1. For the following problem you may find the following equations useful:

\[
n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}} e^{i\vec{G} \cdot \vec{r}} \quad n_{\vec{G}} = \frac{1}{V_c} \int d^3 \vec{r} n(\vec{r}) e^{-i\vec{G} \cdot \vec{r}}
\]

\[
f = \int d^3 \vec{r} n(\vec{r}) e^{-i\vec{G} \cdot \vec{r}} \quad S_{\vec{G}} = \sum_{j} f_{j} e^{-i\vec{G} \cdot \vec{r}}
\]

\[
n\lambda = 2d \sin \theta \quad \Delta \vec{k} = \vec{G}
\]

(a) In the hypothetical 2D crystal structure shown below, the large and small atoms are of different types, respectively gallium (Z=31) and arsenic (Z=33). Draw the outline of one unit cell. Write expressions for the primitive translation vectors \( \mathbf{a}_1 \) and \( \mathbf{a}_2 \) and draw these on the figure. Draw and label lattice planes of Miller indices \((1,0)\) \((0,1)\) \((1,1)\) \((1,2)\) \((2,1)\). Write the unit cell basis \( \{\mathbf{R}_i, Z_i\} \).

**Answer:** \( \mathbf{a}_1 = 2\hat{x} \) and \( \mathbf{a}_2 = 1\hat{y} \). Basis is Ga (Z=31) at \( \mathbf{R}_1 = (0, 0) \) and As (Z=33) at \( \mathbf{R}_2 = \frac{1}{2}\mathbf{a}_1 \).
(b) Write expressions for the primitive reciprocal lattice vectors \( \mathbf{b}_1 \) and \( \mathbf{b}_2 \). On the axes shown below, plot points at the locations of diffraction peaks of Miller indices \((1,0) \ (0,1) \ (1,1) \ (1,2) \ (2,1)\). Please be careful to place the points accurately, and label them. For each peak state the position in reciprocal space and the value of the structure factor \( S_G \).

**Answer:**
Recall the definition of \( \mathbf{b}_i \): \( \mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij} \). Thus \( \mathbf{b}_1 = \pi \hat{x}, \mathbf{b}_2 = 2\pi \hat{y} \). A peak of Miller indices \((hk)\) is a position \( \mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 \). Noting that \( \mathbf{G} \cdot \mathbf{R}_1 = 0 \) and \( \mathbf{G} \cdot \mathbf{R}_2 = h\pi \), and setting \( f_i = Z_i \), we have

\[
S_G = \begin{cases} 
64 & h \text{ (even)} \\
-2 & h \text{ (odd)} 
\end{cases}
\]

(c) Owing to electronegativity differences, arsenic can draw an electron from gallium. What extinctions (vanishing peaks) would occur in this case?

**Answer:**
In this case \( f_1 = f_2 = 32 \), so \( S_G = 0 \) for odd values of \( h \).
2. (adapted from Kittel #3.8) Recall the Voigt notation,

\[
\begin{array}{cccc}
xx & \rightarrow & 1 \\
zy & \rightarrow & 4 \\
yy & \rightarrow & 2 \\
zx & \rightarrow & 5 \\
zz & \rightarrow & 3 \\
xy & \rightarrow & 6 \\
\end{array}
\]

and the fact that for cubic symmetry the elastic tensor has only three independent constants, \(C_{11}\), \(C_{12}\), and \(C_{44}\). Consider the following figure of an \(L \times L \times L\) cube stretched by \(dx > 0\) that spontaneously shrinks by \(dy = dz < 0\). Stresses lie along the \(x\) direction but not \(y\) or \(z\). The material is a cubic crystal whose symmetry axes are aligned with the cube.

\(\text{L+dx} \quad \text{L} \quad \text{L+dy}\)

(a) Derive an expression for the Poisson ratio \(\nu \equiv -dy/dx\) in terms of the constants \(C_{ij}\).

**Answer:**
Consider \(\sigma_2 = C_{21}e_1 + C_{22}e_2 + C_{23}e_3\). Recall that \(C_{21} = C_{23} = C_{12}\) and \(e_3 = e_2 = dy/L\). We are given that \(e_1 = dx/L\) and \(\sigma_2 = 0\). Hence the Poisson ratio

\[
\nu = \frac{C_{12}}{C_{11} + C_{12}}
\]

(b) Derive an expression for the Young’s modulus \(E \equiv \sigma_1/e_1\).

**Answer:** Using the known symmetries, we have \(\sigma_1 = C_{11}e_1 + C_{12}e_2 + C_{12}e_2\), and from part (a) we have \(e_2 = -\nu e_1\). Hence

\[
E = C_{11} - \frac{2C_{12}^2}{C_{11} + C_{12}}
\]
3. (Adapted from Kittel, “Elastic waves in cubic crystals”)  
(a) Elastic waves propagating with $\mathbf{K}$ in the cubic [hkl] direction exhibit one longitudinally polarized mode and two transversely polarized modes only for special values of [hkl]. State these values and briefly justify your assertion without calculation.

**Answer:**

Special polarizations depend on rotational symmetries. The high symmetry directions in a cubic crystal are: [100] (4x), [110] (2x), and [111] (3x). Cyclic permutations of the indices are implicit.

(b) For what values of [hkl] do the two transverse sound velocities equal each other? Briefly justify your answer without calculation.

**Answer:**

For $\mathbf{K}$ along a four-fold symmetry axis, a 90° rotation about $\mathbf{K}$ converts one transverse mode into the other, hence their velocities are equal. Similarly, for $\mathbf{K}$ along a three-fold symmetry axis, a 120° rotation leaves the sound velocity invariant, while mixing the two transverse modes. Hence their velocities must be equal. In contrast, a 180° rotation about a two-fold axis does not mix the transverse modes so in general their velocities will differ.