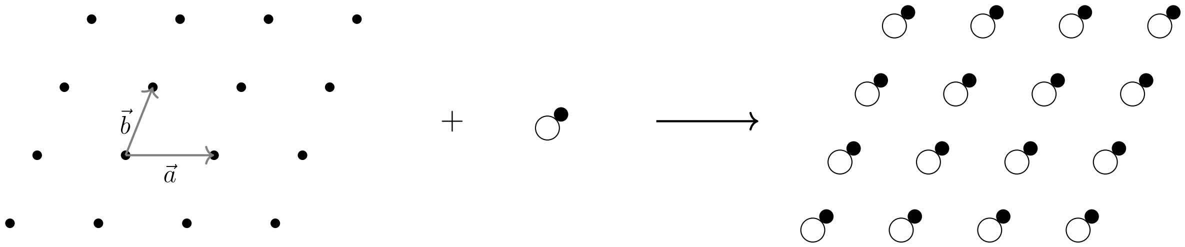
2
Crystallography

- **Space lattice**: array of points in space such that the environment about each point is the same.
- **Basis**: A unit assembly of atoms or molecules that are identical in composition

Space lattice can be constructed with two vectors: $\vec{a}, \vec{b}$ (also known as translational vectors) And it defines space lattice as:

$$T = n_1\vec{a} + n_2\vec{b}$$

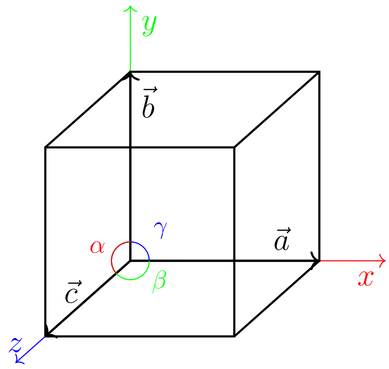


Space Lattice Basis Crystal

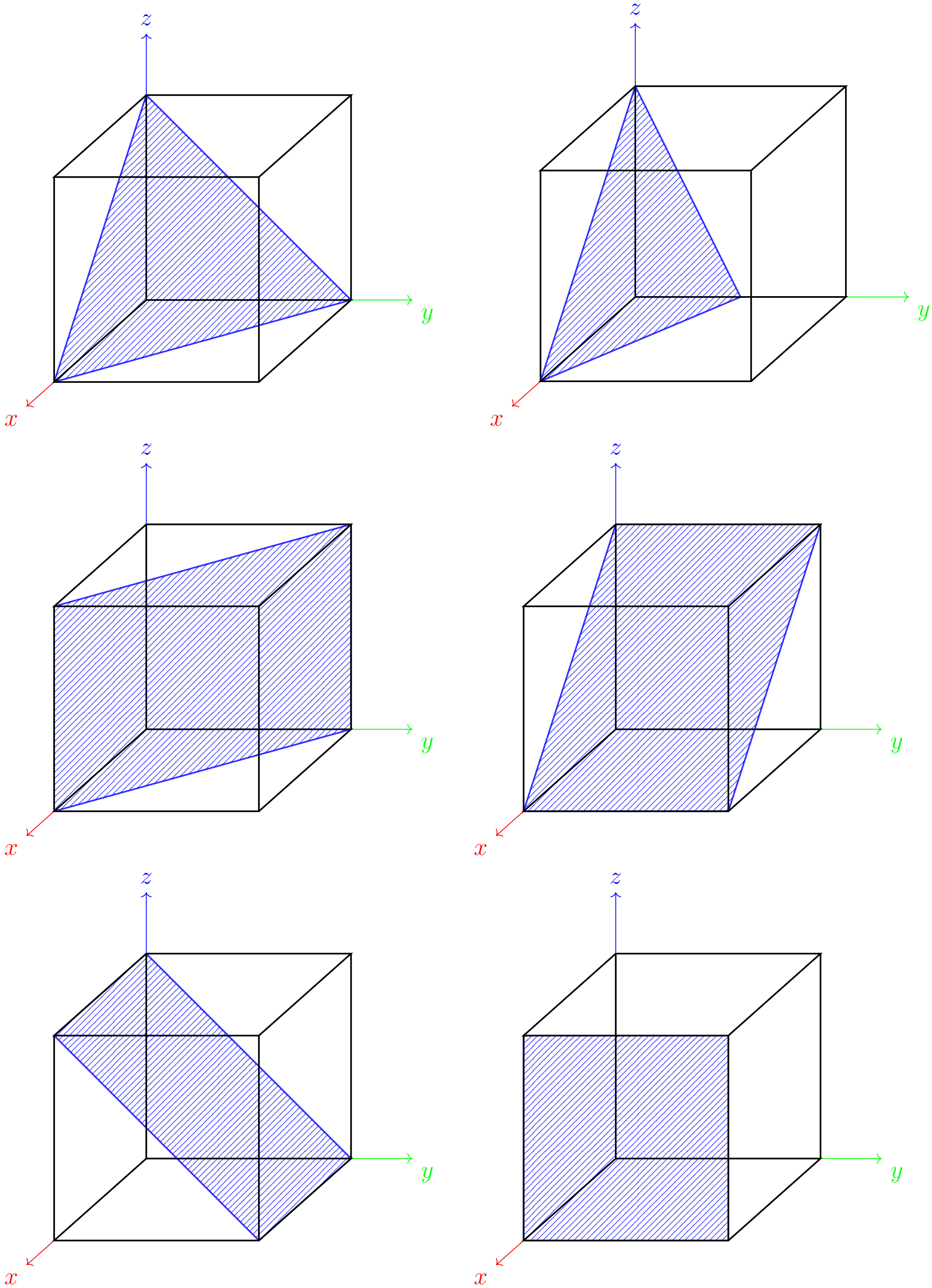
Unit cell

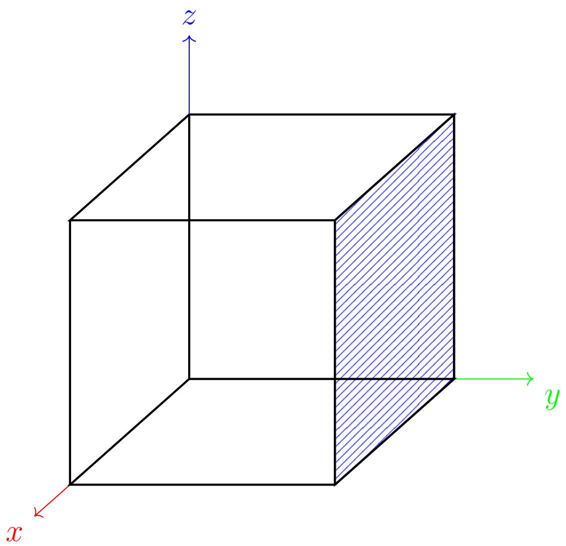
It is the smallest repeatable unit of a crystal. A unit cell is characterised by 6 parameters:

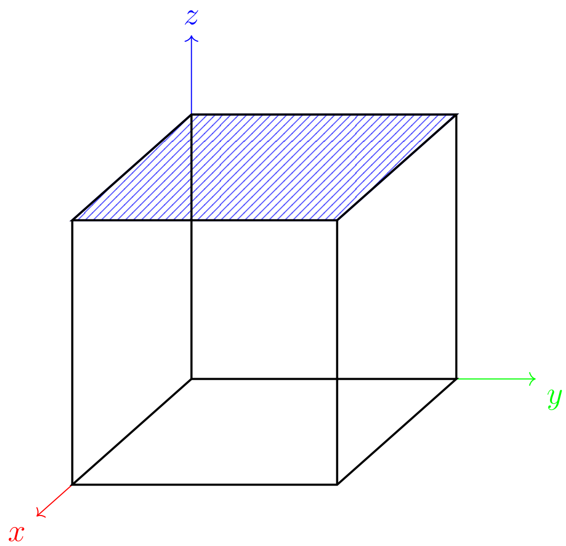
- lattice coefficients: a, b, c
- interfacial angles: α, β, γ



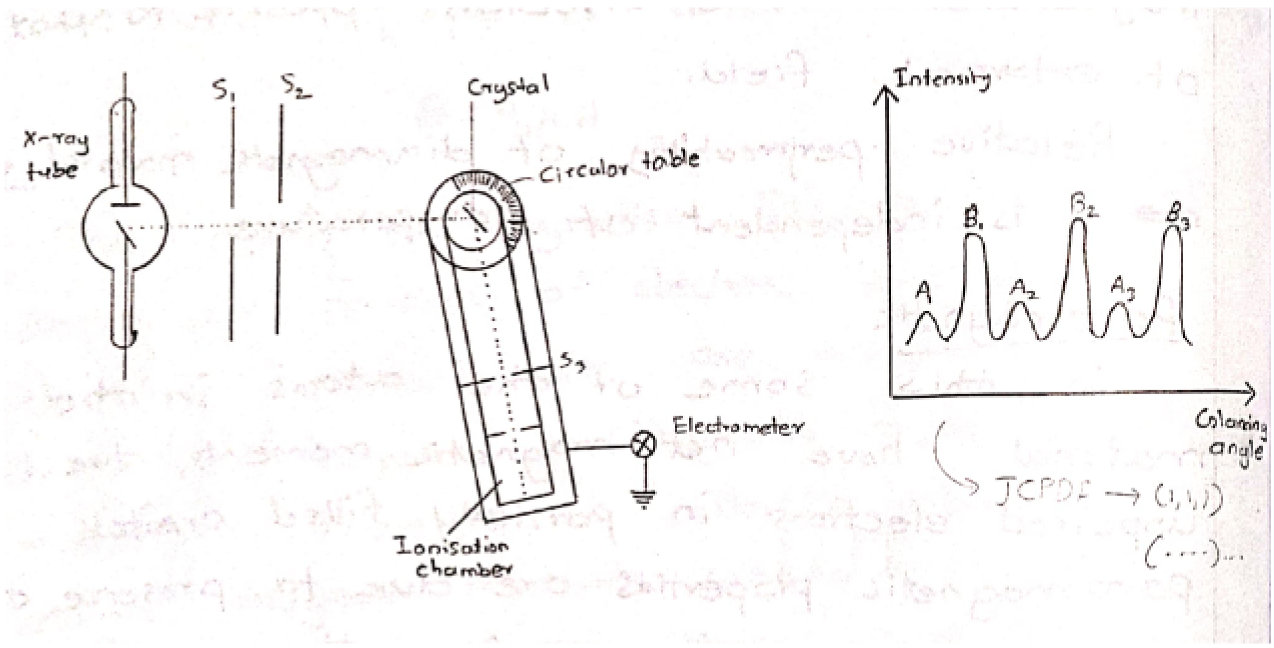
Miller Indices







Bragg's X-ray spectrometer



Components

- Source of X-rays
- Crystal held on a circular table which is graduated and provided with vernier.
- A detector (Ionisation chamber)

Operation

1. X-ray from X-ray tube, limited by two narrow slits: S_1 and S_2 are allowed to fall upon crystel.

2. The crystal is mound on the circular table which can rotate above a vertical und its position can be determined by vernier.
3. The table is provided with a radial arm which carries an ionisation chamber.
4. The ionisation chamber is connected to a electrometer to measure the ionisation current. Hence we can measure the intensity of X-ray beam diffracted in the direction of ionisation chamber.
5. S_3 is another slit to limit the width of diffracted beam.

To begin with, the glancing angle θ for the incident beam is kept very small, the ionisation chamber is adjusted to recieve the reflected beam till the rate of deflection is maximum. The glancing angle and intensity of diffracted beam are detected. The glancing angle is increased in equal steps by rotating the crystal table. The ionization current is noted for different glancing angles. The graph of ionisation current against glancing angle obtained is called X-ray spectrum. The prominent peaks, A_1, A_2 & A_3 refer to X-rays of wavelength λ. The glancing angles $\theta_1, \theta_2, \theta_3$ Corresponding to peaks A_1, A_2 & A_3 which are obtained from the graph. It is found that $\sin(\theta_1) : \sin(\theta_2) : \sin(\theta_2)$ is $1 : 2 : 3$ that is A_1, A_2 & A_3 refer to first, second & third order reflections of same wavelength, similarly B_1, B_2 & B_3 are such peaks for 1^{st}, 2^{nd} and 3^{rd} order for other wavelength. So Bragg experimentally verified

$$2d\sin(\theta) = n\lambda$$

2 Monochromatic X-rays of wavelength 1.5Å, are incident on a crystal having interplar ar spacing 1.6Å. Find highest order for which bragg's reflection maximum can be seen.

Answer

$n\lambda = 2d\sin(\theta)$

$\therefore n = 2\dfrac{d}{\lambda}\sin(\theta) = 2 \times \dfrac{1.6}{1.5}\sin(\theta)$

For $n_{max}, \theta = 90^\circ$

$\therefore n_{\max} = 2 \times \dfrac{1.6}{1.5} = 2.13$

For integer values (n = 2), $\theta = 69^\circ$

3 A beam of X-rays of wavelength 0.071n m is diffracted by (110) plane with lattice constant, 0.28 nm. Find glancing angle for $2^{\mathbf{nd}}$ order diffraction

Answer

$2\lambda = 2d\sin(\theta), d = 0.28/\sqrt{3} = 0.198\text{nm}$

$\theta = \sin^{-1}(\lambda/d) = \sin^{-1}(0.071/0.198)$

$\theta = 21.01^\circ$

4 Calculate glancing angle at (110) plane of a cubic crystal having axial length 0.26 nm corresponding to $2^{\mathbf{nd}}$ order diffraction maxima, for x-ray of wavelength 0.065 nm

Answer
Axial length $= a$

$$2\lambda = 2d \cdot \sin(\theta)$$
$$\theta = \sin^{-1}\left(\frac{0.065}{0.185}\right) = 20.69^{\circ}$$

5 Bragg's angle for reflection from (111) plane in FCC crystal is 19.2° for an X-ray of wavelength 1.54 Å

Answer
(Assume that $n = 1$, if its not given in the question)

$$n \cdot \lambda = 2d\sin(\theta)$$
$$1.54\text{Å} = 2d\sin(19.2^{\circ})$$
$$\Rightarrow d = 2.341$$

$\therefore$ Cube length a=$2.391\sqrt{3} = 4.05\text{Å}$