

Introduction to Condensed Matter Physics

Introduction to Condensed Matter Physics notes by [K. Sreeman Reddy](#). Taken from [The Oxford Solid State Basics](#).

1. [Geometry of Solids](#)
 1. [Lattices in 3D](#)
 1. [Body-Centered Cubic \(bcc\) Lattice](#)
 2. [Face-Centered Cubic \(fcc\) Lattice](#)
 3. [Sphere Packing](#)
 2. [Reciprocal Lattice](#)
 1. [RL as a Fourier Transform](#)
 1. [For any function with the periodicity of the lattice](#)
 2. [Structure factor](#)
 2. [RL Points as Families of Lattice Planes](#)
 1. [Miller Indices](#)
 3. [Brillouin zone](#)
 3. [X-Rays & Periodic lattice](#)
 4. [Bloch's theorem](#)
 5. [Tight binding Model](#)
 6. [Drude model](#)
 1. [Assumptions](#)
 2. [Theory](#)
 3. [E](#)
 4. [E and B](#)
 1. [Hall effect](#)
 5. [E AC field](#)
 6. [Thermal Transport](#)
 7. [Free electron or Sommerfeld model](#)
 8. [Debye](#)
 9. [Semi classical model](#)
 10. [Appendix](#)

Geometry of Solids

Lattice: A lattice is

- an infinite set of points **defined by integer sums** of a set of linearly independent primitive lattice vectors.

$$\mathbf{R}_{[n_1 n_2 n_3]} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$$

- an infinite set of vectors where **addition of any two vectors** in the set gives a third vector in the set.
- a set of points where the **environment of any given point is equivalent** to the environment of any other given point.

In 2D and 3D, the choice of primitive lattice vectors is **not unique** as any set of independent vectors which span the space will work.

Unit cell: A unit cell is a region of space such that when many identical units are stacked together it tiles (completely fills) all of space and reconstructs the full structure.

- The choice of a unit cell is not unique.
- a **conventional unit cell** is a unit cell which is simpler to work (e.g. has orthogonal axes) with but is not a primitive unit cell.

Primitive unit cell: A primitive unit cell for a periodic crystal is a unit cell containing **exactly one lattice point**.

- Of course while counting lattice points we should **consider the fraction of point** in the cell.

Wigner–Seitz cell: Given a lattice point, the set of all points in space which are **closer to that given lattice point than to any other** lattice point constitute the Wigner–Seitz cell of the given lattice point.

- **always** gives a primitive unit cell.
- draw perpendicular bisectors (perpendicular-bisecting planes in 3D) to lines connecting a point to all of its possible near neighbors (not just its nearest neighbors)

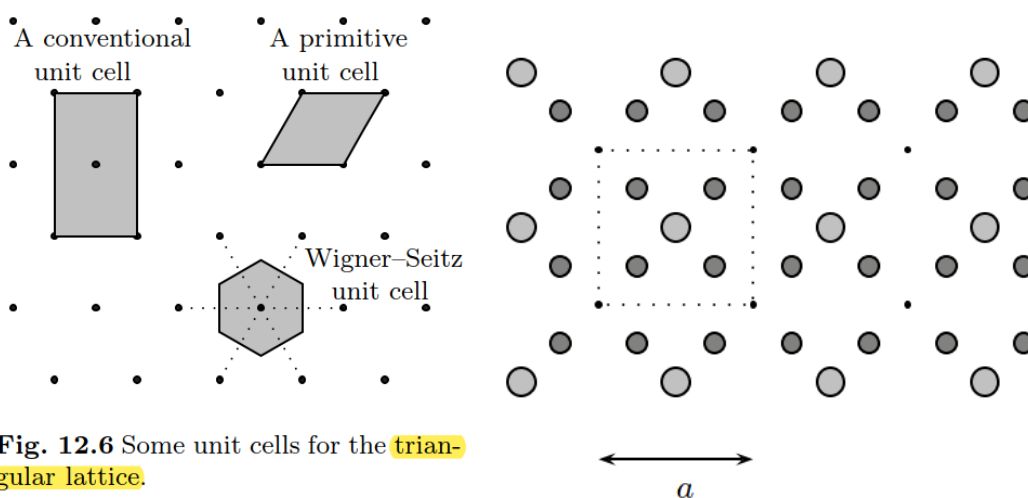


Fig. 12.6 Some unit cells for the **triangular lattice**.

Basis: The description of objects in the unit cell with respect to the reference lattice point in the unit cell is known as a basis.

- the positions of the atoms in the crystal are **“the lattice plus the basis”**.

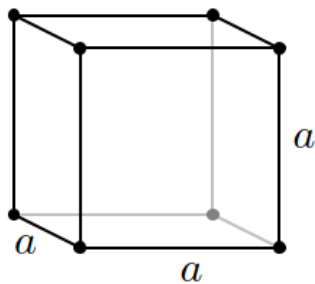
- In the above right pictures the smallest black dots are lattice points and adding basis to a point we get a unit cell.

coordination number of a lattice (frequently called Z or z) is the number of nearest neighbors any point of the lattice has

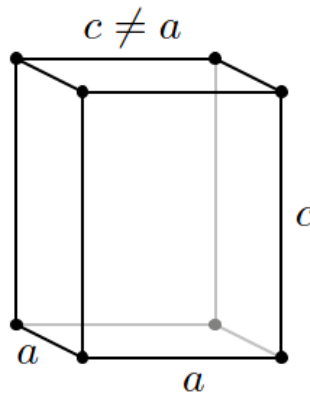
Lattices in 3D

$$[uvw] = u\mathbf{a}_1 + v\mathbf{a}_2 + w\mathbf{a}_3$$

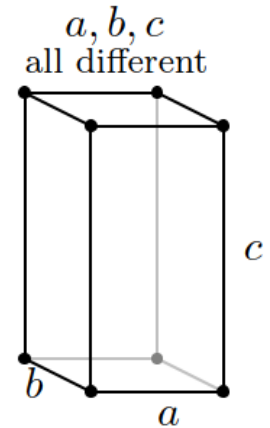
- The following 3 lattices have **orthogonal** axes



Cubic
unit cell



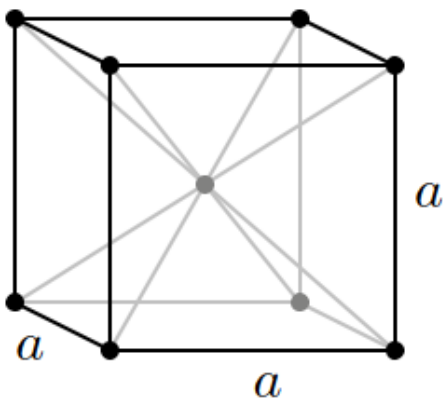
Tetragonal
unit cell



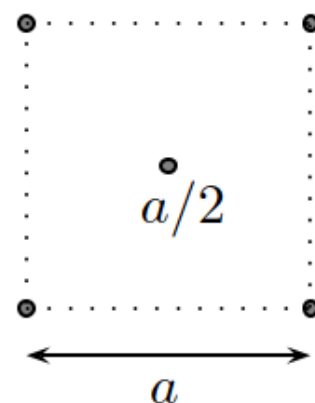
Orthorhombic
unit cell

For simple cubic lattice $Z = 6$: or 6 **nearest neighbors**.

Body-Centered Cubic (bcc) Lattice



Body-centered cubic
unit cell



Plan view

- $Z = 8$
- the conventional unit cell contains two ($2 = 8 \times 1/8 + 1$) lattice points
- 2 interpenetrating simple cubic lattices displaced from each other by $[1/2, 1/2, 1/2]$

- simple cubic lattice with a basis of two atoms per conventional cell
- local environment of every point is same

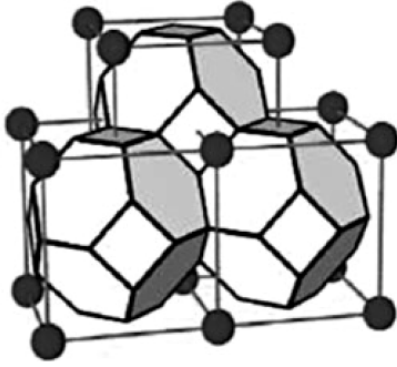
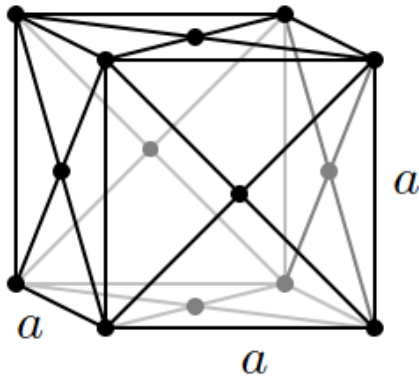


Fig. 12.14 The Wigner–Seitz cells of the bcc lattice pack together to tile all of space. Note that the structure of the bcc lattice is that of two interpenetrating simple cubic lattices.

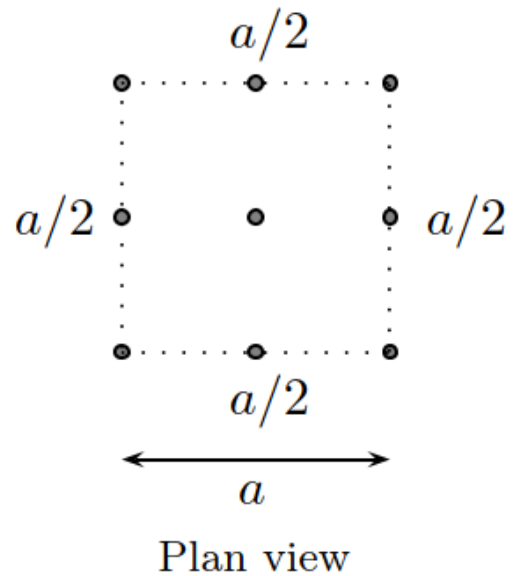
$$\mathbf{R}_{\text{corner}} = [n_1, n_2, n_3] \quad \mathbf{R}_{\text{center}} = [n_1, n_2, n_3] + \left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right]$$

$$\mathbf{a}_1 = [1, 0, 0] \quad \mathbf{a}_2 = [0, 1, 0] \quad \mathbf{a}_3 = \left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right]$$

Face-Centered Cubic (fcc) Lattice



Face-centered cubic
unit cell



- $Z=12$
- simple cubic lattice + lattice point in the center of every face
- conventional unit cell contains exactly four ($4= 8 \times 1/8 + 6 \times 1/2$) lattice points
- either all 3 coordinates are integers (in units of a), or 2 of the 3 coordinates are half-odd integers and the remaining 1 coordinate is an integer.

- simple cubic lattice with a basis of 4 atoms per conventional unit cell

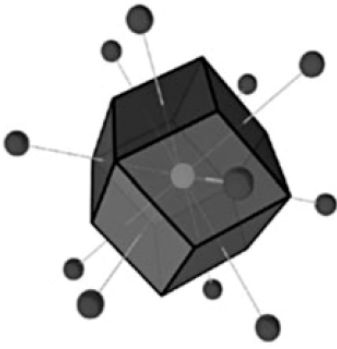


Fig. 12.16 The Wigner–Seitz cell of the fcc lattice (this shape is a “rhombic dodecahedron”). Each face is the perpendicular bisector between the central point and one of its 12 nearest neighbors.

$$\begin{aligned} \mathbf{R}_{\text{corner}} &= [n_1, n_2, n_3] & \mathbf{R}_{\text{face-xy}} &= [n_1, n_2, n_3] + \left[\frac{1}{2}, \frac{1}{2}, 0 \right] \\ \mathbf{R}_{\text{face-xz}} &= [n_1, n_2, n_3] + \left[\frac{1}{2}, 0, \frac{1}{2} \right] & \mathbf{R}_{\text{face-yz}} &= [n_1, n_2, n_3] + \left[0, \frac{1}{2}, \frac{1}{2} \right]. \\ \mathbf{a}_1 &= \left[\frac{1}{2}, \frac{1}{2}, 0 \right] & \mathbf{a}_2 &= \left[\frac{1}{2}, 0, \frac{1}{2} \right] & \mathbf{a}_3 &= \left[0, \frac{1}{2}, \frac{1}{2} \right] \end{aligned}$$

Sphere Packing

- bcc and fcc lattices are realized much more frequently in nature than simple cubic as they more tightly packed and energetically favored.
- fcc and hexagonal close packed have the **maximum possible** packing fraction.

Reciprocal Lattice

Given a (direct) lattice of points \mathbf{R} , a point \mathbf{G} is a point in the **reciprocal lattice** if and only if

$$e^{i\mathbf{G}\cdot\mathbf{R}} = 1$$

for all points \mathbf{R} of the direct lattice.

- the reciprocal lattice is a lattice in reciprocal space
- the primitive lattice vectors of the reciprocal lattice are defined by

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$$

$$\mathbf{b}_1 = \frac{2\pi \mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_2 = \frac{2\pi \mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_3 = \frac{2\pi \mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

- an arbitrary point in reciprocal space can be expressed as (m_i are integers)

$$\mathbf{G} = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3$$

- The important physics of vibrational waves and electron waves in solids is best described in reciprocal space.
- Direct lattice exists in **real-space** and is what one would commonly understand as a physical lattice (e.g., a lattice of a crystal) but the reciprocal lattice exists in **reciprocal space** or **momentum space** or **K-space** (momentum and position are Pontryagin duals).

RL as a Fourier Transform

Let $\rho(\mathbf{r})$ be a function with a delta function at each lattice point

$$\rho(\mathbf{r}) = \sum_{\mathbf{R}} \delta^D(\mathbf{r} - \mathbf{R})$$

$$\mathcal{F}[\rho(\mathbf{r})] = \int d\mathbf{r} e^{i\mathbf{k} \cdot \mathbf{r}} \rho(\mathbf{r}) = \sum_{\mathbf{R}} \int d\mathbf{r} e^{i\mathbf{k} \cdot \mathbf{r}} \delta^D(\mathbf{r} - \mathbf{R}) = \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}}$$

$$= \frac{(2\pi)^D}{v} \sum_{\mathbf{G}} \delta^D(\mathbf{k} - \mathbf{G})$$

In the last step we used **Poisson resummation formula**. Here D is the dimension, v is the volume of the unit cell, R and G are the set of direct and reciprocal lattice points.

For any function with the periodicity of the lattice

Let $\rho(\mathbf{r}) = \rho(\mathbf{r} + \mathbf{R})$

$$\mathcal{F}[\rho(\mathbf{r})] = \int d\mathbf{r} e^{i\mathbf{k} \cdot \mathbf{r}} \rho(\mathbf{r})$$

Any point in space \mathbf{r} as the sum of a lattice point \mathbf{R} and a vector \mathbf{x} within the unit cell

$$\mathcal{F}[\rho(\mathbf{r})] = \sum_{\mathbf{R}} \int_{\text{unit-cell}} d\mathbf{x} e^{i\mathbf{k} \cdot (\mathbf{x} + \mathbf{R})} \rho(\mathbf{x} + \mathbf{R}) = \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} \int_{\text{unit-cell}} d\mathbf{x} e^{i\mathbf{k} \cdot \mathbf{x}} \rho(\mathbf{x}).$$

The sum of exponentials, as in Eq. 13.5, just gives a sum of delta functions yielding

Structure factor

$$\mathcal{F}[\rho(\mathbf{r})] = (2\pi)^D \sum_{\mathbf{G}} \delta^D(\mathbf{k} - \mathbf{G}) S(\mathbf{k})$$

$$S(\mathbf{k}) = \int_{\text{unit-cell}} \mathbf{d}\mathbf{x} e^{i\mathbf{k}\cdot\mathbf{x}} \rho(\mathbf{x})$$

RL Points as Families of Lattice Planes

A lattice plane (or crystal plane) is a plane containing at least three non-collinear (and **therefore an infinite number** of) points of a lattice.

The families of lattice planes are in one-to-one correspondence with the possible directions of reciprocal lattice vectors, to which they are normal. Further, the spacing between these lattice planes is $d = 2\pi/|\mathbf{G}_{\min}|$ where \mathbf{G}_{\min} is the minimum length reciprocal lattice vector in this normal direction.

- $\mathbf{G} \cdot \mathbf{r} = 2\pi m$ is a family of parallel equally spaced planes with every point in lattice belonging to some plane, **but may not be a family of lattice planes** as not every plane needs to contain a lattice point.

Miller Indices

Useful notation to describe lattice planes or reciprocal lattice vectors

- (hkl)
- To represent a family of lattice plane, one should take the shortest reciprocal lattice vector in the given direction, meaning h, k, and l should have no common divisors

Important Comment: For any cubic lattice (simple cubic, fcc, or bcc) it is conventional to choose \hat{a}_i to be $a\hat{x}$, $a\hat{y}$, and $a\hat{z}$ with a the cube edge length. For the primitive (simple) cubic case these are primitive reciprocal lattice vectors, but for the fcc and bcc case, they are not. So in the **fcc and bcc** cases **not all integer sets of Miller indices (hkl) are reciprocal lattice vectors**.

Brillouin zone

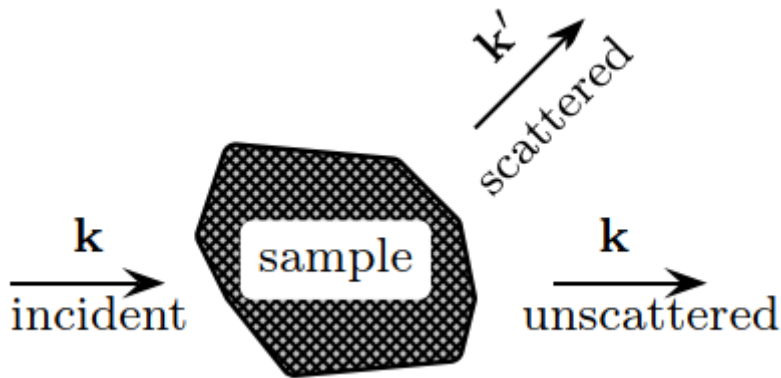
A Brillouin zone is any primitive unit cell of the reciprocal lattice.

- $\mathbf{k} \rightarrow \mathbf{k} + \mathbf{G}$ nothing changes
- includes each physically different crystal momentum exactly once

Start with the reciprocal lattice point $\mathbf{G} = 0$. All \mathbf{k} points which are closer to 0 than to any other reciprocal lattice point define the **first Brillouin zone** (like Wigner–Seitz cell). Similarly all \mathbf{k} points where the point 0 is the second closest reciprocal lattice point to that point constitute the **second Brillouin zone**, and so forth. Zone boundaries are defined in terms of this definition of Brillouin zones.

- If you cross only one perpendicular bisector, you Brillouin zone number changes by 1.

X-Rays & Periodic lattice



Bloch's theorem

Tight binding Model

Drude model

- 1900: Paul Drude realized that he could apply Boltzmann's kinetic theory of **gases** to understanding electron motion within metals.
- classical model

Assumptions

SS

1. Electrons have a scattering time τ (phenomenological parameter as it is hard to predict). The probability of scattering within a time interval dt is dt/τ .
2. After scattering the electron returns to $\mathbf{p} = 0$.
3. $\mathbf{F} = -e(\mathbf{E} + \mathbf{v} \times \mathbf{B})$

AM

4. During collisions interactions are ignored between e^- , e^- and e^- , *ion*.
5. Independent electron approximation: neglects long-range interaction between the electrons. (better than \downarrow approximation)
6. Free electron approximation: neglects long-range interaction between e^- , *ion*.
7. e^- , e^- is not important. But e^- , *ion* is important.
8. e^- s achieve thermal equilibrium only through collisions.
9. Just after collision the $\langle v \rangle = 0$ is 0 but $\langle v^2 \rangle \propto T$.

Theory

$$\mathbf{p}(t_0 + dt) = \left(1 - \frac{dt}{\tau}\right) [\mathbf{p}(t_0) + \mathbf{f}(t)dt + O(dt^2)] + \frac{dt}{\tau} (\mathbf{g}(t_0) + \mathbf{f}(t)dt + O(dt^2))$$

Transport equation:

$$\frac{d}{dt}\mathbf{p}(t) = \mathbf{f}(t) - \frac{\mathbf{p}(t)}{\tau}$$

E

$$V = IR$$

$$\mathbf{E}l = \mathbf{j}A \frac{\rho l}{A} \Rightarrow \mathbf{E} = \rho \mathbf{j} \Rightarrow \mathbf{j} = \sigma \mathbf{E}$$

$$\mathbf{J} = \frac{n(Avdt)q}{Adt} = nq\langle \mathbf{v} \rangle$$

At time $t = t_0 + dt$ the average electron's momentum will be

$$\langle \mathbf{p}(t_0 + dt) \rangle = \left(1 - \frac{dt}{\tau}\right) (\langle \mathbf{p}(t_0) \rangle + q\mathbf{E} dt),$$

and then

$$\frac{d}{dt}\langle \mathbf{p}(t) \rangle = q\mathbf{E} - \frac{\langle \mathbf{p}(t) \rangle}{\tau},$$

$$\langle \mathbf{p}(t) \rangle = q\tau\mathbf{E}(1 - e^{-t/\tau}) + \langle \mathbf{p}(0) \rangle e^{-t/\tau}$$

in steady state

$$\langle \mathbf{p} \rangle = q\tau\mathbf{E}$$

$$\Rightarrow \mathbf{J} = \left(\frac{nq^2\tau}{m}\right) \mathbf{E}$$

$$\Rightarrow \sigma_0 = \frac{nq^2\tau}{m}$$

Note that we cannot write

$$\frac{1}{2}m\langle \mathbf{v} \rangle^2 = qE\langle \mathbf{v} \rangle\tau$$

because $1/2\langle \mathbf{v} \rangle\tau$ is the distance travelled.

Q: Let at $t=0$ an electron collides and $p=0$ it will next collide at $t = \tau$. Just before collision it will have $V = q\tau E/m$. But that is the maximum velocity reached in between these collisions. So the average

should be $V = 0.5q\tau E/m$. What is the flaw in this argument?

A:

E and B

Hall effect

$$R_H = \frac{E_y}{j_x B_z}$$

or

$$\mathbf{E} = -R_H(\mathbf{J}_c \times \mathbf{B})\mathbf{E} = -R_H(\mathbf{J}_c \times \mathbf{B})$$

$$R_H = \frac{E_y}{j_x B} = \frac{V_H t}{IB} = \frac{\rho_{yx}}{|B|} = -\frac{1}{ne}$$

- determines the sign of the charge carriers.

E AC field

Let

$$E(t) = \Re(E_0 e^{i\omega t});$$

$$J(t) = \Re(\sigma(\omega) E_0 e^{i\omega t}).$$

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

$$\nabla \times (\nabla \times \mathbf{E}) = \nabla(\nabla \cdot \mathbf{E}) - \nabla^2 \mathbf{E} = -\nabla^2 \mathbf{E}$$

since $\nabla \cdot \mathbf{E} = 0$ (no charge)

$$\nabla \times (\nabla \times \mathbf{E}) = \nabla \times \left(-\frac{\partial \mathbf{B}}{\partial t} \right) = \nabla \times (-1(-i\omega \mathbf{B})) = i\omega(\mu_0 \left(\mathbf{J} + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right))$$

Thermal Transport

- made two mistakes that roughly cancel each other
- a specific heat that is way too large, but we have also used a velocity that is way too small

Free electron or Sommerfeld model

- 1927: Sommerfeld added **Fermi–Dirac statistics** (1926) to the classical Drude model.

Debye

Semi classical model

Appendix

➤ There are atoms at all eight corners and all six faces.

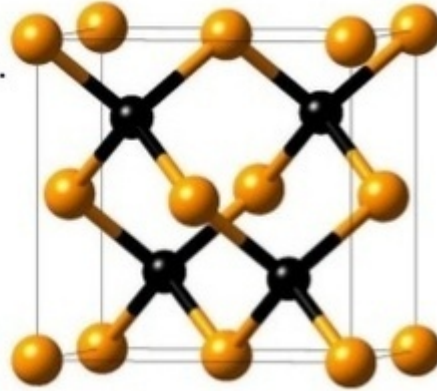
$$\begin{aligned}n_{fcc} &= (1/8 \times 8 \text{ corner atoms}) + (1/2 \times 6 \text{ face atoms}) \\ &= 1+3 \\ &= 4 \text{ atoms.}\end{aligned}$$

➤ In addition to that there are 4 full atoms inside the unit cell.

Total number of atoms present in a unit cell.

$$\begin{aligned}n &= 4+4 \\ &= 8\end{aligned}$$

$$r = ?$$



$$\mathcal{F}[\rho(\mathbf{r})] = \int d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} \rho(\mathbf{r}) = \sum_n \int d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} \delta(\mathbf{r} - a\mathbf{n}) = \sum_n e^{i\mathbf{k}\cdot a\mathbf{n}}$$

$$e^{i\mathbf{G}\cdot\mathbf{R}} = e^{i(m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3) \cdot (n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3)} = e^{2\pi i(n_1m_1 + n_2m_2 + n_3m_3)}$$

$$\mathcal{F}[\rho(\mathbf{r})] = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} = \frac{(2\pi)^D}{v} \sum_{\mathbf{G}} \delta^D(\mathbf{k} - \mathbf{G})$$