2.14

<u>bcc</u>

$$\delta_0 = (0,0,0)\cdot a$$
$$\delta_1 = \left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)\cdot a$$

$$F = \sum_j f_{a_j} e^{i\vec{s}\vec{\delta_j}} = f_a\left[1 + e^{i(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)\cdot \delta_1}\right]$$

$$= f_a\left[1 + e^{i\pi(h+k+l)}\right]$$

$\Rightarrow$ when $h+k+l$ = odd $\quad F = 0$

$\Rightarrow$ (100), (111), (210) will be missing

<u>fcc</u>

$$\delta_0 = (0,0,0)a$$
$$\delta_1 = \left(\frac{1}{2},\frac{1}{2},0\right)a$$
$$\delta_2 = \left(0,\frac{1}{2},\frac{1}{2}\right)a$$
$$\delta_3 = \left(\frac{1}{2},0,\frac{1}{2}\right)a$$

$$\Rightarrow F = 1 + e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(h+l)}$$

$\Rightarrow F \neq 0$ if h, k, l are all even or all odd

$\Rightarrow$ (100), (110), (210), (211) are missing

2.16

$f_{Cs} = 3 f_{Cl}$

Cs in the corner, Cl in the center.

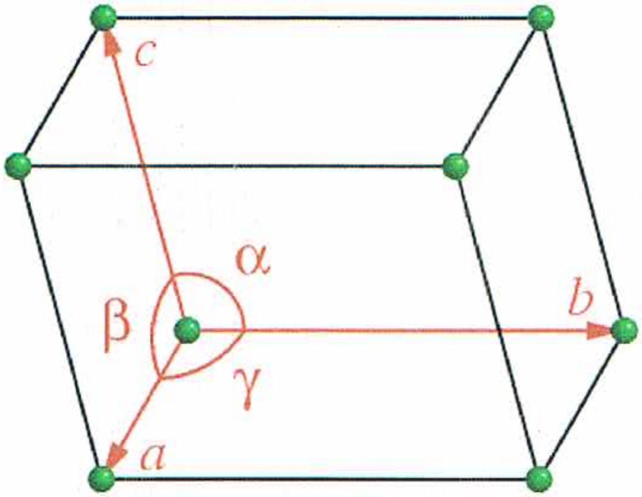
$$F_{100} = f_{Cs} + f_{Cl}\, e^{2\pi i \left(\frac{1}{2}h + \frac{1}{2}k + \frac{1}{2}e\right)} =$$
$$= f_{Cl}\left(3 + e^{i\pi(h+k+e)}\right) = 2 f_{Cl}$$

Cl in the corner, Cs in the center

$$F_{100} = f_{Cl} + 3 f_{Cl}\, e^{i\pi(h+k+e)} = -2 f_{Cl}$$

In both cases, we notice that $f_{Cs} \neq f_{Cl}$, so the lattice can no longer be regarded as th bcc lattice with all the same atoms in the unit cell.

2.20



$a = 4\ A$

$b = 6\ A$

$c = 8\ A$

$\alpha = \beta = 90^\circ$

$\gamma = 120^\circ$

a) $\vec{a} = a(1,0,0)$

$\vec{b} = b(\cos 120^\circ, \sin 120^\circ, 0) = b\left(-\frac{1}{2}, \frac{\sqrt{3}}{2}, 0\right)$

$\vec{c} = c(0,0,1)$

$$\Omega_c = |\vec{a}(\vec{b}\times\vec{c})| = |\vec{b}(\vec{c}\times\vec{a})| = abc\,\frac{\sqrt{3}}{2}$$

$$\vec{a}^* = \frac{2\pi\ \cancel{b}\cancel{c}}{\left(\frac{\sqrt{3}}{2}\right)a\cancel{b}\cancel{c}} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 1 \end{vmatrix} = \frac{4\pi}{\sqrt{3}a}\cdot\frac{\sqrt{3}}{2}\hat{x} + \frac{4\pi}{\sqrt{3}a}\,\frac{1}{2}\hat{y} =$$

$$= \frac{2\pi}{a}\hat{x} + \frac{2\pi}{\sqrt{3}a}\hat{y}$$

$$\vec{b}^* = \frac{2\pi\ \cancel{c}\cancel{a}}{\left(\frac{\sqrt{3}}{2}\right)\cancel{a}b\cancel{c}} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{vmatrix} = \frac{4\pi}{\sqrt{3}\,b}\hat{y} = \frac{2\pi}{3\sqrt{3}}\hat{y}$$

$$\vec{c}^* = \frac{2\pi\ \cancel{a}b}{\left(\frac{\sqrt{3}}{2}\right)\cancel{a}bc} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & 0 & 0 \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \end{vmatrix} = \frac{4\pi}{\sqrt{3}c}\,\frac{\sqrt{3}}{2}\hat{z} = \frac{2\pi}{c}\hat{z} = \frac{\pi}{4}\hat{z}$$

b) Volume of the real cell:

$$\Omega_c = abc\,\frac{\sqrt{3}}{2} = 4 \cdot 6 \cdot 8 \cdot \frac{\sqrt{3}}{2} = 166.27\ A^3$$

Volume of the reciprocal cell

$$\frac{(2\pi)^3}{\Omega_c} = \frac{(2\pi)^3\ 2}{abc\sqrt{3}} = 1.49\ A^{-3}$$

c) The spacing between the (210) planes

$$d_{210} = \frac{1}{\left(\frac{2^2}{4^2} + \frac{1}{6^2}\right)^{\frac{1}{2}}} = 1.89\ \mathring{A}$$

d) The Bragg angle θ for refraction from the above planes.

$$2 d_{210} \sin\theta = \lambda$$

$$\Rightarrow \theta = \sin^{-1}\left(\frac{\lambda}{2 d_{210}}\right)$$

2.21

$$\gamma = \frac{dV}{V}$$

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

$$\frac{d}{d\theta}\left(2d\sin\theta\right) = \frac{d\lambda}{d\theta}$$

$$d\cos\theta + \sin\theta\,\frac{d(d)}{d\theta} = 0$$

$$d\theta = -\tan\theta\,\frac{d(d)}{d}$$

some constant

$$V = c\,d^3$$

$$dV = 3d^2\,d(d) \Rightarrow \frac{d(d)}{d} = \frac{dV}{3d^3} = \frac{dV}{3V} = \frac{\gamma}{3}$$

$$\Rightarrow d\theta = -\frac{\gamma}{3}\tan\theta$$

3.2 Since both longitudinal (compressional) and transverse (shear) waves can be transmitted by the solid, and since their speeds are different, we replace v_s in (3.20) by

$$\frac{3}{v_s^3} = \left(\frac{1}{v_e^3} + \frac{2}{v_t^3}\right)$$

$$\Rightarrow \quad g(\omega) = \frac{V}{2\pi^2} \omega^2 \left(\frac{1}{v_e^3} + \frac{2}{v_t^3}\right)$$

3.4

$$Z = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp\left(-\frac{1}{k_B T}\left[\frac{p^2}{2m} + \frac{1}{2} k x^2\right]\right) dp\, dx =$$

$$= \int_{-\infty}^{\infty} \exp\left(-\frac{p^2}{2 m k_B T}\right) dp \int_{-\infty}^{\infty} \exp\left(-x^2\left(\frac{k}{k_B T}\right)\right) dx$$

$$k = m\omega^2 \qquad \beta = \frac{1}{k_B T}$$

$$= \sqrt{2 m k_B T \pi}\ \sqrt{\pi k_B T / m\omega^2} = \pi k_B T / \omega = \frac{\pi}{\beta\omega}$$

$$E = -\frac{\partial}{\partial\beta} \ln Z = \frac{1}{\beta} = k_B T$$

3.8

$$E = \frac{3V}{2\pi^2 v_s^3} \int_0^{\omega_D} \frac{\hbar\omega^3}{e^{\hbar\omega/k_BT}-1}\, d\omega$$

$$C_V = \left(\frac{dE}{dT}\right)_V = \frac{3V}{2\pi^2 v_s^3} \int_0^{\omega_D} \frac{\hbar\omega^3 \, \frac{\hbar\omega}{k_B}\, \frac{1}{T^2}\, e^{\hbar\omega/k_BT}}{\left(e^{\hbar\omega/k_BT}-1\right)^2}\, d\omega$$

$$= \frac{3V\ \hbar^2}{2\pi\, v_s^3\, k_B T^2} \int_0^{\omega_D} \frac{\omega^4\, e^{\hbar\omega/k_BT}}{\left(e^{\hbar\omega/k_BT}-1\right)^2}\, d\omega$$

$$x = \frac{\hbar\omega}{k_BT} \qquad \Theta_D = \frac{\hbar\omega_D}{k} \qquad \Rightarrow \quad \omega = \frac{x k_B T}{\hbar}$$

$$C_V = \frac{3V\hbar^2}{2\pi v_s^3 k_B T^2}\frac{(k_BT)^5}{\hbar^5} \int^{\Theta_D/T} \frac{x^4\, e^x dx}{(e^x-1)^2} =$$

$$= \frac{3V\ k_B^4\, T^3}{2\pi\, v_s^3\, \hbar^3} \int_0^{\Theta_D/T} \frac{x^4 e^x dx}{(e^x-1)^2}$$

$$\omega_D = v_s\,(6\pi^2 n)^{1/3} = v_s\left(6\pi^2 \frac{N_A}{V}\right)^{1/3}$$

$$\Rightarrow v_s^3 = \left(\frac{\Theta_D k_B}{\hbar}\right)^3 \frac{V}{N_A\ 6\pi^2}$$

$$\Rightarrow C_V = \frac{3V\hbar^2\ k_B^4\ T^3\ N_A \cdot 6\pi\hbar^3}{2\pi\ V\ \Theta_D^3\ k_B^3\ \hbar^3} \int^{\Theta_D/T} \frac{x^4 e^x dx}{(e^x-1)^2} =$$

$$= 9R\left(\frac{T}{\Theta_D}\right)^3 \int_0^{\Theta_D/T} \frac{x^4 e^x \cancel{dx}}{(e^x-1)^2}\, dx$$