

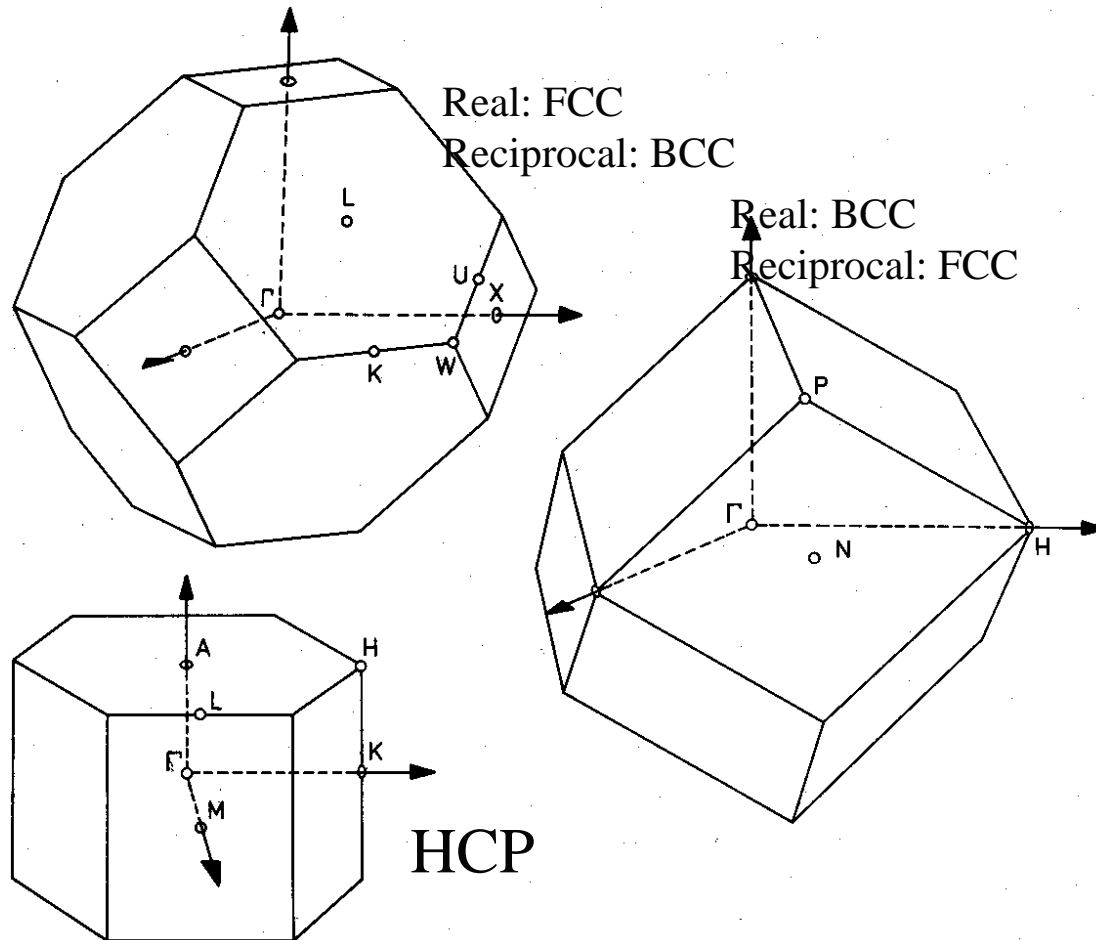
PAPER-A: CONDENSED MATTER PHYSICS
(B.Sc. Semester-V)

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CONTENTS

- ❑ Brillouin zones and its construction in two and three dimensions,
- ❑ Structure factor and atomic form factor

Brillouin zones for FCC, BCC, HCP



Structure and Atomic Form Factors

Recall that the scattering amplitude equals to

$$F = \int_{cell} dV n(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} = NS_G$$

where S_G is the **structure factor** defined as an integral over a single unit cell.

If we write the electron density as a superposition of the electron densities in the cell, taking into account the of atoms per basis, we have

where s is the of atoms in the unit cell.

$$n(\mathbf{r}) = \sum_{j=1}^s n_j(\mathbf{r} - \mathbf{r}_j)$$

Substituting this back gives

$$\begin{aligned} S_G &= \sum_{j=1}^s \int_{cell} dV n_j(\mathbf{r} - \mathbf{r}_j) e^{-i\mathbf{G} \cdot \mathbf{r}} \\ &= \sum_{j=1}^s e^{-i\mathbf{G} \cdot \mathbf{r}_j} \int_{cell} dV n_j(\rho) e^{-i\mathbf{G} \cdot \rho} = \sum_{j=1}^s e^{-i\mathbf{G} \cdot \mathbf{r}_j} f_j \end{aligned}$$

where f_j is the **atomic form factor**. Now if we specify \mathbf{G} and \mathbf{r}_j as

we get:

$$\mathbf{G} = v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3 \quad \text{and} \quad \mathbf{r}_j = x_j \mathbf{a}_1 + y_j \mathbf{a}_2 + z_j \mathbf{a}_3$$

Note that S_G can be complex, because the scattering intensity involves the magnitude squared of S_G .

$$S_G = \sum_{j=1}^s f_j e^{-2\pi i(x_j v_1 + y_j v_2 + z_j v_3)}$$

- The atomic form factor can also be written in the following form for spherically-symmetric electron density

$$f_j = 4\pi \int_0^{\infty} n_j(r) r^2 \frac{\sin(Gr)}{Gr} dr$$

- That means that when $n(r)=Zd(r)$, then $f_j=Z$, i.e. f_j is the ratio of radiation amplitude scattered by the electron distribution to that scattered by a localized electron.

□ Examples of Structure Factor Calculations

(a) BCC lattice

For a BCC lattice, we have two atoms per unit cell located at (000) and $(\frac{1}{2} \frac{1}{2} \frac{1}{2})$. The structure factor is then:

$$S_G = \left[1 + e^{-\pi i(v_1+v_2+v_3)} \right] f$$

- ❑ The structure factor is maximum $S_G = 2f$ when the sum of the indices is even, i.e. $v_1+v_2+v_3=2n$.
- ❑ The structure factor is $S_G = 0$ when the sum of the indices is odd, i.e. $v_1+v_2+v_3=2n+1$.

(b) FCC lattice

For a FCC lattice, we have four atoms per unit cell located at (000) , $(0 \frac{1}{2} \frac{1}{2})$, $(\frac{1}{2} 0 \frac{1}{2})$ and $(\frac{1}{2} \frac{1}{2} 0)$. The structure factor is then:

$$S_G = \left[1 + e^{-\pi i(v_1+v_2)} + e^{-\pi i(v_1+v_3)} + e^{-\pi i(v_2+v_3)} \right] f$$

- ❑ When all indices are even or odd, then $S_G = 4f$.
- ❑ When the indices are partially even and partially odd, then $S_G = 0$.
- ❑ To summarize, in a FCC lattice, no reflections occur when the indices are partially even and partially odd.

Basis and Bravais Structure Factor Terms

$$F = \sum_{n=1}^{N_p} e^{2\pi i \mathbf{g} \cdot \mathbf{r}_n} \sum_{m=1}^{N_b} f_m e^{2\pi i \mathbf{g} \cdot \mathbf{r}_m} = F_{BR} F_{BA}$$

The following simple table giving the integer values of F_{BR} for the different types of centering translations. Keep in mind that these are valid for any crystal system.

Centering type	Missing Reflections ($F_{BR} = 0$)	Possible Reflections ($F_{BR} \neq 0$)	Bravais Term F_{BR} for possible reflections
P (primitive)	None	All	1
I (body-centered)	($h + k + l$) odd	($h + k + l$) even	2
A (base-centered on A face)	($k + l$) odd	($k + l$) even	2
B (base-centered on B face)	($h + l$) odd	($h + l$) even	2
C (base-centered on C face)	($h + k$) odd	($h + k$) even	2
F (face-centered)	hkl mixed	hkl unmixed	4

CONCLUSION

X-rays are electromagnetic radiation of wavelength about 1 Å (10^{-10} m), which is about the same size as an atom.

The discovery of X-rays in 1895 enabled scientists to probe crystalline structure at the atomic level. X-ray diffraction has been in use in two main areas, for the fingerprint characterization of crystalline materials and the determination of their structure. Each crystalline solid has its unique characteristic X-ray powder pattern which may be used as a "fingerprint" for its identification. Once the material has been identified, X-ray crystallography may be used to determine its structure, i.e. how the atoms pack together in the crystalline state and what the interatomic distance and angle are etc. X-ray diffraction is one of the most important characterization tools used in solid state chemistry and materials science.

We can determine the size and the shape of the unit cell for any compound most easily using X-ray diffraction.

REFERENCES

- Introduction To Solid State Physics- Kittel
- Elementary Solid state Physics- Omar
- Solid state Physics- S. O. Pillai