Problem # 1
Using the atomic positions given in the problem.

$$F_{hkl} = f_c\left(e^{-2i\pi(0h+0k+0l)} + e^{-2i\pi\left(\frac{h}{2}+\frac{k}{2}\right)} + e^{-2i\pi\left(\frac{h}{2}+\frac{l}{2}\right)} + e^{-2i\pi\left(\frac{k}{2}+\frac{l}{2}\right)} + e^{-2i\pi\left(\frac{h}{4}+\frac{k}{4}+\frac{l}{4}\right)} + e^{-2i\pi\left(\frac{3h}{4}+\frac{3k}{4}+\frac{l}{4}\right)} + e^{-2i\pi\left(\frac{3h}{4}+\frac{k}{4}+\frac{3l}{4}\right)} + e^{-2i\pi\left(\frac{h}{4}+\frac{3k}{4}+\frac{3l}{4}\right)}\right)$$

$$F_{hkl} = f_c\left(1 + e^{-i(h+k)\pi} + e^{-i(h+l)\pi} + e^{-i(k+l)\pi} + e^{-i\frac{\pi}{2}(h+k+l)} + e^{-i\frac{\pi}{2}(3h+3k+l)} + e^{-i\frac{\pi}{2}(h+3k+3l)} + e^{-i\frac{\pi}{2}(3h+k+3l)}\right)$$

$$F_{hkl} = f_c\left(1 + (-1)^{h+k} + (-1)^{k+l} + (-1)^{h+l} + (-1)^{\frac{h+k+l}{2}} + (-1)^{\frac{(3h+3k+l)}{2}} + (-1)^{\frac{(h+3k+3l)}{2}} + (-1)^{\frac{(3h+k+3l)}{2}}\right)$$

- the first four terms generally cancel unless h, k, l are all odd or all even.

When starting from the transmitted beam, diffraction will be observed at scattering vectors $|\vec{s}| = \left(\frac{h^2 + k^2 + l^2}{a^2} \right)^{1/2}$ for which F_{hkl} is not zero.

Planes	$\lvert \vec{S}_{hkl} \rvert$	F_{hkl}
{100}	$\frac{1}{a}$	0
{110}	$\frac{\sqrt{2}}{a}$	0
1 {111}	$\frac{\sqrt{3}}{a}$	$(4 - 4i) f_c$
{200}	$\frac{2}{a}$	0
{120}	$\frac{\sqrt{5}}{a}$	0
2 {220}	$\frac{2\sqrt{2}}{a}$	$8 f_c$
3 {311}	$\frac{\sqrt{11}}{a}$	$(4 + 4i) f_c$
4 {400}	$\frac{4}{a}$	$8 f_c$

Note that if h, k, l are mixed the reflection is systematically absent (shown for (1 0 0) (1 1 0) (1 2 0).)

You can also show easily that

$$\left.\begin{array}{ll} (2\,2\,1) & |\vec{S}| = \frac{\sqrt{9}}{d} \\ (3\,0\,0) & |\vec{S}| = \frac{\sqrt{9}}{d} \\ (3\,1\,0) & |\vec{S}| = \frac{\sqrt{10}}{d} \\ (2\,2\,2) & |\vec{S}| = \frac{\sqrt{12}}{d} \\ (3\,2\,0) & |\vec{S}| = \frac{\sqrt{13}}{d} \\ (3\,2\,1) & |\vec{S}| = \frac{\sqrt{14}}{d} \end{array}\right\} \text{ are absent}$$

the first four reflections are
$\{1\,1\,1\}$ $\{2\,2\,0\}$ $\{3\,1\,1\}$ $\{4\,0\,0\}$

② If the structure is Fe S.

$$F_{hkl} = \overset{24\bar{e}}{f_{Fe^{2+}}}\left(1 + (-1)^{h+k} + (-1)^{k+l} + (-1)^{h+l}\right) +$$

$$\underset{18\bar{e}}{f_{S}}\left((-1)^{\frac{h+k+l}{2}} + (-1)^{\frac{(3h+3k+l)}{2}} + (-1)^{\frac{(h+3k+3l)}{2}} + (-1)^{\frac{(3h+k+3l)}{2}}\right).$$

some of the F_{hkl} terms that were zero for diamond will no longer be zero

FeS will have non-zero values for the following (hkl) planes.

$\{111\}$ $F_{111} = 4 f_{Fe^{2+}} - 4i f_{S^{2-}}$

$\{200\}$ $F_{200} = 4 f_{Fe^{2+}} - 4 f_{S^{2-}}$

$\{220\}$ $F_{220} = 4 f_{Fe^{2+}} + 4 f_{S^{2-}}$

$\{311\}$ $F_{311} = 4 f_{Fe^{2+}} + 4i f_{S^{2-}}$

Part c) see solution given as handout.

Note that in Problem # 6 the Bragg or Glancing angle (i.e. θ) was 6°. The diffraction angle (i.e 2θ) would be 12°.

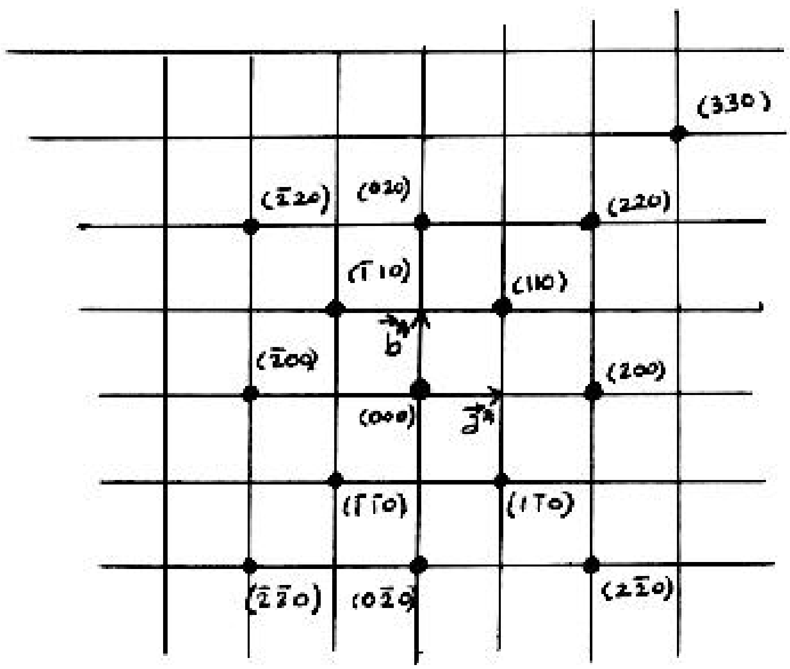
Problem # 7

Body centered cubic crystal oriented with [001] direction parallel to direction of electron beam.

Ewald sphere has a radius $\frac{1}{\lambda}$ ⇒ Since λ is very small then the radius of the sphere is very large → Ewald sphere is a plane.

The direction of the incident electron beam is parallel to [001]. Since the crystal is bcc, [001] of the crystal is parallel to $\vec{z}^*$ ([001] ⊥ (001) for cubic crystals and $\vec{c}^*$ the normal to (001) planes is parallel to $\vec{z}$)

⇒ The Ewald plane contains $\vec{a}^*$, $\vec{b}^*$



bcc crystal
(h, k, l) all odd are systematically absent.

$\left.\begin{array}{l}(1,0,0)\\(0,1,0)\\(1,2,0)\\(2,1,0)\\(3,0,0)\\(0,3,0)\\\text{etc}\end{array}\right\}$ absent

Solution for Imperfections:

① View the Formation of an MgO Schottky Defect as the following reaction

$$\text{Null} \longrightarrow V_{Mg^{2+}} + V_{O^{2-}}$$ one vaccancy of Mg^{2+} + one vacancy of O^{2-}

$$[V_{Mg^{2+}}][V_{O^{2-}}] = \exp\left[-\frac{\Delta G_s^{\circ}}{RT}\right]$$

since $[V_{Mg^{2+}}] = [V_{O^{2-}}]$ then

$$x = [V_{Mg^{2+}}] = [V_{O^{2-}}] = \exp\left[-\frac{\Delta G_s^{\circ}}{2R}\right]$$

$x = 4.2\ 10^{-51} \simeq 0$ at 300 K.

$x = 2.4\ 10^{-12}$ at 1300 K.

$x = 2.7\ 10^{-7}$ at 230 K.

② Energy of a Dislocation $\propto |\vec{b}|^2$.

in bcc $\quad a\langle 100\rangle \quad |\vec{b}|^2 = a^2$

$\quad \frac{a}{2}\langle 111\rangle \quad |\vec{b}|^2 = \frac{3}{4}a^2$.

$\Rightarrow \frac{a}{2}\langle 111\rangle$ dislocation (Burger vector) is less energetic than $a\langle 100\rangle$

$\Rightarrow \frac{a}{2}\langle 111\rangle$ forms in preference over $a\langle 100\rangle$

③ bcc

(110)	$[\bar{1}11]\ [1\bar{1}1]$
$(\bar{1}10)$	$[111]\ [11\bar{1}]$
(101)	$[\bar{1}11]\ [11\bar{1}]$
$(\bar{1}01)$	$[111]\ [1\bar{1}1]$
(011)	$[1\bar{1}1]\ [11\bar{1}]$
$(0\bar{1}1)$	$[111]\ [\bar{1}11]$

see attached picture to visualize.
(next page)

fcc.

(111)	$[\bar{1}10]\ [\bar{1}01]\ [0\bar{1}1]$
$(\bar{1}11)$	$[110]\ [101]\ [0\bar{1}1]$
$(1\bar{1}1)$	$[110]\ [\bar{1}01]\ [011]$
$(11\bar{1})$	$[\bar{1}10]\ [101]\ [011]$

④ ⓐ $\vec{b}_T = \vec{b}_1 + \vec{b}_2$

$$= \frac{a}{6}[\bar{1}2\bar{1}] + \frac{a}{6}[1\bar{1}2]$$

$$\vec{b}_T = \frac{a}{6}[011]$$

ⓑ $$|\vec{b}_T|^2 = \frac{a^2}{36}(1+1) = \frac{a^2}{18}$$

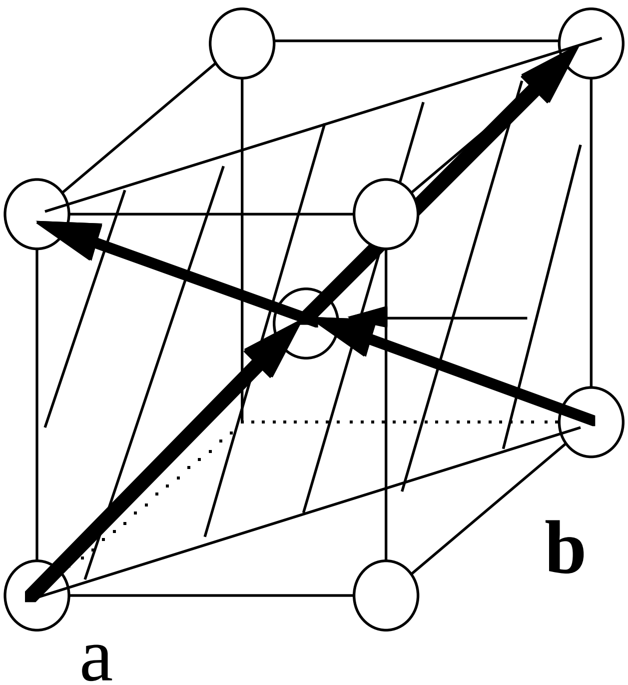
$$|\vec{b}_1|^2 + |\vec{b}_2|^2 = \frac{a^2}{36}\left[(1+4+1)+(1+1+4)\right]$$

$$= \frac{6a^2}{18} > \frac{a^2}{18}$$

$\Rightarrow$ combination of dislocations is feasible.

Example of Slip System:
Slip plane + Burgers vector in the Slip Plane

bcc structure



(110) Slip plane is a densely-packed plane (containing densely packed directions).

Burgers vectors: (a/2)<111> are in the slip plane and their length is equal to an interatomic distance along the most densely packed directions.

c) The resulting dislocation cannot glide in (111) or ($\bar{1}$11) because it is not parallel to either plane –

$\vec{b}_T$ is not parallel to either plane, because $\vec{b}_T$ is not normal to either plane normals

$(111) \perp [111]$
$(\bar{1}11) \perp [\bar{1}11]$

$[111] \not\perp \frac{a}{6}[011]$ since $\frac{a}{6}(1\times0+1\times1+1\times1) \neq 0$

$[\bar{1}11] \not\perp \frac{a}{6}[011]$ since $\frac{a}{6}(\bar{1}\times0+1\times1+1\times1) \neq 0$