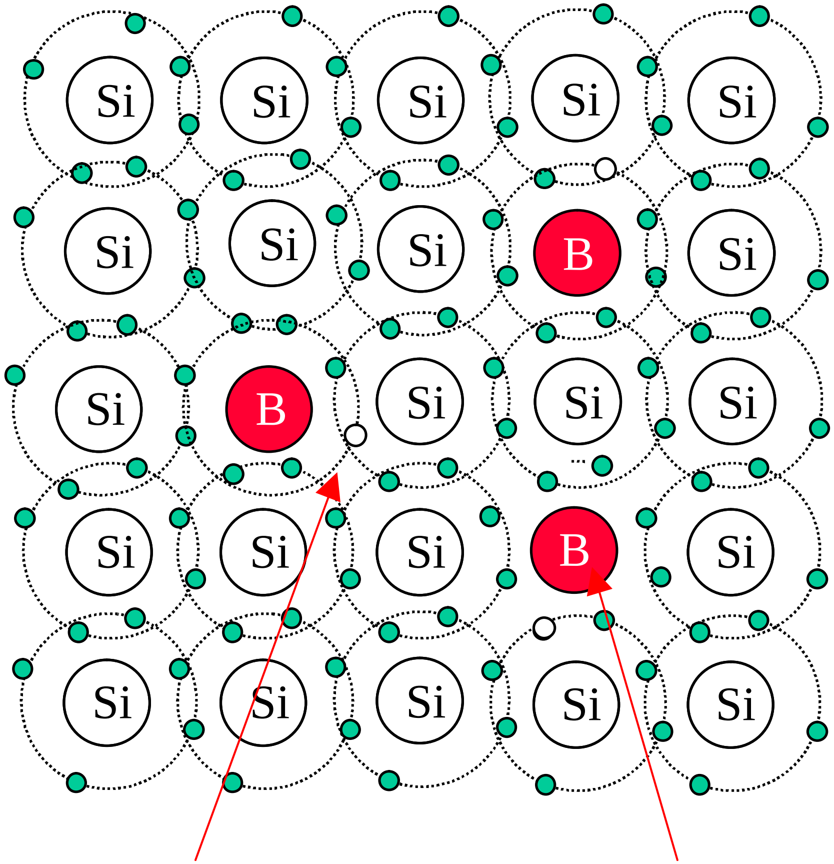


Figure 2.24

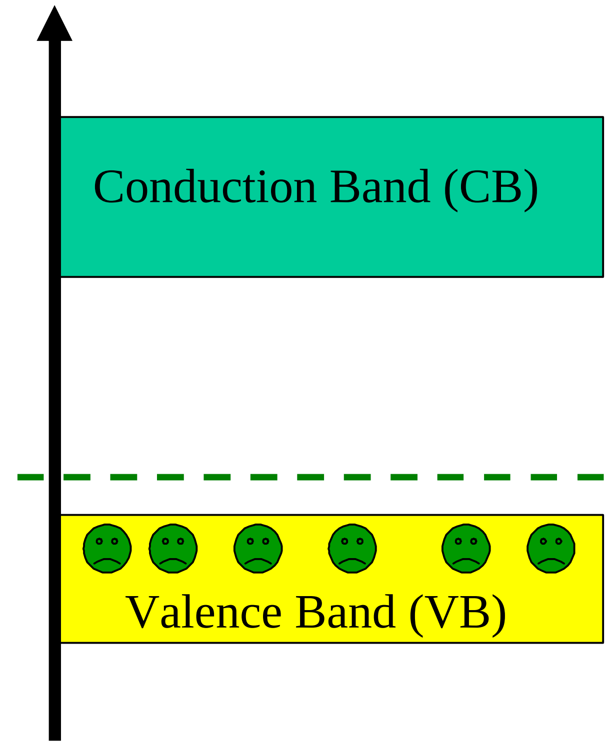
Holes in p-Type Silicon with Boron Dopant

Acceptor atoms provide a deficiency of electrons to form p-type silicon.



+ Hole

Boron atom serves as p-type dopant



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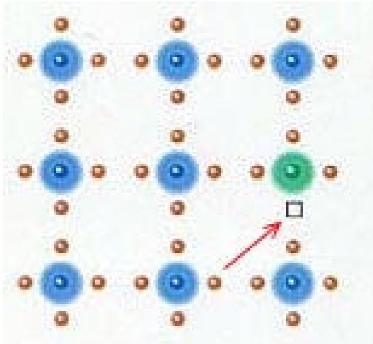
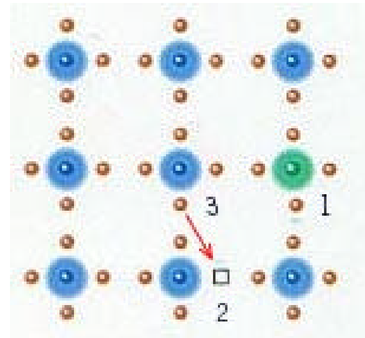
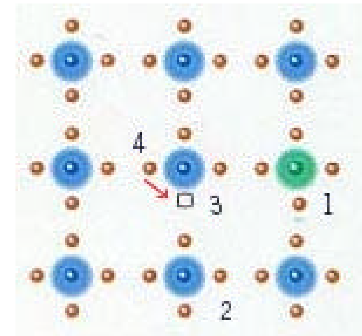
"Hole Movement in Silicon"



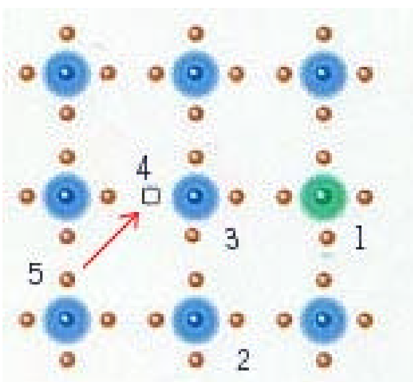
Boron is neutral, but nearby electron may jump to fill bond site.



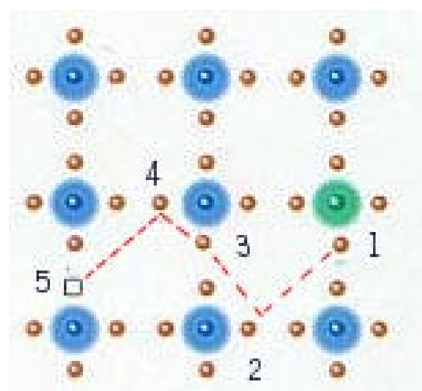
Boron is now a negative ion.



Only thermal energy to kick electrons from atom to atom.



Hole moved from 2 to 3 to 4, and will move to 5.



The empty silicon bond sites (holes) are thought of as being *positive*, since their presence makes that region positive.

Conduction in p-Type Silicon

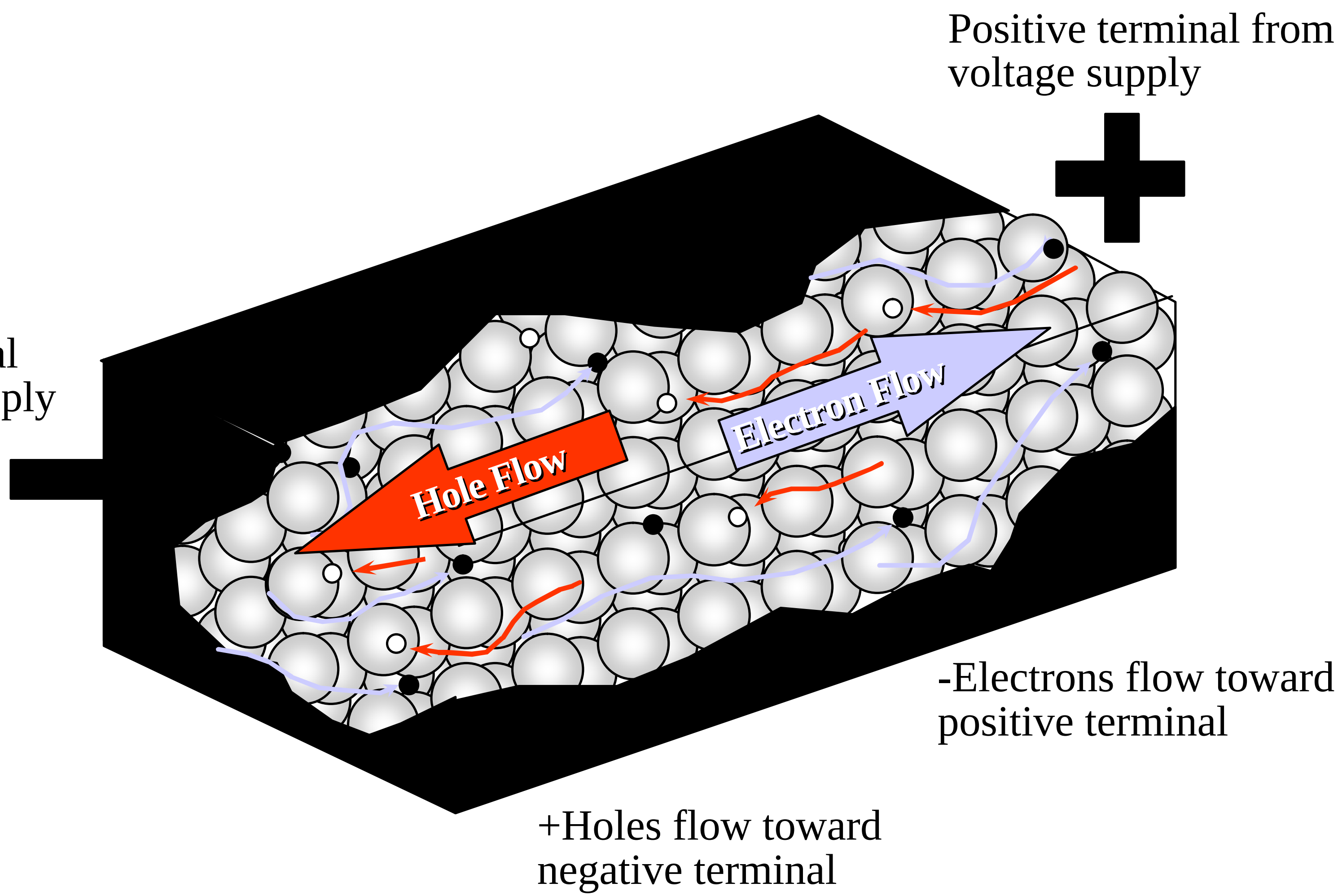


Figure 2.26

Outline

- Silicon and Silicon crystal structure
- Defect types in silicon crystals
- Silicon doping (Dopants = Defects)
- Radiation induced defects
  - Point defects and clusters
  - Particle dependence
  - Defect kinetics
  - Example of DLTS measurement

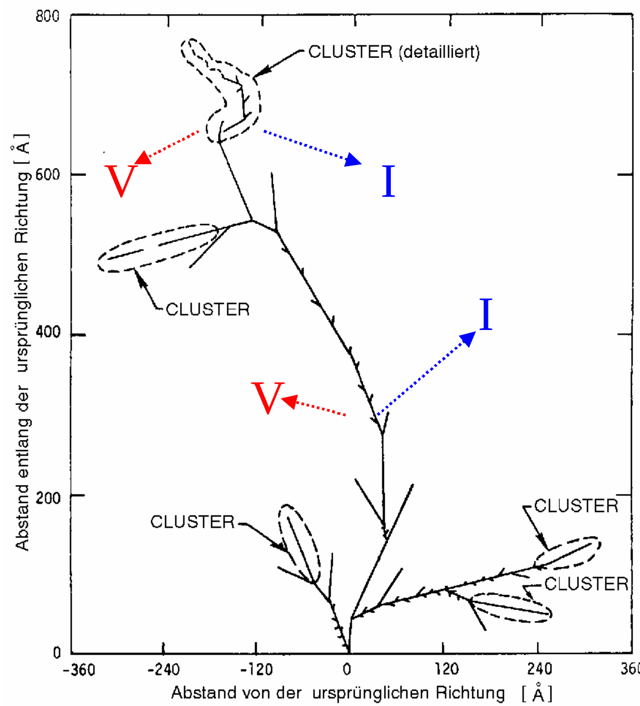
- What are defects doing to detectors?
- How to measure defects?
- Coffee

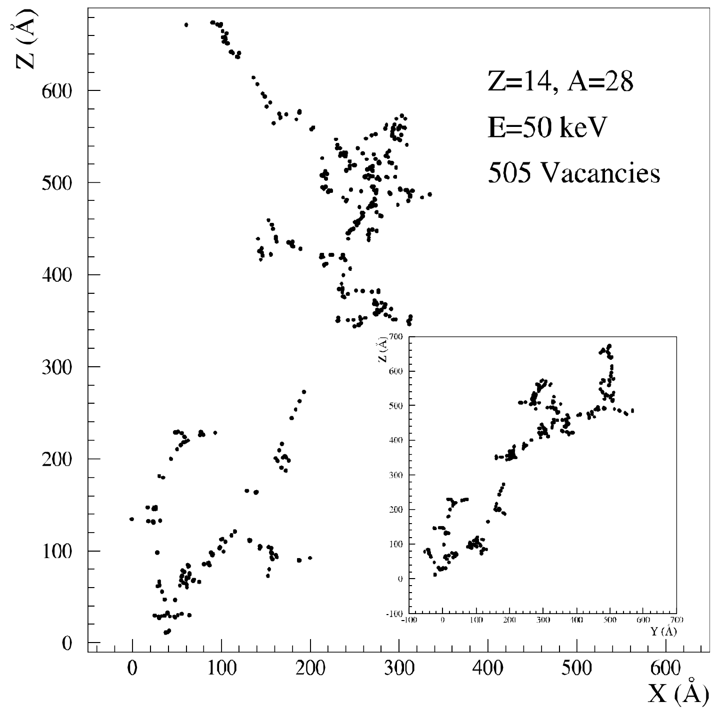
Radiation Damage – Microscopic Effects

- **Spatial distribution of vacancies created by a 50 keV Si-ion in silicon.**
  (typical recoil energy for 1 MeV neutrons)

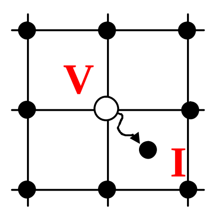
M.Huhtinen 2001

van Lint 1980





particle → Si_s → E_K>25 eV

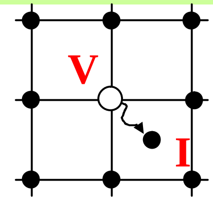


Vacancy + Interstitial → *point defects (V-O, C-O, ..)*

→ E_K > 5 keV *point defects and clusters of defects*

Radiation Damage – Microscopic Effects

particle → Si_S → E_K>25 eV



Vacancy + **I**nterstitial → *point defects (V-O, C-O, ..)*

E_K > 5 keV *point defects and clusters of defects*

- **^{60}Co-gammas**
  - Compton Electrons with max. $E_\gamma \approx$1 MeV (<u>no cluster production</u>)
- **Electrons**
  - E_e > 255 keV for displacement
  - E_e > 8 MeV for cluster
- **Neutrons (elastic scattering)**
  - E_n > 185 eV for displacement
  - E_n > 35 keV for cluster

Only point defects ⟷ point defects & clusters ⟷ Mainly clusters

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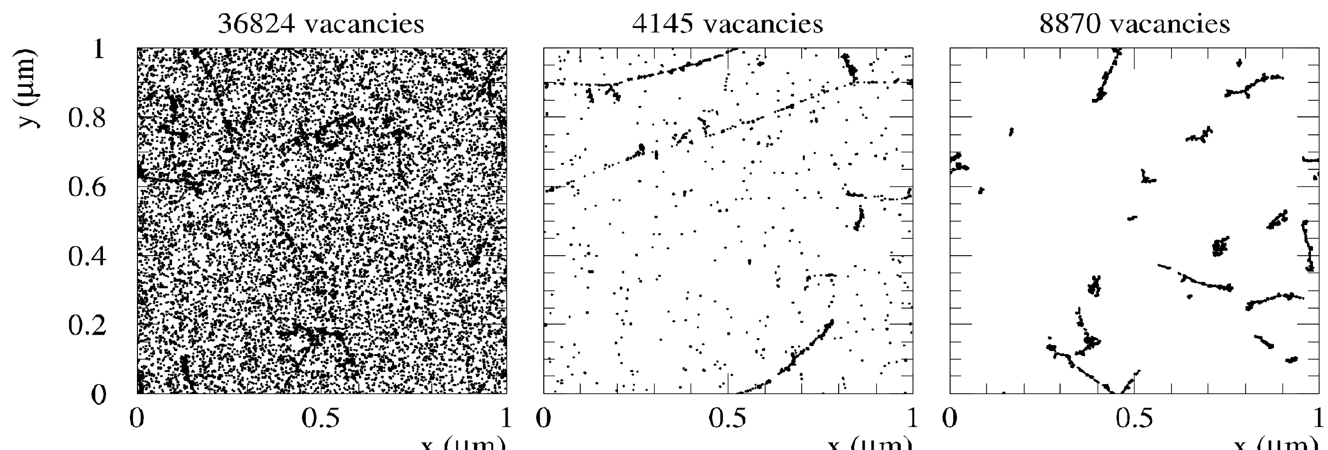
Simulation:

Initial distribution of vacancies in (1mm)^3 after 10^{14} particles/cm^2

[Mika Huhtinen NIMA 491(2002) 194]

10 MeV protons | **24 GeV/c protons** | **1 MeV neutrons**



Primary Damage and secondary defect formation

- **Two basic defects**

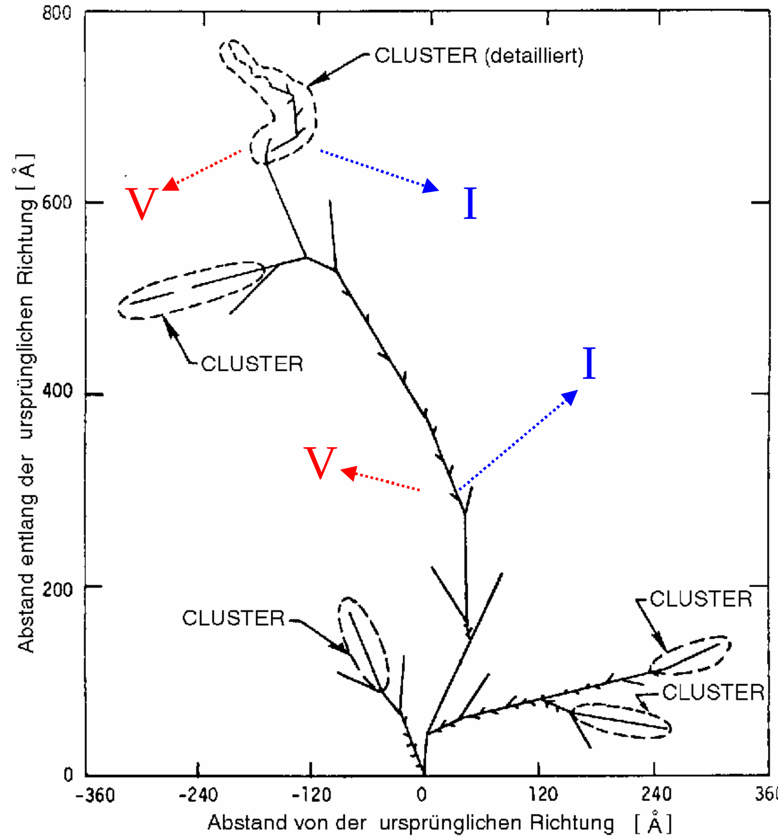
  I - Silicon Interstitial   V - Vacancy

- **Primary defect generation**

  I, I_2 higher order I (?)
  Þ **I** -CLUSTER **(?)** ⇐

  V, V_2, higher order V (?)   **Damage?!**
  Þ **V** -CLUSTER **(?)** ⇐

- **Secondary defect generation**



Main impurities in silicon: Carbon (C_s)
Oxygen (O_i)

$I+C_s$ ® C_i ⇒ C_i+C_s ® C_iC_S
C_i+O_i ® C_iO_i
C_i+P_s ® C_iP_S

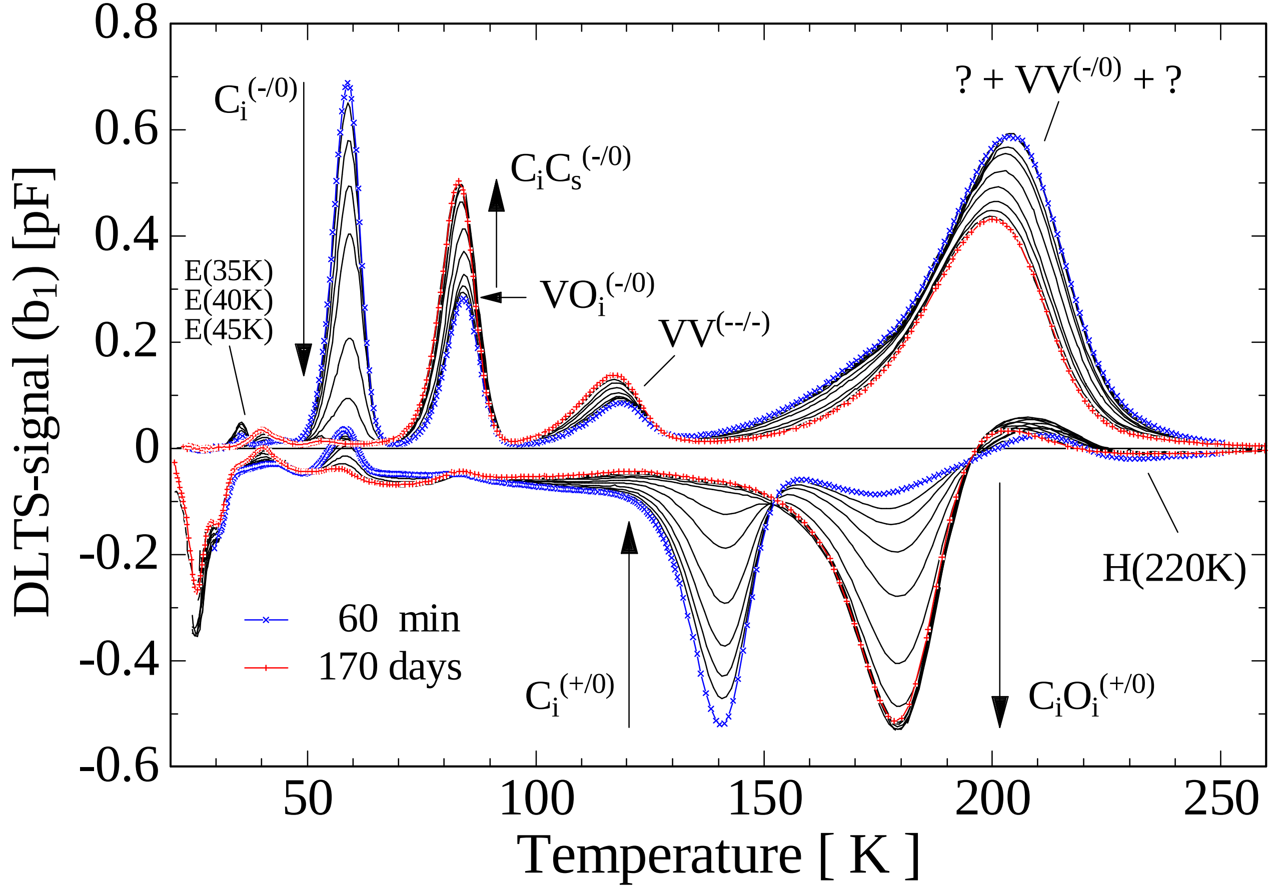
$V+V$ ® V_2 $V+V_2$ ® V_3
$V+O_i$ ® VO_i ⇒ $V+VO_i$ ® $\underline{V_2O_i}$ ⇐ **Damage?! (“V_2O-model”)**
$V+P_s$ ® VP_s

$I+V_2$ ® V $I+VO_i$ ® O_i ....

Example of defect spectroscopy

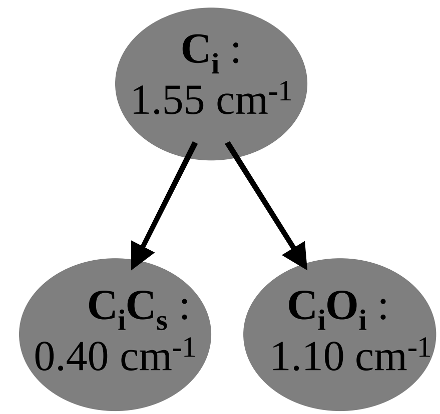
- neutron irradiated -

Deep Level Transient Spectroscopy



Introduction Rates

N_t/F_{eq}:



example : F_{eq} = 1´10^{14} cm^{-2}

defects » 1´10^{14} cm^{-3}

space charge » 5´10^{12}cm^{-3}

- **Introduction rates of main defects » 1 cm^{-1}**
- **Introduction rate of negative space charge » 0.05 cm^{-1}**

Outline

- **Silicon and Silicon crystal structure**
- **Defect types in silicon crystals**
- **Silicon doping (Dopants = Defects)**
- **Radiation induced defects**
- **What are defects doing to detectors?**
- **How to measure defects?**
- **Coffee**

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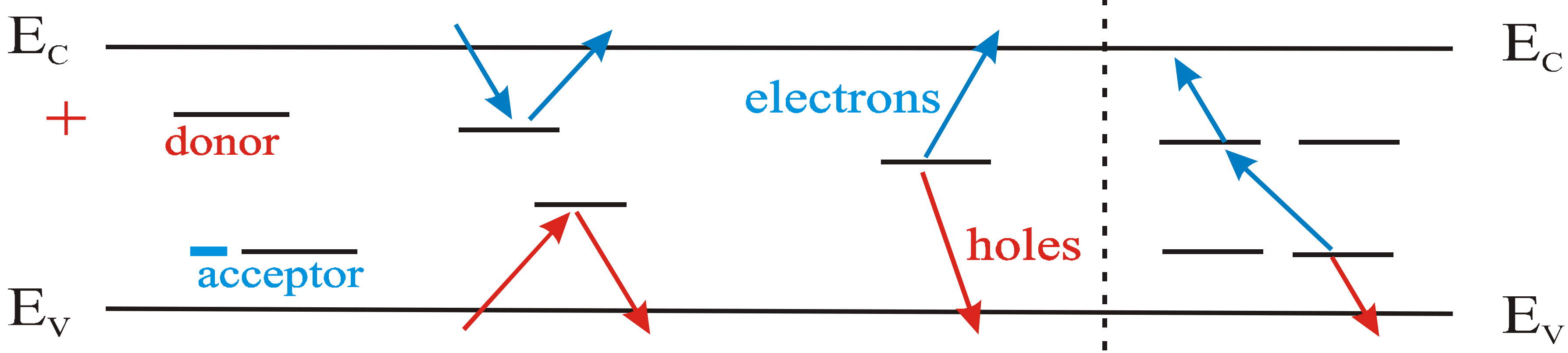
Impact of Defects on Detector properties

Shockley-Read-Hall statistics
(standard theory)

Inter-center charge
transfer model
(inside clusters only)



charged defects
Þ N_{eff} , V_{dep}
e.g. donors in upper and acceptors in lower half of band gap

Trapping (e and h)
Þ CCE
shallow defects do not contribute at room temperature due to fast detrapping

generation
Þ leakage current
Levels close to midgap most effective

enhanced generation
Þ leakage current
Þ space charge

Impact on detector properties can be calculated if all defect parameters are known:

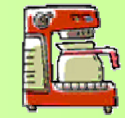
$s_{n,p}$: cross sections **DE : ionization energy** **N_t : concentration**

Outline

- **Silicon and Silicon crystal structure**
- **Defect types in silicon crystals**
- **Silicon doping   (Dopants = Defects)**
- **Radiation induced defects**
- **What are defects doing to detectors?**
- **How to measure defects?**
  - **Some measurement techniques …**
  - **Deep Level Transient Spectroscopy**

- **Coffee**

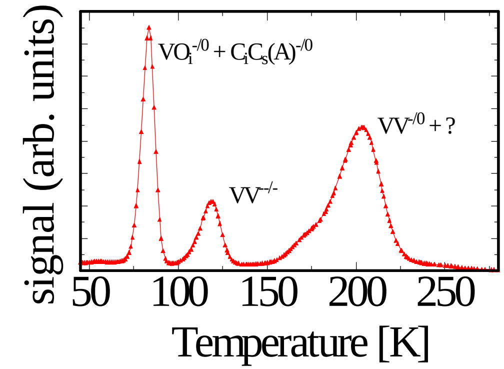
How to measure defects in silicon?



- **Structure and Chemical Configuration**
  - **TEM – Transmission Electron Spectroscopy**
  - **EPR – Electron Paramagnetic Resonance**
- **Optical properties (local vibrational modes)**
  - **FTIR – Fourier Transform Infrared spectroscopy**
- **Electrical Properties**
  - **PL - Photoluminescence**
  - **TSC – Thermally Stimulated Current**
  - **DLTS – Deep Level Transient Spectroscopy**
- **Binding energy and migration**
  - **Annealing experiments**

CERN TA1/SSD — Deep Level Transient Spectroscopy

- simplified working principle -

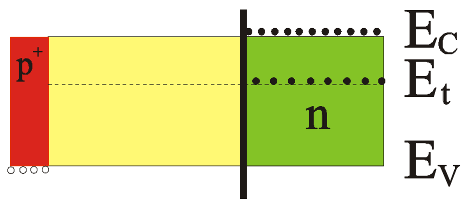


a) Stabilize temperature

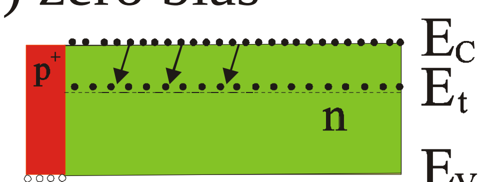
b) Variation of voltage

→ **Measurement of capacitance transient**

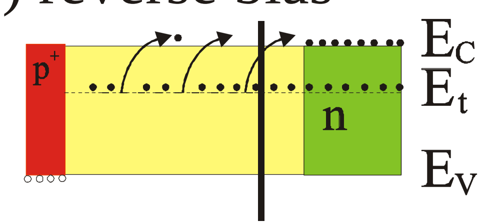
1) reverse bias

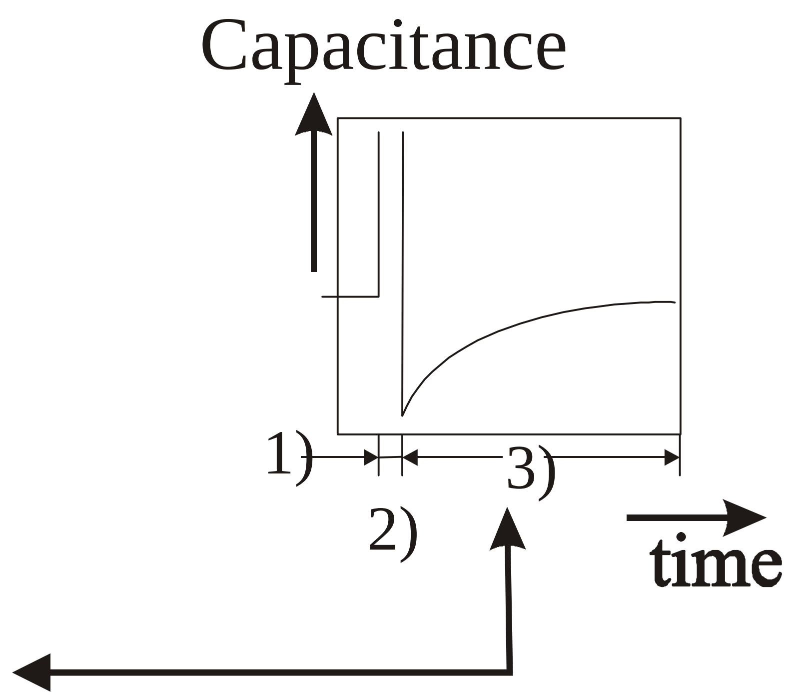


2) zero bias



3) reverse bias



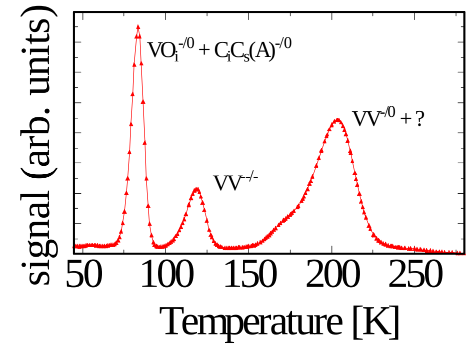


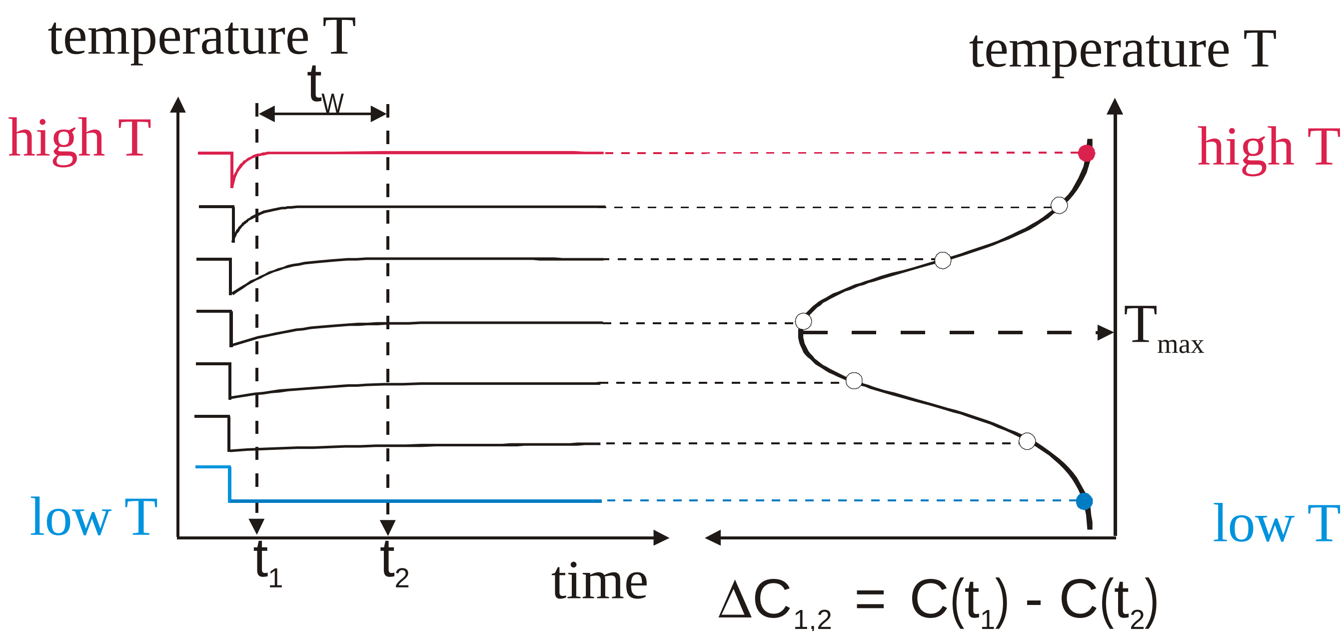
$C \propto \frac{1}{W} \propto \sqrt{N_{eff}}$

Deep Level Transient Spectroscopy

- simplified working principle -

c) Measure capacitance transients at many temperatures
→ DLTS - spectrum





c) Analyze the DLTS-spectra ("Arrhenius Plots")

Þ **extract defect parameters :**

E_t	**position in bandgap**
s_n, s_p	**cross sections for electrons and holes**
N_t	**defect concentration**

Coffee !!!!!

Coffee !!!!!