2021 Fall ECE606 - Homework 1 Solutions

Problem 1 (a)

The blue hexagonal unit cells were overlayed onto the graphene nanoribbon to aid in the determination of the number of carbon atoms per unit cell. Each point of a hexagonal unit cell contains an atom that is shared with two other unit cells. As a result, each of the six points in the hexagonal unit contains $\frac{1}{3}$ of an atom.

$$\frac{\text{atoms}}{\text{hexagonal unit cell}} = \left(\frac{1}{3}\right) 6 = 2 \tag{1}$$

Problem 1 (b)

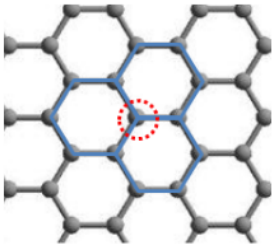


Figure 1: Graphene Unit Cells

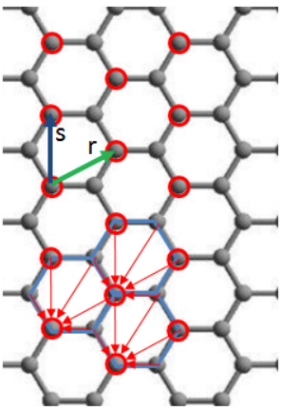


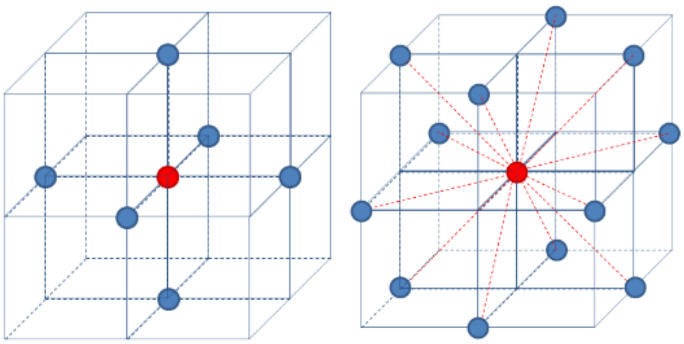
Figure 2: Graphene Basis Vectors $\vec{r}$ and $\vec{s}$

Basis vectors for the graphene structure can be found by using a hexagonal unit cell. As shown in Figure 2, each unit cell depicted in light blue can be thought of as a single point collapsed on the lower left point of the cell. Performing this on each hexagonal structure, a grid of 2D points is created as depicted by the red circles. In order to construct the original lattice, basis vectors $\vec{r}$, depicted in green, and $\vec{s}$, depicted in blue, are needed. These basis vectors can be used to move to any point relative to an origin by using the vector

$$p = a\vec{s} + b\vec{r} \tag{2}$$

where a and b are integers.

Problem 2



(a) Nearest (b) Second Nearest

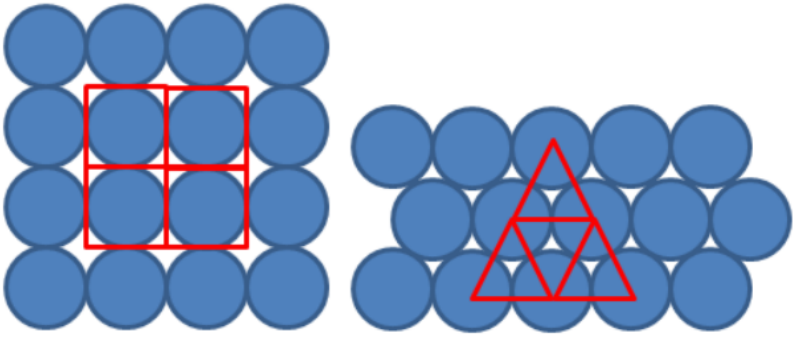
Figure 3: Simple cubic Bravais lattice nearest and second nearest neighbours

An arrangement of simple cubic Bravais lattices are depicted in Figure 3. Consider the nearest neighbors to the red point in Figure 3a. There are a total of 6 nearest neighbors that can be described by the following set of position vectors, with $a\hat{x}$, $a\hat{y}$, $a\hat{z}$ as basis vectors, using the red point as the origin:

$$r_1 = a\hat{x} \tag{3}$$
$$r_2 = -a\hat{x} \tag{4}$$
$$r_3 = a\hat{y} \tag{5}$$
$$r_4 = -a\hat{y} \tag{6}$$
$$r_5 = a\hat{z} \tag{7}$$
$$r_6 = -a\hat{z} \tag{8}$$

Now consider the second nearest neighbors to the red point in Figure 3b. There are a total of 12 second nearest neighbors at a distance of $\sqrt{2}a$ away where a is the lattice constant. The following set of position vectors, using the $a\hat{x}$, $a\hat{y}$, $a\hat{z}$ as basis vectors, describe the locations of the second nearest neighbors using the red point as the origin:

$$r_1 = a\hat{x} + a\hat{y} \tag{9}$$
$$r_2 = a\hat{x} - a\hat{y} \tag{10}$$
$$r_3 = -a\hat{x} + a\hat{y} \tag{11}$$
$$r_4 = -a\hat{x} - a\hat{y} \tag{12}$$
$$r_5 = a\hat{x} + a\hat{z} \tag{13}$$
$$r_6 = a\hat{x} - a\hat{z} \tag{14}$$
$$r_7 = -a\hat{x} + a\hat{z} \tag{15}$$
$$r_8 = -a\hat{x} - a\hat{z} \tag{16}$$
$$r_9 = a\hat{y} + a\hat{z} \tag{17}$$
$$r_{10} = a\hat{y} - a\hat{z} \tag{18}$$
$$r_{11} = -a\hat{y} + a\hat{z} \tag{19}$$
$$r_{12} = -a\hat{y} - a\hat{z} \tag{20}$$
$$\tag{21}$$



(a) Square (b) Triangle

Figure 4: 2D Lattice Packing Fraction

Problem 3 (a)

First, consider the packing fraction for the 2D square Bravais lattice shown in Figure 4a. The unit cell, depicted in red, contains a complete circle. Let the unit cell length be given by a. The area for the square unit cell is a^2 while the area of the circle is $\pi a^2/4$. This produces the following packing fraction:

$$\text{square lattice packing fraction} = \frac{\text{circle area}}{\text{unit area}} = \frac{\frac{\pi a^2}{4}}{a^2} = \frac{\pi}{4} \tag{22}$$

Problem 3 (b)

Now consider the packing fraction for the 2D triangular Bravais lattice shown in Figure 4b. The unit cell depicted in red contains a portion of three circles. The unit cell as shown has sides of length a and is therefore an equilateral triangle. This means that each fraction of a circle contained in the unit cell is given by $60/360 = 1/6$. Therefore, there is a total of $3(1/6) = 1/2$ circles per unit area. The area of an equilateral triangle is given by $\sqrt{3}a^2/4$. This produces the following packing fraction:

$$\text{triangular lattice packing fraction} = \frac{\text{circle area}}{\text{unit area}} = \frac{\frac{0.5\pi a^2}{4}}{\frac{\sqrt{3}a^2}{4}} = \frac{\pi}{2\sqrt{3}} \tag{23}$$

Problem 3 (c)

This shows that the triangular lattice is more closely packed than the square lattice as $2\sqrt{3} < 4$.

Problem 4

The first step in the process is to find the norm of an arbitrary plane. Consider an arbitrary plane:

$$a_1 x + b_1 y + c_1 y = d_1 \tag{24}$$

An arbitrary vector in this plane can be describe by the following column vector letting y and z be represented by free variables t and r respectively:

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \frac{d_1 - b_1 t - c_1 r}{a_1} \\ t \\ r \end{bmatrix} = \begin{bmatrix} \frac{d_1}{a_1} \\ 0 \\ 0 \end{bmatrix} + t \begin{bmatrix} \frac{-b_1}{a_1} \\ 1 \\ 0 \end{bmatrix} + r \begin{bmatrix} \frac{-c_1}{a_1} \\ 0 \\ 1 \end{bmatrix} \tag{25}$$

The last two column vectors are independent and span the plane shifted from the origin by the first column vector. These vectors form a basis for the plane. Any vectors orthogonal to these vectors are normal to the plane. Therefore the normal vectors are found by finding the left null space of the basis vectors.

$$\begin{bmatrix} \frac{-b_1}{a_1} & 1 & 0 \\ \frac{-c_1}{a_1} & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{26}$$

$$\begin{bmatrix} 1 & \frac{-a_1}{b_1} & 0 \\ c_1 & 0 & -a_1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{27}$$

$$\begin{bmatrix} 1 & \frac{-a_1}{b_1} & 0 \\ 0 & \frac{a_1 c_1}{b_1} & -a_1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{28}$$

Letting $z = r$ it is seen that $y = b_1 r/c_1$ and $x = a_1/c_1 r$. Absorbing $1/c_1$ into the arbitrary r, any vector of the form

$$r \begin{bmatrix} a_1 \\ b_1 \\ c_1 \end{bmatrix} \tag{29}$$

will be normal to the plane, as is well known. Letting $r = 1$, a normal vector can be directly obtained from (a_1, b_1, c_1). It is also known that the cosine of the angle between two vectors (and for normals to planes, the cosine of the angle between the two planes) is given by

$$cos(\theta) = \frac{v_1 \cdot v_2}{|v_1||v_2|} \tag{30}$$

Now let the vectors $v_1 = (a_1, b_1, c_1)$ and $v_2 = (a_2, b_2, c_2)$ be the normals of two arbitrary planes. This yields

$$cos(\theta) = \frac{a_1 a_2 + b_1 b_2 + c_1 c_2}{\sqrt{a_1^2 + b_1^2 + c_1^2}\sqrt{a_2^2 + b_2^2 + c_2^2}} \tag{31}$$

The problem is now to show that the miller indices are equal to the normal vectors or $(h_i, k_i, l_i) = (a_i, b_i, c_i)$. Consider again the original equation for an arbitrary plane. The process outlined for finding the miller indices $[hkl]$ will be followed:

1. Find the intercepts and divide by the cell length along the respective axis

$$x = \frac{d_1}{a_1}, y = \frac{d_1}{b_1}, z = \frac{d_1}{c_1} \tag{32}$$

2. Invert the intercepts

$$x^{-1} = \frac{a_1}{d_1}, y^{-1} = \frac{b_1}{d_1}, z^{-1} = \frac{c_1}{d_1} \tag{33}$$

3. Find the smallest possible set of whole numbers (multiply by d_1)

$$h = d_1 x^{-1} = a_1, h = d_1 y^{-1} = b_1, h = d_1 z^{-1} = c_1 \tag{34}$$

4. Enclose the set in brackets $(hkl) = (a_1 b_1 c_1)$

This shows the the procedure to find the miller indices is equivalent to finding the norm of the chosen plane.In essence, the miller procedure amounts to finding the plane equation and taking the coefficients a_1, b_1, c_1. As a result

$$cos(\theta) = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\sqrt{h_2^2 + k_2^2 + l_2^2}} \tag{35}$$

Problem 5 (a)

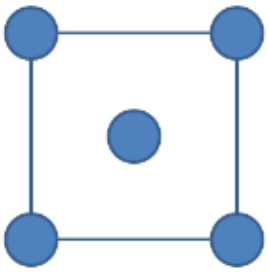


Figure 5: (100) plane for Silicon

Figure 5 represents the 2D cross-section of the (100) plane of a Si unit cell. As shown there are a total of $(4)(1/4) + 1 = 2$ atoms for an area of a^2 where a is the lattice constant (edge of plane). This means there are 2 atoms/a^2 or 2 atoms/2.9495×10^{-16}cm^2 $= 6.781 \times 10^{14}$ atoms/cm^2 where a silicon lattice constant of $a = 5.43095$ angstroms was used.

$$\frac{\text{atoms}}{\text{cm}^2} = 6.781 \times 10^{14} \tag{36}$$

Problem 5 (b)

Figure 6 represents the 2D cross-section of the (110) plane of a Si unit cell. As shown there are a total of $(4)(1/4) + 2 + 2(1/2) = 4$ atoms for an area of $a \times \sqrt{2}a = \sqrt{2}a^2$. These values come from the four atoms on the four corners which are each shared with three neighboring cells, 2 atoms contained within the cell, and 2 atoms at the top and bottom shared between 1 neighboring cell. The area comes from the normal height of the cell a and the diagonal of the unit cell base $\sqrt{2}a$, where a represents the lattice constant in cm.

$$\frac{\text{atoms}}{\text{cm}^2} = \frac{4}{\sqrt{2}a^2} = 9.589 \times 10^{14} \tag{37}$$

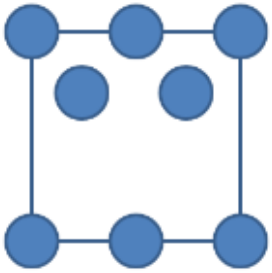


Figure 6: (110) plane for Silicon

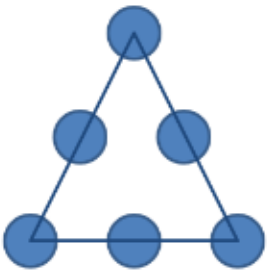


Figure 7: (111) plane for Silicon

Figure 7 represents the 2D cross-section of the (111) plane of a Si unit cell. As shown there are a total of $(3)(1/6) + 3(1/2) = 2$ atoms for an area of $\sqrt{3}(\sqrt{2}a)^2/4 = \sqrt{3}a/2$. These values come from the 3 atoms on the3 corners which are each shared with 5 neighboring cells and the 3 atoms shared between 1 neighboring cell. The area comes from the equilateral triangle unit cell with side $\sqrt{2}a$, where a represents the lattice constant in cm.

$$\frac{\text{atoms}}{\text{cm}^2} = \frac{2}{\sqrt{3}a^2/2} = 7.830 \times 10^{14} \tag{38}$$

Problem 6

Each BCC unit cell contains a total of $1 + (1/8)8 = 2$atoms. Each iron atom has a mass of 55.845 amu or 9.273×10^{-26}kg. Evaluating the following proportion will find the lattice constant a:

$$\frac{(2)(9.273 \times 10^{-26}\text{kg})}{a^3} = 800\frac{\text{kg}}{\text{m}^3} \tag{39}$$

$$\frac{(2)(9.273 \times 10^{-26}\text{kg})}{800\frac{\text{kg}}{\text{m}^3}} = a^3 \tag{40}$$

$$2.318 \times 10^{-29}\text{m}^3 = a^3 \tag{41}$$

$$a = 2.851\text{Å} \tag{42}$$

Problem 7 (a)(b)

The nearest and second nearest neighbours for a BCC lattice are shown in Figures 9a and 9b respectively. As can be seen, there are 8 nearest neighbors. Using the unit cell described in Figure 8 and corresponding basis vectors, the nearest neighbors can be described using the red point as the origin as follows

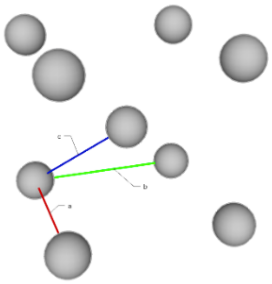
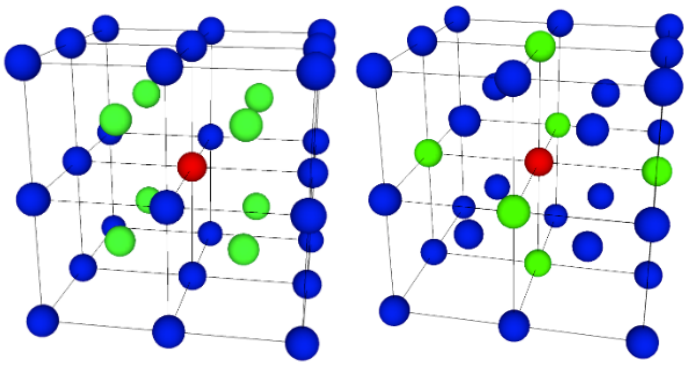


Figure 8: BCC unit cell with basis vectors $[\hat{a}, \hat{b}, \hat{c}]$



(a) Nearest (b) Second Nearest

Figure 9: BCC Bravais lattice nearest and second nearest neighbours

$$
\begin{aligned}
r_1 &= \hat{c} \\
r_2 &= -\hat{a} + \hat{c} \\
r_3 &= -\hat{b} + \hat{c} \\
r_4 &= -\hat{a} - \hat{b} + \hat{c} \\
r_5 &= -\hat{c} \\
r_6 &= \hat{a} - \hat{c} \\
r_7 &= \hat{b} - \hat{c} \\
r_8 &= \hat{a} + \hat{b} - \hat{c}
\end{aligned}
$$

There are a total of 6 next nearest neighbors described by the following position coordinates using the red point as the origin

$$
\begin{aligned}
r_1 &= \hat{a} \\
r_2 &= \hat{b} \\
r_3 &= -\hat{a} \\
r_4 &= -\hat{b} \\
r_5 &= 2\hat{c} - \hat{a} - \hat{b} \\
r_6 &= -2\hat{c} + \hat{a} + \hat{b}
\end{aligned}
$$

The nearest and second nearest neighbours for a FCC lattice are shown in Figures 11a and 11b respectively. The figures shows that there are 12 nearest neighbors. Using the unit cell described in Figure 10 and corresponding basis vectors, the nearest neighbors can be described using the red point as the origin as follows

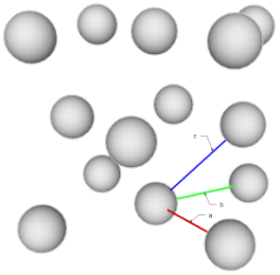
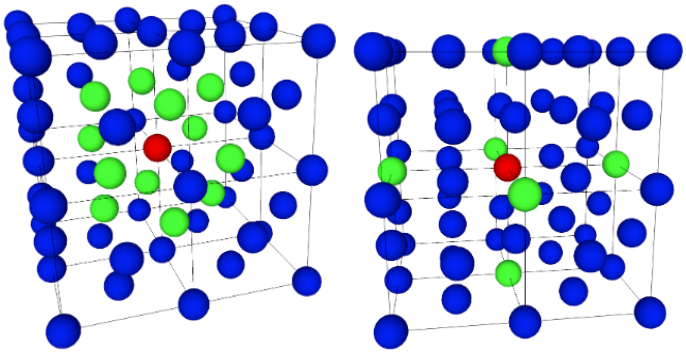


Figure 10: FCC unit cell with basis vectors $[\hat{a}, \hat{b}, \hat{c}]$



(a) Nearest (b) Second Nearest

Figure 11: FCC Bravais lattice nearest and second nearest neighbours

$$
\begin{aligned}
r_1 &= \hat{a} \\
r_2 &= \hat{b} \\
r_3 &= -\hat{a} \\
r_4 &= -\hat{b} \\
r_5 &= \hat{c} \\
r_6 &= -\hat{a} - \hat{b} + \hat{c} \\
r_7 &= -\hat{a} + \hat{c} \\
r_8 &= -\hat{b} + \hat{c} \\
r_9 &= -\hat{c} \\
r_{10} &= \hat{a} + \hat{b} - \hat{c} \\
r_{11} &= \hat{a} - \hat{c} \\
r_{12} &= \hat{b} - \hat{c}
\end{aligned}
$$

There are a total of 6 second nearest neighbors described by the following position coordinates using the red point as the origin

$$
\begin{aligned}
r_1 &= \hat{a} + \hat{b} \\
r_2 &= \hat{a} - \hat{b} \\
r_3 &= -\hat{a} + \hat{b} \\
r_4 &= -\hat{a} - \hat{b} \\
r_5 &= 2\hat{c} - \hat{a} - \hat{b} \\
r_6 &= -2\hat{c} + \hat{a} + \hat{b}
\end{aligned}
$$

Problem 7 (c)

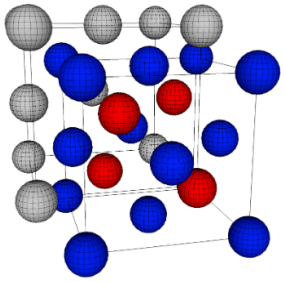


Figure 12: Diamon lattice represented by two FCC unit cells

Silicon is classified as a diamond lattice. A diamond lattice is two FCC lattices interlocked with one another as shown in Figure 12. This figure has the first FCC unit in blue and the portion of the second FCC cell within the first shown in red.

Problem 7 (d)

The atoms within the silicon unit cell are partitioned as follows: 4 atoms are from the interlocked FCC cell, $(1/8)8 = 1$ atoms are from the 8 corners, and $(1/2)6 = 3$ atoms are from the faces. This results in a total of 8 silicon atoms per unit cell.

Problem 7 (e)

The fractional coordinates for the cells are as follows. Using the back-bottom left blue atom as the origin, the relative positions of the bottom and top corner atoms can be described as fractions of the lattice constant a:

$$
\begin{aligned}
r_1 &= (0, 0, 0) \\
r_2 &= (1, 0, 0) \\
r_3 &= (0, 1, 0) \\
r_4 &= (1, 1, 0) \\
r_5 &= (0, 0, 1) \\
r_6 &= (1, 0, 1) \\
r_7 &= (0, 1, 1) \\
r_8 &= (1, 1, 1)
\end{aligned}
$$

The 6 atoms on the faces are described as follows:

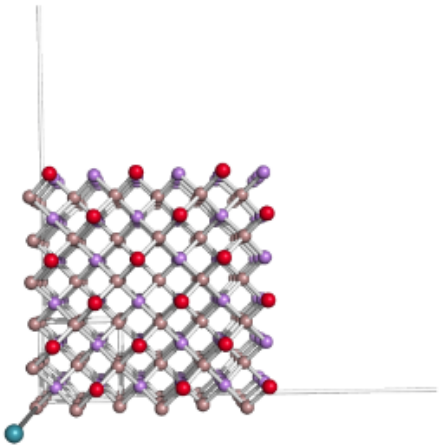
$$
\begin{aligned}
r_9 &= (0.5, 0.5, 0) \\
r_{10} &= (0.5, 0, 0.5) \\
r_{11} &= (0, 0.5, 0.5) \\
r_{12} &= (0.5, 1, 0.5) \\
r_{13} &= (1, 0.5, 0.5) \\
r_{14} &= (0.5, 0.5, 1)
\end{aligned}
$$

The inner silicon atoms are described as follows:

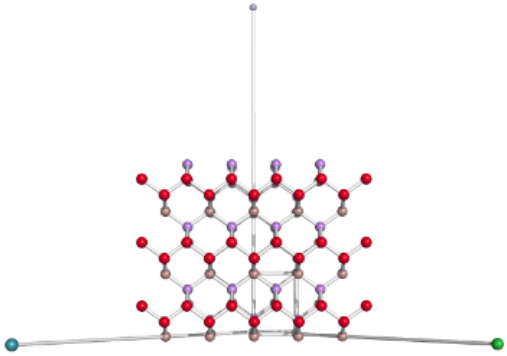
$$
\begin{aligned}
r_{15} &= (0.25, 0.25, 0.25) \\
r_{16} &= (0.75, 0.75, 0.25) \\
r_{17} &= (0.75, 0.25, 0.75) \\
r_{18} &= (0.25, 0.75, 0.75)
\end{aligned}
$$

These numbers represent the fractional (fraction of the lattice constant a) coordinates relative to an origin.

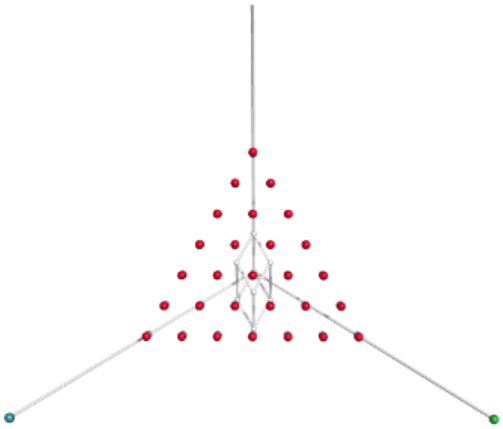
Problem 8



(a) GaAs Zinc Blende in [100] direction



(b) GaAs Zinc Blende in [110] direction



(c) GaAs Zinc Blende in [111] direction

Figure 13: Zinc Blende crystal system from three different directions