Solution.

1.

With respect to a simple cubic, fcc has four lattice points in a cell and hence four members in the basis :

$$\vec{r}_i = \left\{\vec{0}, \frac{1}{2}(\vec{a}_1 + \vec{a}_2), \frac{1}{2}(\vec{a}_1 + \vec{a}_3), \frac{1}{2}(\vec{a}_2 + \vec{a}_3)\right\}$$

If $\vec{K} = h\vec{b}_1 + k\vec{b}_1 + \ell\vec{b}_1$

$$\therefore S_{\vec{K}} = \sum_i e^{i\vec{K}\cdot\vec{r}_i} = \exp(0) + \exp(\frac{1}{2}\cdot h\cdot 2\pi + \frac{1}{2}\cdot k\cdot 2\pi) + \exp(\frac{1}{2}\cdot h\cdot 2\pi + \frac{1}{2}\cdot \ell\cdot 2\pi) + \exp(\frac{1}{2}\cdot k\cdot 2\pi + \frac{1}{2}\cdot \ell\cdot 2\pi)$$

$$= 1 + \exp(h+k)\pi + \exp(h+\ell)\pi + \exp(k+\ell)\pi$$

$$= \begin{cases} 4 & \text{if } h, k, \ell \text{ are all odd or all even} \\ 0 & \text{otherwisw} \end{cases}$$

Condition for diffraction : $\underline{\underline{h, k, \ell \text{ are all odd or all even}}}$

Bragg's law : $2d\sin\theta = \lambda$. The first peak corresponds to the smallest θ and hence the longest d.

$$d = \frac{a}{\sqrt{h^2 + k^2 + \ell^2}}$$

d is longest for the (111) peak (all odd). <u>Hence the first peak is the (111) peak.</u>

(b) $\theta = 25.38^o$, $2d\sin\theta = \lambda \Rightarrow 2d\sin 25.38^o = 1.789\,\mathring{A}$

$$\Rightarrow d = 2.087\,\mathring{A}$$

$$d = \frac{a}{\sqrt{h^2 + k^2 + \ell^2}} \Rightarrow a = 2.087\,\mathring{A}\times\sqrt{3} = \underline{\underline{3.615\,\mathring{A}}}$$

(c) Lattice constant at 1200K $= 3.615\,\mathring{A}[1 + 1.91\times10^{-5}\times(1200-300)]$

$$= 3.677\,\mathring{A}$$

$$d = \frac{a}{\sqrt{h^2 + k^2 + \ell^2}} = \frac{3.677\,\mathring{A}}{\sqrt{3}} = 2.123\,\mathring{A}$$

$$2d\sin\theta = \lambda \Rightarrow 2\times 2.123\,\mathring{A}\times\sin\theta = 1.789\,\mathring{A} \Rightarrow \sin\theta = 0.4213$$

$$\Rightarrow \sin\theta = \underline{\underline{24.92^o}}$$

2.

$\omega = 2\pi\nu$ and $k = \dfrac{2\pi}{\lambda}$, hence the dispersion relation is given by

$$\left(\frac{\omega}{2\pi}\right)^2 = \frac{2\pi\sigma}{\rho}\left(\frac{k}{2\pi}\right)^3 \quad \Rightarrow \omega^2 = \frac{\sigma k^3}{\rho}$$

For a two dimensional system, the density of state is given by

$$D(\omega)d\omega = \frac{1}{A}\frac{2\pi k dk}{\frac{(2\pi)^2}{A}}$$