NAME: SOLUTIONS

33-448 Solid State Physics Midterm #1 Wednesday, Feb. 10, 2016

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

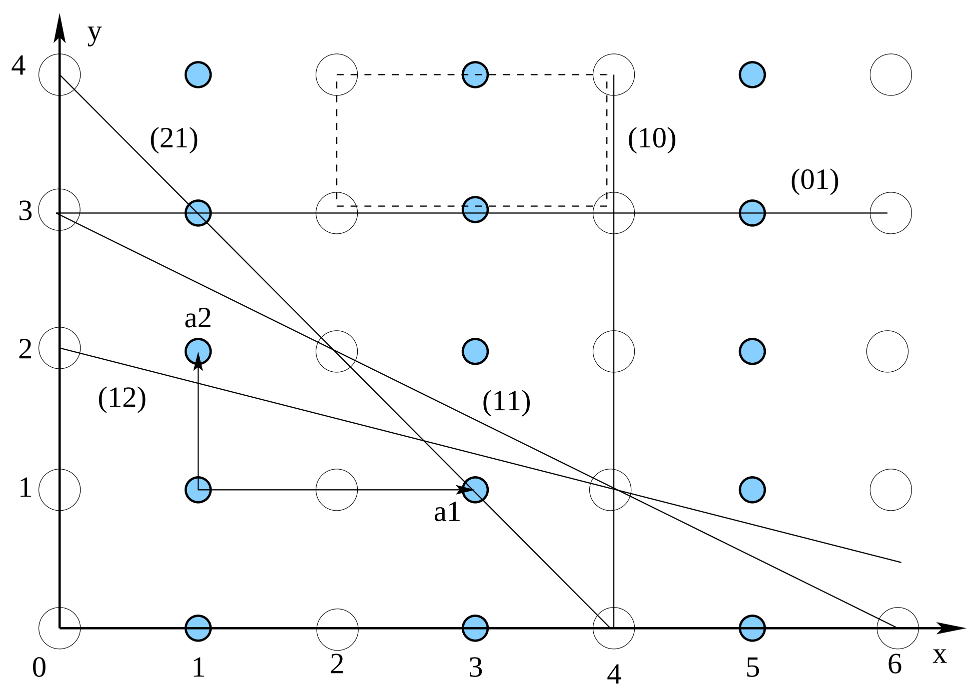
$$n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \qquad n_{\vec{G}} = \frac{1}{V_c}\int d^3\vec{r}\, n(\vec{r}) e^{-i\vec{G}\cdot\vec{r}}$$

$$f = \int d^3\vec{r}\, n(\vec{r}) e^{-i\vec{G}\cdot\vec{r}} \qquad S_{\vec{G}} = \sum_j f_j e^{-i\vec{G}\cdot\vec{r}}$$

$$n\lambda = 2d\sin\theta \qquad \Delta\vec{k} = \vec{G}$$

(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: $\mathbf{a}_1 = 2\hat{\mathbf{x}}$ and $\mathbf{a}_2 = 1\hat{\mathbf{y}}$. Basis is Ga (Z=31) at $\mathbf{R}_1 = (0,0)$ and As (Z=33) at $\mathbf{R}_2 = \frac{1}{2}\mathbf{a}_1$.

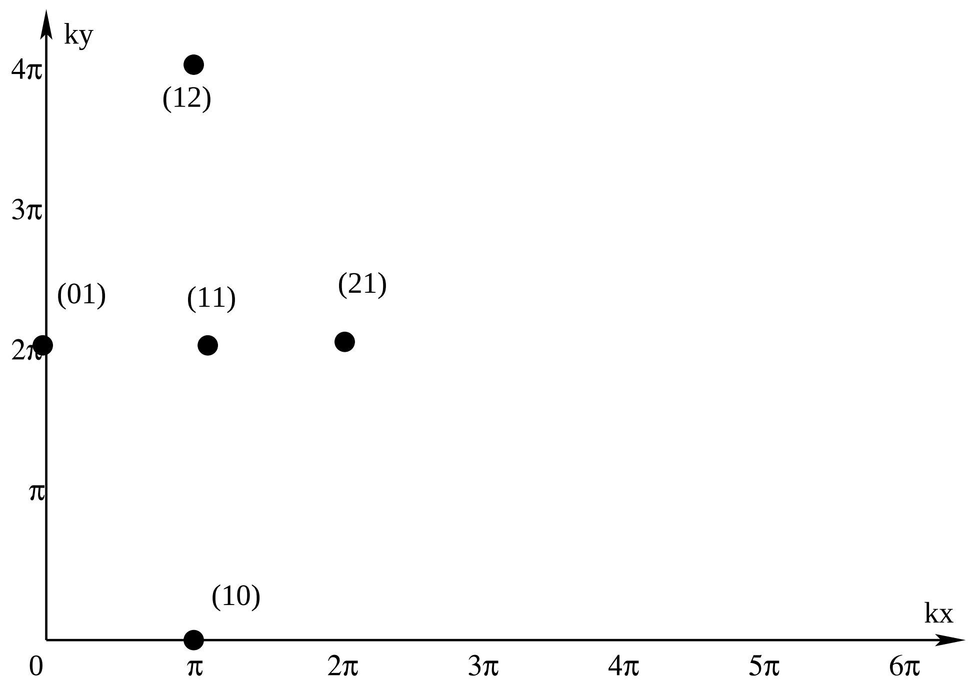


(b) Write expressions for the primitive reciprocal lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$. On the axes shown below, plot points at the locations of diffraction peaks of Miller indices (1,0) (0,1) (1,1) (1,2) (2,1). Please be careful to place the points accurately, and label them. For each 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 $\mathbf{b}_1 = \pi\hat{\mathbf{x}}, \mathbf{b}_2 = 2\pi\hat{\mathbf{y}}$. 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

$$S_{\mathbf{G}} = \begin{cases} 64 & h \text{ (even)} \\ -2 & h \text{ (odd)} \end{cases}$$



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

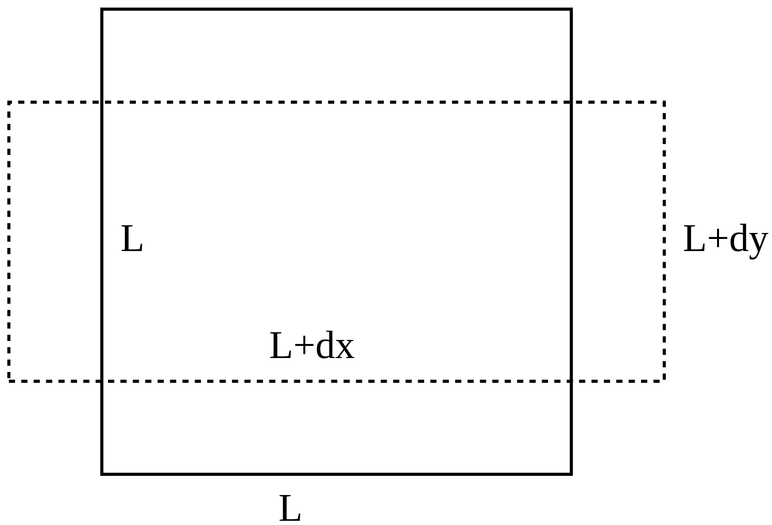
Answer:

In this case $f_1 = f_2 = 32$, so $S_{\mathbf{G}} = 0$ for odd values of h.

2. (adapted from Kittel #3.8) Recall the Voigt notation,

$$xx \to 1 \qquad yz \to 4$$
$$yy \to 2 \qquad zx \to 5$$
$$zz \to 3 \qquad xy \to 6$$

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 $LxLxL$ 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.



(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 **K** in the cubic $[hkl]$ direction exhibit one longitudinally polarized mode and two transversely polarized modes only for special values of $[hkl]$. States 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 **K** along a four-fold symmetry axis, a 90° rotation about **K** converts one transverse mode into the other, hence their velicities are equal. Similarly, for **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.