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

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CONTENTS

- ❑Reciprocal lattices of SC, BCC and FCC,
- ❑Bragg's law in reciprocal lattice,

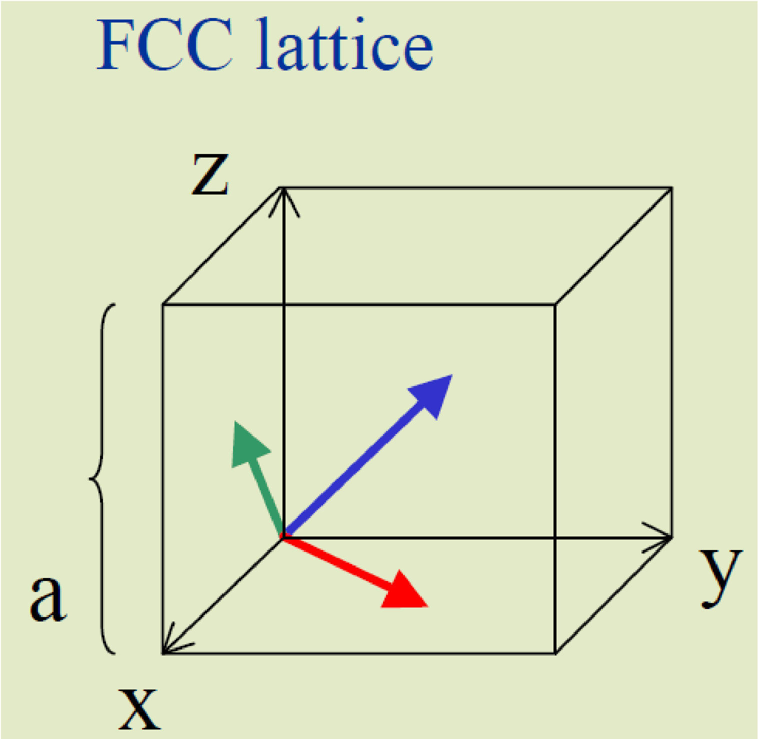
Reciprocal Lattice of Simple Cubic

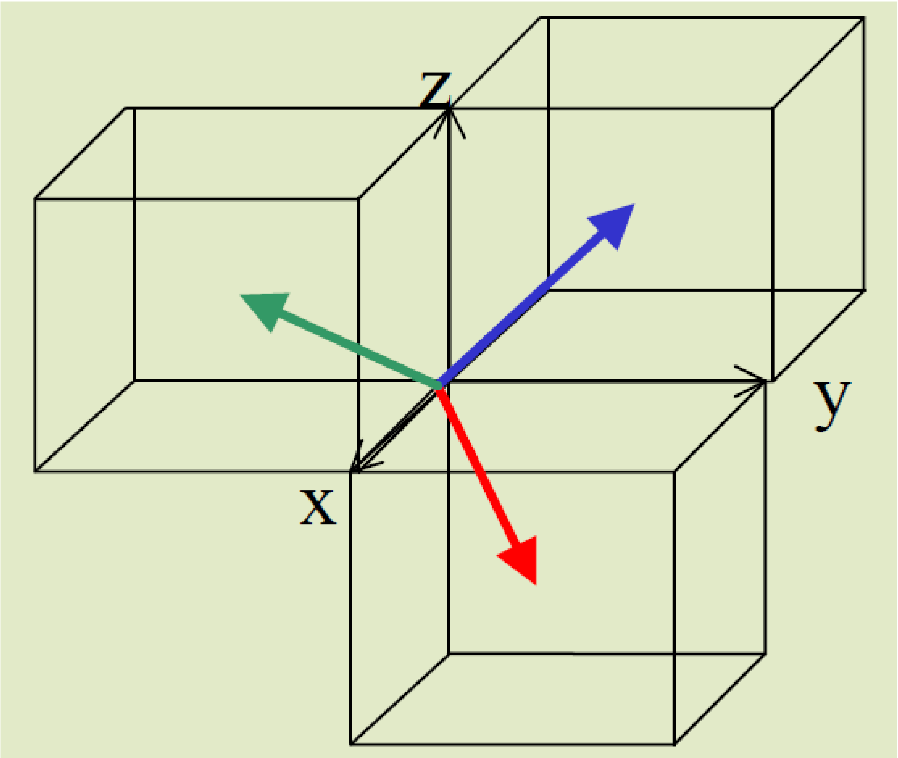
- The simple cubic Bravais, with cubic primitive cell of side *a*, has for its reciprocal a simple cubic lattice with a cubic primitive cell of side (in the crystallographer's definition).
- The cubic lattice is therefore said to be self-dual, having the same symmetry in reciprocal space as in real space

Example

(1) Find the primitive unit cell of the selected structure

(2) Identify the unit vectors





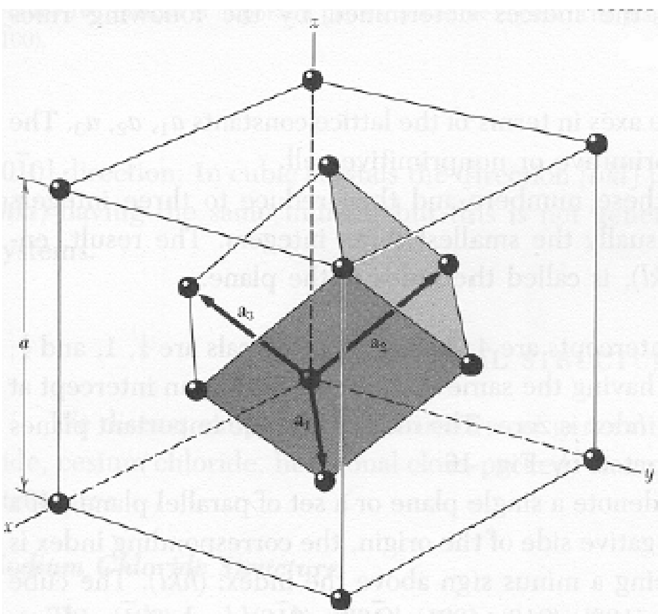
$\frac{1}{2}a(\hat{x}+\hat{y})$ $\frac{1}{2}a(\hat{y}+\hat{z})$ $\frac{1}{2}a(\hat{x}+\hat{z})$

$\frac{1}{2}a(-\hat{x}+\hat{y}+\hat{z})$ $\frac{1}{2}a(\hat{x}-\hat{y}+\hat{z})$ $\frac{1}{2}a(\hat{x}+\hat{y}-\hat{z})$

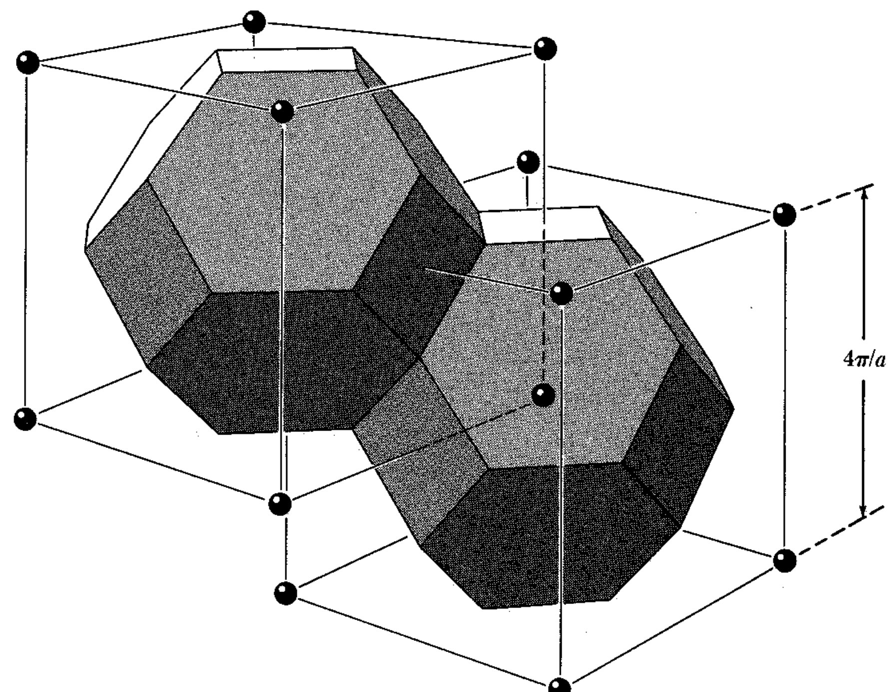
Face-centered cubic

The reciprocal lattice to an FCC lattice is the body-centered cubic (BCC) lattice.

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



FCC in real space



BCC in fourier space

$$\vec{a} = \frac{a}{2}(\hat{x} + \hat{z}) \qquad \vec{b} = \frac{a}{2}(\hat{x} + \hat{y}) \qquad \vec{c} = \frac{a}{2}(\hat{y} + \hat{z})$$

$$V = \vec{a} \cdot (\vec{b} \times \vec{c}) = \frac{a}{2}(\hat{x} + \hat{z}) \cdot \left[\frac{a}{2}(\hat{x} + \hat{y}) \times \frac{a}{2}(\hat{y} + \hat{z}) \right]$$

$$\left[\frac{a}{2}(\hat{x} + \hat{y}) \times \frac{a}{2}(\hat{y} + \hat{z}) \right] = \frac{a^2}{4}(\hat{z} + (-\hat{y}) + \hat{x})$$

$$\underline{V} = \vec{a} \cdot (\vec{b} \times \vec{c}) = \frac{a}{2}(\hat{x} + \hat{z}) \cdot \frac{a^2}{4}(\hat{x} - \hat{y} + \hat{z}) = \frac{a^3}{8} \times 2 = \underline{\frac{a^3}{4}}$$

Volume of F.C.C. is a^3. There are four atoms per unit cell! $\rightarrow$ the volume for the primitive of a F.C.C. structure is ?

$$\vec{a}^* = \frac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})} = \frac{\frac{a}{2}(\hat{x}+\hat{y})\times\frac{a}{2}(\hat{y}+\hat{z})}{a^3/4}$$

$$= \frac{\frac{a^2}{4}(\hat{x}+\hat{y})\times(\hat{y}+\hat{z})}{a^3/4} = \frac{(\hat{x}+\hat{y})\times(\hat{y}+\hat{z})}{a}$$

$$= \frac{\hat{z}+(-\hat{y})+\hat{x}}{a} = \frac{\hat{x}-\hat{y}+\hat{z}}{a}$$

Similarly,

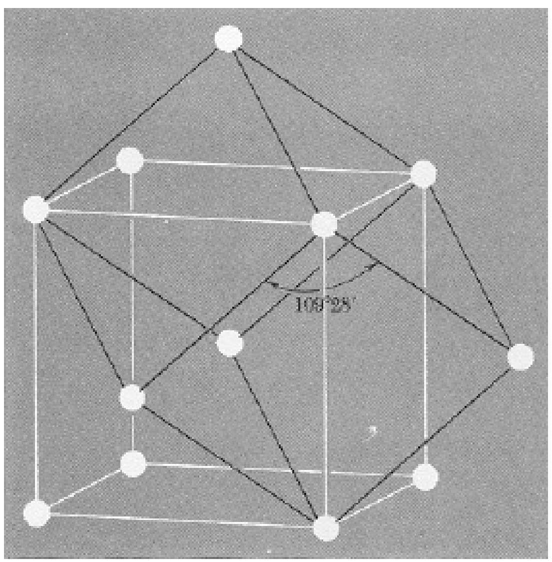
$$\vec{b}^* = \frac{\hat{x}+\hat{y}-\hat{z}}{a} \qquad \vec{c}^* = \frac{-\hat{x}+\hat{y}+\hat{z}}{a}$$

$$\frac{\hat{x}-\hat{y}+\hat{z}}{a}, \frac{\hat{x}+\hat{y}-\hat{z}}{a}, \frac{-\hat{x}+\hat{y}+\hat{z}}{a} \rightarrow \text{B.C.C.}$$

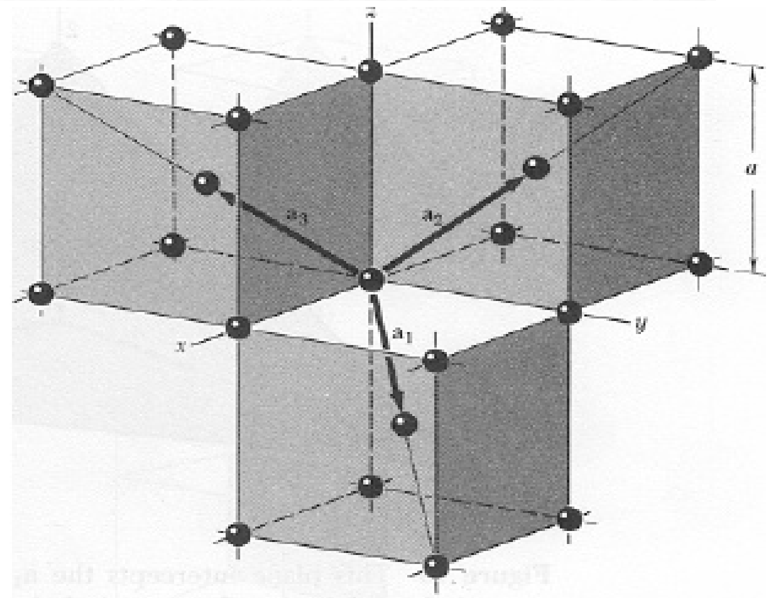
Body-centered cubic

The reciprocal lattice to an BCC lattice is the face-centered cubic (FCC) lattice.

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



FCC in real space



Primitive Translation Vectors:

$$\mathbf{a}_1 = \tfrac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}) \; ; \qquad \mathbf{a}_2 = \tfrac{1}{2}a(-\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}) \; ;$$

$$\mathbf{a}_3 = \tfrac{1}{2}a(\hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}}) \; .$$

Using primitive translation vector to do the reciprocal lattice calculation:
Case: FCC → BCC

$$\frac{\hat{x}-\hat{y}+\hat{z}}{a}, \frac{\hat{x}+\hat{y}-\hat{z}}{a}, \frac{-\hat{x}+\hat{y}+\hat{z}}{a}$$

$$\vec{a}^* \qquad \vec{b}^* \qquad \vec{c}^*$$

$$\frac{1}{d_{hkl}^2} = (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)\cdot(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)$$

$$= h^2\vec{a}^*\cdot\vec{a}^* + hk\vec{a}^*\cdot\vec{b}^* + hl\vec{a}^*\cdot\vec{c}^*$$

$$+ hk\vec{b}^*\cdot\vec{a}^* + k^2\vec{b}^*\cdot\vec{b}^* + kl\vec{b}^*\cdot\vec{c}^*$$

$$+ hl\vec{c}^*\cdot\vec{a}^* + kl\vec{c}^*\cdot\vec{b}^* + l^2\vec{c}^*\cdot\vec{c}^*$$

$$\vec{a}^* \cdot \vec{a}^* = \frac{\hat{x} - \hat{y} + \hat{z}}{a} \cdot \frac{\hat{x} - \hat{y} + \hat{z}}{a} = \frac{3}{a^2}$$

$$\vec{a}^* \cdot \vec{b}^* = \vec{b}^* \cdot \vec{a}^* = \frac{\hat{x} - \hat{y} + \hat{z}}{a} \cdot \frac{\hat{x} + \hat{y} - \hat{z}}{a} = \frac{-1}{a^2}$$

$$\vec{a}^* \cdot \vec{c}^* = \vec{c}^* \cdot \vec{a}^* = \frac{\hat{x} - \hat{y} + \hat{z}}{a} \cdot \frac{-\hat{x} + \hat{y} + \hat{z}}{a} = \frac{-1}{a^2}$$

$$\vec{b}^* \cdot \vec{b}^* = \frac{\hat{x} + \hat{y} - \hat{z}}{a} \cdot \frac{\hat{x} + \hat{y} - \hat{z}}{a} = \frac{3}{a^2}$$

$$\vec{b}^* \cdot \vec{c}^* = \vec{c}^* \cdot \vec{b}^* = \frac{\hat{x} + \hat{y} - \hat{z}}{a} \cdot \frac{-\hat{x} + \hat{y} + \hat{z}}{a} = \frac{-1}{a^2}$$

$$\vec{c}^* \cdot \vec{c}^* = \frac{-\hat{x} + \hat{y} + \hat{z}}{a} \cdot \frac{-\hat{x} + \hat{y} + \hat{z}}{a} = \frac{3}{a^2}$$

$$\frac{1}{d_{hkl}^2} = (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)\cdot(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)$$

$$= \frac{3h^2}{a^2} - \frac{hk}{a^2} - \frac{hl}{a^2} - \frac{hk}{a^2} + \frac{3k^2}{a^2} - \frac{kl}{a^2} - \frac{hl}{a^2} - \frac{kl}{a^2} + \frac{3l^2}{a^2}$$

$$= \frac{1}{a^2}[3(h^2 + k^2 + l^2) - 2(hk + kl + hl)]$$

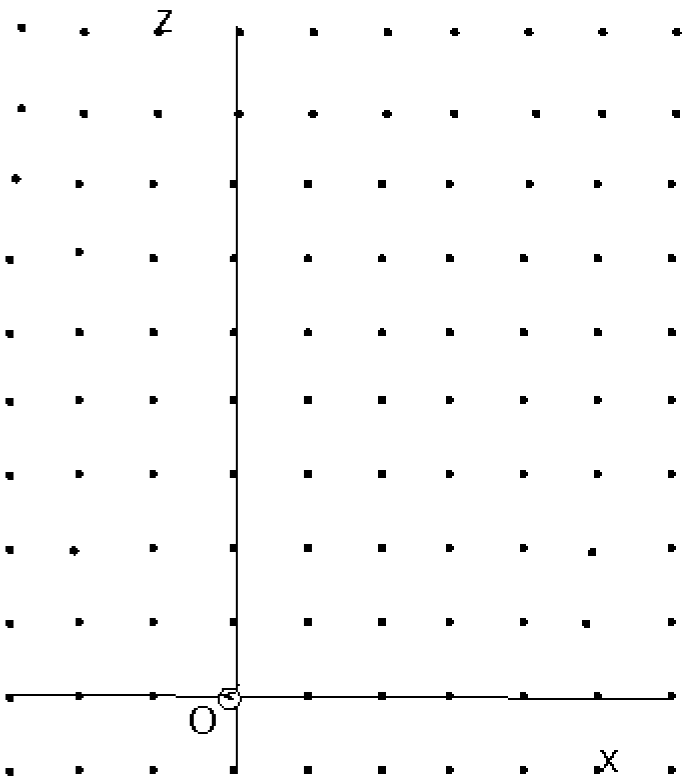
not $\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} = \frac{h^2 + k^2 + l^2}{a^2}$ Why?

(hkl) defined using unit cell!

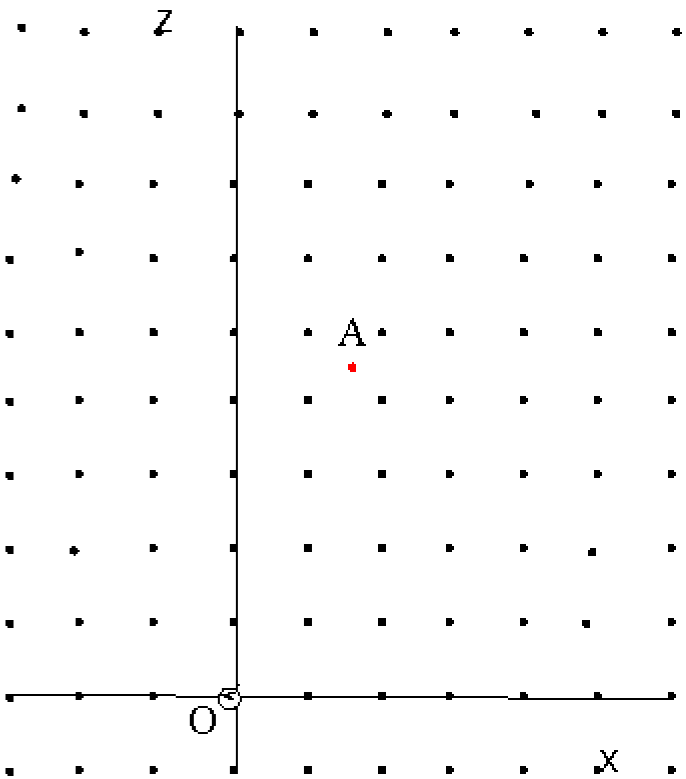
(hkl) is defined using primitive cell!

(HKL)

Bragg law in Reciprocal Lattice (Ewald Construction)

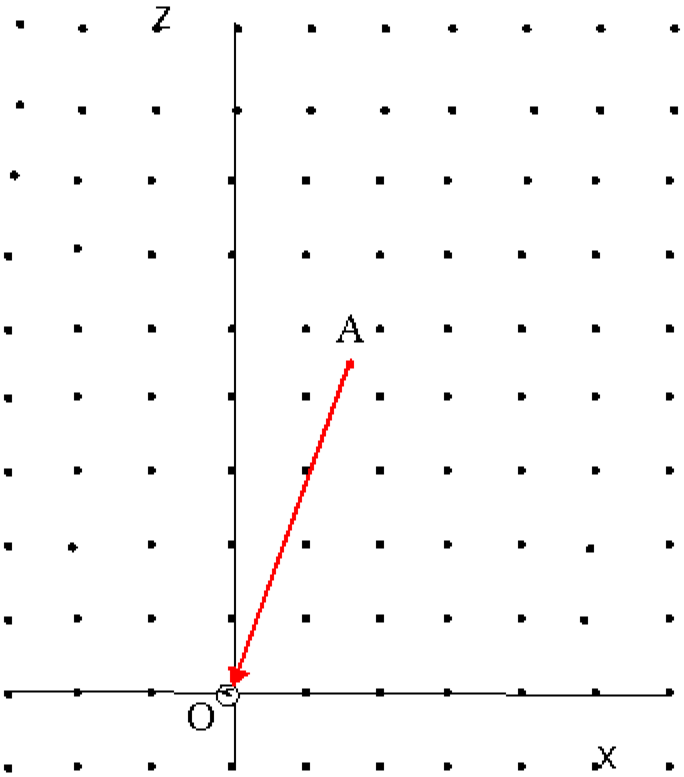


Chose a point according to the orientation of the specimen with respect to the incident beam.

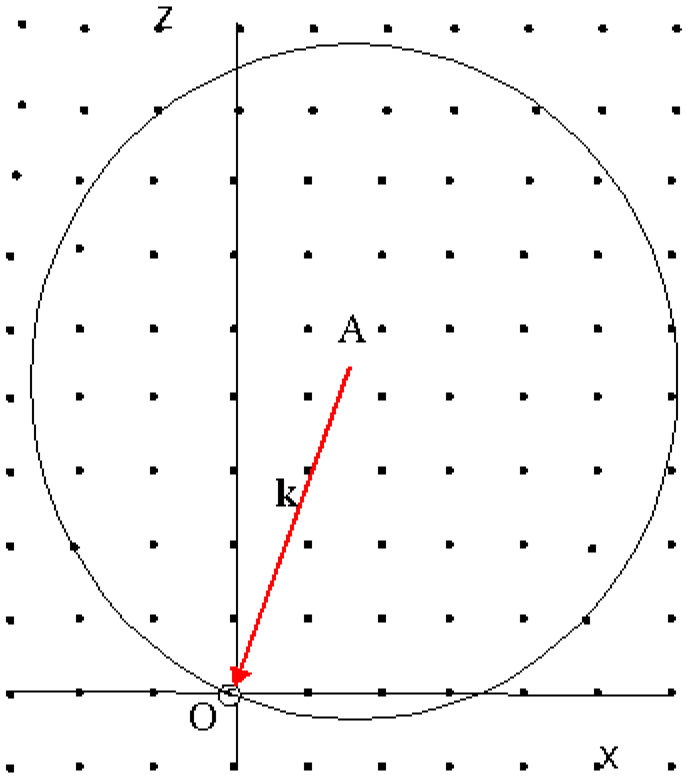


Draw a vector AO in the incident direction of length 2p/l terminating at the origin

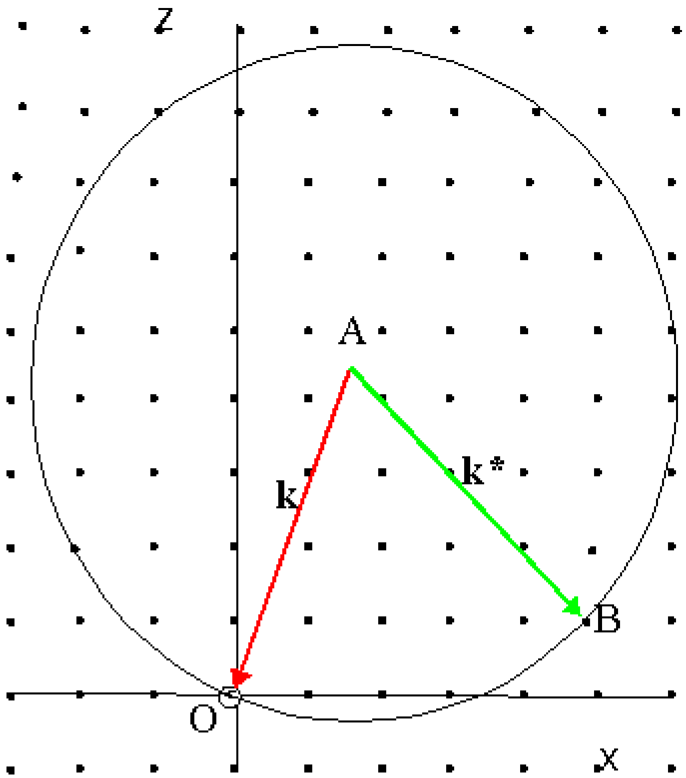
(Ewald Construction)



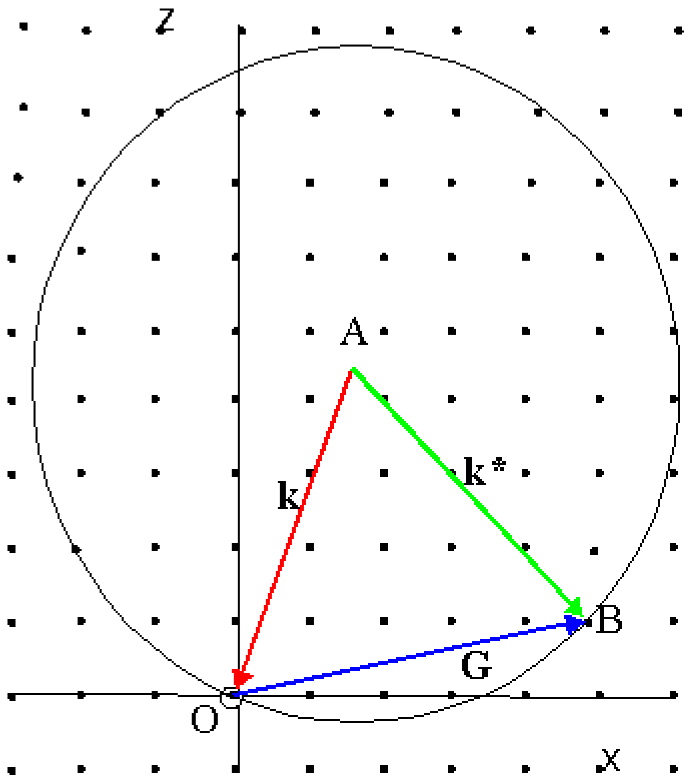
Construct a circle of radius 2p/l with center at A. Note whether this circle passes through any point of the reciprocal lattice; if it does....



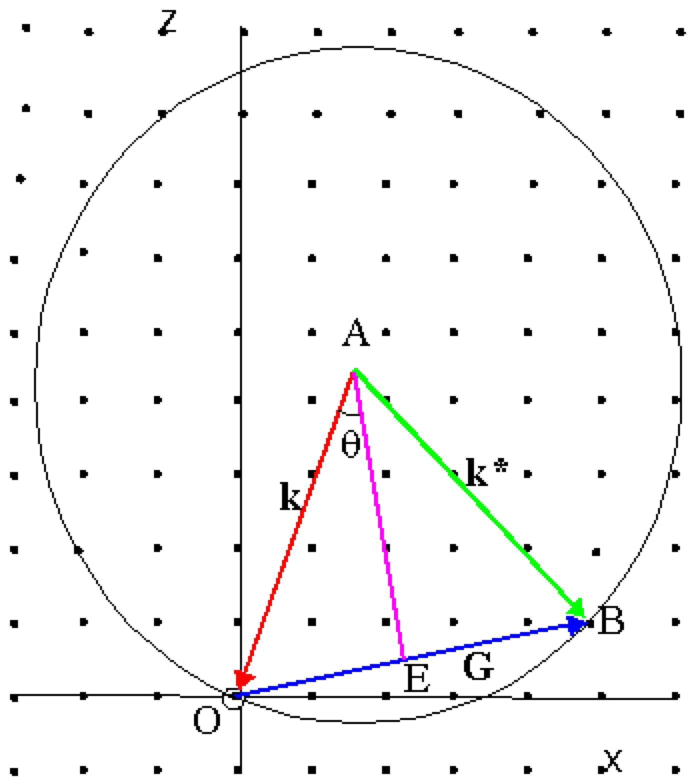
Draw a vector AB to the point of the intersection



Draw a vector OB to the point of the intersection



Draw a line AE perpendicular to OB



Complete the construction to all the intersection points in the same fashion

REFERENCES

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