Solved problems on Bragg's Law

1] X rays of unknown wavelength give first order Bragg reflection at glancing angle 20° width (2 1 2) planes of copper having FCC structure. Find the wavelength of X rays if lattice constant of copper is 3.615 A°

→ $d = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{3.615A°}{\sqrt{2^2+1^2+2^2}} = 1.205A°$

$\lambda = \frac{2d\sin\theta}{n} = \frac{2\times 1.205 \times \sin 20°}{1} = 0.8244°$

2] The first order diffraction is found to occur at a glancing angle of 9°. Calculate the wavelength of X ray and the glancing angle for 2nd order diffraction if spacing between adjacent plane is 2.51 A°.

→

(i) $\lambda = \frac{2d\sin\theta}{n} = \frac{2\times 2.51\times \sin 9°}{1} = 0.7853A°$

(ii) $\sin\theta = \frac{n\lambda}{2d} = \frac{2\times 0.7853}{2\times 2.51} = 0.3129$

$\theta = \sin^{-1}(0.3129) = 18.23°$

3] The Bragg angle for (220) reflection from nickel is 38.2°, when X rays of wavelength 1.54 A° are employed in a diffraction experiment. Determine the lattice parameter of nickel

→

$d = \frac{n\lambda}{2\sin\theta} = \frac{1\times 1.54}{2\sin 38.2°} = 1.245A°$

$a = h\sqrt{h^2+k^2+l^2} = 1.245 \times \sqrt{2^2+2^2+0^2} = 1.245\sqrt{8} = 3.52\,A^\circ$

4] Calculate the longest wavelength that can be analysed by a rock salt crystal of spacing $d = 2.82\,A^\circ$ in the 1^{st} order.

→

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

$\lambda_{max} = \frac{2d\sin\theta}{n}$ → max = 1

$\lambda_{max} = \frac{2d}{n} = \frac{2 \times 2.82}{1} = 5.64\,A^\circ$

5] Calculate the maximum order of diffraction if X rays of wavelength of $0.819\,A^\circ$ is incident on a crystal of lattice spacing 0.282 nm.

→ for n_{max} → $\sin\theta = 1$ → $2d = \cancel{n_{max}}\, n_{max}\lambda$

$\therefore\ n_{max} = \frac{2d}{\lambda} = \frac{2 \times 0.282 \times 10^{-9}}{0.819 \times 10^{-10}} = 6.886 < 7$

$\therefore\ n_{max} = 6$

6] If X rays of wavelength $1.549\,A^\circ$ is reflected from a crystal with interplanar spacing $4.255\,A^\circ$. Calculate the smallest glancing angle and higest order of reflection that can be observed.

→ (i) for θ_{min} → n must be min → $n = 1$

$\sin\theta_{min} = \frac{n\lambda}{2d} = \frac{1 \times 1.549}{2 \times 4.255} = 0.182$

$\theta_{min} = \sin^{-1}(0.182) = 10.48^\circ$

(ii) for n_{max} → $\sin\theta = 1$ → $n_{max} = \frac{2d}{\lambda} = \frac{2 \times 4.255}{1.549}$

$n_{max} = 5.49 < 6$ $\therefore\ n_{max} = 5$

7] Monochromatic high energy X rays are incident on a crystal. If 1st order reflection is observed at an angle 3.4°, at what angle would second order reflection to be expected?

→ $2d\sin\theta = n\lambda$

$$\sin\theta = \frac{n\lambda}{2d}$$ same

const.

$$\sin\theta \propto n$$

$$\frac{\sin\theta_1}{\sin\theta_2} = \frac{n_1}{n_2} \longrightarrow \frac{\sin 3.4°}{\sin\theta_2} = \frac{1}{2}$$

$$\sin\theta_2 = 2\sin 3.4° = 0.1186$$

$$\theta_2 = \sin^{-1}(0.1186) = 6.81°$$

8] The unit cell dimension 'a' of NaCl lattice is 5.63Å. If X ray beam of wavelength 1.1Å fall on a family of planes with a separation of $(d/\sqrt{5})$. How many others of diffraction are observable?

→ $$n_{max} = \frac{2d\sin\theta}{\lambda} \overset{=1}{=} \frac{2d}{\lambda} = \frac{2 \times 5.63}{\sqrt{5} \times 1.1} = 4.578 < 5$$

$$\therefore \quad n_{max} = 4$$

Four orders of diffraction is observable.

9] Monochromatic X ray beam of wavelength $\lambda = 5.8189$ Å is reflected strongly for a glancing angle of $\theta = 75.86°$ in the 1st order by certain planes of cubic crystal of lattice constant 3Å. Determine Miller indices of possible planes.

→ $2d\sin\theta = n\lambda$

$$d = \frac{n\lambda}{2\sin\theta} = \frac{1 \times 5.8189}{2\sin 75.86°} = 3Å$$

$$\sqrt{h^2+k^2+l^2} = \frac{a}{d} = \frac{3}{3} = 1$$

$\therefore \quad h^2+k^2+l^2 = 1$

The possible Miller indices are $(100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1})$.

10] In comparing the wavelengths of two monochromatic X ray lines it is found that line A gives 1st order Bragg's maximum at glancing angle of 30° to the smooth face of crystal. Line B of known wavelength of 0.97Å gives 3rd order maximum at a glancing angle of 60° with same face of crystal. Find the wavelength of line A.

→

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

$$\lambda = \frac{\overset{\text{const.}}{2d}\,\overset{\text{same}}{\sin\theta}}{n}$$

$$\lambda \propto \frac{\sin\theta}{n}$$

$$\frac{\lambda_1}{\lambda_2} = \frac{\sin\theta_1}{n_1} \cdot \frac{n_2}{\sin\theta_2} = \frac{\sin 30^\circ}{1} \times \frac{3}{\sin 60^\circ} = \frac{1}{2} \times \frac{3\times 2}{\sqrt{3}} = \sqrt{3}$$

$$\lambda_1 = \lambda_2\sqrt{3} = 0.97\times\sqrt{3} = 1.68\text{Å}$$

11] An X ray beam of wavelength 0.71Å is diffracted by a FCC crystal of density $1.99\times10^3\ kg/m^3$. Calculate interplanar spacing for (200) planes and glancing angle for 2nd order reflection from these planes if the molecular weight of the crystal is 74.6 amu.

→

$$\rho = \frac{\text{mass}}{\text{volume}} = \frac{nM}{N_A a^3}$$

$$a = \left(\frac{nM}{\rho N_A}\right)^{1/3} = \left(\frac{4\times 74.6}{1.99\times10^3\times6.02\times10^{26}}\right)^{1/3} = 6.26\text{Å}$$

$$d_{200} = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{6.26}{\sqrt{2^2+0^2+0^2}} = 3.13\text{Å}$$

$$\sin\theta = \frac{n\lambda}{2d} = \frac{2\times 0.71}{2\times 3.13} = 0.2268$$

$$\therefore \quad \theta = \sin^{-1}(0.2268) = 13.11^\circ$$

Solved problems based on interplanar spacing

1] Calculate the interplanar spacing for a (321) plane in a simple cubic lattice whose lattice constant is 4.2 A°

→ $$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{4.2}{\sqrt{3^2+2^2+1^2}} = 1.122\,A^\circ$$

2] Silver has FCC structure and its atomic radius is 1.441 A°. Find the spacing of (220) plane.

→ $$a = \frac{4r}{\sqrt{2}} = \frac{4\times 1.441}{\sqrt{2}}\,A^\circ$$

$$d_{hkl} = \frac{4\times 1.441}{\sqrt{2}\sqrt{2^2+2^2+0^2}} = \frac{4\times 1.441}{\sqrt{2}\sqrt{8}} = 1.441\,A^\circ$$

3] The interplanar spacing of (110) plane is 2A° for FCC crystal. Find atomic radius.

→ $$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$a = d_{110}\sqrt{1^2+1^2+0^2} = 2\sqrt{2}\,A^\circ$$

$$r = \frac{\sqrt{2}a}{4} = \frac{\sqrt{2}\times 2\sqrt{2}}{4} = 1\,A^\circ$$

4] Calculate the interplanar spacing for (220) plane of a bcc iron with atomic radius 1.24 A°.

→ $\cancel{r = \frac{\sqrt{3}a}{4}}$ $$a = \frac{4r}{\sqrt{3}} = \frac{4\times 1.24}{\sqrt{3}} = 2.86\,A^\circ$$

$$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{2.86}{\sqrt{2^2+2^2+0^2}} = \frac{2.86}{\sqrt{8}}$$

$$\therefore d_{220} = 1.01\,A^\circ$$

5] Determine lattice constant for FCC lead crystal of radius 1.746 Å. Also find the spacing of
(i) (111) planes (ii) (200) planes (iii) (220) plane

→ $a = \frac{4r}{\sqrt{2}} = \frac{4 \times 1.746}{\sqrt{2}} = 4.938 \text{Å}$

(i) $d_{111} = \frac{4.938}{\sqrt{1^2+1^2+1^2}} = 2.851 \text{Å}$

(ii) $d_{2000} = \frac{4.938}{\sqrt{2^2+0^2+0^2}} = 2.469 \text{Å}$

(iii) $d_{220} = \frac{4.938}{\sqrt{2^2+2^2+0^2}} = 1.746 \text{Å}$

6] In a simple cubic crystal
(i) find the ratio of intercepts of three axes by (1 2 3) plane
(ii) Find the ratio of spacing of (110) & (111) planes

→

(i) $x_{int} : y_{int} : z_{int} = \frac{a}{h} : \frac{b}{k} : \frac{c}{l} = \frac{a}{1} : \frac{a}{2} : \frac{a}{3} = 1 : \frac{1}{2} : \frac{1}{3}$

(ii) $\frac{d_{110}}{d_{111}} = \frac{a/\sqrt{1^2+1^2+0^2}}{a/\sqrt{1^2+1^2+1^2}} = \frac{\sqrt{3}}{\sqrt{2}} = 1.225$

7] Deduce Miller indices of a set of parallel plane which makes intercept in the ratio of a:2b on x & y axes & parallel to z axis. Also calculate the interplanar spacing of the plane taking the lattice to be cubic ~~with~~ with a=b=c=5Å.

→ $x_{int} : y_{int} : z_{int} = a : 2b : \infty$

$pa : qb : rc = a : 2b : \infty$

$(h\ k\ l) = (1/p\ \ 1/q\ \ 1/r) = (1/1\ \ 1/2\ \ 1/\infty)$

$(h\ k\ l) = (2\ \ 1\ \ 0)$

$$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}} =$$

$$d_{210} = \frac{5}{\sqrt{2^2+1^2+0^2}} = \frac{5}{\sqrt{5}} = \sqrt{5}\,A^\circ$$

8] What is the family of planes $\{hkl\}$ with an interplanar spacing of $d = 1.246\,A^\circ$ in nickel with $a = 3.524\,A^\circ$

→ $$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$\sqrt{h^2+k^2+l^2} = \frac{a}{d_{hkl}} = \frac{3.524}{1.246} = 2.828$$

$$h^2+k^2+l^2 = 8$$

$$\therefore \{hkl\} = \{220\}$$

9] The density of copper is 8980 kg/m³ and unit cell dimension is 3.61 A°. Atomic weight of copper is 63.54. Determine crystal structure. Calculate atomic radius and interplanar spacing of (110) plane.

→ (i) $$\rho = \frac{mass}{Volume} = \frac{nM}{N_A a^3}$$

$$n = \frac{\rho N_A a^3}{M} = \frac{8980 \times 6.02\times10^{26} \times (3.61\times10^{-10})^3}{63.54} = 4 \Rightarrow FCC$$

(ii) $$r = \frac{\sqrt{2}a}{4} = \frac{\sqrt{2}\times 3.61}{4} = 1.276\,A^\circ$$

(iii) $$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$d_{110} = \frac{3.61}{\sqrt{1^2+1^2+0^2}} = 2.553\,A^\circ$$

Sketching a lattice plane

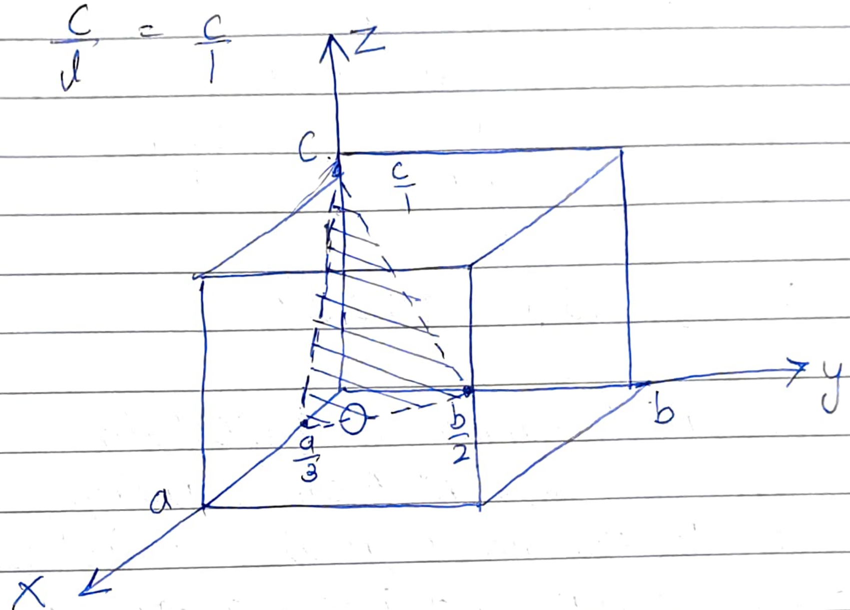
* Mark x_{int}, y_{int}, z_{int} & join these points.

1] Draw (3 2 1) plane.

$x_{int} = \frac{a}{h} = \frac{a}{3}$

$y_{int} = \frac{b}{k} = \frac{b}{2}$

$z_{int} = \frac{c}{l} = \frac{c}{1}$

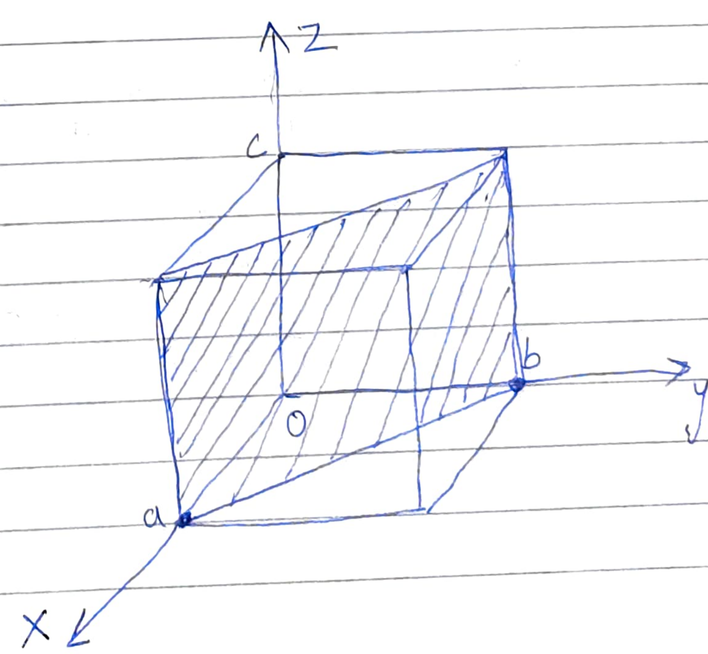


2] Draw (1 1 0) plane

$x_{int} = \frac{a}{h} = \frac{a}{1}$

$y_{int} = \frac{b}{k} = \frac{b}{1}$

$z_{int} = \frac{c}{l} = \frac{c}{0} = \infty$

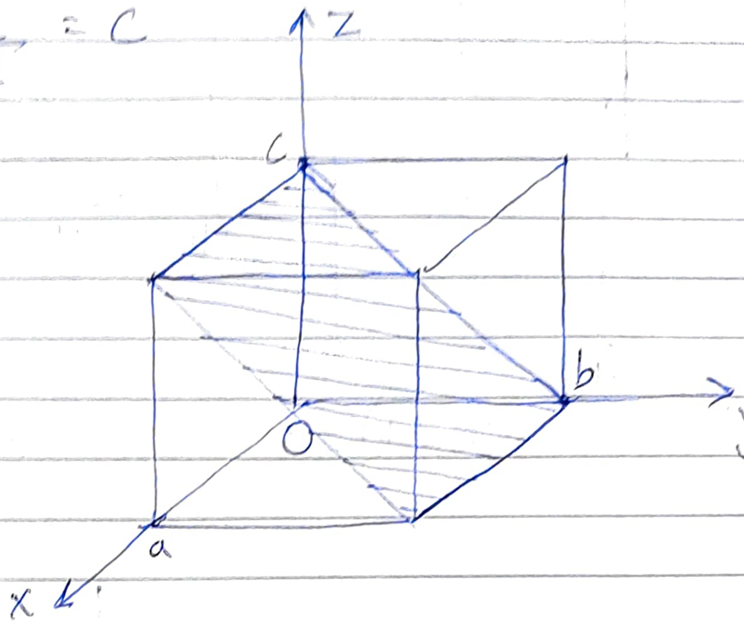


3] Draw a] ~~100~~ (011) plane   b] (101) plane

a] $x_{int} = \frac{a}{h} = \infty$

$y_{int} = \frac{b}{k} = b$

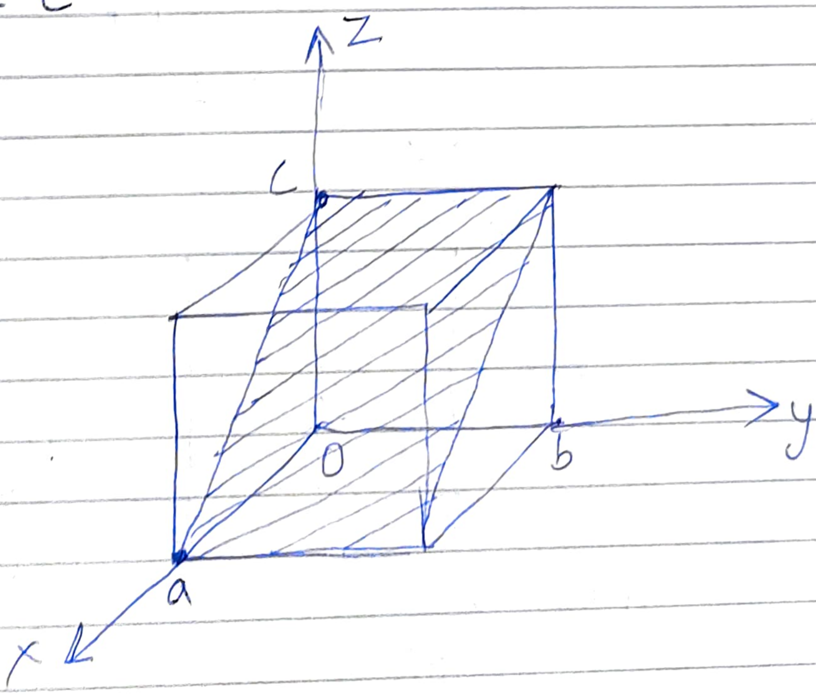
$z_{int} = \frac{c}{l} = c$



b] $x_{int} = a/h = a$

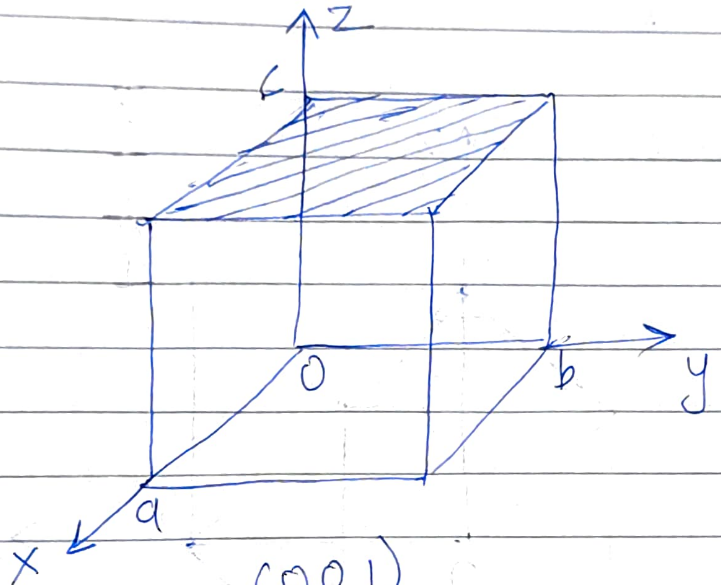
$y_{int} = b/k = \infty$

$z_{int} = c/l = c$

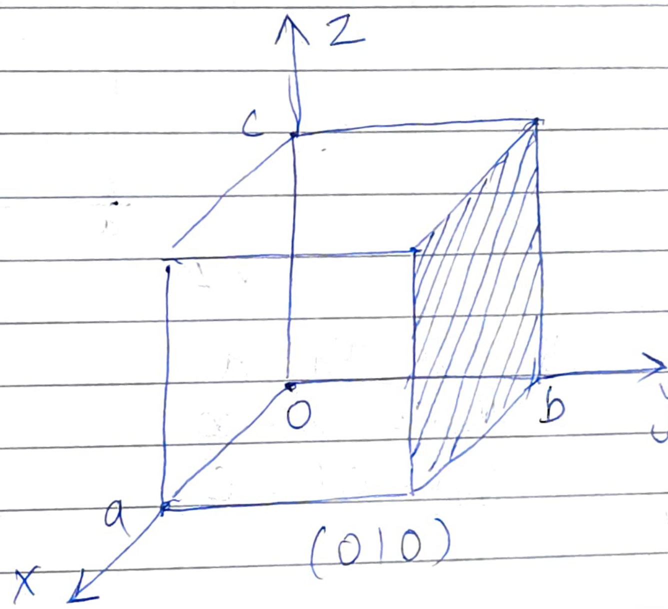


4]

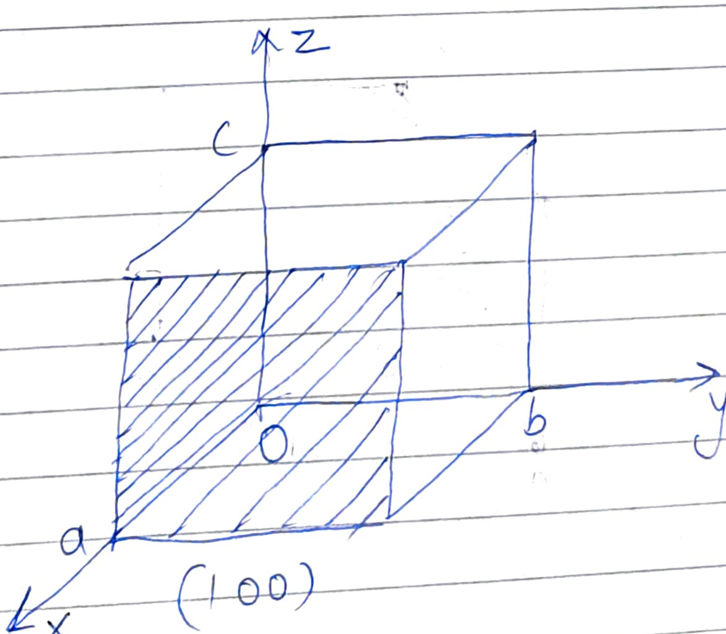
Draw	(1 0 0)	(0 1 0)	(0 0 1)
$x_{int} = a/h$	a	∞	∞
$y_{int} = b/k$	∞	b	∞
$z_{int} = c/l$	∞	∞	c



(0 0 1)



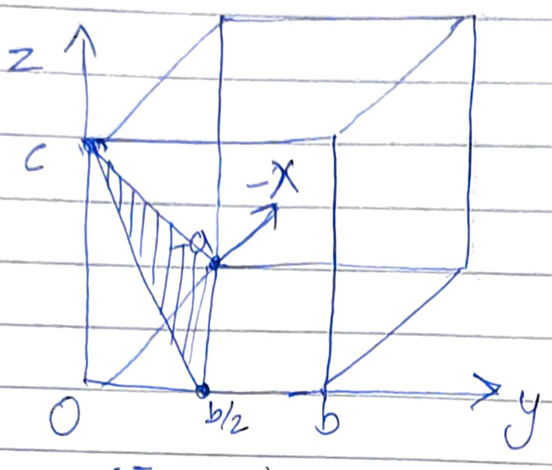
(0 1 0)



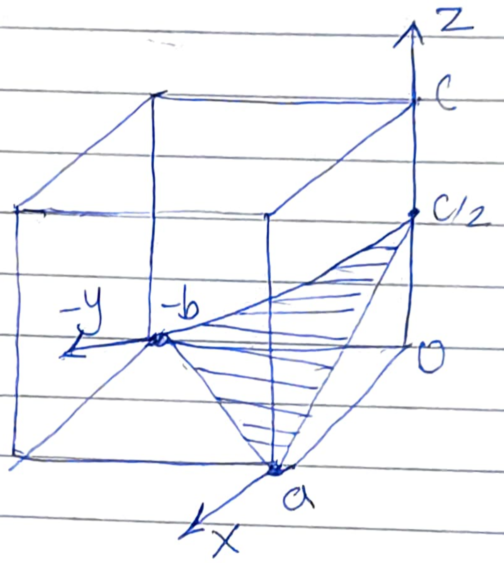
(1 0 0)

5] Draw

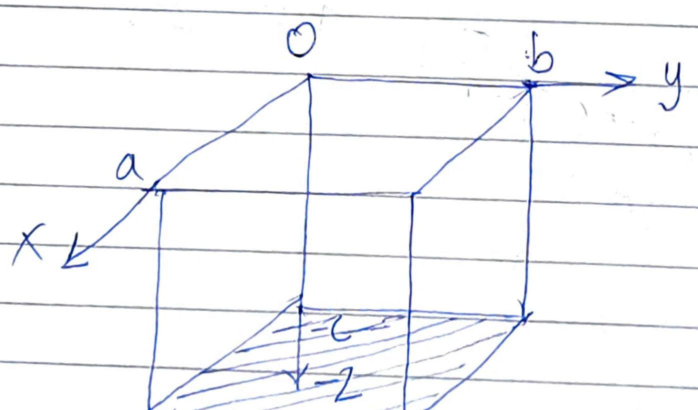
	$(\bar{1}21)$	$(1\bar{1}2)$	$(00\bar{1})$
$x_{int} = a/h$	$-a$	a	∞
$y_{int} = b/k$	$b/2$	$-b$	∞
$z_{int} = c/l$	c	$c/2$	$-c$



$(\bar{1}\,2\,1)$



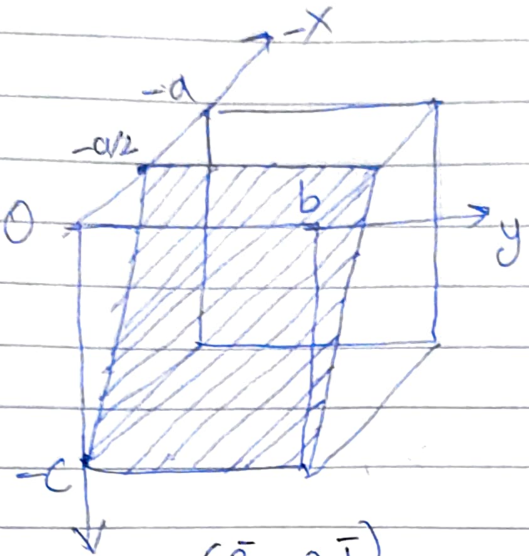
$(1\,\bar{1}\,2)$



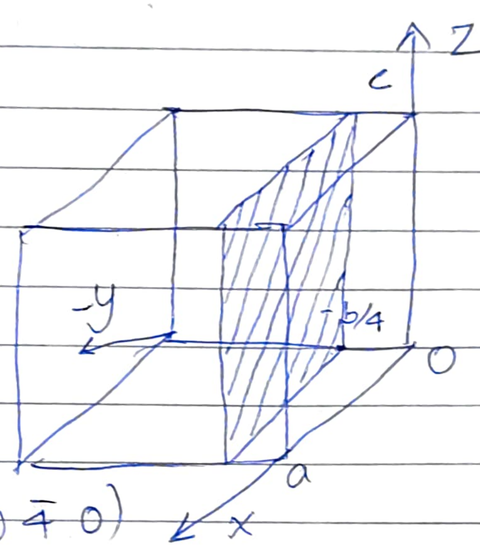
$(0\,0\,\bar{1})$

6] Draw

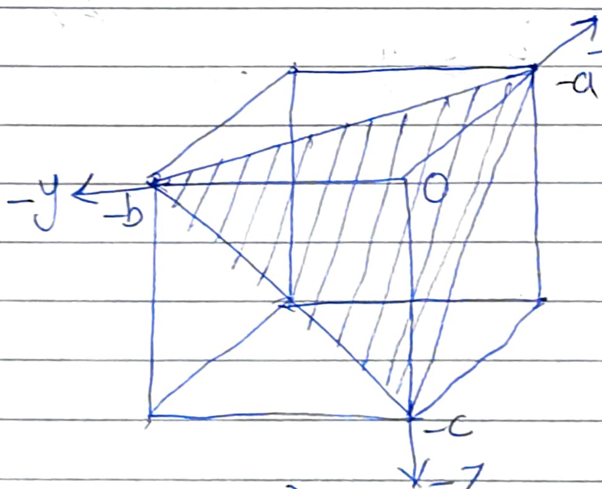
	$(\bar{2}\,0\,\bar{1})$	$(0\,\bar{4}\,0)$	$(\bar{1}\,\bar{1}\,\bar{1})$
$x_{int} = a/h$	$-a/2$	∞	$-a$
$y_{int} = b/k$	∞	$-b/4$	$-b$
$z_{int} = c/l$	$-c$	∞	$-c$



$(\bar{2}\ 0\bar{1})$



$(0\,\bar{4}\,0)$



$(\bar{1}\ \bar{1}\ \bar{1})$

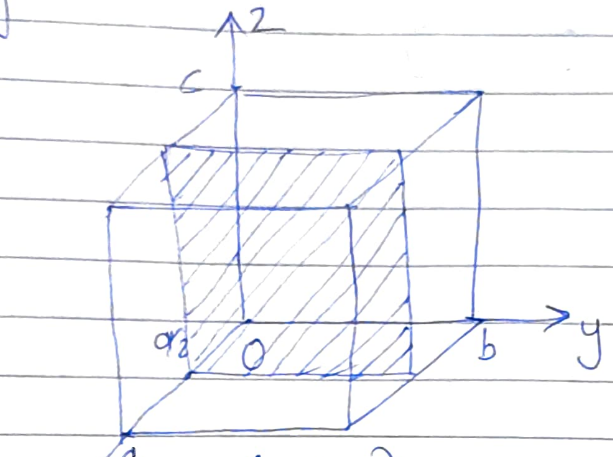
7] Draw following planes

a] (200) b] (020) c] (002)

d] (220) e] (202) f] (022)

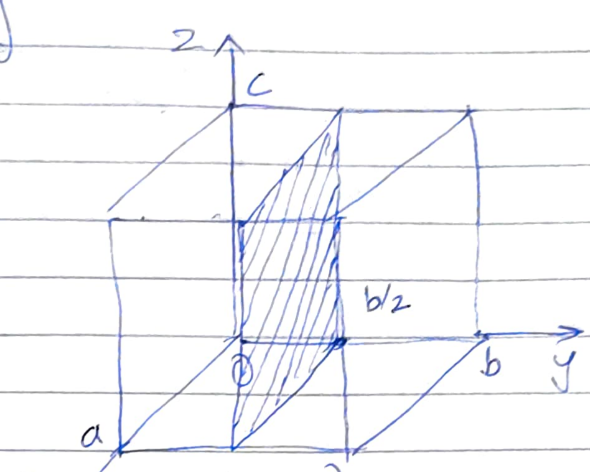
g] (222)

a]



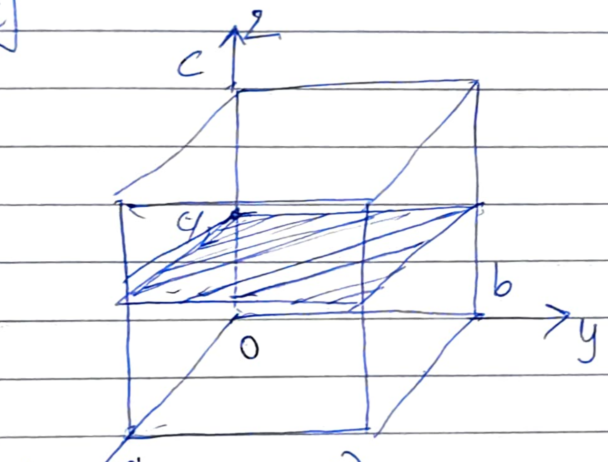
(200)

b]



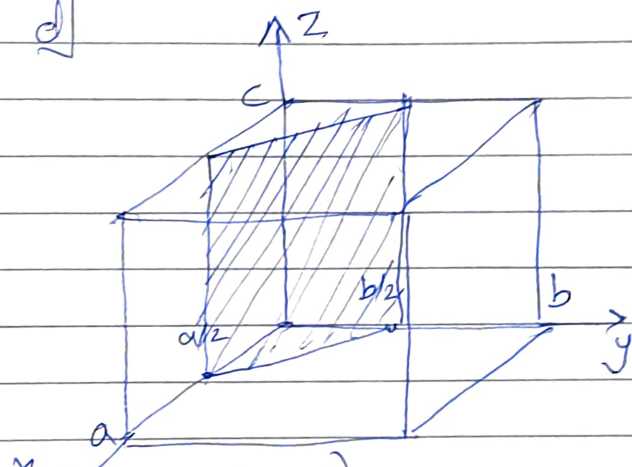
(020)

c]



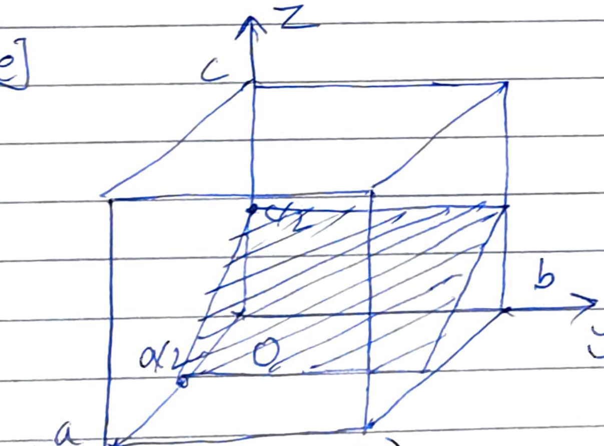
(002)

d]



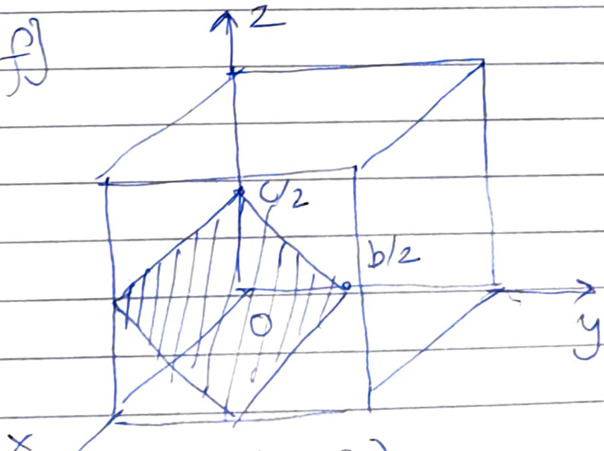
(220)

e]



(202)

f]



(022)

9]