Quantum and Solid State Physics

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Contents

Part I
Quantum Physics

1 Lecturer Information

Asia Shapira

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2 Required Reading

1. Griffiths, D. Introduction to quantum mechanics

3 Additional Reading

1. Tang: Fundamentals of quantum mechanics, Cambridge press.

2. Miller, Quantum mechanics for scientists and engineers.

4 Waves

Waves

Mechanical   Electromagnetic

Need medium for propagation   Do not need medium for propagation
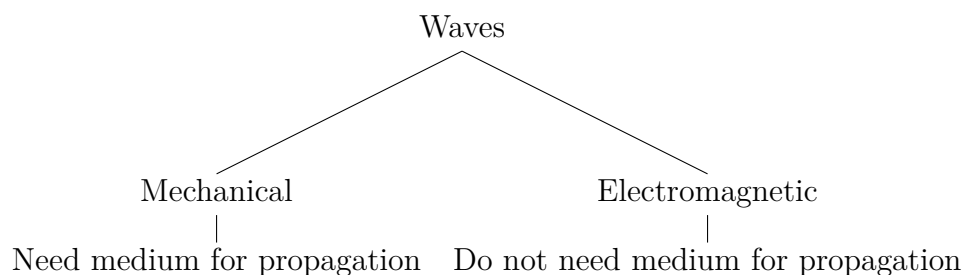
4.1 1D Wave Equation

Definition 1 (1D wave equation)**.** The equation

$$\frac{\partial^2 \psi}{\partial t^2} = v^2 \frac{\partial^2 \psi}{\partial x^2}$$

where ψ is a function of x and t, and v is the velocity of the wave, is called a 1D wave equation.

5   Harmonic Waves

Definition 2 (Harmonic waves)**.** If a wave satisfies the equation

$$\psi(x,t) = A\cos(kx - \omega t + \varphi)$$

it is called a harmonic wave.
A is called the amplitude of the wave.
k is called the wave number, or spatial frequency of the wave.
ω is called the angular frequency of the wave.

Definition 3 (Wavelength)**.** For a harmonic wave, a number λ, such that

$$\psi(x) = \psi(x + \lambda)$$

is called the wavelength of the wave.
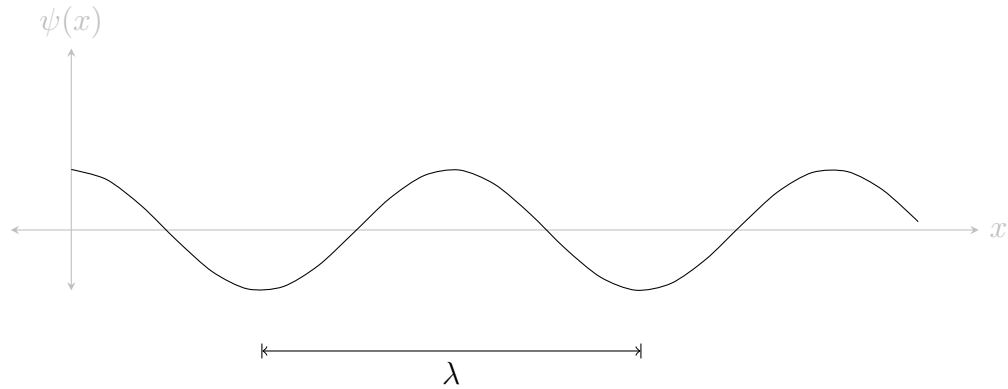
Definition 4 (Time period)**.** For a harmonic wave, a number T, such that

$$\psi(t) = \psi(t + T)$$

is called the time period of the wave.

4
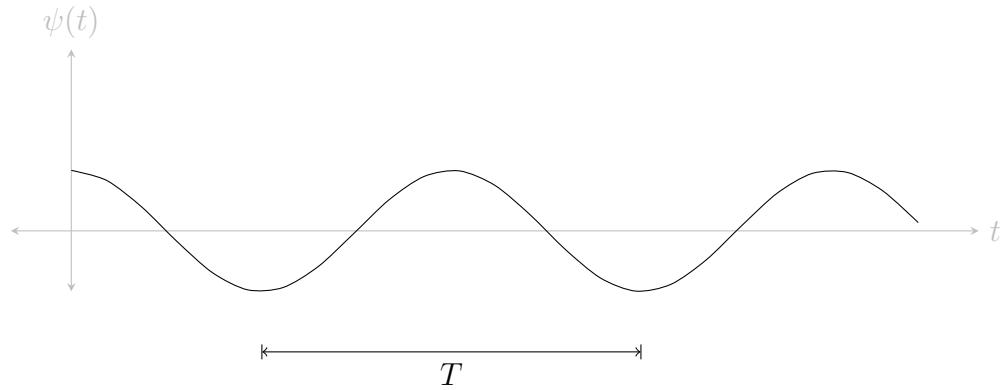
Theorem 1.

$$k = \frac{2\pi}{\lambda}$$

where k is the wave number, and λ is the wavelength.

Proof. If $t = 0$,

$$\psi(x) = A\cos(kx)$$

By the definition of wavelength,

$$\psi(x) = \psi(x + \lambda)$$
$$\therefore A\cos(kx) = A\cos\left(k(x + \lambda)\right)$$
$$\therefore k\lambda = 2\pi$$
$$\therefore k = \frac{2\pi}{\lambda}$$

□

Theorem 2.

$$\omega = \frac{2\pi}{T}$$

where ω is the angular frequency, and T is the time period.

Proof. If $x = 0$,

$$\psi(t) = A\cos(\omega t)$$

By the definition of wavelength,

$$\psi(t) = \psi(t + T)$$
$$\therefore A\cos(\omega t) = A\cos\left(\omega(t + T)\right)$$
$$\therefore \omega T = 2\pi$$
$$\therefore \omega = \frac{2\pi}{T}$$

□

5.1 Complex Representation of Waves

Let

$$\widetilde{\psi} = A e^{i(kx - \omega t + \varphi)}$$

Then,

$$\psi = \Re\{\widetilde{\psi}\}$$

5.2 Interference of Waves

Theorem 3. *Wave equations are linear, i.e. if ψ_1 and ψ_2 are solutions to the equation, then $\psi_1 + \psi_2$ is also a solution to the equation.*

5.2.1 Interference of Waves with a Phase Difference

Let

$$\psi_1 = A\cos(kx - \omega t + \varphi)$$
$$\psi_2 = A\cos(kx - \omega t)$$

Therefore,

$$\because \cos a + \cos b = 2\cos\left(\frac{a+b}{2}\right)\cos\left(\frac{a-b}{2}\right)$$

$$\begin{aligned}
\psi_3 &= \psi_1 + \psi_2 \\
&= A\cos(kx - \omega t + \varphi) + A\cos(kx - \omega t) \\
&= 2A\cos\left(\frac{\varphi}{2}\right)\cos\left(kx + \omega t + \frac{\varphi}{2}\right)
\end{aligned}$$

Therefore, the resultant wave is a wave with amplitude $2A\cos\left(\frac{\varphi}{2}\right)$ and phase $\frac{\varphi}{2}$.

6 Young's Double Slit Experiment (1801)

This experiment provided substantial proof that light behaves like a wave.
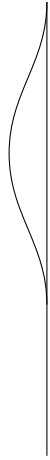
Figure 1: Intensity of light with only first slit open

Figure 2: Intensity of light with only second slit open

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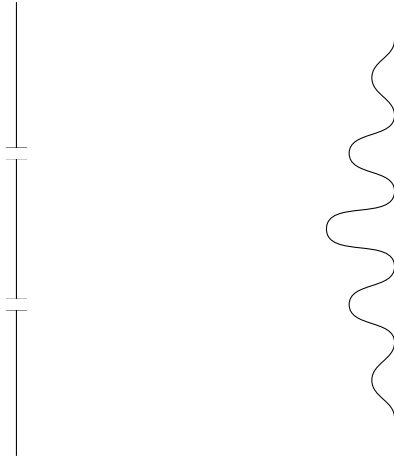
Figure 3: Intensity of light with both slits open

6.1 YDSE with Classical Particles

If the double slit experiment is performed with classical particles, instead of waves, the intensities add up. There is no fringe pattern, as observed in the experiment with waves.

7 The Photoelectric Effect

The first experiment in which the photoelectric effect was observed was performed by Hertz in 1887.

Two metallic plates, acting as electrodes were arranged as shown. They were connected to a voltage source ΔV, as shown.
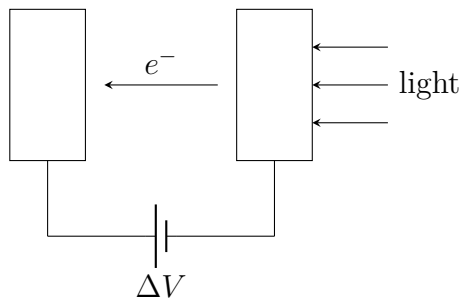
The results observed were as shown.

1. The relationship between ΔV and the current in the wire was observed to be as shown.

The conclusions were as follows.

(a) If the light intensity is constant, a specific amount of electrons is emitted. Therefore, the current is constant, and independent of ΔV.

(b) If $\Delta V >> 0$, all electrons emitted reached the other plate, and hence contributed to the current.
If $\Delta V < 0$, some electrons were unable to reach the other plate, and hence did not contribute to the current.

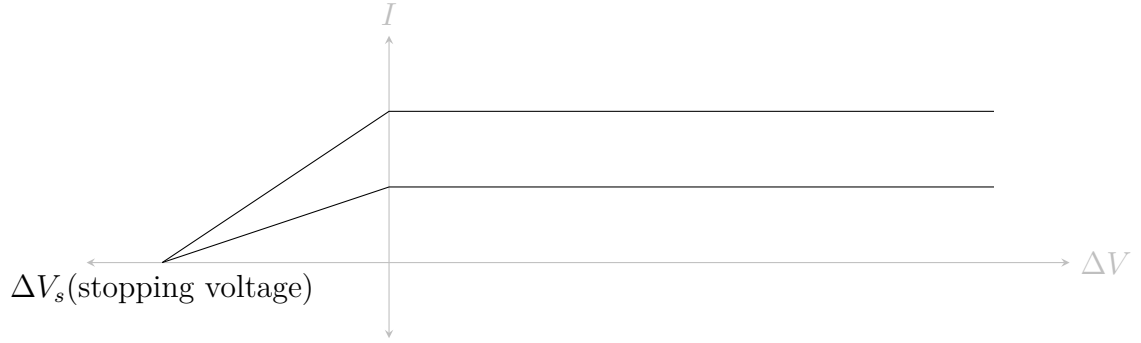(c) ΔV_s is not dependent on the intensity of the light.

As the energy of an electron is conserved,

$$E_{K_i} + E_{P_i} = E_{K_f} + E_{P_f}$$

Therefore, if the electron barely reaches the other plate, i.e. if the voltage is ΔV_s

$$E_{K_i} + 0 = (-e)(-\Delta V_s)$$
$$\therefore e\Delta V_s = E_K$$

Therefore, as ΔV_s is independent of the intensity of light, the kinetic energy of the emitted electrons is also independent of the intensity of light.

2. The relationship between the kinetic energy of the emitted electrons, and the frequency of the incident light was observed to be as shown.
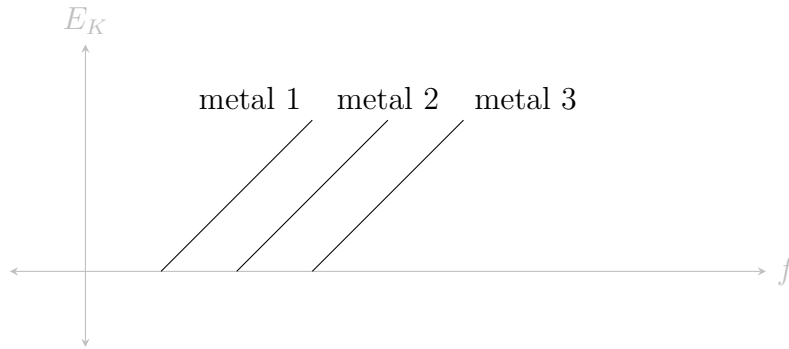
The conclusions were as follows.

(a) There is a cutoff frequency, i.e. a frequency below which no electrons are emitted.

(b) The kinetic energy of the emitted electrons is linearly dependent on the frequency of light.

These conclusions were inconsistent with the accepted notion of light being a wave.

7.1 Einstein's Explanation of the Photoelectric Effect (1905)

According to Einstein's explanation, light is a stream of particles, called photons. Each photon has energy equal to hf, where h is Planck's constant, and f is the frequency of the light, which is in fact a property of the wave nature of the light. This theory can explain the conclusions of Hertz's experiment, which could not be explained by classical theories.

According to the explanation, each material has a property called the work function (W). The fact that there exists a cutoff voltage is justified due to this energy barrier. For an electron to be emitted, it needs to be provided energy to overcome this barrier. The cutoff frequency is such that all energy in a photon of this frequency to be used to overcome the work function. Therefore,

$$hf_{\text{cutoff}} = W$$

Also, as each photon provides all its energy to a single electron, increasing the intensity of light just increases the number of electrons emitted, but does not increase the kinetic energy of the emitted electrons.

8 Quantum Particles

Definition 5 (Momentum of a quantum particle)**.** The momentum of a quantum particle is defined as

$$p = \frac{E}{c}$$

where E is the energy of the particle.

Theorem 4 (Einstein Equation)**.**

$$E = mc^2 + pc$$

Definition 6. The reduced Planck's constant is defined as

$$\hbar = \frac{h}{2\pi}$$

where h is Planck's constant.

Theorem 5.

$$E = \hbar\omega$$
$$p = \hbar k$$

Proof.

$$E = hf$$
$$= h\frac{\omega}{2\pi}$$
$$= \hbar\omega$$

$$p = \frac{E}{c}$$
$$= \frac{h}{\lambda}$$
$$= \frac{h}{2\pi}k$$
$$= \hbar k$$

$\square$

8.1 de Broglie Wavelength

According to de Broglie's theory, particles have waves associated with them. Therefore, according to this theory,

$$\lambda = \frac{h}{p}$$
$$= \frac{h}{mv}$$
$$f = \frac{E}{h}$$

where m is the mass of the particle and v is its velocity.

Therefore, according to this theory, particles must exhibit wave-like behaviour. Hence, if the double slit experiment is performed with particles, the pattern observed must be similar to the fringe pattern observed with waves.

If the double slit experiment is performed with a single electron emitted at a time, over a long period of time, a fringe-like pattern, made up of dots corresponding to single electrons, is observed. This is consistent with de Broglie's theory.

Exercise 1.

Find the de Broglie wavelength of an electron moving at $10^7 \mathrm{m\,s^{-1}}$.

Solution 1.

$$\lambda = \frac{h}{mv}$$
$$= \frac{6.63 \times 10^{-34} \mathrm{J\,s}}{(9.11 \times 10^{-31} \mathrm{kg})\left(10^7 \mathrm{m\,s^{-1}}\right)}$$
$$= 7.27 \times 10^{-11} \mathrm{m}$$
$$= 72 \mathrm{pm}$$

Exercise 2.

Find the de Broglie wavelength of a rock of 50 g, thrown with a speed of 40 $\mathrm{m\,s^{-1}}$.

Solution 2.

$$\lambda = \frac{h}{mv}$$
$$= \frac{6.63 \times 10^{-34}}{(50 \times 10^{-3})\,(40)}$$
$$= 3.3 \times 10^{-34} \mathrm{m}$$

¡++¿

8.2   Impact of Observation on the Result of Experiments

If 100% of the electrons are observed to determine which slit they pass through, the pattern observed is exactly like the pattern observed with classical particles.

If only some electrons are observed, say 70%, then those 70% electrons behave like classical particles, and the rest behave like a wave. Therefore, the effective result is a superposition both of these pattern.

Therefore, the outcome of the experiment is affected by the fact that the particles are being observed.

The reason behind this is that the act of observation involves interacting with the particles, usually in the form of the particle being hit by photons, which are necessary for the observer to make the observations.

Classical particles are not affected by this factor on such a large scale, as their mass is much larger than that of quantum particles.

9   Schrödinger Equation

Theorem 6 (Schrödinger Equation).

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\right) \psi(x,t)$$

Proof. Let the wave be given by

$$\psi(x,t) = A e^{i(kx - \omega t)}$$

Differentiating with respect to time,

$$\frac{\partial \psi(x,t)}{\partial t} = -i\omega \psi(x,t)$$

$$= -i\frac{E}{\hbar} \psi(x,t) \qquad \qquad \because \omega = \frac{E}{\hbar}$$

$$= -\frac{i}{\hbar} \left(\frac{p^2}{2m} + E_P\right) \psi(x,t) \qquad \qquad \text{where } E_P = V(x) \text{ is the potential energy of the particle}$$

$$= -\frac{i}{\hbar} \left(\frac{p^2}{2m} + V(x)\right) \psi(x,t) \qquad \qquad (1)$$

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Differentiating with respect to x,

$$\frac{\partial \psi(x,t)}{\partial x} = ik\psi(x,t)$$

$$\therefore \frac{\partial^2 \psi(x,t)}{\partial x^2} = (ik)(ik)\psi(x,t)$$

$$= -k^2 \psi(x,t)$$

$$= -\frac{p^2}{\hbar^2}\psi(x,t)$$

$$\therefore -h^2 \frac{\partial^2 \psi(x,t)}{\partial x^2} = p^2 \psi(x,t)$$

$$\therefore -\frac{h^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial x^2} = \frac{p^2}{2m}\psi(x,t) \tag{2}$$

Therefore, solving the above equations simultaneously,

$$\frac{\partial \psi(x,t)}{\partial t} = -\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\right)\psi(x,t)$$

$$\therefore i\hbar \frac{\partial \psi(x,t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\right)\psi(x,t)$$

$\square$

10 Basic Postulates of Quantum Mechanics

1. $\psi(x,t)$ describes the configuration of the system.

2. The probability of finding the particle between x and $x + \mathrm{d}x$ at time t is

$$|\psi(x,t)|^2 = \psi(x,t)\psi^*(x,t)$$

where ψ^* is the complex conjugate of of ψ,

3. If $\psi_1(x,t)$ and $\psi_2(x,t)$ are solutions to the Schrödinger equation, then $\alpha\psi(x,t) + \beta\psi(x,t)$ is also a solution to the Schrödinger equation.

11 Properties of $\psi(x,t)$

1. $\displaystyle\int_{-\infty}^{\infty} |\psi(x,t)|^2 \, \mathrm{d}x = 1$

$|\psi(x,t)|^2$ is the probability of the particle being in the neighbourhood of

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x. Therefore, the equation is obvious, as the probability of the particle being in the entire universe must be 1.

2. $|\psi(x,t)|$ is a single valued function.
   This is obvious, as the probability of the particle existing at a point in space must have exactly one value.

Part II
Solid State Physics

1 Lecturer Information

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2 Required Reading

1. Streetman, B. Solid State Electronic Devices

3 Additional Reading

1. Kittel, Introduction to solid state physics, John Wiley & Sons.

2. Pierret. Advanced semiconductor Fundamentals, Prentice Hall.

3. Ashcroft, Solid State Physics, Harcourt college publishers.

4 Electrons

Definition 7 (Particle nature of electrons)**.** An electron behaves as a negatively charged charge carrying particle.
The magnitude of the charge on it is

$$q = 1.602 \times 10^{-19} \text{C}$$

Its mass is

$$m_0 = 9.11 \times 10^{-31} \text{kg}$$

Definition 8 (Wave nature of electrons)**.** Electrons exhibit wave-like properties, in addition to particle-like properties.
The energy transmitted by a wave is

$$E = h\nu$$
$$= \frac{hc}{\lambda}$$

where

$$h = \text{Planck's constant} \left(6.626 \times 10^{-34}\right)$$
$$\nu = \text{frequency}$$
$$c = \text{speed of light}$$
$$\lambda = \text{wavelength}$$

5 Semiconductors

Law 1 (Ohm's Law). *The voltage across two points on a conductor is directly proportional to the current through the conductor. The constant of proportionality is called the resistance of the conductor.*

$$\frac{V}{I} = R$$

Law 2 (Microscopic Ohm's Law).

$$\overrightarrow{J} = \sigma \overrightarrow{E}$$

where $\overrightarrow{J}$ is the current density, σ is the conductivity, $\overrightarrow{E}$ is the electric field in the resistor.

Definition 9 (Resistivity). If

$$R = \rho \frac{L}{A}$$

where R is the resistance of the resistor, L is the length of the resistor, and A is the cross-sectional area of the resistor, then ρ is called the resistivity of the resistor.
$\sigma = \frac{1}{\rho}$ is called the conductivity of the resistor.
They are constant for a particular material.

Conductors   Semiconductors   Insulators ρ

10^{-5} 10^{6}
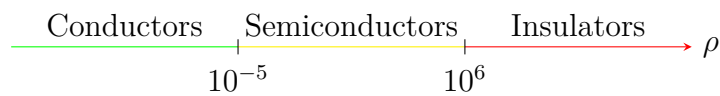
5.1 Control Factors

The major factors which affect the conductivity of a material are

1. Temperature

2. Chemical composition

   (a) Atomic bonding

   (b) Crystal structure

   (c) Charge carriers in the crystal

3. Optical effects

4. Doping

5.2 Chemical Makeup

II	III	IV	V	VI
	B	C	N	O
	Al	Si	P	S
Zn	Ga	Ge	As	
Cd	In			

Silicon is usually used as a semiconductor, as it

1. is easily available, hence economical

2. performs better at higher temperatures
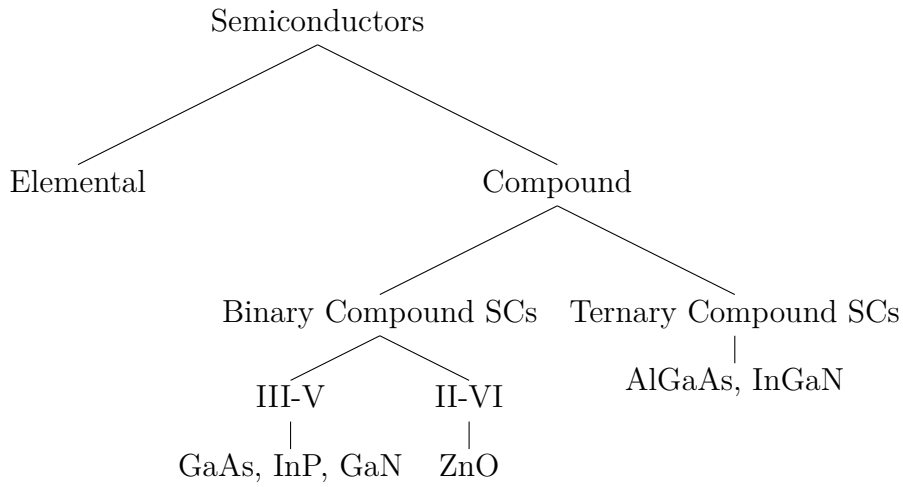
3. can be converted to silica on heating

Figure 4: Classification of Semiconductors

Exercise 3.

A sample of Germanium has resistivity $\rho = 0.46\Omega\text{m}$. The dimensions of the sample are

$$l = 50\mu\text{m}$$
$$h = 0.2\mu\text{m}$$
$$w = 1\mu\text{m}$$

Find the resistance of the sample and the conductivity of the material.

Solution 3.

$$\rho = 0.46\Omega\,\text{m}$$
$$= 46\Omega\,\text{cm}$$

Therefore,

$$\sigma = \frac{1}{\rho}$$
$$= \frac{1}{46\Omega\,\text{cm}}$$
$$= 0.022\Omega^{-1}\,\text{cm}^{-1}$$

Therefore,

$$l = 50\mu\text{m}$$
$$= 50 \times 10^{-4}\text{cm}$$

Therefore,

$$R = \rho \frac{l}{A}$$
$$= 11500 \times 10^{-4} \Omega$$

Exercise 4.

A sample of Germanium has resistivity σ. The dimensions of the sample are as shown.
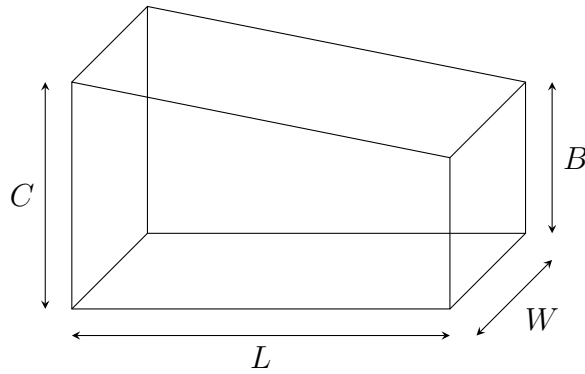
Find the relationship between R and σ.

Solution 4.

Consider a slice with height h, width w, and thickness $\mathrm{d}x$. Therefore, the cross-sectional area of the elemental slice is

$$\mathrm{d}A = wh$$
$$= w \left(\frac{B - C}{L} x + C \right)$$
$$= w \left(\frac{Bx - C(L - x)}{L} \right)$$

Therefore,

$$\mathrm{d}R = \frac{\mathrm{d}x}{\sigma w h}$$
$$= \frac{L \, \mathrm{d}x}{\sigma w \left(Bx - C(L - x) \right)}$$

6 Types of Materials

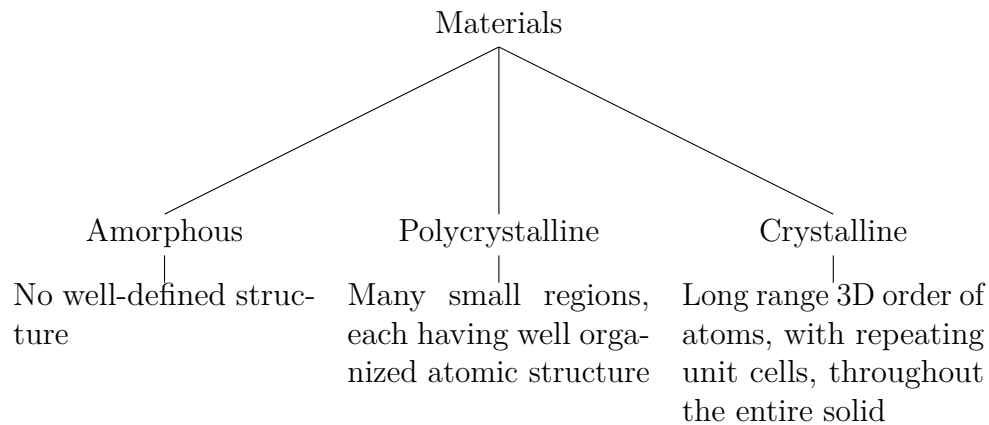Atoms tend to arrange themselves in such a way that the resultant energy is minimized.

Materials

Amorphous — No well-defined structure

Polycrystalline — Many small regions, each having well organized atomic structure

Crystalline — Long range 3D order of atoms, with repeating unit cells, throughout the entire solid

Figure 5: Classification of Materials

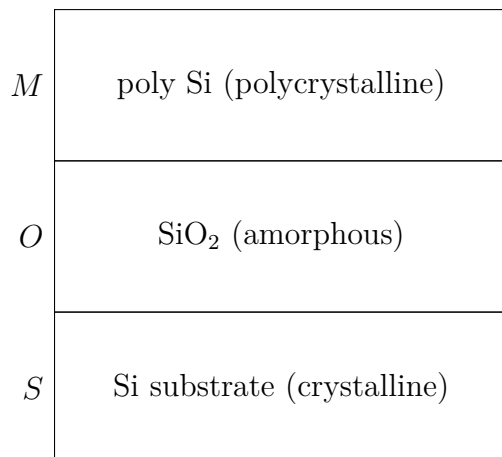Semiconductor devices can use all of these types of materials.

M | poly Si (polycrystalline)

O | SiO$_2$ (amorphous)

S | Si substrate (crystalline)

Figure 6: MOS which uses all three types of materials

7 Bohr's Model

According to Bohr's model of the atom, electrons can have discrete energy levels only. The electrons in an atom are arranged in the order of filling

electronic shells, given by the Aufbau Principle.

The energy of a free electron is called E_{vac}. This is used as a reference energy.
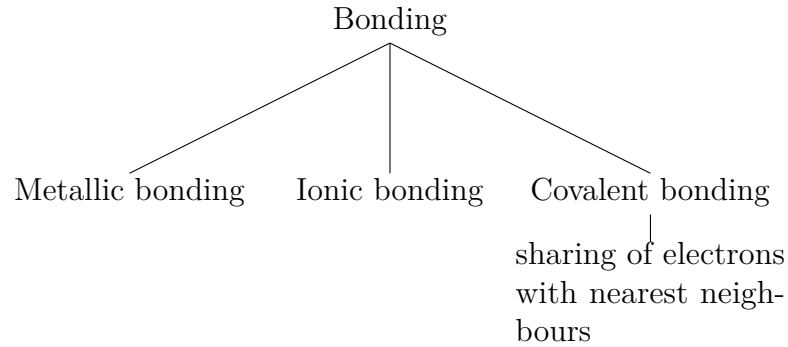
8 Atomic Bonding

Figure 7: Types of Atomic Bonds
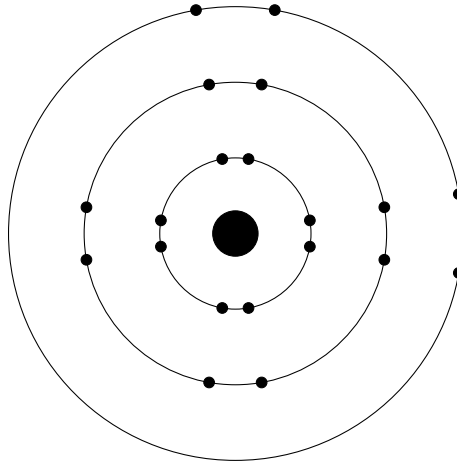
8.1 Covalent Bonds in Silicon

Figure 8: Arrangement of electrons in a silicon atom, in shells according to Bohr's model

In a silicon crystal, the silicon atoms are packed tightly and periodically, i.e. in a repeating pattern. The atomic density for silicon is approximately 10^{23} atoms per cm^3.

This arrangement of silicon atoms in crystalline form acts as a conductor only
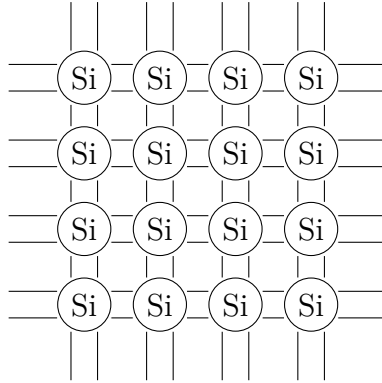
Figure 9: 2D model of bonding in silicon

at certain temperatures. At low temperatures, i.e. around 0 K, the electrons are tightly bound, and hence the crystal behaves as an insulator. However, at higher temperatures, the additional thermal energy may be sufficient to break bonds, and hence produce free electrons.

This property of silicon and other semiconductors makes it possible to control their conductivity.

9 Basics of Crystal Structure

Definition 10 (Crystal lattice). The periodic arrangement of atoms in a crystal is called crystal lattice.

Definition 11 (Lattice constant). The distance between two adjacent atoms in a crystal lattice is called the lattice constant.
It is denoted by a.
It is determined by the attractive and repulsive forces acting on the atoms.
The lattice constant corresponds to the lowest energy in the crystal.
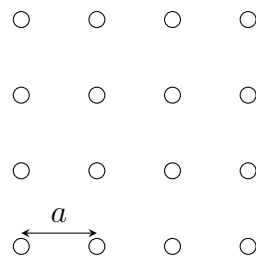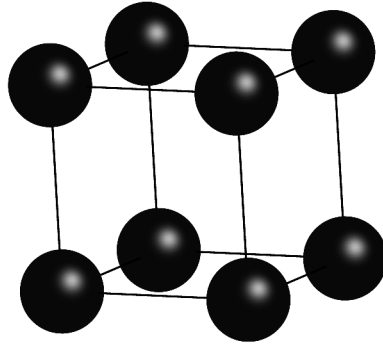

Figure 10: Crystal lattice and lattice constant

Definition 12 (Unit cell). A volume which is repeated throughout the crystal is called the unit cell. It is used to represent the entire crystal lattice.

Definition 13. The atomic packing factor defined to be

$$\text{APF} = \frac{\text{volume filled by atoms}}{\text{total volume of unit cell}}$$

9.1 Simple Cubic Lattice

The number of atoms per unit cell are

$$\text{atoms per unit cell} = \underbrace{\frac{1}{8}}_{\text{atoms per corner}} \times \underbrace{8}_{\text{number of corners}}$$

$$= 1$$

The atomic packing factor is

$$\text{APF} = \frac{\overbrace{\frac{4}{3}\pi r^3}^{\text{volume of 1 atom}} \times \overbrace{1}^{\text{number of atoms}}}{\underbrace{a^3}_{\text{volume of unit cell}}} = \frac{\overbrace{\frac{4}{3}\pi \left(\frac{a}{2}\right)^3}^{\text{volume of 1 atom}} \times \overbrace{1}^{\text{number of atoms}}}{\underbrace{a^3}_{\text{volume of unit cell}}}$$
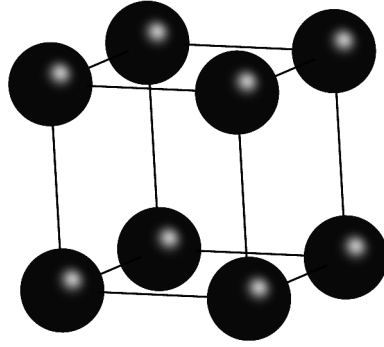
$$= \frac{\pi}{6}$$

Figure 11: Simple cubic lattice (SC)

9.2   Face Centred Cubic Lattice

The number of atoms per unit cell are

$$\text{atoms per unit cell} = \underbrace{\frac{1}{8}}_{\text{atoms per corner}} \times \underbrace{8}_{\text{number of corners}} + \underbrace{\frac{1}{2}}_{\text{atoms per face}} \times \underbrace{6}_{\text{number of faces}}$$

$$= 4$$

The atomic packing factor is

$$\text{APF} = \frac{\overbrace{\frac{4}{3}\pi r^3}^{\text{volume of 1 atom}} \times \overbrace{1}^{\text{number of atoms}}}{\underbrace{a^3}_{\text{volume of unit cell}}} = \frac{\overbrace{\frac{4}{3}\pi \left(\frac{a}{2\sqrt{2}}\right)^3}^{\text{volume of 1 atom}} \times \overbrace{4}^{\text{number of atoms}}}{\underbrace{a^3}_{\text{volume of unit cell}}}$$
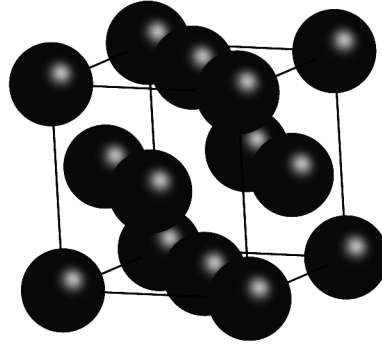
$$= \frac{\pi}{3\sqrt{2}}$$

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Figure 12: Face centred cubic lattice (FCC)

9.3 Body Centred Cubic Lattice

The number of atoms per unit cell are

$$\text{atoms per unit cell} = \underbrace{\frac{1}{8}}_{\text{atoms per corner}} \times \underbrace{8}_{\text{number of corners}} + \underbrace{1}_{\text{atom at centre}}$$
$$= 2$$

10 Basics of Crystal Growth

Definition 14. Epitaxy is the growth of layers, called epitaxial layers, on top of a thicker substrate layer.
Homoepitaxy is growing an epitaxial layer of the same material as the substrate. Heteroepitaxy is growing an epitaxial layer of a material different from the substrate.
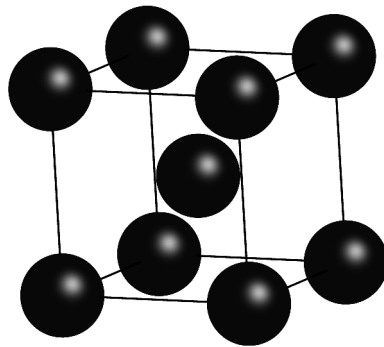
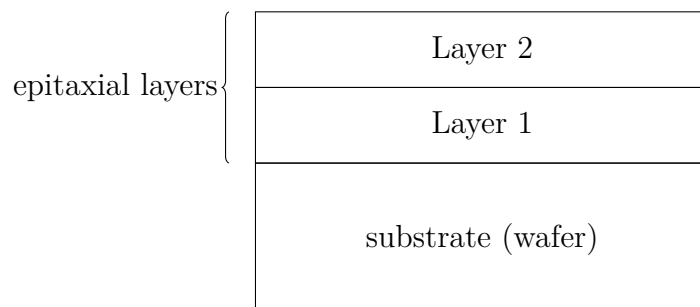Figure 13: Body centred cubic lattice (BCC)

Figure 14: Epitaxial layers

Due to different properties of the materials which make up the substrate and epitaxial layers, there are certain constraints on the possible combinations. These factors include

1. lattice constants

2. crystal structure

10.1 Lattice Matching

If there is a difference between the lattice constants of the materials of two adjacent layers, there is a stress or strain generated, due to the interaction of the different lattices.
To minimize this stress, a technique called lattice matching is used.

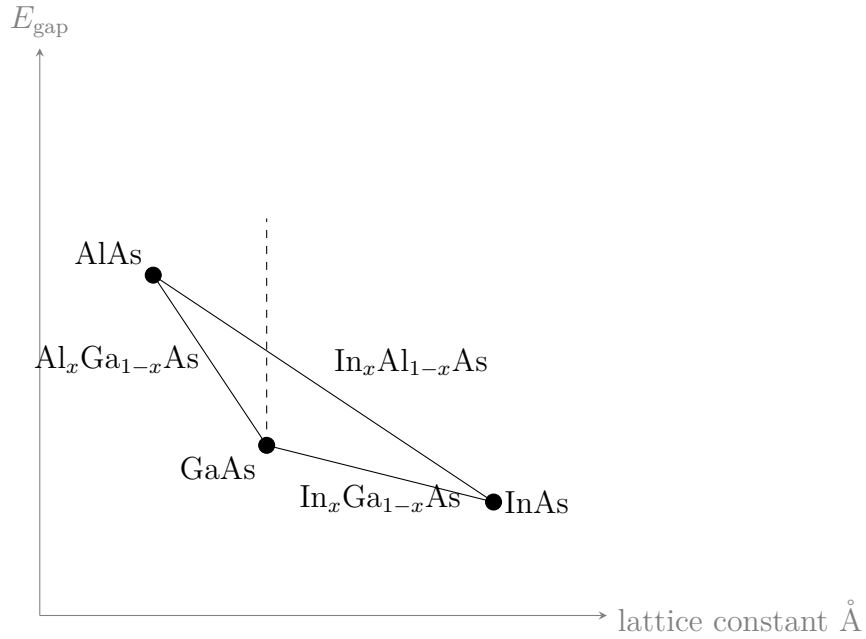Suppose the lattice constants of AlAs, InAs, and GaAs are as shown in the graph.

Figure 15: Lattice matching

If the substrate used is GaAs, and the epitaxial layer is made of InAlAs, then the composition of the epitaxial layer of InAlAs can be determined graphically.
The straight line connecting the points representing AlAs and InAs represents all possible values of $In_xAl_{1-x}As$, with x varying from 0 to 1, with 0 corresponding to AlAs, and 1 corresponding to InAs.
Therefore, the ideal material for the epitaxial layer, is the composition of $In_xAl_{1-x}As$ with lattice constant equal to that of GaAs.

11 Thermal Motion

Definition 15. The energy needed to break a bond and free an electron is called the binding energy, or the ionization energy.