Solid State Physics

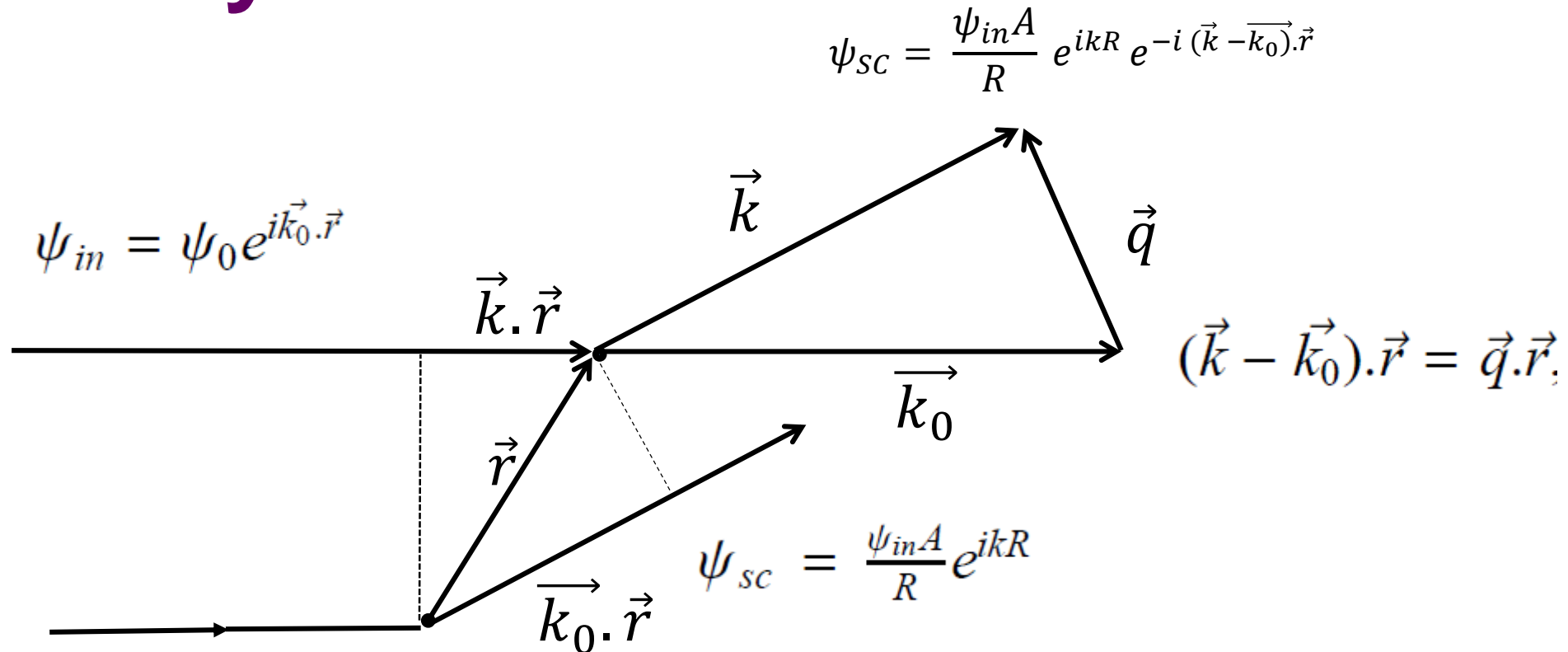## Lecture – UG III,

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X-ray diffraction

$$\psi_{SC} = \frac{\psi_{in}A}{R} \, e^{ikR} \, e^{-i\,(\vec{k} - \vec{k_0}).\vec{r}}$$

$$\psi_{in} = \psi_0 e^{i\vec{k_0}.\vec{r}}$$

$$\vec{k}$$

$$\vec{k}.\vec{r}$$

$$\vec{q}$$

$$\vec{k_0}$$

$$(\vec{k} - \vec{k_0}).\vec{r} = \vec{q}.\vec{r}.$$

$$\vec{r}$$

$$\vec{k_0}.\vec{r}$$

$$\psi_{SC} = \frac{\psi_{in}A}{R} e^{ikR}$$

: Scattering vector: $\left| \vec{q} \right| = \frac{4\pi sin\theta}{\lambda}$

Scattered wave due to N independent scatterers

$$\psi_{sc} = \frac{\psi_{in}A}{R}e^{ikR}\sum_{i=1}^{N}e^{-i\vec{q}.\vec{r_i}}$$
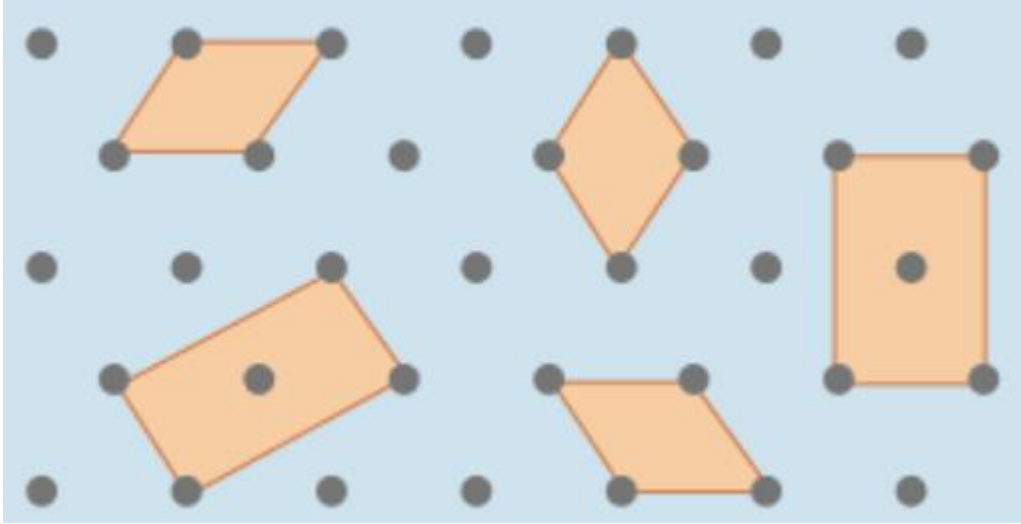
Where, r_i is the position of ith scatterer.

$$\psi_{SC} = \frac{\psi_{in}A}{R}e^{ikR}\int\sum\delta(r-r_i)e^{-i\vec{q}.\vec{r}}d\vec{r}$$

Continuous electron density function $\rho(\vec{r}) = \sum_{i=1}^{N}\delta(\vec{r}-\vec{r_i})$

$$\psi_{sc} = \frac{\psi_{in}A}{R}e^{ikR}\int\rho(\vec{r})e^{-i\vec{q}.\vec{r}}d\vec{r}$$

$$I(\vec{q}) = |\psi_{sc}|^2 = |\frac{\psi_{in}A}{R}\int\rho(\vec{r})e^{-i\vec{q}.\vec{r}}d\vec{r}|^2$$

Bravais Lattices

Two dimensional lattices and different unit cell

Diffraction by periodic object

Electron density $\rho(r) = \rho_{lattice} \otimes \rho_{basis}$

Scattered intensity $I(q) = S(q)P(q)$,

where $S(q) = |F_{lattice}|^2$ and $P(q) = |F_{basis}|^2$

$F_{lattice}$ and F_{basis} are the Fourier transforms of $\rho_{lattice}$ and ρ_{basis}, respectively

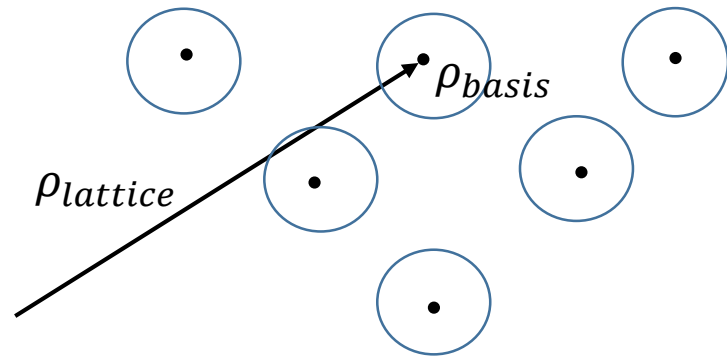$S(q)$ ⟶ Structure factor: Positions in the reciprocal space, where intensities of sampled:

$P(q)$ ⟶ Form factor: Intensity at each of these positions

$$\rho_{lattice}(\vec{r}) = \sum_{n_1}\sum_{n_2}\sum_{n_3} \delta(\vec{r} - n_1\vec{a} - n_2\vec{b} - n_3\vec{c})$$

$$\rho_{basis}(\vec{r}) = \sum_{j=1}^{N} \rho_j(\vec{r} - \vec{r_j})$$

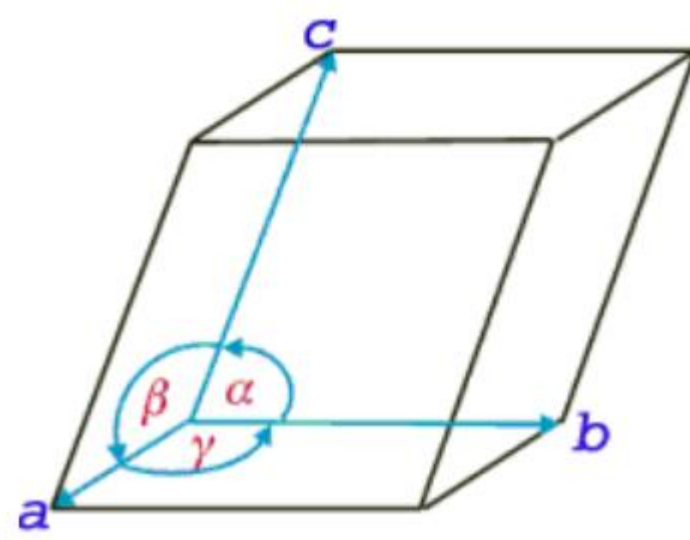$$F_{lattice}(\vec{q}) = \sum_{h}\sum_{k}\sum_{l} \delta(\vec{q} - h\vec{a}^* - k\vec{b}^* - l\vec{c}^*)$$

$$F_{basis}(\vec{q}) = \sum_{j=1}^{N} f_j e^{-i\vec{q}.\vec{r_j}}$$

$$f_j = \int \rho_j(\vec{r}) e^{-i\vec{q}.\vec{r}} d\vec{r}.$$

ρ_{basis}

$\rho_{lattice}$

$$I(\vec{q}) \propto | \int \rho(\vec{r}) e^{-i\vec{q}.\vec{r}} d\vec{r} |^2 = \frac{1}{(\vec{a} \times \vec{b}.\vec{c})^2} | F_{basis}(\vec{q}) |^2 \sum_{h,k,l} \delta(\vec{q} - h\vec{a}^* - k\vec{b}^* - l\vec{c}^*).$$
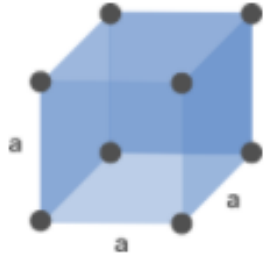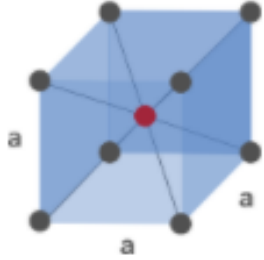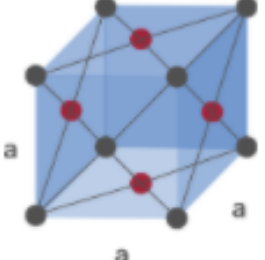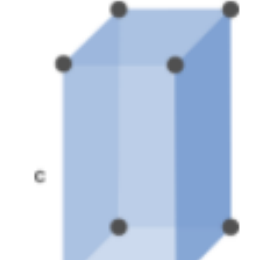
Reciprocal and Real lattice
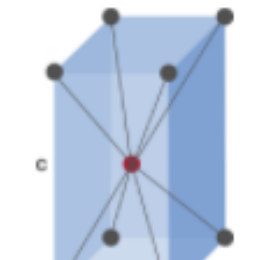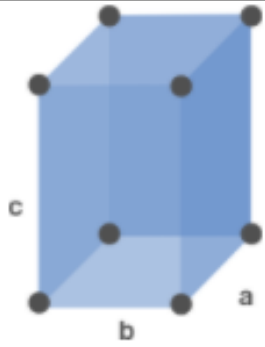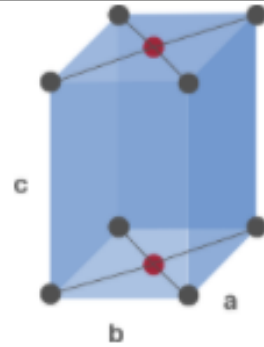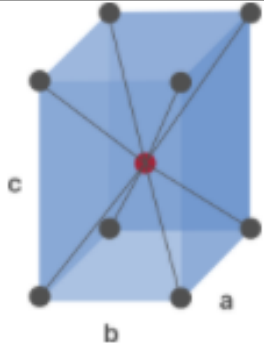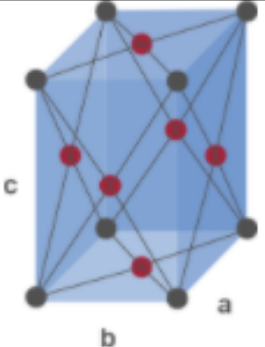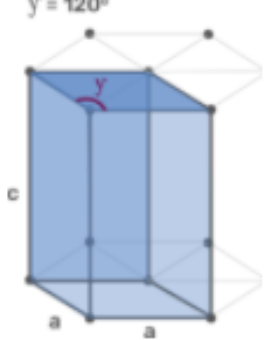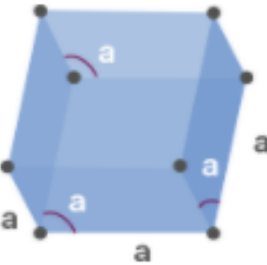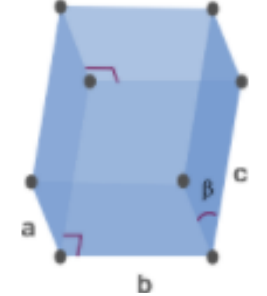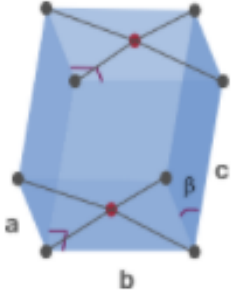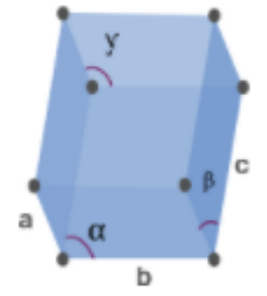
$$a^* = \frac{b \times c}{V}; \quad \cos \alpha^* = \frac{\cos \beta . \cos \gamma - \cos \alpha}{\sin \beta . \sin \gamma} \quad ; \quad a^* \text{ perpendicular to: } b, c$$

$$b^* = \frac{c \times a}{V}; \quad \cos \beta^* = \frac{\cos \alpha . \cos \gamma - \cos \beta}{\sin \alpha . \sin \gamma} \quad ; \quad b^* \text{ perpendicular to: } c, a$$

$$c^* = \frac{a \times b}{V}; \quad \cos \gamma^* = \frac{\cos \alpha . \cos \beta - \cos \gamma}{\sin \alpha . \sin \beta} \quad ; \quad c^* \text{ perpendicular to: } a, b$$

14 Bravais lattices

Lattice System	Primitive (P)	Base Centered (C)	Body centered (I)	Face centered (F)	Total
Cubic a = b = c α= β=γ=90°		-			3
Tetragonal a = b ≠ c α= β=γ=90°		-		-	2
Orthorhombic a ≠ b ≠ c α= β=γ=90°					4

Hexagonal a = b ≠ c α=120°,β=γ=90°		-	-	-	1
Rhombohedral a = b = c α= β=γ≠ 90°		-	-	-	1
Monoclinic		-	-	2
Triclinic		-	-	-	1
Total					14

14 Bravais Lattices and 7crystal systems

Crystal family	Lattice system	Volume
	Triclinic	$abc\sqrt{1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma}$
	Monoclinic	$abc \sin \beta$
	Orthorhombic	abc
	Tetragonal	$a^2 c$
Hexagonal	Rhombohedral	$a^3 \sqrt{1 - 3\cos^2 \alpha + 2\cos^3 \alpha}$
Hexagonal	Hexagonal	$\dfrac{\sqrt{3}}{2} a^2 c$
	Cubic	a^3

$$bcc : \mathrm{V} = \frac{1}{2} a^3$$

$$fcc : \mathrm{V} = \frac{1}{4} a^3$$

Characteristics of crystal structure

Structure	a_0 versus r	Atoms per Cell	Coordination Number	Packing Factor	Examples
Simple cubic (SC)	$a_0 = 2r$	1	6	0.52	Polonium (Po), α-Mn
Body-centered cubic	$a_0 = 4r/\sqrt{3}$	2	8	0.68	Fe, Ti, W, Mo, Nb, Ta, K, Na, V, Zr, Cr
Face-centered cubic	$a_0 = 4r/\sqrt{2}$	4	12	0.74	Fe, Cu, Au, Pt, Ag, Pb, Ni
Hexagonal close-packed	$a_0 = 2r$ $c_0 \approx 1.633a_0$	2	12	0.74	Ti, Mg, Zn, Be, Co, Zr, Cd

Millar indices
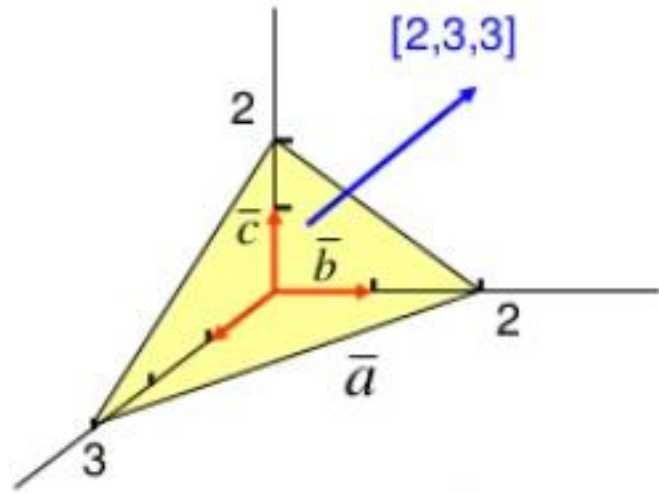
Plane intercepts axes at $3\bar{a}, 2\bar{b}, 2\bar{c}$

Reciprocal numbers are: $\dfrac{1}{3}, \dfrac{1}{2}, \dfrac{1}{2}$

Indices of the plane (Miller): (2,3,3)

Indices of the direction: [2,3,3]

[2,3,3]

2

$\bar{c}$

$\bar{b}$

$\bar{a}$

2

3

(200)

(100)

(110)

(111)

($\bar{1}$00)
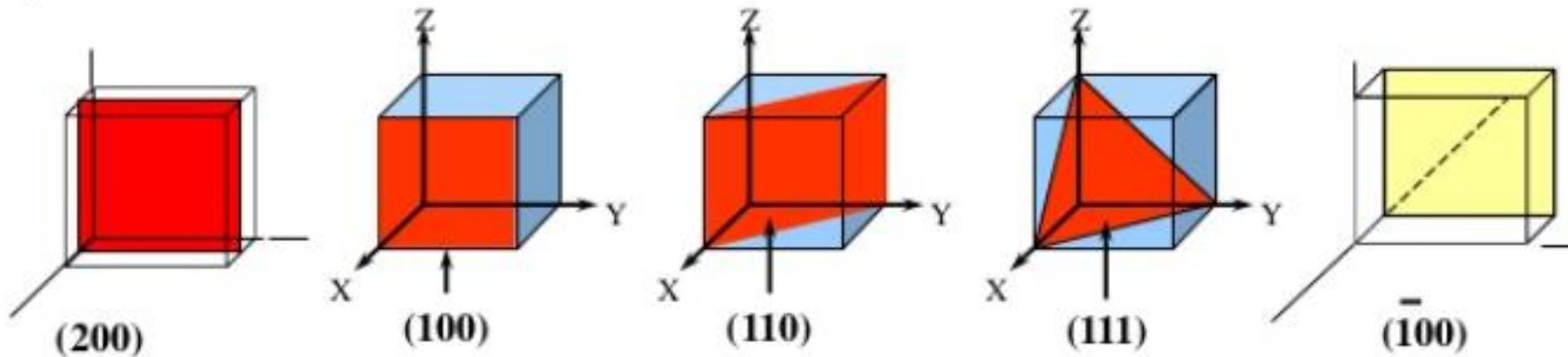
Diffraction condition

A reciprocal vector can be written as $\vec{G} = a^* h + b^* k + c^* l$

A set of reciprocal vector **G** determines the possible x-ray reflections
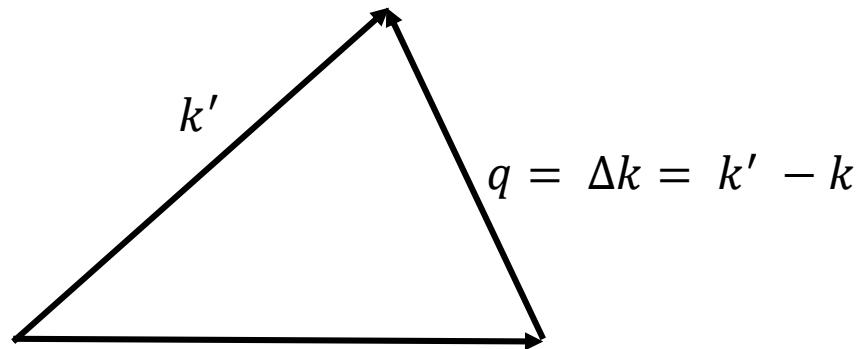
Scattering amplitude

$$F = \int \rho(r) \exp[-i\,(k' - k).r]\,dV$$

$$= \int \rho(r) \exp[-iqr]\,dV$$

$$= \sum_G \int \rho_G\, e^{iG.r} \exp[-iqr]\,dV$$

$$= \sum_G \int \rho_G \exp[-i(q - G)r]\,dV$$

$q = \Delta k = k' - k$

$$\boxed{\vec{q} = \vec{G}}$$

$$\rho(r) = \sum_G \rho_G\, e^{iG.r}$$

As electron density is a periodic function of ρ(r).

In elastic scattering of a photon its energy $\hbar\omega$ is conserved, so that the frequency $\omega' = ck'$ of the emergent beam is equal to the frequency of the incident beam. Thus the magnitudes k and k' are equal, and $k^2 = k'^2$, a result that holds also for elastic scattering of electron and neutron beams. From (21) we found $\Delta\mathbf{k} = \mathbf{G}$ or $\mathbf{k} + \mathbf{G} = \mathbf{k}'$, so that the **diffraction condition** is written as $(\mathbf{k} + \mathbf{G})^2 = k^2$, or

$$2\mathbf{k}.\mathbf{G} + G^2 = 0$$

$$2|k||G| \sin\theta = G^2$$

$$2.\,2\frac{\pi}{\lambda} \sin\theta = \frac{2\pi}{d_{hkl}}$$

$$\boxed{2d_{hkl} \sin\theta = \lambda}$$

Brillouin Zone

$$k \cdot \frac{1}{2}G = \left(\frac{1}{2}G\right)^2$$

Reciprocal Lattice to bcc Lattice

The primitive translation vectors of the bcc lattice (Fig. 12) are

$$\mathbf{a_1} = \tfrac{1}{2}a(-\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}) \; ; \quad \mathbf{a_2} = \tfrac{1}{2}a(\hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}}) \; ; \quad \mathbf{a_3} = \tfrac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}) \; ,$$

where a is the side of the conventional cube and $\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}$ are orthogonal unit vectors parallel to the cube edges. The volume of the primitive cell is

$$V = |\mathbf{a_1} \cdot \mathbf{a_2} \times \mathbf{a_3}| = \tfrac{1}{2}a^3 \; .$$

The primitive translations of the reciprocal lattice are defined by (13). We have, using (28),

$$\mathbf{b_1} = (2\pi/a)(\hat{\mathbf{y}} + \hat{\mathbf{z}}) \; ; \qquad \mathbf{b_2} = (2\pi/a)(\hat{\mathbf{x}} + \hat{\mathbf{z}}) \; ; \qquad \mathbf{b_3} = (2\pi/a)(\hat{\mathbf{x}} + \hat{\mathbf{y}}) \; .$$
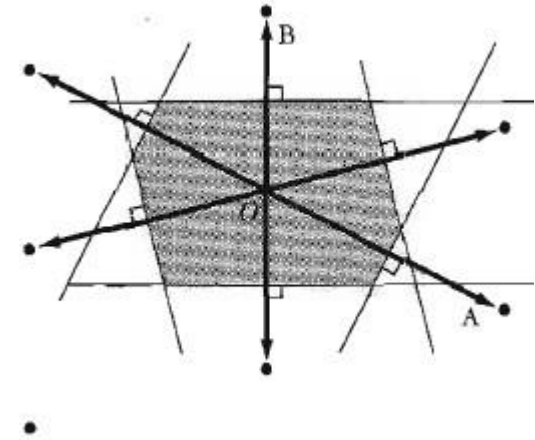
fcc Lattice
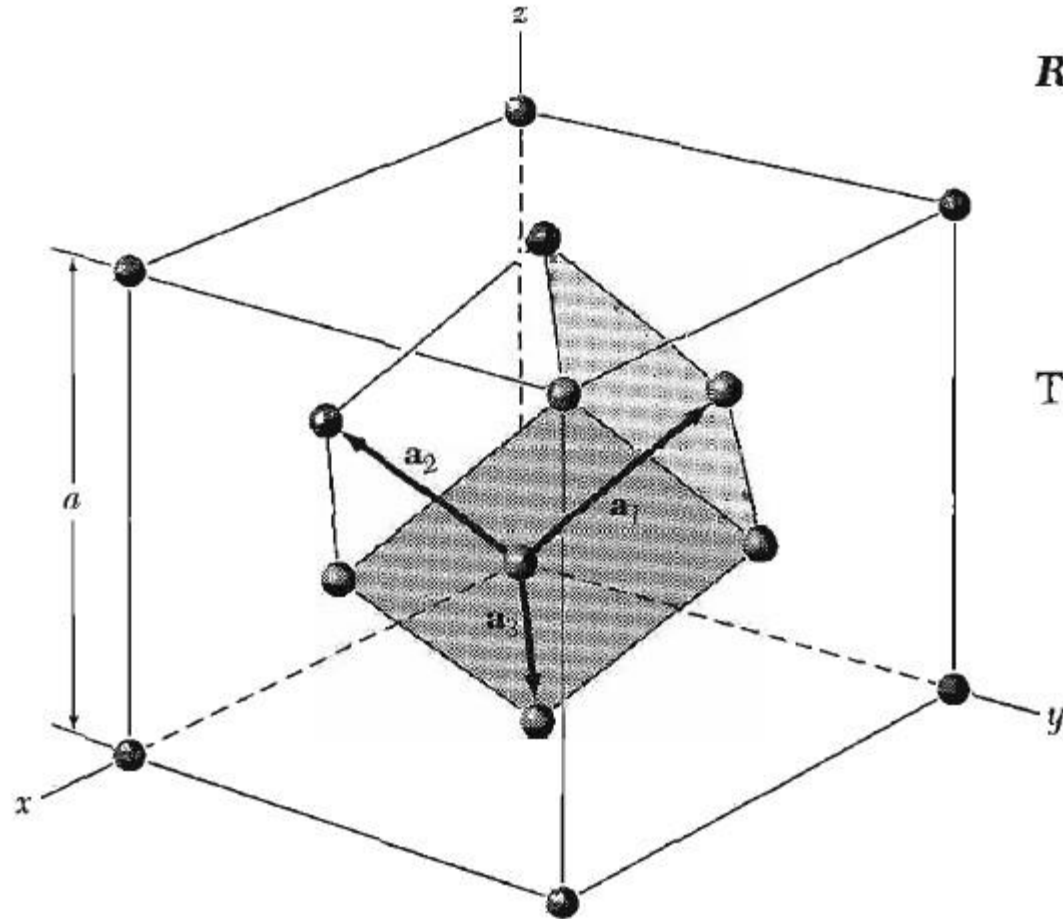
Reciprocal Lattice to fcc Lattice

The primitive translation vectors of the fcc lattice of Fig. 14 are

$$\mathbf{a}_1 = \frac{1}{2}a(\hat{\mathbf{y}} + \hat{\mathbf{z}}) \;;\quad \mathbf{a}_2 = \frac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{z}}) \;;\quad \mathbf{a}_3 = \frac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{y}}) \;.$$

The volume of the primitive cell is

$$V = |\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3| = \frac{1}{4}a^3 \;.$$

The primitive translation vectors of the lattice reciprocal to the fcc lattice are

$$\mathbf{b}_1 = (2\pi/a)(-\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}) \;;\qquad \mathbf{b}_2 = (2\pi/a)(\hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}}) \;;$$
$$\mathbf{b}_3 = (2\pi/a)(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}) \;.$$

Form factor and structure factor

Scattering amplitude per unit cell

$$F = \int dV \, \rho(r) \exp(-i \, G.r)$$

$$= \sum \int dV \, \rho_j \left(r - r_j \right) \exp(-i \, G.r)$$

$$= \sum \int dV \, \rho_j \left(R \right) \exp(-i \, G.R) \exp(-iG.r_j)$$

$$= \sum f_j \exp(-iG.r_j)$$

If r_j is the vector at the centre of the atom,
then $\rho_j \left(r - r_j \right)$ is the contribution of electron
Density associated with the jth atom in the cell
Therefore, $\rho(r) = \sum_j \rho_j \left(r - r_j \right)$
Let $r - r_j = R$

Where, $f_j = \int \rho(R) \exp(-iG.R) dV$ f_j **is known as atomic form factor**

F is the structure factor of the basis

Structure factor

$$r_j = x_j a + y_j b + z_j c \ , \quad G = ha^* + kb^* + lc^*, \quad G.r_j = 2\pi \ (hx_j + ky_j + lz_j)$$

$$F(h,k,l) = \sum f_j \exp(-i2\pi \ (hx_j + ky_j + lz_j)$$

Structure factor of bcc lattice

Positions of the atoms are $x_1 = 0, y_1 = 0, z_1 = 0$ and $x_2 = 1/2, y_2 = 1/2, z_2 = 1/2$

$$F(h,k,l) = f \ [1 + \ \exp(-i\pi \ (h + k + l)]$$

F = 0 when *h + k + l* is odd integer
      = 2f when *h + k + l* is even integer

Structure factor

Metallic sodium has a bcc structure. The diffraction pattern does not contain lines such as (100), (300), (111), or (221), but lines such as (200), (110), and (222) will be present;

Structure factor of the fcc lattice

Positions of the atoms are (0,0,0), (0, ½, ½), (1/2, 0, ½), (1/2, 1/2., 0)

$$F(h, k, l) = f\,[1 + \exp(-i\pi\,(h + k) + \exp(-i\pi\,(k + l) + \exp(l + h)]$$

If all indices are even integers, $S = 4f$; similarly if all indices are odd integers. But if only one of the integers is even, two of the exponents will be odd multiples of $-i\pi$ and S will vanish. If only one of the integers is odd, the same argument applies and S will also vanish. Thus in the fcc lattice no reflections can occur for which the indices are partly even and partly odd.

Diffraction profile for fcc lattice
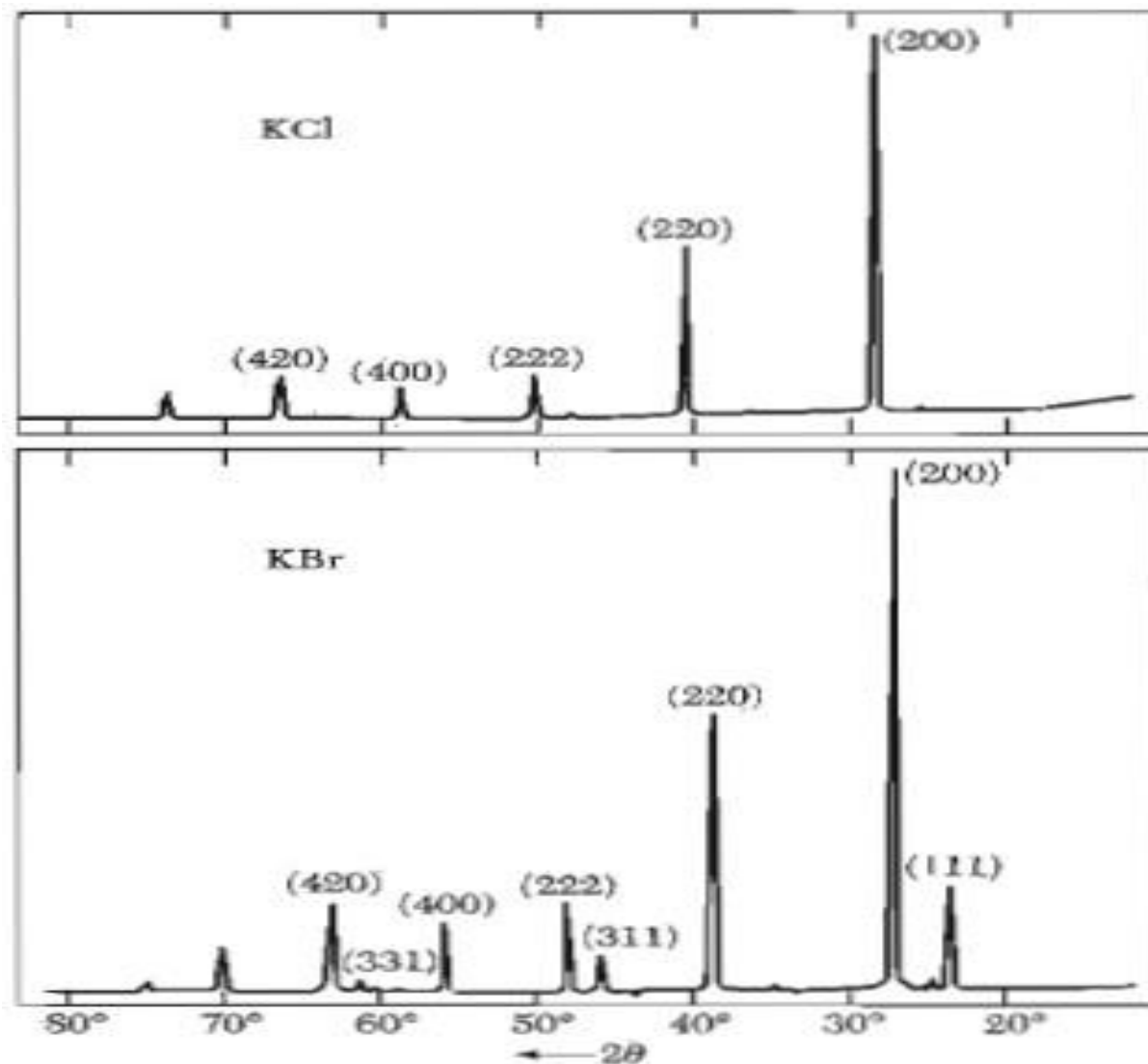
Atomic form factor

f_j Measures the scattering power of jth atom in the unit cell. Therefore, value of f depends on the number of electrons, rather electron density of the jth atom.

Scattered radiation from a single atom, i.e, form factor

$$\boldsymbol{f_j = \int dV \, \rho_j \, (r) \, \exp(-iG.r)}$$

For spherically symmetric electron density, we write $f_j = 2\pi \int dr r^2 \, \rho_j \, (r) \frac{\sin Gr}{Gr}$

If electron density is concentrated at r = 0, Gr = 0 and $f_j = Z$, total number of electron

In the forward scattering $G = 0$, and again $f = Z$

Crystal binding

➤ Van der Waal crystal or crystals of inert gases (0.1 eV/atom)

➤ Ionic crystal (8 eV/atom)

➤ Covalent crystal (~ 4-5 eV/atom)

➤ Metal (~ 5 eV/atom)
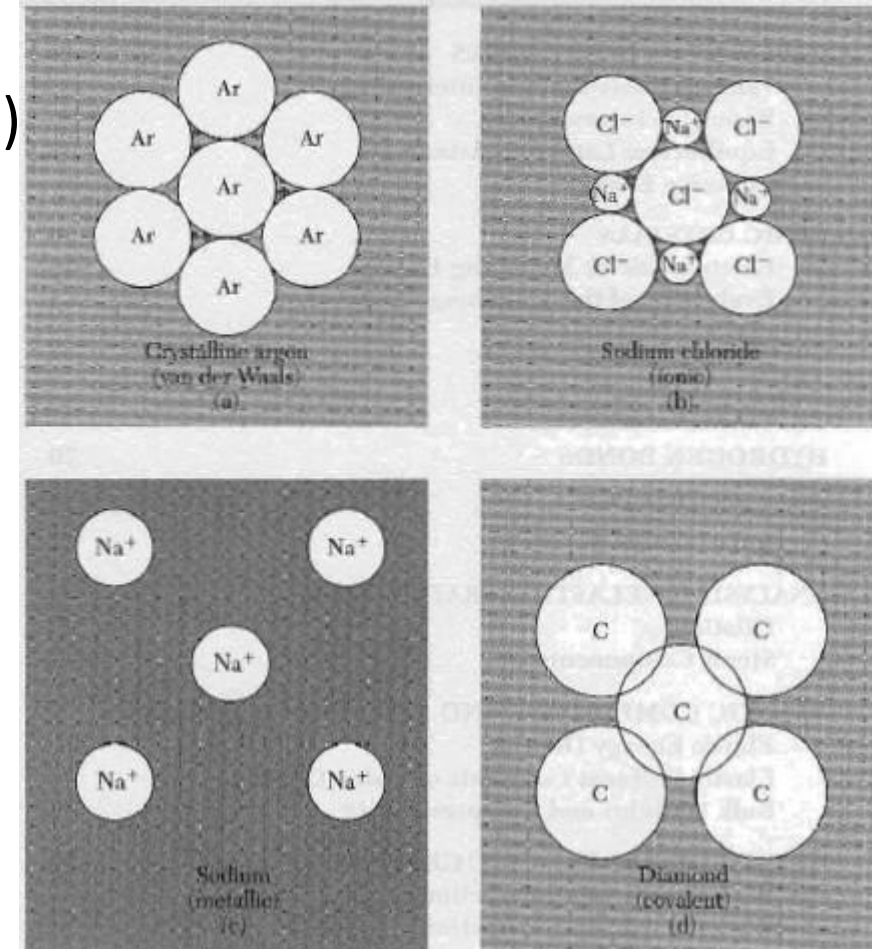
Electrical conductivity: Drude model

Basic assumptions:

1. Between collisions the interaction of a given electron, both with the others and with the ions is neglected.
   The neglect of electron-electron interactions between collisions is known as the *independent electron approximation* and neglect of electron-ion interaction is known as *free electron approximation*.

2. Collisions in the Drude model as in kinetic theory, are instantaneous events that abruptly alter the velocity of an electron.

The Drude model

Nucleus
Core electrons
Valence electrons

(a)

Ion { Nucleus, Core }
Conduction electrons

(b)

24
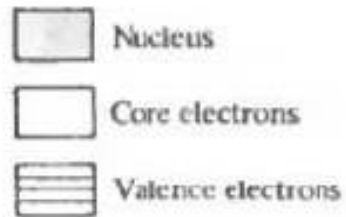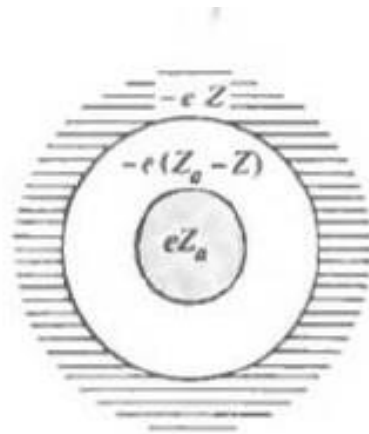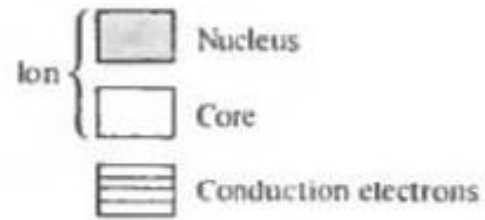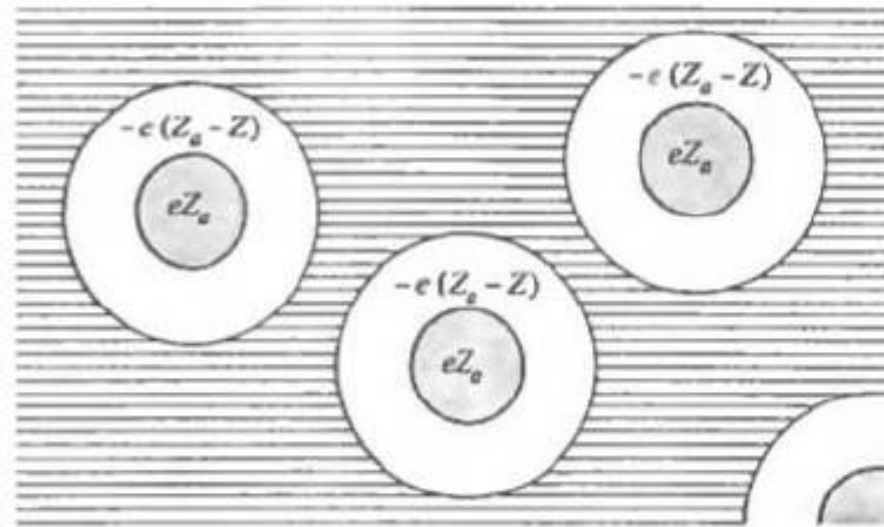
DC electrical conductivity of a metal

The resistivity ρ is defined to be the proportionality constant between the electric field E at
A point in the metal and the current density j that it induces:

$$E = \rho j$$

If n electrons per unit volume all move with velocity v, then the current density they
give rise to will be parallel to v , the electron carries a charge $-e$ the charge crossing
 A in the time dt Will be $-nevAdt$ and hence the current density

$$j = -nev$$

In the presence of a field E, electrons will acquire the additional velocity $= -\dfrac{eEt}{m}$. For a random
collisions, there will no effect on the initial velocity of the electrons,
Therefore

$$v = -\frac{eE\tau}{m} ; j = \left(\frac{ne^2\tau}{m}\right) E \quad \text{as } j = \frac{E}{\rho} = \sigma \text{ E } , \text{Therefore,} \quad \boxed{\sigma = \frac{ne^2\,\tau}{m}}$$

AC electrical conductivity of a metal

Metal is subjected to a time dependent electric field in the form

$$E(t) = Re\ (E(\omega)e^{-i\omega t}$$

Equation of motion of the electron

$$\frac{dp}{dt} = -\frac{p}{\tau} - eE$$

Assume the steady state solution as $p(t) = -Re\ (p(\omega)e^{-i\omega t}$

$$-i\omega p(\omega) = -\frac{p(\omega)}{\tau} - eE(\omega)\ ;\ j = -\frac{nep}{m}$$

$$j(t) = Re\big(j(\omega)e^{-i\omega t}\big)\ ;\ j(\omega) = -\frac{-nep(\omega)}{m} = \frac{\left(\frac{ne^2}{m}\right)E(\omega)}{\frac{1}{\tau} - i\omega}$$

$$j(\omega) = \sigma(\omega)E(\omega)\ ;\qquad \sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau}\ ,\qquad \sigma_0 = \frac{ne^2\tau}{m}$$

Thermal conductivity of a metal

The Drude model assumes that the bulk of the thermal current in a metal is carried by the conduction electrons.

If there are no source or sink to maintain the temperature grandient, the thermal energy will flow opposite to the Temperature gradient. Therefore, the thermal current j can be written as

$$j = -K \, \nabla T$$

Where, K is the constant, identified as thermal conductivity.

If heat flows in the positive x direction, $j = -K \dfrac{dT}{dx}$

Consider a one dimensional model and electrons can move only x direction

temperature side of x, and half from the low. If $\varepsilon(T)$ is the thermal energy per electron in a metal in equilibrium at temperature T, then an electron whose last collision was at x' will, on the average, have a thermal energy $\varepsilon(T[x'])$. The electrons arriving at x from the high-temperature side will, on the average, have had their last collision at

Thermal conductivity……

$x - v\tau$, and will therefore carry a thermal energy per electron of size $\varepsilon(T[x - v\tau])$. Their contribution to the thermal current density at x will therefore be the number of such electrons per unit volume, $n/2$, times their velocity, v, times this energy, or $(n/2)v\varepsilon(T[x - v\tau])$. The electrons arriving at x from the low-temperature side, on the other hand, will contribute $(n/2)(-v)[\varepsilon(T[x + v\tau])]$, since they have come from the positive x-direction and are moving toward negative x. Adding these together gives

$$j = \frac{1}{2}nv[\varepsilon(T[x - v\tau]) - \varepsilon(T[T + v\tau])]$$

$$= nv^2\tau\frac{d\varepsilon}{dT}\left(-\frac{dT}{dx}\right)$$

$$= \frac{1}{3}v^2\tau c_v(-\nabla T) \quad \text{In 3 dimension}$$

$$\langle v_x{}^2\rangle = \langle v_y{}^2\rangle = \langle v_z{}^2\rangle = \frac{1}{3}v^2$$

$$n\frac{d\varepsilon}{dT} = \frac{N}{V}\frac{d\varepsilon}{dT} = \frac{1}{V}\frac{dE}{dT} = c_v. \text{ The electronic specific heat}$$

$$K = \frac{1}{3}v^2\tau c_v$$

Wiedemann and Franz law

$$\frac{K}{\sigma} = \frac{\frac{1}{3} c_v m v^2}{n e^2}$$

$$\frac{K}{\sigma} = \frac{3}{2} \left(\frac{k_B}{e}\right)^2 T$$

$$L = \frac{K}{\sigma T} = \frac{3}{2} \left(\frac{k_B}{e}\right)^2 = 1.24 \times 10^{-13} \ \left(\frac{erg}{esu-K}\right)^2$$

$$= 1.11 \times 10^{-8} \ \text{watt-ohm}/K^2$$

L is called Lorentz number. The theoretical value is in rather good agreement with experimental data in the high temperature region.

Wiedemann and Franz law is being predicted reasonably well. This is the Success of Drude model

Success of Drude model!

The success of Drude model was wholly fortuitous and was so impressive as to spur further investigations with the model.

Major drawbacks:

- No electronic contribution to the specific heat remotely comparable to $\frac{3}{2}nK_B$ was ever observed.

- At room temperature, no electronic contribution to the specific heat indeed was found.

- Classical gas law cannot be applied to the electron gas in a metal, as electrons for Fermions. Therefore, value of mean square electronic speed must have been erroneous.

Actual electronic contribution to the specific heat is about 100 times smaller that the classical prediction, but The mean square electronic speed is about 100 times larger.

Hall effect

$$\boldsymbol{F} = -e(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B})$$

B_z

j_x

E_x

e^-

j_x
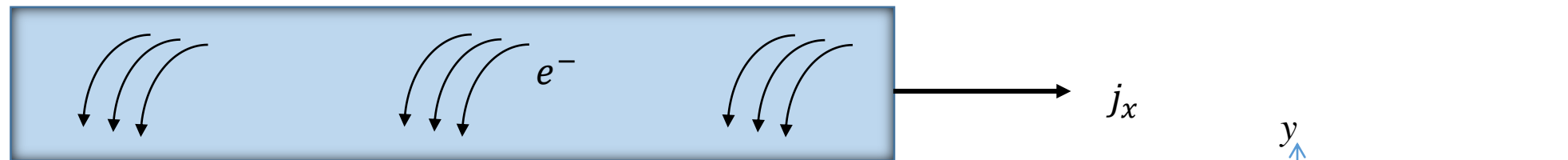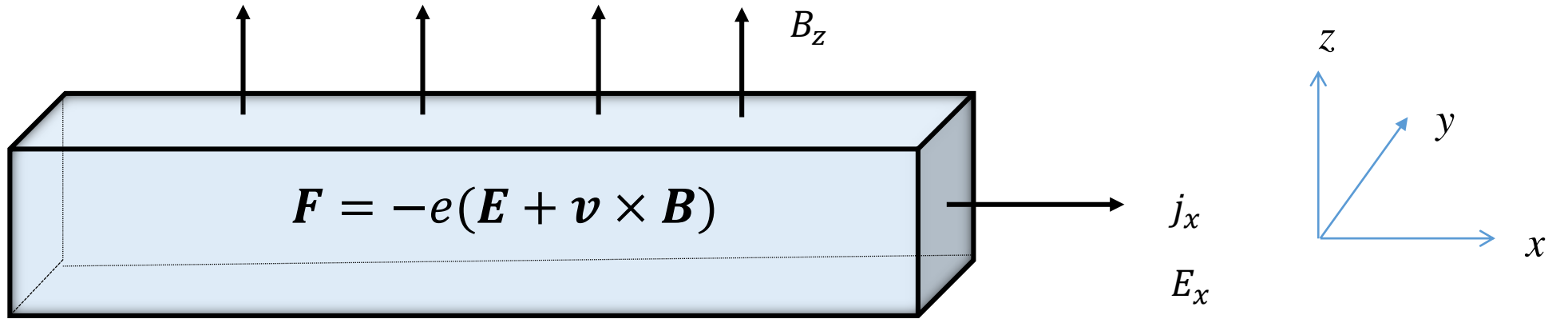
X-Y Plane

Drift velocity is in steady state

$+ + + + + + + + + + + + + +$
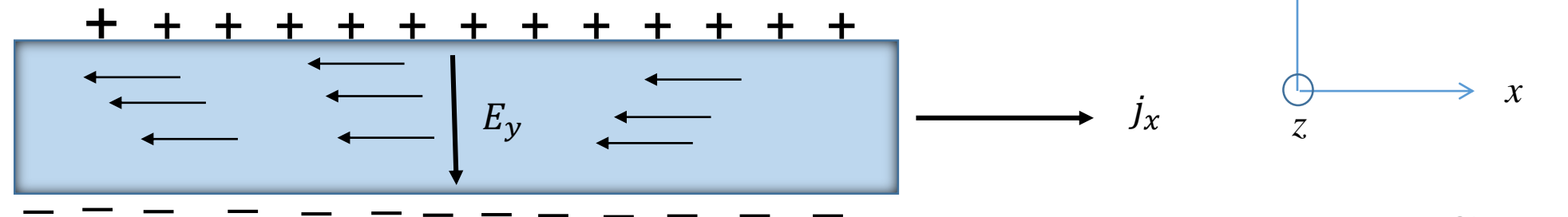
E_y

j_x

$- - - - - - - - - - - - - -$

Motion of electrons in magnetic field: Hall effect

Equation of motion of electrons

$$\frac{dp}{dt} + \frac{p}{\tau} = \mathrm{F} = -\mathrm{e}\,(\mathrm{E} + \mathrm{v} \times B)$$

$$m\left(\frac{d}{dt} + \frac{1}{\tau}\right) v = -\mathrm{e}\,(\mathrm{E} + \mathrm{v} \times B)$$

In a steady state, time derivatives are zero

$$m\left(\frac{d}{dt} + \frac{1}{\tau}\right) v_x = -\mathrm{e}\,(E_x + B v_y)$$

$$m\left(\frac{d}{dt} + \frac{1}{\tau}\right) v_y = -\mathrm{e}\,(E_y - B v_x)$$

$$m\left(\frac{d}{dt} + \frac{1}{\tau}\right) v_z = -\mathrm{e}\,(E_z)$$

$$v_x = -\frac{e\tau E_x}{m} - \omega_c \tau v_y$$

$$v_y = -\frac{e\tau E_y}{m} + \omega_c \tau v_x$$

$$v_z = -\frac{e\tau E_z}{m}$$

$$\omega_c = \frac{eB}{m}$$, is known as cyclotron frequency

Hall effect

Hall field developed in y direction due to accumulation of electrons cancels out the Lorentz force due to the magnetic field. Therefore $v_y = 0$

$$E_y = -\omega_c \tau m v_x / e\tau = \omega_c \tau m \frac{e\tau E_x}{m} / e\tau = \omega_c \tau E_x = \frac{eB\tau}{m} E_x$$

The Hall coefficient is defines as $R_H = \dfrac{E_y}{j_x B} = -\dfrac{\frac{eB\tau E_x}{m}}{\frac{ne^2 \tau E_x B}{m}} = -\dfrac{1}{ne}$

Failures of free electron model

Striking deficiencies of the model were due to use of classical statistics in describing the conduction electrons.

❑ Inadequacies in the free electron transport coefficients

    i.   The hall coefficient

    ii. The Magnetoresistance

    iii. The Thermoelectric field

    iv. The Wiedemann Franz law

    v.   Temperature dependence of the DC conductivity

    vi. Directional dependence of DC conductivity

    vii. AC conductivity

❑ Inadequacies in the static Thermodynamics predictions

    i.   Linear term in the specific heat

    ii. Cubic term in the specific heat

    iii. The compressibility of metal

Lattice Vibration

Why do lattice vibrate?

At any finite temperature, atoms within the crystal are not static, rather vibrate about their mean position due to thermal energy. It is the thermal agitation which impels atoms to vibrate.

Why do we study lattice vibration?

A major contribution to the specific heat of materials is the lattice vibration. Quantisation of lattice vibration is known as phonons. Behaviour of the specific heat with temperature is best described by a popular Debye T^3 law which is the consequence of lattice vibration. Therefore, in order to obtain insights into the thermal properties of solids, it is desirable and necessary to study the lattice vibration of solids.

Why did Einstein's theory of lattice vibration fail to explain empirical behaviour of specific heat?

Although, the Einstein's description of specific heat was able to explain the qualitative behaviour with temperature, it fails to explain the exact empirical nature of the curve at very low temperature. This is because of the over-simplified model Introduced by him. He considered the atoms within the crystal vibrate independently with simple harmonic manner.

Lattice vibration with monatomic basis

Lattice vibration of the crystal results in an elastic wave propagating within the crystal. We want to find out the frequency of the wave in terms of wave vector.
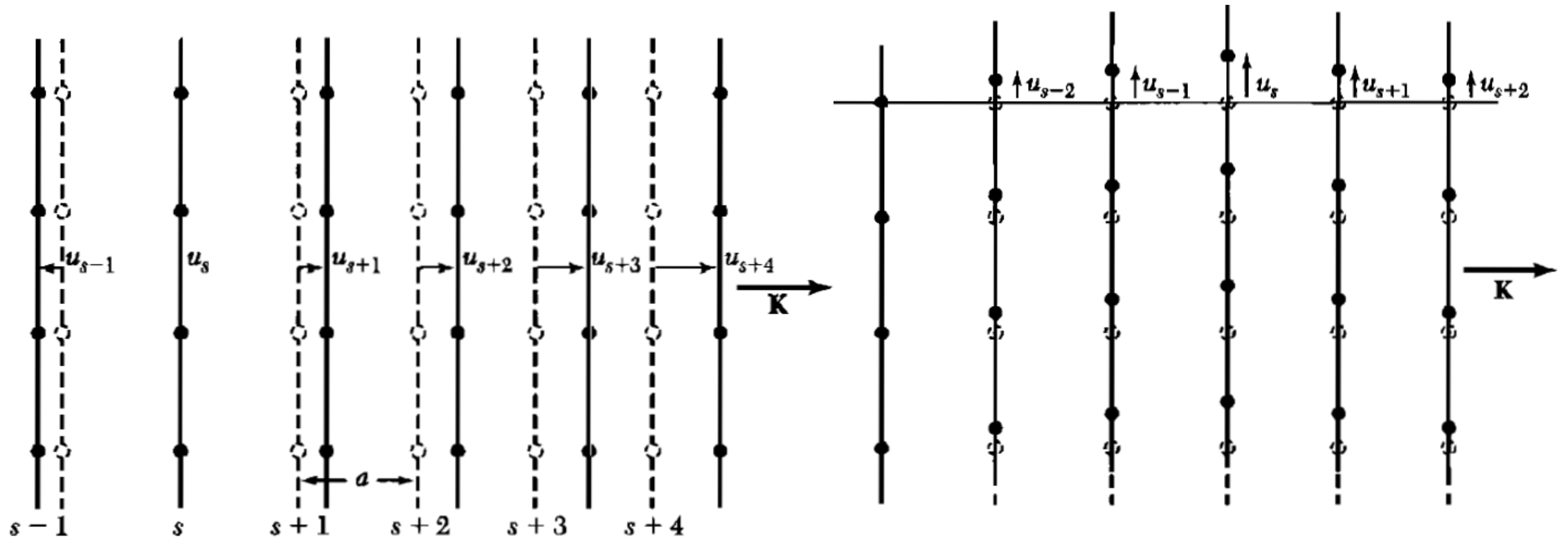
Assuming the force on the plane *s* caused by the displacement of the place *s+p* is proportional to the difference $u_{s+p} - u_s$, The force can be written as

$$F_s = C(u_{s+1} - u_s) + C(u_{s-1} - u_s) \text{ ....} \quad (1)$$

Considering nearest neighbour interaction, the equation of motion of the vibration of plane s is

$$M \frac{d^2 u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s) \text{ ... .} \quad (2)$$

Look for the solutions with all displacements having the time dependence $\exp(-i\omega t)$

Then $\frac{d^2 u_s}{dt^2} = -\omega^2 u_s$ and (2) becomes

$$-M\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s) \ . \quad (3)$$

$$u_{s\pm1} = u \exp(isKa) \exp(\pm iKa) \ , \tag{4}$$

Using Eq. (4) , Eq. (3) can be expressed as

$$-\omega^2 Mu \exp(isKa) = Cu\{\exp[i(s + 1)Ka] + \exp[i(s - 1)Ka] - 2 \exp(isKa)\} \ . \tag{5}$$

$$\omega^2 M = -C[\exp(iKa) + \exp(-iKa) - 2] \ . \tag{6}$$

$$\omega^2 = (2C/M)(1 - \cos Ka) \ . \tag{7}$$

The boundary of the first Brillouin zone lies at $K = \pm\pi/a$. We show from (7) that the slope of ω versus K is zero at the zone boundary:

$$d\omega^2/dK = (2Ca/M) \sin Ka = 0 \tag{8}$$

at $K = \pm\pi/a$, for here $\sin Ka = \sin (\pm\pi) = 0$. The special significance of phonon wavevectors that lie on the zone boundary is developed in (12) below.

By a trigonometric identity, (7) may be written as

$$\omega^2 = (4C/M) \sin^2 \tfrac{1}{2} Ka \ ; \qquad \omega = (4C/M)^{1/2} |\sin \tfrac{1}{2} Ka| \ . \tag{9}$$

References

1. Introduction to Solid State Physics: Charles Kittel

2. Solid State Physics: Neil W. Ashcropt and N. David Mermin

3. Solid State Physics: Adrianus J. Dekker