Homework 2 Solutions

Problem 1

1×1 cell:

The crystal structure of graphene is a hexagonal lattice with a two-atom basis. The 1×1 cell is defined by the primitive vectors

$$\mathbf{a}_1 = a\left(0,\, -\sqrt{3}\right) \tag{1}$$

$$\mathbf{a}_2 = a\left(\frac{3}{2},\, \frac{\sqrt{3}}{2}\right), \tag{2}$$

where a is the distance between nearest-neighbor carbon atoms in the honeycomb lattice. The primitive lattice vectors are illustrated in Figure 1. There are two atoms in this cell, located at

$$\boldsymbol{\tau}_A = (0,\, 0) \tag{3}$$

$$\boldsymbol{\tau}_B = (a,\, 0)\,. \tag{4}$$

We can find the reciprocal lattice vectors using $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$. Doing so yields

$$\mathbf{b}_1 = \frac{2\pi}{a}\left(\frac{1}{3},\, -\frac{1}{\sqrt{3}}\right) \tag{5}$$

$$\mathbf{b}_2 = \frac{2\pi}{a}\left(\frac{2}{3},\, 0\right) \tag{6}$$

.

$\sqrt{3} \times \sqrt{3}$R30 cell

The $\sqrt{3} \times \sqrt{3}R30$ cell of graphene is illustrated in Figure 2. The lattice vectors for this cell are

$$\mathbf{a}_1' = a\left(\frac{3}{2}, -\frac{3\sqrt{3}}{2}\right) \tag{7}$$

$$\mathbf{a}_2' = a\left(\frac{3}{2}, \frac{3\sqrt{3}}{2}\right). \tag{8}$$

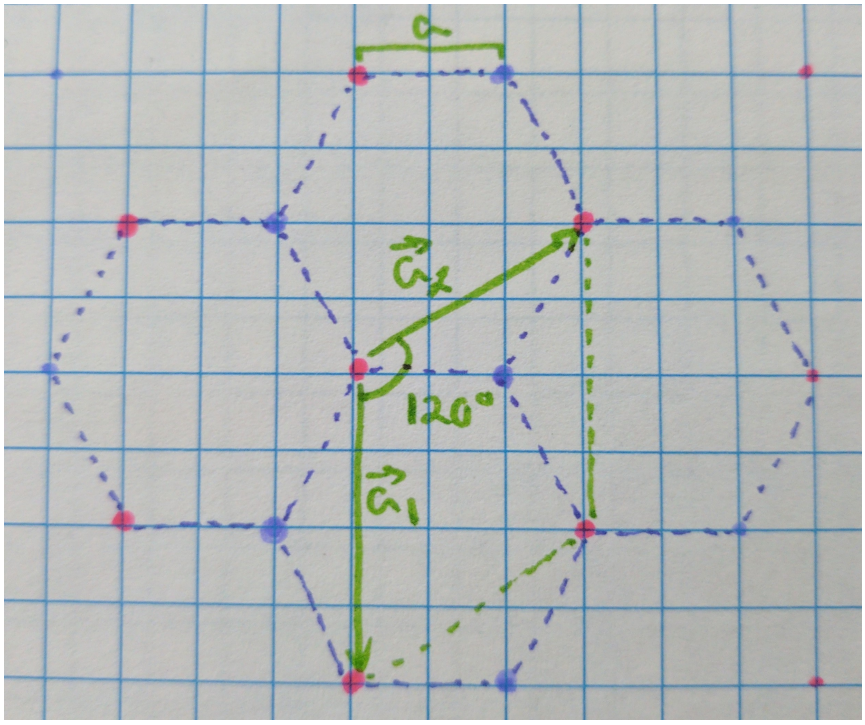

Figure 1: Graphene 1×1 cell.

There are six atoms in this cell, located at

$$\boldsymbol{\tau}_1 = (0,\, 0) \tag{9}$$
$$\boldsymbol{\tau}_2 = a\,(1,\, 0) \tag{10}$$
$$\boldsymbol{\tau}_3 = a\left(\frac{3}{2},\, \frac{\sqrt{3}}{2}\right) \tag{11}$$
$$\boldsymbol{\tau}_4 = a\left(\frac{3}{2},\, -\frac{\sqrt{3}}{2}\right) \tag{12}$$
$$\boldsymbol{\tau}_5 = a\left(1,\, \sqrt{3}\right) \tag{13}$$
$$\boldsymbol{\tau}_6 = a\left(1,\, -\sqrt{3}\right). \tag{14}$$

If this isn't clear to you, note that not all of the atoms in the cell in the illustration are unique. There are only 3 unique atoms on the corners and sides of the cell–the others are periodic images. The other 3 atoms are inside the cell.

Problem 2

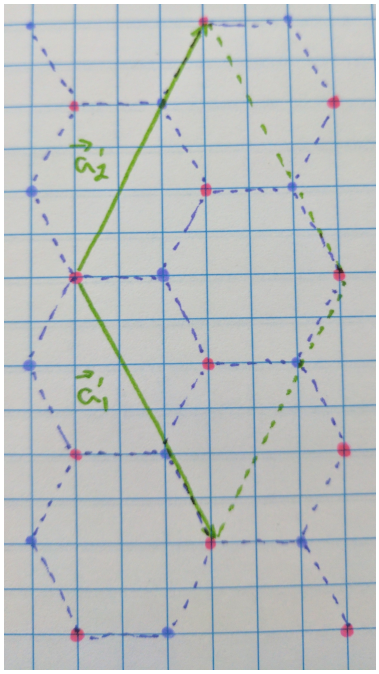

Figure 2: Graphene $\sqrt{3} \times \sqrt{3}R30$ cell.

We can find the bond angle using elementary vector analysis. In the conventional cell, two of the nearest neighbors of the atom at the origin are in the $\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}}$ and $-\hat{\mathbf{x}}-\hat{\mathbf{y}}+\hat{\mathbf{z}}$ directions. We can find the angle between these two vectors using $\theta = \arccos\left(\frac{\mathbf{a}\cdot\mathbf{b}}{|\mathbf{a}||\mathbf{b}|}\right)$. The argument of the inverse cosine is then $-1/3$, which gives us an angle of

$$\boxed{\theta = 109.471^\circ = 1.911\,\text{rad}} \tag{15}$$

Problem 3

The reciprocal lattice vectors for the primitive fcc cell are (see **Problem 4**)

$$\mathbf{b}_1' = \frac{4\pi}{a}\frac{1}{2}\left(\hat{\mathbf{y}}+\hat{\mathbf{z}}-\hat{\mathbf{x}}\right) \tag{16}$$

$$\mathbf{b}_2' = \frac{4\pi}{a}\frac{1}{2}\left(\hat{\mathbf{z}}+\hat{\mathbf{x}}-\hat{\mathbf{y}}\right) \tag{17}$$

$$\mathbf{b}_3' = \frac{4\pi}{a}\frac{1}{2}\left(\hat{\mathbf{x}}+\hat{\mathbf{y}}-\hat{\mathbf{z}}\right), \tag{18}$$

where the primes are to distinguish these vectors from the conventional cell's reciprocal lattice vectors. In the conventional cell basis, the planes (100) and (001) are normal to the reciprocal lattice vectors $\mathbf{b}_1 = \frac{2\pi}{a}\hat{\mathbf{x}}$ and $\mathbf{b}_3 = \frac{2\pi}{a}\hat{\mathbf{z}}$. To find the miller indices in terms of the reciprocal lattice vectors of the primitive cell, we need to find the linear combination of reciprocal lattice

vectors that will equal the vectors in the conventional cell. Multiplying $\mathbf{b}_2'$ and $\mathbf{b}_3'$ by 1/2 and adding them together yields

$$\frac{1}{2}\left(\mathbf{b}_2' + \mathbf{b}_3'\right) = \mathbf{b}_1 = \frac{2\pi}{a}\hat{\mathbf{x}}. \tag{19}$$

Removing the factor of 1/2, we can therefore write the (100) plane in the miller indices of the primitive cell as $(011)'$. We can do the same for the (001) plane. Altogether, we have

$$\boxed{\begin{array}{l}(100) \to (011)' \\ (001) \to (110)'\end{array}} \tag{20}$$

Problem 4

Recall that the reciprocal lattice vectors are given in terms of the primitive lattice vectors by

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \tag{21}$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \tag{22}$$

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \tag{23}$$

Applying these formulas, we find that the reciprocal lattice of the simple cubic lattice is a simple cubic lattice with side lengths $2\pi/a$. The reciprocal lattice of an fcc lattice is a bcc lattice with side lengths $4\pi/a$, and the reciprocal lattice of a bcc lattice is an fcc lattice with side lengths $4\pi/a$. Explicitly, the reciprocal lattice vectors are

$$\boxed{\begin{array}{llll}
\text{sc:} & \mathbf{b}_1 = \dfrac{2\pi}{a}\hat{\mathbf{x}}, & \mathbf{b}_2 = \dfrac{2\pi}{a}\hat{\mathbf{y}}, & \mathbf{b}_3 = \dfrac{2\pi}{a}\hat{\mathbf{z}} \\
\text{fcc:} & \mathbf{b}_1 = \dfrac{4\pi}{a}\dfrac{1}{2}\left(\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}\right), & \mathbf{b}_2 = \dfrac{4\pi}{a}\dfrac{1}{2}\left(\hat{\mathbf{z}} + \hat{\mathbf{x}} - \hat{\mathbf{y}}\right), & \mathbf{b}_3 = \dfrac{4\pi}{a}\dfrac{1}{2}\left(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}\right) \\
\text{bcc:} & \mathbf{b}_1 = \dfrac{4\pi}{a}\dfrac{1}{2}\left(\hat{\mathbf{y}} + \hat{\mathbf{z}}\right), & \mathbf{b}_2 = \dfrac{4\pi}{a}\dfrac{1}{2}\left(\hat{\mathbf{x}} + \hat{\mathbf{z}}\right), & \mathbf{b}_3 = \dfrac{4\pi}{a}\dfrac{1}{2}\left(\hat{\mathbf{x}} + \hat{\mathbf{y}}\right)
\end{array}} \tag{24}$$

Problem 5

Recall that the structure factor is given by

$$S_{\mathbf{K}} = \sum_{j=1}^{n} \exp\left(i\mathbf{K} \cdot \mathbf{d}_j\right). \tag{25}$$

The conventional cell of diamond has 8 atoms located at

$$\mathbf{d}_1 = (0,\, 0,\, 0) \tag{26}$$
$$\mathbf{d}_2 = \frac{a}{2}(1,\, 1,\, 0) \tag{27}$$
$$\mathbf{d}_3 = \frac{a}{2}(0,\, 1,\, 1) \tag{28}$$
$$\mathbf{d}_4 = \frac{a}{2}(1,\, 0,\, 1) \tag{29}$$
$$\mathbf{d}_5 = \frac{a}{4}(1,\, 1,\, 1) \tag{30}$$
$$\mathbf{d}_6 = \frac{a}{4}(3,\, 1,\, 3) \tag{31}$$
$$\mathbf{d}_7 = \frac{a}{4}(1,\, 3,\, 3) \tag{32}$$
$$\mathbf{d}_8 = \frac{a}{4}(3,\, 3,\, 1) \tag{33}$$

where a is the side length of the cell. Because the conventional cell is cubic, a general reciprocal lattice vector can be written

$$\mathbf{K} = \frac{2\pi}{a}\left(\nu_1\mathbf{x} + \nu_2\mathbf{y} + \nu_3\mathbf{z}\right). \tag{34}$$

Plugging these into the expression for the structure factor yields

$$\begin{aligned} S_{\mathbf{K}} &= 1 + e^{i\pi(\nu_1+\nu_2)} + e^{i\pi(\nu_2+\nu_3)} + e^{i\pi(\nu_1+\nu_3)} \\ &\quad + e^{\frac{i\pi}{2}(\nu_1+\nu_2+\nu_3)} + e^{\frac{i\pi}{2}(3\nu_1+\nu_2+3\nu_3)} + e^{\frac{i\pi}{2}(\nu_1+3\nu_2+3\nu_3)} + e^{\frac{i\pi}{2}(3\nu_1+3\nu_2+\nu_3)} \qquad (35) \\ &= 1 + e^{i\pi(\nu_1+\nu_2)} + e^{i\pi(\nu_2+\nu_3)} + e^{i\pi(\nu_1+\nu_3)} \\ &\quad + e^{\frac{i\pi}{2}(\nu_1+\nu_2+\nu_3)}\left[1 + e^{i\pi(\nu_1+\nu_2)} + e^{i\pi(\nu_2+\nu_3)} + e^{i\pi(\nu_1+\nu_3)}\right] \\ &= \left(1 + e^{\frac{i\pi}{2}(\nu_1+\nu_2+\nu_3)}\right)\left(1 + e^{i\pi(\nu_1+\nu_2)} + e^{i\pi(\nu_2+\nu_3)} + e^{i\pi(\nu_1+\nu_3)}\right) \\ &= \left[1 + i^{(\nu_1+\nu_2+\nu_3)}\right]\left[1 + (-1)^{(\nu_1+\nu_2)} + (-1)^{(\nu_2+\nu_3)} + (-1)^{(\nu_1+\nu_3)}\right]. \qquad (36) \end{aligned}$$

If ν_1, ν_2, and ν_3 are all even or all odd, the second factor is non-zero. When they are all odd, the first factor is also non-zero. If they are all even *and* are equal to a multiple of 4, the first factor is non-zero. The structure factor is zero when $\nu_1 + \nu_2 + \nu_3 = 2(2k+1)$ or when one (two) of the ν_i are even (odd) and the last one is odd (even).

Problem 6

The Wigner-Seitz cells for the 2D square, rectangular, and hexagonal lattices are shown in Figures 3, 4, and 5.

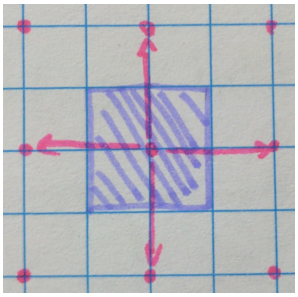

Figure 3: Wigner-Seitz cell of the 2D square lattice.

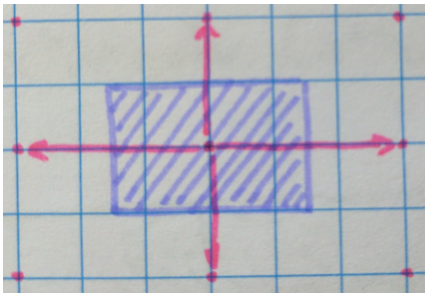

Figure 4: Wigner-Seitz cell of the 2D rectangular lattice.

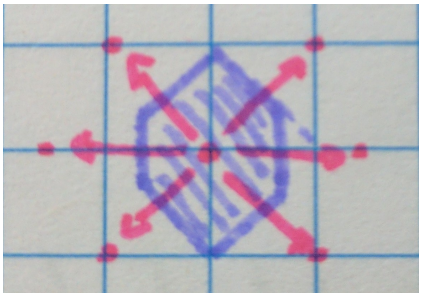

Figure 5: Wigner-Seitz cell of the 2D hexagonal lattice