上海交通大学
SHANGHAI JIAO TONG UNIVERSITY

Lecture 3

Semiconductor physics I

The Crystal Structure of Solids

- **Semiconductor materials**
- **Types of solids**
- **Space lattices**
- **Atomic Bonding**
- **Imperfection and doping in solids**

Semiconductor

Semiconductors definition

A group of materials having conductivities between those of metals and insulators.

Semiconductor classification

--- Group IV elemental materials

Si （硅）

Ge （锗）

--- compound materials of group III and group IV elements.

GaAs （砷化镓）–common compound semiconductor for high-speed and optical divices.

GaP （磷化镓）

InP （磷化铟）

--- three-element compound semiconductor

	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
	13 Al	14 Si	15 P	16 S
IIB				
30 Zn	31 Ga	32 Ge	33 As	34 Se
48 Cd	49 In	50 Sn	51 Sb	52 Te

Fig Periodic table.

Intrinsic silicon (本征硅)

✓ **Pure silicon crystal**

	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
IIB	13 Al	14 Si	15 P	16 S
30 Zn	31 Ga	32 Ge	33 As	34 Se
48 Cd	49 In	50 Sn	51 Sb	52 Te

periodic table (元素周期表)

- **Si**
- in Column IV of the periodic table with atomic number 14
- by far the most common semiconductor used in ICs.

Other group IV technologies:

- **Carbon nanotube （碳纳米）**
- **Graphene （石墨烯）**

TYPES OF SOLIDS

According to the size of an ordered region within the material, there are three types of solids:

(a) amorphous（不规则的)

(b) polycrystalline （多晶）

(c) single crystal （单晶）--- the best electrical properties due to without grain boundaries .

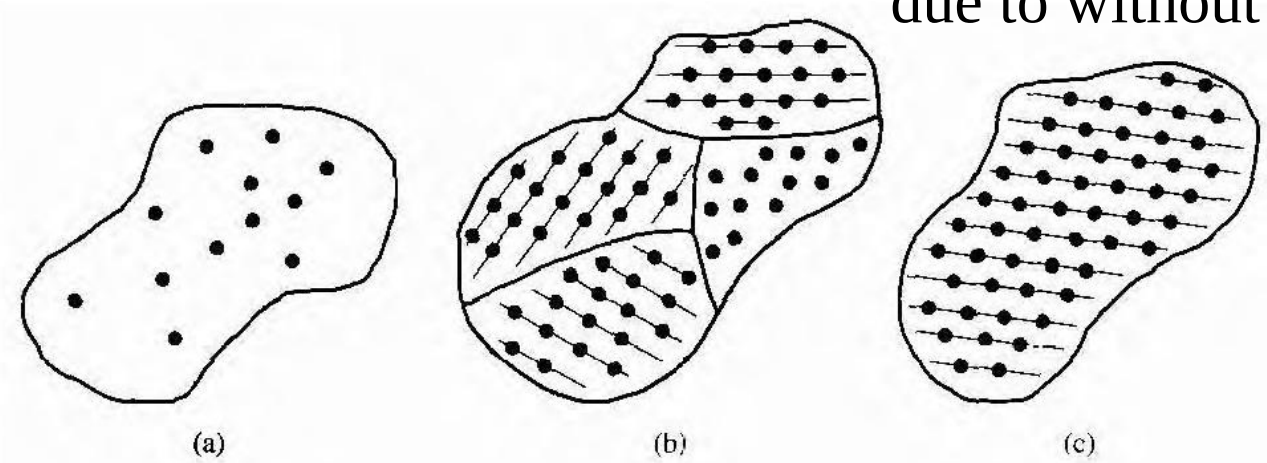


Fig Schematics of three general types of crystals:
(a) amorphous, (b) polycrystalline, (c) single crystal.

SPACE LATTICES（晶格）

- **Lattice of the single crystal**

  --- the periodic arrangement of atoms in the crystal.

- **Primitive cell/ unit cell （原胞/晶胞）**

  --- the smallest unit cell that can be repeated to form the lattice.

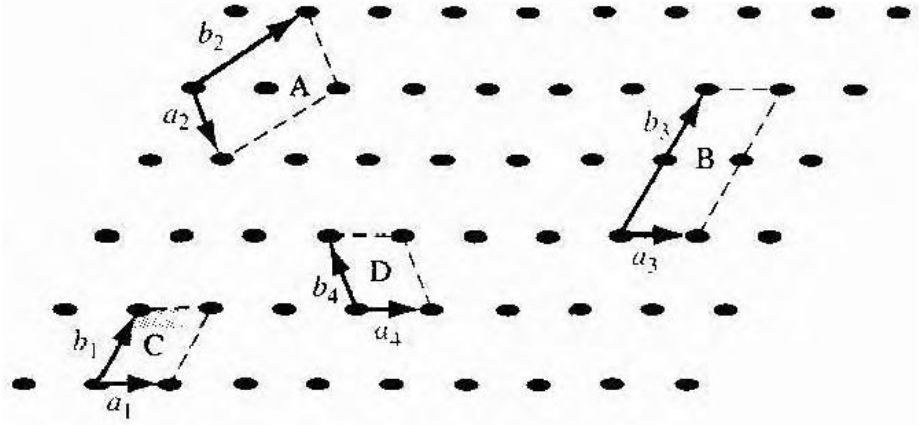


Fig Two-dimensional representation of a single-crystal lattice showing various possible unit cells

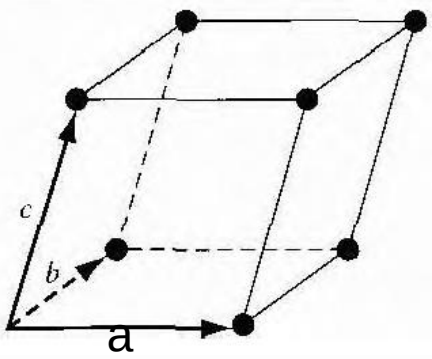


Fig A generalized primitive unit cell.

lattice point （格点）

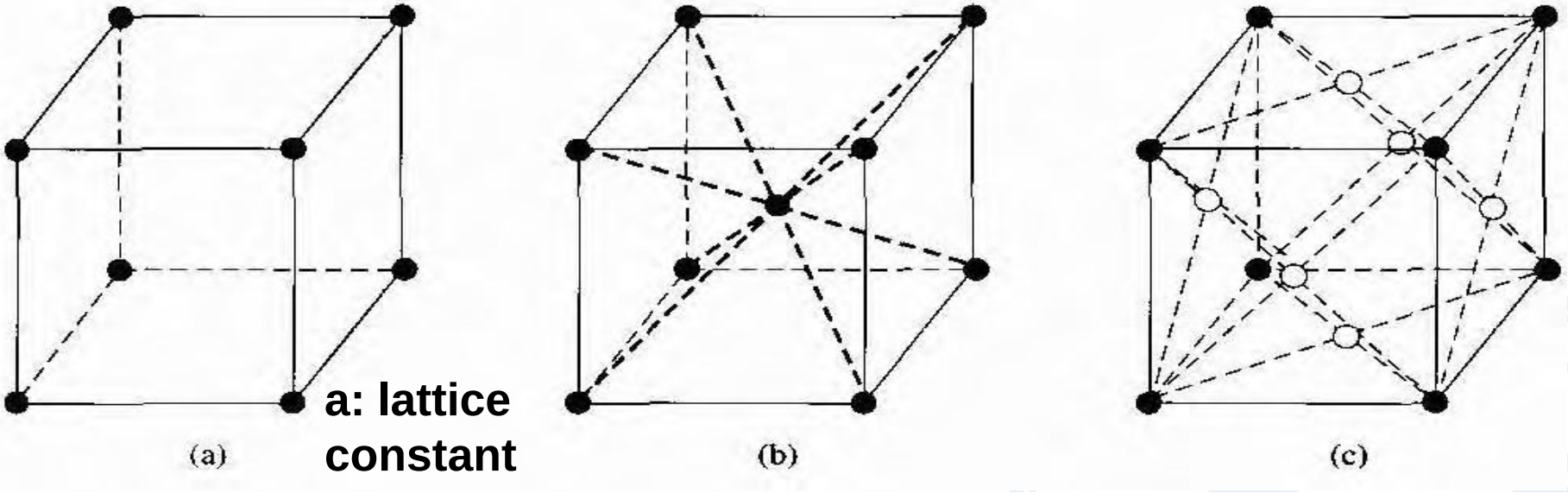
--- to represent a particular atomic array by a dot.

--- its location expressed using the vector

$$\boxed{\vec{r} = p\vec{a} + q\vec{b} + s\vec{c}}$$

where p, q, and s are positive integers.

Basic Crystal Structures



a: lattice constant

Figure Three lattice types: (a) simple cubic.
(b) body-centered cubic.
(c) face-centered cubic.

Volume density （体密度） of atoms

- **Volume density of atoms is determined by**

--- the crystal structure of a material

--- its lattice dimensions

Example: Consider a single-crystal material that is a body-centered cubic with a lattice constant $a = 5\,A = 5 \times 10^{-8} cm$. Compute its volume density.

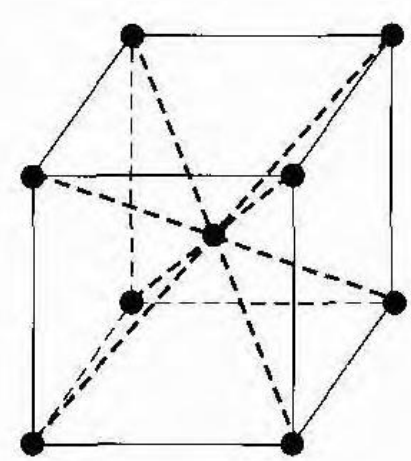


Fig body-centered cubic

Solution:

A corner atom is shared by eight unit cells

⇒The eight corner atoms then contribute an equivalent of one atom to the unit cell.

\+ the body centered atom

=> each unit cell contains an equivalent of two atoms

$$Density = \frac{2 atoms}{(5 \times 10^{-8})^3} = 1.6 \times 10^{22}\, atoms / cm^3$$

Crystal Planes and Miller Indices
（晶格平面与密勒指数）

- **Why to describe crystal planes?**

---The real crystals are not infinitely large, eventually terminating at a surface.

---The surface properties may influence the device characteristics.

Miller Indices

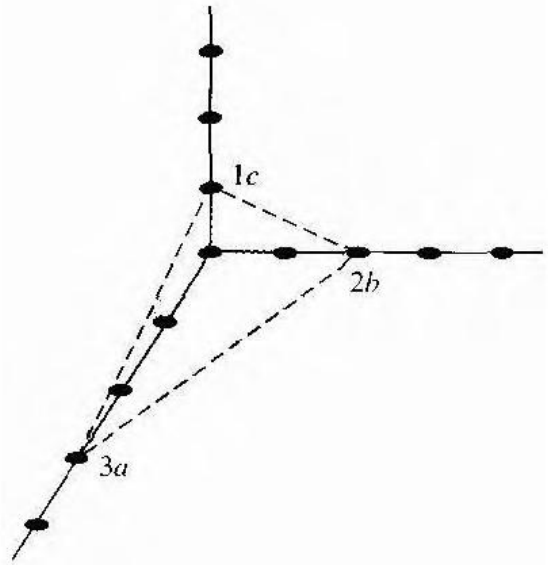


Fig A representative crystal Lattice plane.

1. The intercepts of the plane correspond to

   $p = 3$, $q = 2$, and $s = 1$.

2. The reciprocals （倒数） of the intercepts $\left(\frac{1}{3}, \frac{1}{2}, \frac{1}{1}\right)$

3. Multipling by the lowest common denominator yields Miller indices （2,3,6）

* Parallel plates have the same miller indices.

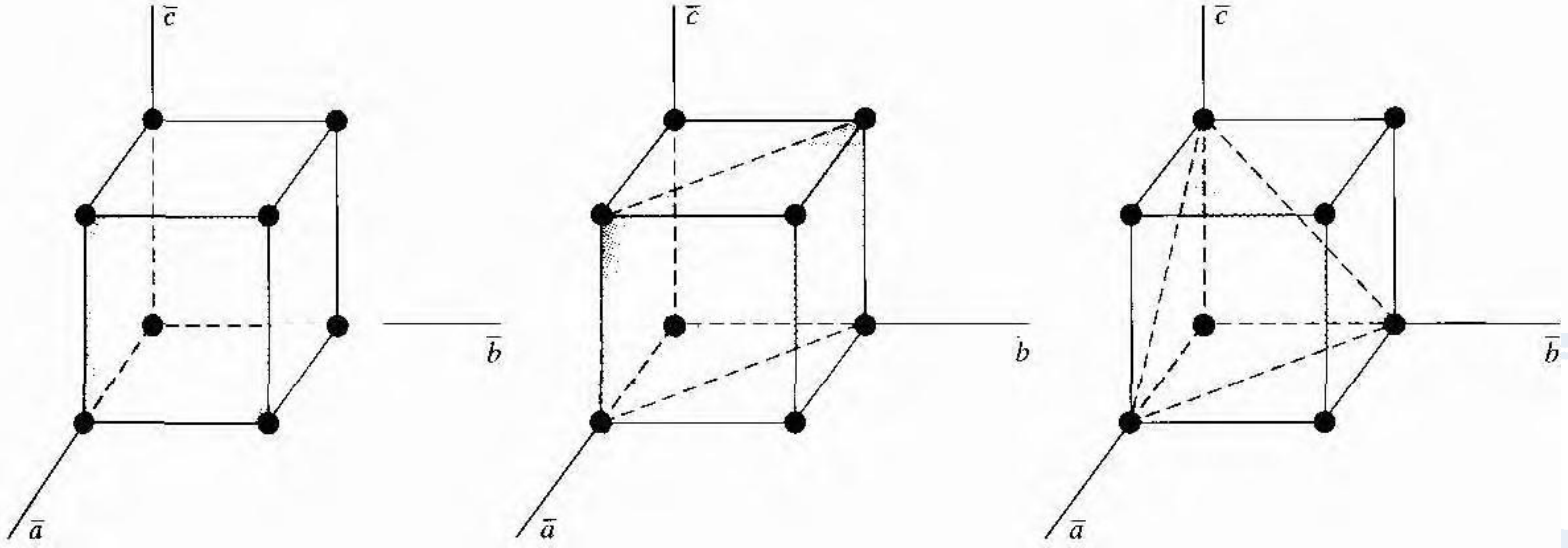


Fig Three lattice planes

(a) (100) plane； (b) (110) plane； (c)(111) plane

Example: Consider the body-centered cubic structure and the (110) plane. Compute the surface density.

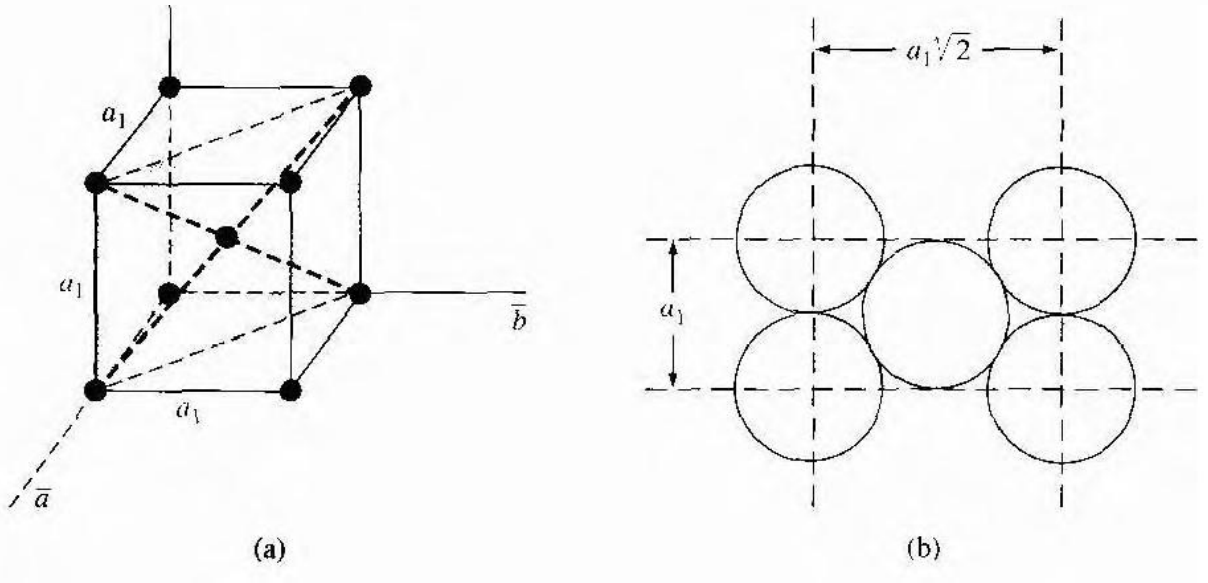


Fig (a) The (110) plane in a body-centered cubic and
(b) The atoms cut by the (110) plane in a body-centered cubic

Solution

The atom at each corner is shared by four similar equivalent lattice planes

⇒The four corner atoms then effectively contribute one atom to this lattice plane.

The atom in the center is completely enclosed in the lattice plane

⇒The lattice plane contains two atoms

$$Surface\ Density = \frac{2atoms}{(a_1)(a_1\sqrt{2})} = \frac{2}{(5\times10^{-8})^2(\sqrt{2})}$$

$$= 5.66\times10^{24}\ atoms/cm^2$$

* Surface density of atoms depends on the plane and generally varies from one crystal plane to another.

Diamond Structure （钻石结构）

- **Silicon and Germanium （锗）, as a group IV elements and have a diamond crystal structure.**

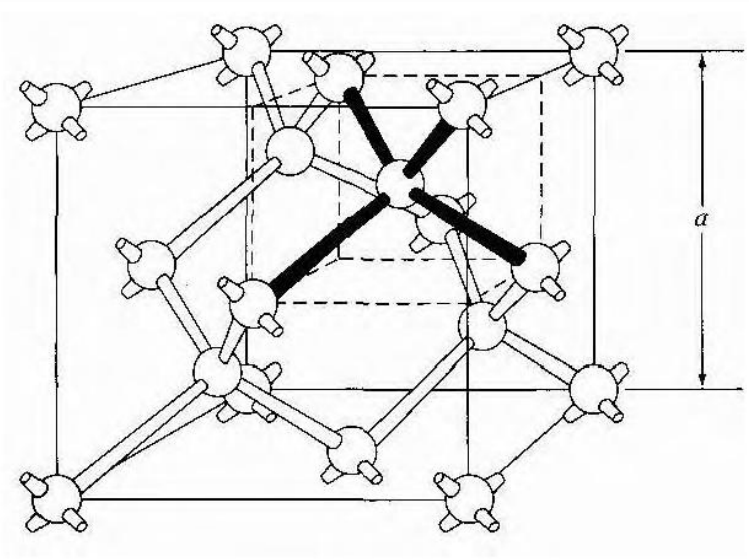


Fig The diamond structure.

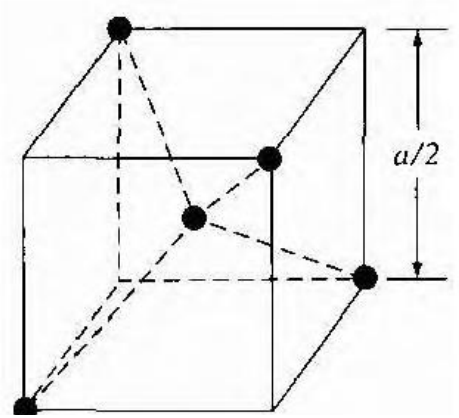


Fig The tetrahedral（四面体）structure of closest neighbors in the diamond lattice.

Every atom in the tetrahedral structure has four nearest neighbors.

Homework1

The lattice constant of silicon is 5.43 A. Calculate the volume density of silicon atoms.

Answer: Si atomic density : 5×10^{22} cm^{-3}

ATOMIC BONDING（原子键）

- Why one particular crystal structure is favored over another for a particular assembly of atoms.
  - A fundamental law of nature
    - the total energy of a system in **thermal equilibrium** （热平衡） tends to reach a minimum value.
  - The interaction that occurs between atoms to form a solid depends on the type of atom or atoms involved.
  - The interaction of various atoms is considered by valence electrons（价电子）（outermost electrons of an atom）

Classification of atomic bonding

☐ *Ionic bonding*（离子键）:

The atoms at the **two extremes of the periodic table** tend to lose or gain valence electrons, thus forming ions to complete outer energy shells.

－The elements in group I tend to lose their one electron and become positively charged.

－ the elements in group VII tend to gain an electron and become negatively charged.

－These oppositely charged ions then experience a coulomb attraction and form a bond referred to as an ionic bond.

□***Covalent bonding***（共价键）：The atoms at the middle of the periodic table tend to **share valence electrons** to complete outer energy shells.

□***Metallic bonding*** （金属键）：the positive **metallic ions** as being surrounded by a sea of negative electrons, the solid being held together by the electrostatic forces.

□**Van *der Waals bond*** （范德华键）*:* is the weakest of the chemical bonds.

solids formed by the Van der Waals bonds have a relatively low melting temperature-in fact, most of these materials are in **gaseous form** at room temperature.

Covalent bonding in Si

- In intrinsic silicon, diamond lattice is formed by the **four valence electrons** associated with each silicon atom.
- These atoms are held in their positions by **covalent bonds**.

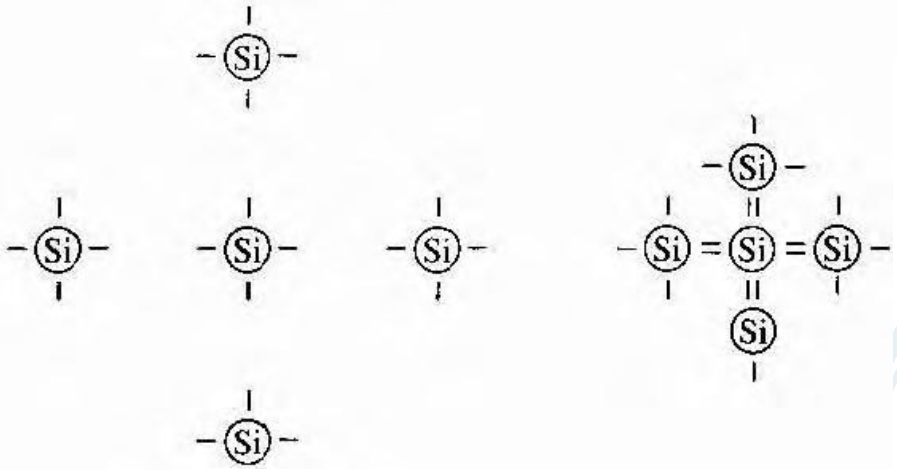
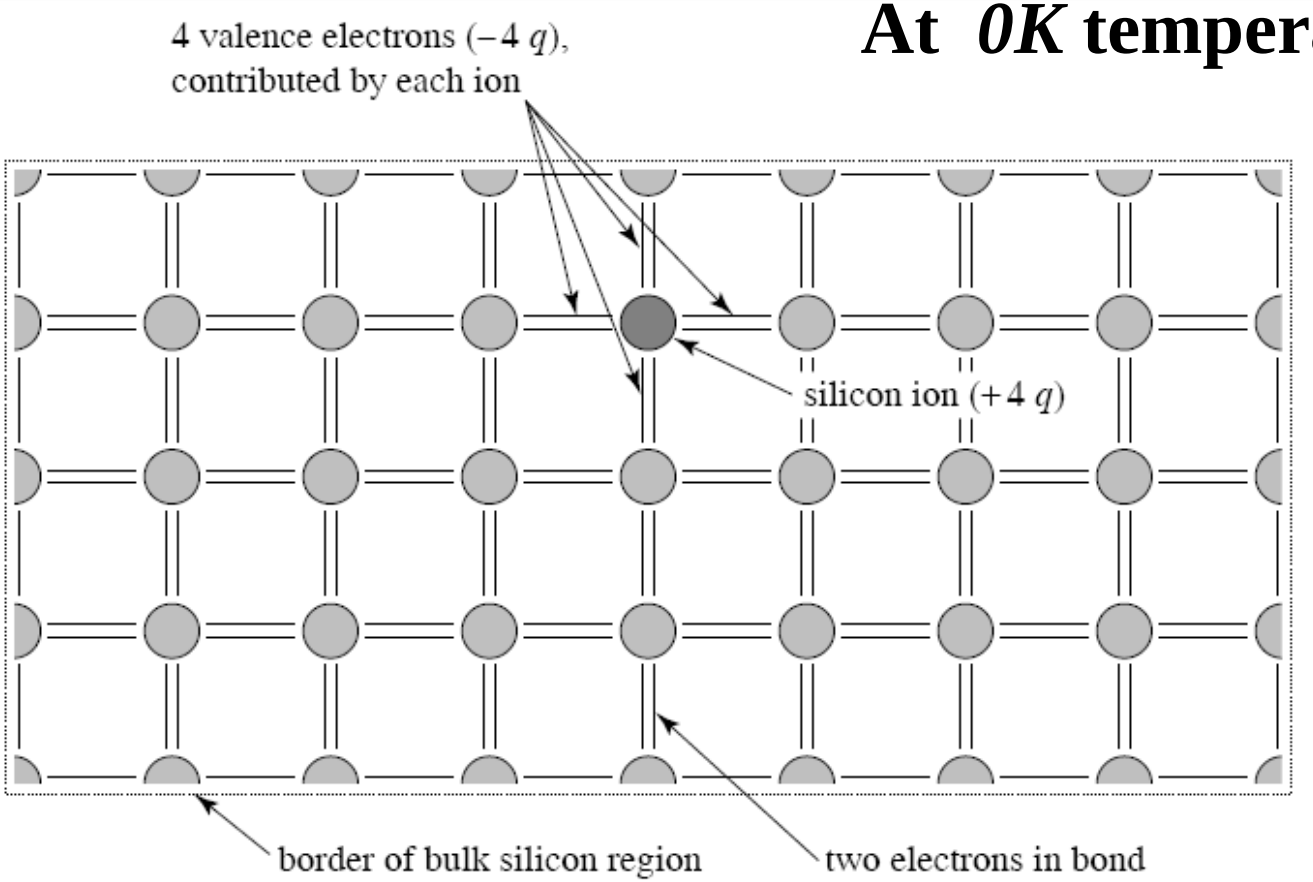


Fig Representation of (a) silicon valence and (b) covalent bonding in the silicon crystal

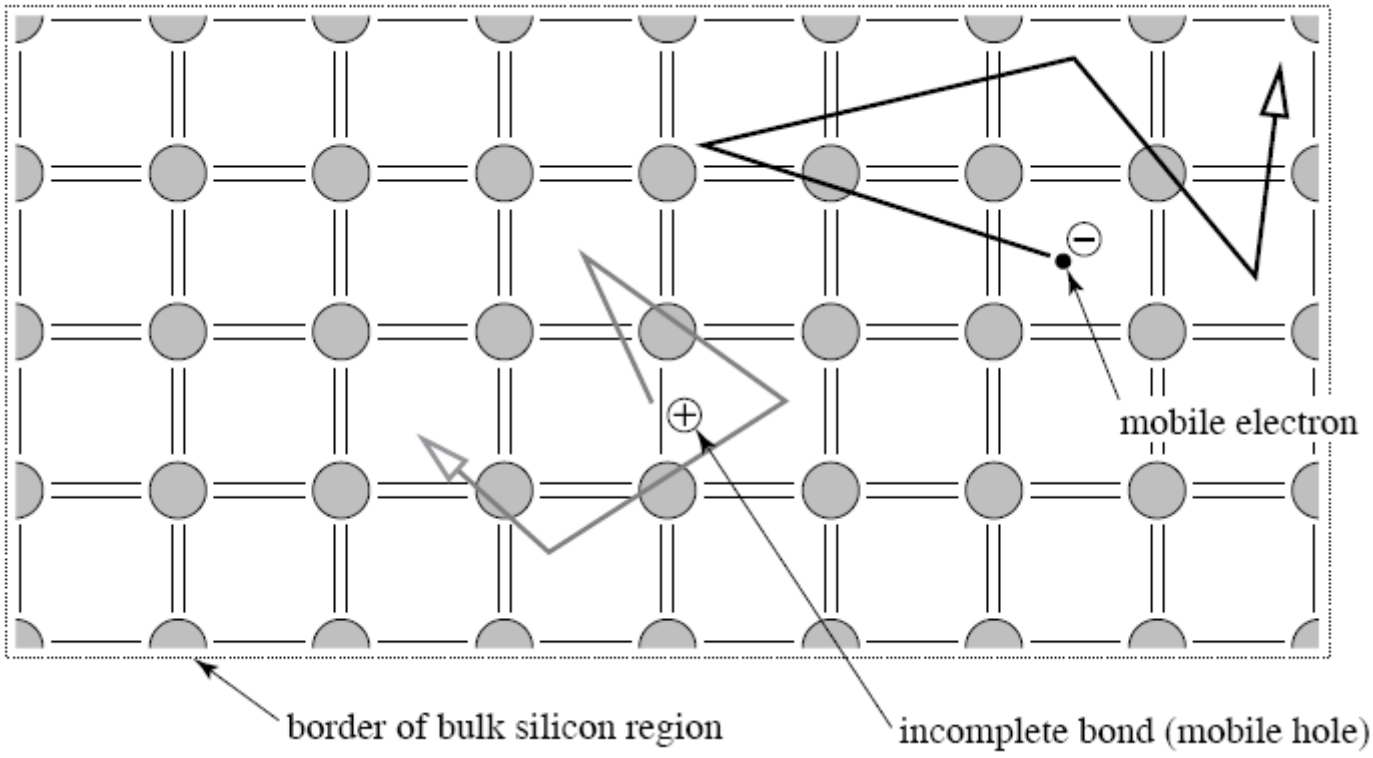
At *0K* temperature



Each atom shares 8 electrons – *low energy situation*

There is no free electron, intrinsic silicon is an insulator .

At finite temperature



Thermal generation

- **lattice vibrations** （晶格振动） occurs
- Some bonds are broken

--- “free” electrons – Mobile negative charge, -1.6×10^{-19} C

--- “free” holes– Mobile positive charge, $+1.6 \times 10^{-19}$ C

Covalent bonding broken:

At high temperature, some of the bonds are broken by **thermal ionization （热电离）**. So some electrons are freed and a positive charge is left with the parent atom.

Electric current:

An electron from the neighboring atom may fills up the "hole" that existed in the ionized atom but creates a new hole in the other atom. This "hole", a positively charged carrier, can also conduct electric current.

In the following, "electron' means free electron

- Not concerned with bonding electrons or core electrons
- Define: n ≡ (free) electron concentration [cm^{-3}]

  p ≡ (free) hole concentration [cm^{-3}]

GENERATION

break-up of covalent bond to form electron and hole pairs
Requires energy from thermal or optical sources (or external sources)

Generation rate: $G = G_{th} + G_{opt} \; / \; cm^{-3} \bullet s^{-1}$

G_{th}: thermal generation rate, which increases exponentially with temperature.
G_{opt} : optical generation occurs when a bond absorbs a photon to break it, which is independent of temperature.

- **In general, atomic density >> *n, p* ⇒ *G ≠ f(n,p)***

☐Recombination

---Thermal ionization results in free electrons and holes in equal number and hence equal concentrations.

---These free electrons and holes move randomly and some of them may be recombined.

RECOMBINATION=formation of covalent bond by bringing together electron and hole

- Releases energy in thermal or optical form
- Recombination rate: $R = [/cm^{-3} \bullet s^{-1}]$
- recombination event requires 1 electron + 1 hole

$$\Rightarrow R \propto n \bullet p$$

☐Generation and recombination most likely take place at surfaces where periodic crystalline structure is broken.

Thermal equilibrium

the recombination rate = the thermal-generation rate.

- Generation rate in thermal equilibrium: $Go = f(T)$
- Recombination rate in thermal equilibrium:

$$Ro \propto n_o \bullet p_o$$

In thermal equilibrium:

$$Go\,(T) = Ro \Rightarrow n_o p_o = k_o G_o\,(T)$$

Mass-action law

$$\boxed{n_0 p_0 = n_i^2(T)}$$

The concentration of free electrons n, is equal to the concentration of holes p.

$$n = p = n_i$$

n_i denotes the concentration of free electrons or holes in intrinsic silicon at a given temperature.

Intrinsic concentration $n_i^2 = BT^3 e^{-E_G/kT}$

B is a material-dependent parameter = 5.4×10^{31} for silicon.

E_G is a parameter know as the bandgap energy =1.12 electron volts (eV), representing the minimum energy required to break a covalent bond and thus generate an electron-hole pair.

k is Boltzmann's constant = 8.62×10^{-5} eV/K

At room temperature $T = 300$ K $n_i = 1.5\times10^{10}$ carriers/cm^3

To place this number in perspective, we note that the silicon crystal has about 5×10^{22} atoms/cm^3

IMPERFECTIONS （缺陷） IN SOLIDS

- **Atomic thermal vibration**

--- lattice vibrates as atom energy is a function of temperature

--- affects some electrical parameters

- **Point defect （点缺陷）**

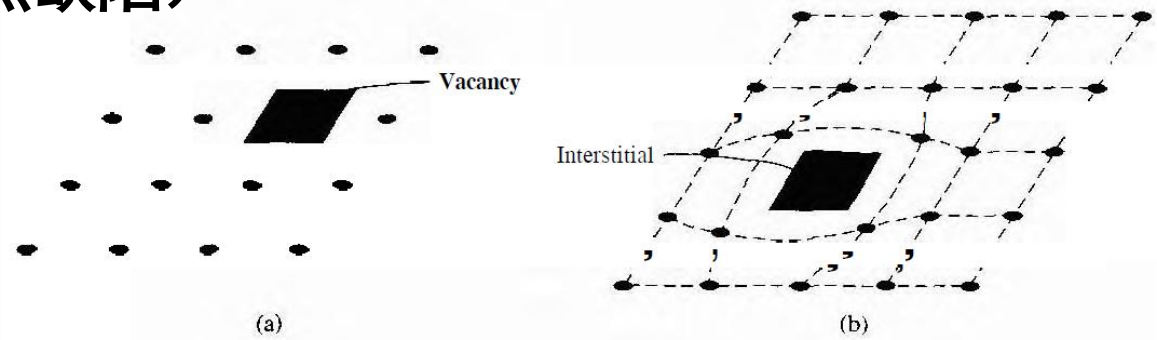


Fig Two-dimensional representation of a single-crystal lattice showing (a) a vacancy （空位） defect (b) an interstitial （填隙） defect.

- Frenkel defect: the vacancy defect and interstitial defect
- Line defect: missing the entire row of atoms

IMPURITIES (杂质) IN SOLIDS

- Foreign atoms, or impurity atoms, may be present in a crystal lattice.

--- ***Substitutional impurities*** （替位杂质）: Impurity atoms may be located at normal lattice sites.

--- ***Interstitial impurities***（填位杂质）: Impurity atoms may also be located between normal sites

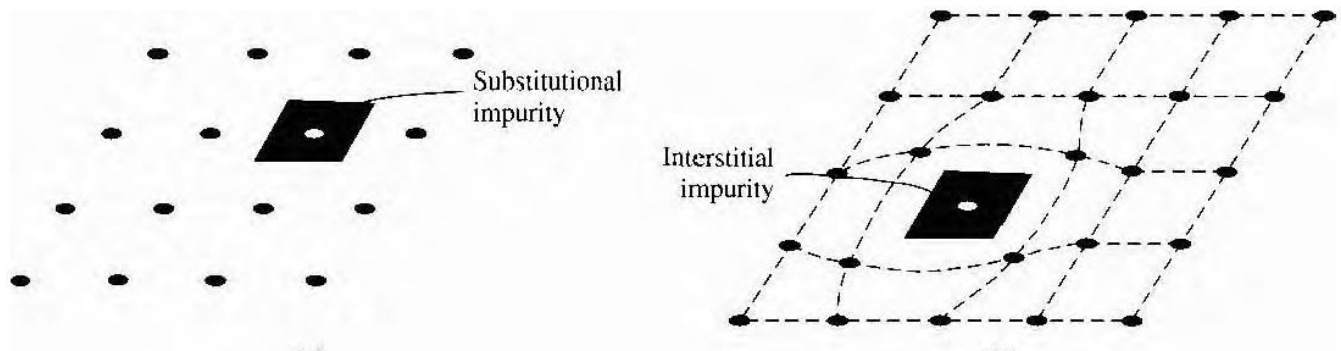


Fig Two-dimensional representation of a single-crystal lattice (a) a substitutional impurity and (b) an interstitial impurity.

Doping

- **Doping （掺杂）**

  --- adding controlled amounts of particular impurity atoms into pure semiconductor material.

  --- favorably altering the electrical characteristics of the material.

- **Two general methods of doping:**

  --- Impurity diffusion （杂质扩散）

  --- Ion implantation （离子注入）

- **Impurity diffusion**

  --- a semiconductor crystal is placed in a high temperature gaseous atmosphere containing the desired impurity atom

- **Ion implantation**

  --- A beam of impurity ions is accelerated to kinetic energies in the range of 50 keV or greater and then directed to the surface of the semiconductor.

  --- takes place at low temperature than impurity diffusion.

  ---Advantage: controlled numbers of impurity atoms introduced into specific regions of the crystal.

  --- Disadvantage: thermal annealing process is required to remove lattice displacement damage.

Doped semiconductors

- Doped semiconductors are materials in which carriers of one kind (electrons or holes) predominate.

  N type: the majority of charge carriers are the electrons

  P type: the majority of charge carriers are the holes

- n-type silicon is formed by introducing impurity atoms of a **pentavalent** （五价的）element such as phosphorus.

  --- Pentavalent element have five valence electrons, four of which form bonds with the neighboring silicon atoms while the fifth becomes a free electron.

  --- the impurity is called **a donor** （施主）.

Doping -Donors

Doping = engineered introduction of foreign atoms to modify semiconductor electrical properties

DONORS:

- Introduce electrons to semiconductors (but not holes)
- For *Si*, group *V* elements with 5 valence electrons (*P As Sb*)

	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
	13 Al	14 Si	15 P	16 S
IIB				
30 Zn	31 Ga	32 Ge	33 As	34 Se
48 Cd	49 In	50 Sn	51 Sb	52 Te

- 4 electrons participate in bonding
- 5th electron easy to release

⇒ at room temperature, each donor releases 1 electron that is available for conduction

- Donor site becomes positively charged (fixed charge)

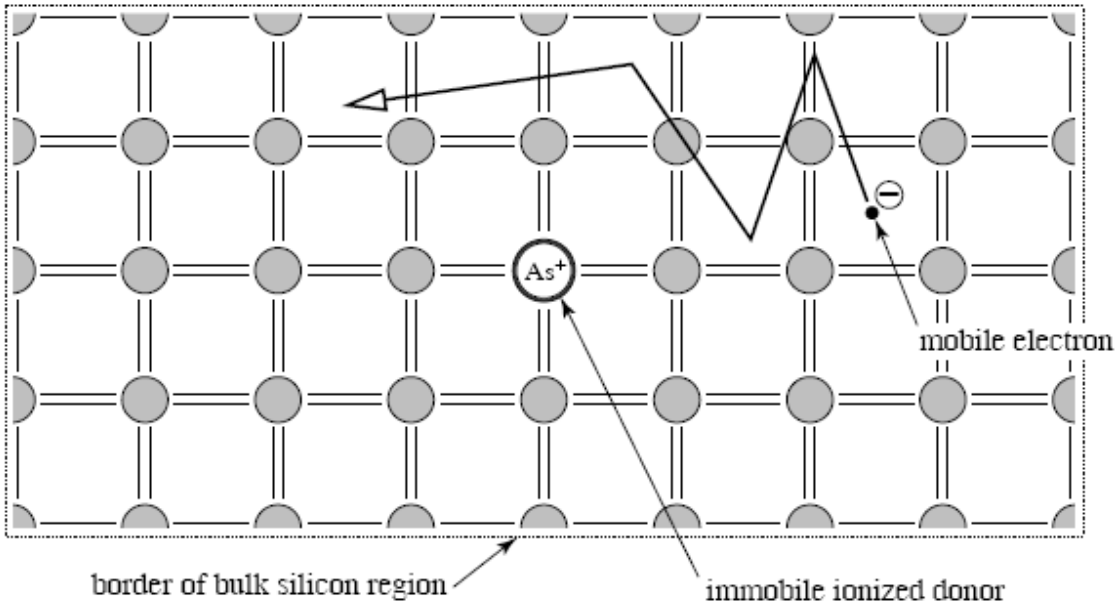


Fig 2D Silicon lattice with As donors.

Define: $N_d \equiv$ donor concentration [cm^{-3}]

In thermal equilibrium the concentration of free electrons in the *n*-type silicon will be

If $N_d << n_i$,doping is irrelevant

– Intrinsic semiconductor $\rightarrow$ $n_{n0} = p_{n_0} = n_i$

If $N_d >> n_i$, doping controls carrier concentration

– Extrinsic semiconductor $\Rightarrow$ $n_{n0} = N_D$

Where the additional subscript 0 denotes thermal equilibrium.

Besides, in thermal equilibrium, $n_0 p_0 = n_i^2$

Thus the concentration of the holes is

$$p_{n0} = \frac{n_i^2}{N_D}$$

(temperature-dependent and donor-concentration-dependent)

Doping : Acceptors （受主）

- Introduce holes to semiconductors (but not electrons)
- Group III elements with 3 valence electrons (B Al Ga In)

	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
	13 Al	14 Si	15 P	16 S
IIB				
30 Zn	31 Ga	32 Ge	33 As	34 Se
48 Cd	49 In	50 Sn	51 Sb	52 Te

- 3 electrons participate in bonding
- 1 bonding site "unsatisfied" making it easy to "accept" neighboring bonding electron to complete all bonds

⇒ at room temperature, each acceptor releases 1 hole that is available for conduction

- Acceptor site becomes negatively charged (fixed charge)

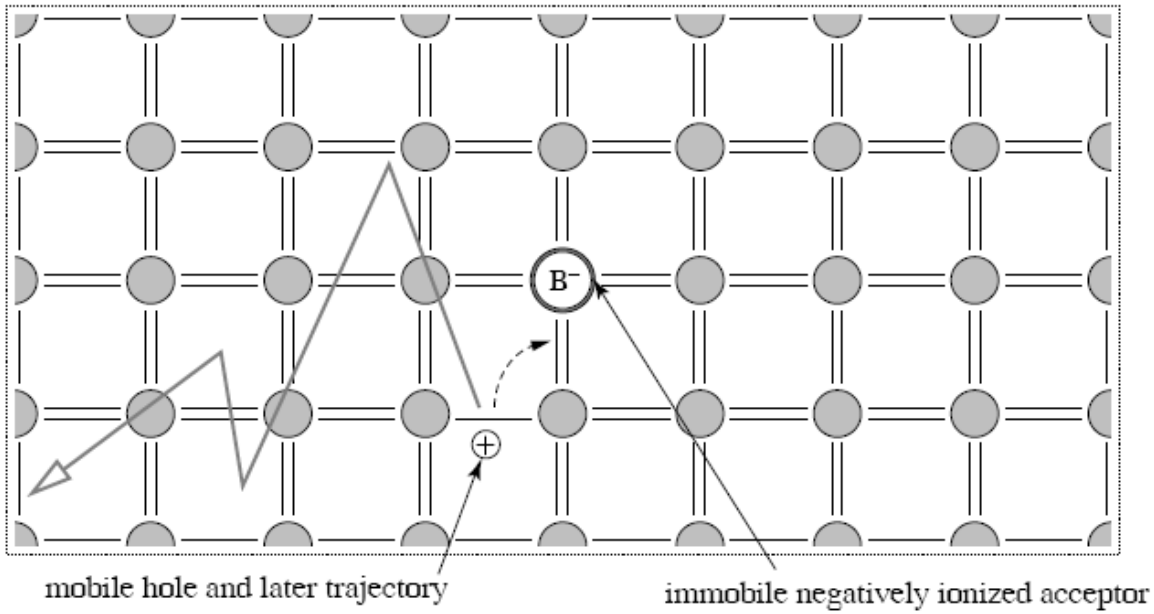


Fig 2D Silicon lattice with Boron donors

The **acceptor** impurity concentration is N_A.

If $N_a >> n_i$, doping controls carrier concentration

– Extrinsic semiconductor

⇒ Under thermal equilibrium, the concentration of the majority holes is

$$p_{p0} = N_A$$

The concentration of the minority electrons, which are generated by thermal ionization, is

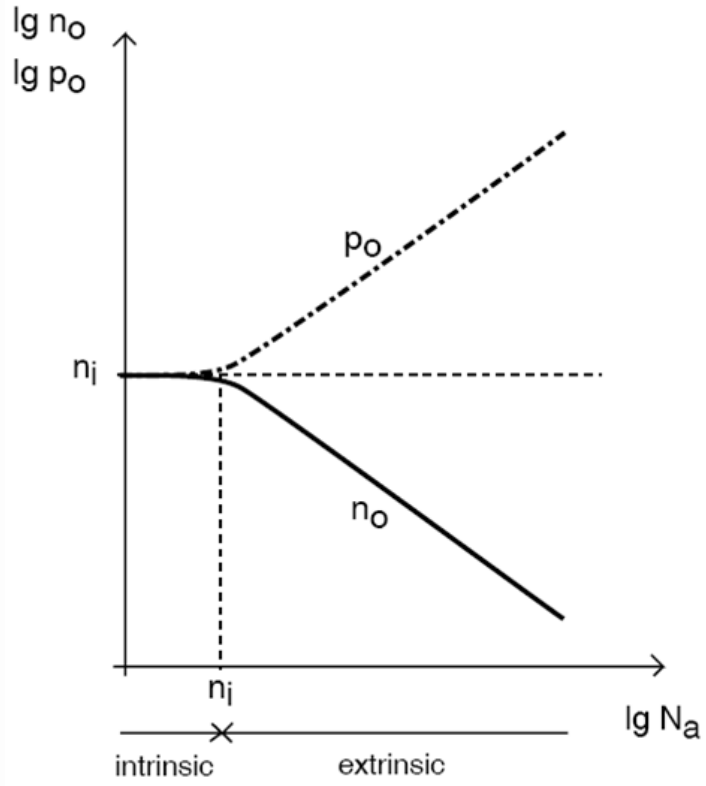
$$n_{p0} = \frac{n_i^2}{N_A}$$

(temperature-dependent and acceptor-concentration-dependent)

Example:

$$N_a = 10^{17}\,cm^{-3} \rightarrow p_0 = 10^{17}\,cm^{-3}, n_0 = 10^3\,cm^{-3}$$

In general: $N_a \approx 10^{15} - 10^{20}\,cm^{-3}$



Holes = majority carriers

Electrons = minority carriers

Donors and acceptors: compensation

- Silicon is often doped with both donors and acceptors.
- To find the equilibrium electron and hole concentrations, we introduce:

Charge neutrality law

$$q(p_0 - n_0 + N_d - N_a) = 0$$

The semiconductor remains charge neutral when it has been doped
⇒ Overall charge neutrality must be satisfied.

Charge Neutrality (电中性)

It should be mentioned that a piece of n-type or p-type silicon is electrically neutral: **the majority free carriers** are neutralized by **bound charges** associated with the impurity atoms.

In general:

$$\rho = q(p_0 - n_0 + N_d - N_a)$$

Let us examine this for $N_d = 10^{17}\,cm^{-3}, N_a = 0$

We solved this in an earlier example

$$n_0 = N_d = 10^{17}\,cm^{-3}, p_0 = \frac{n_i^2}{N_d} = 10^3\,cm^{-3}$$

Hence: $\rho \neq 0$!!

What is wrong?

Nothing wrong!

We just made the approximation when we assumed that $n_0 = N_d$

We should really solve the following system of equations(for $N_a = 0$):

$$\begin{cases} p_0 - n_0 + N_d = 0 \\ n_0 p_0 = n_i^2 \end{cases} \Rightarrow n_0 = N_d + \frac{n_i^2}{n_0}$$

Small enough to be neglected

Error in most practical circumstances too small to matter!

Example

1 Find the thermal equilibrium electron and hole concentrations at room temperature for a bulk silicon region doped with donors at $N_d=10^{14}\text{cm}^{-3}$ and with acceptors at $N_a=5\times10^{13}\text{cm}^{-3}$.

Solution:

The sample is n-type semiconductor since the donor concentration exceeds the acceptor concentration.

=>the donor concentration

$$N_d - N_a = 10^{14}\,\text{cm}^{-3} - 5\times10^{13}\,\text{cm}^{-3} = 5\times10^{13}\,\text{cm}^{-3} >> n_i$$

=>the electron concentration

$$n_0 \cong N_d - N_a = 5\times10^{13}\,\text{cm}^{-3}$$

According to the mass-action law, the hole concentration is

$$p_0 = \frac{n_i^2}{n_0} = 2\times10^{6}\,\text{cm}^{-3}$$

Homework2

Now consider a bulk n-type silicon sample with $N_d=10^{14}\text{cm}^{-3}$. We would like to add acceptors to make the hole concentration $p_0=10^{13}\text{cm}^{-3}$.

Question:
What acceptor doping concentration N_a is needed?
What is the electron concentration?

Summary

Why are IC's made of Silicon?
SILICON IS A SEMICONDUCTOR
— a very special class of materials

- Two types of "carriers" (mobile charge particles):
  – electrons and holes
- Carrier concentrations can be controlled over many orders of magnitude by addition "dopants"
  – selected foreign atoms
- Important Equations under Thermal Equilibrium conditions
  – Charge neutrality $p_0 - n_0 + N_d - N_a = 0$
  – Law of mass action $n_0 p_0 = n_i^2$