ECE606 Homework 1

September 6, 2012

1

Problem

Graphene is a 2D crystal with carbon atoms arranged in a honeycomb structure as shown below. Using the

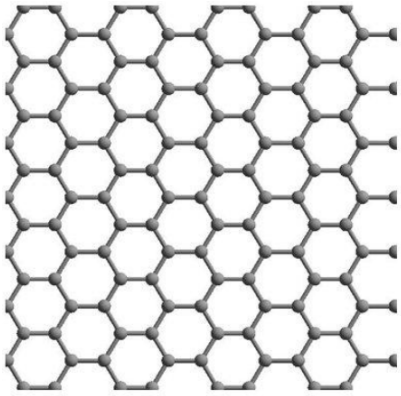


Figure 1: Graphene Nanoribbon

above information and picture, answer the following questions

a) Assuming that the unit cell is a hexagon of carbon atoms, how many atoms of carbon are there in each unit cell?
b) What are the basis vectors needed to reproduce the whole crystal in 2D space?

Solution

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 1/3 of an atom.

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

b

Basis vectors for the graphene structure can be found by using a hexagonal unit cell. As shown in Figure 3, 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

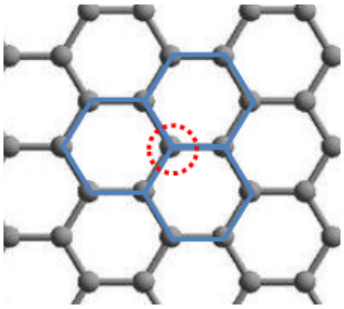


Figure 2: Graphene Unit Cells

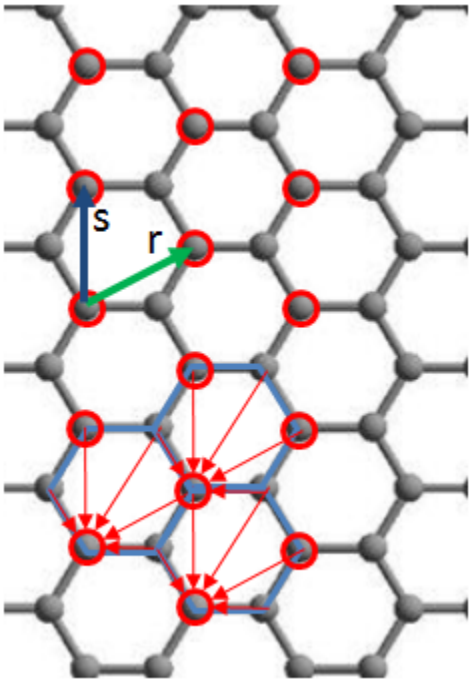


Figure 3: Graphene Basis Vectors $\vec{r}$ and $\vec{s}$

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

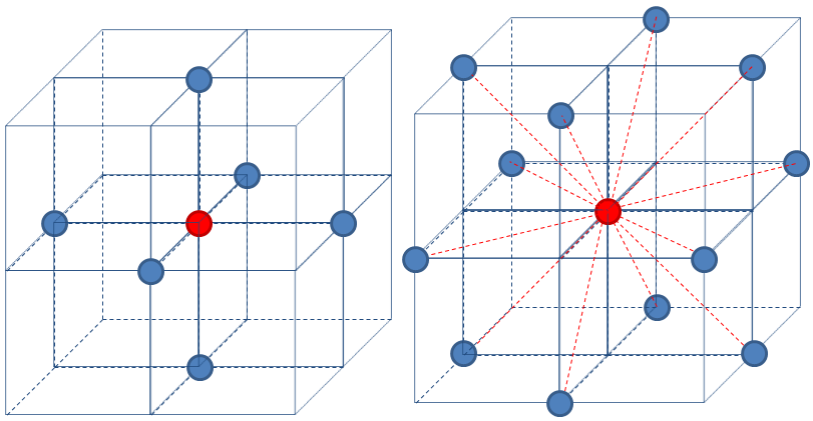
$$p = a\vec{s} + b\vec{r} \tag{2}$$

Where a and b are integers.

2

Problem

Find the number and relative positions of all nearest and second-nearest neighbours of a lattice point in a simple cubic Bravais lattice.



(a) Nearest (b) Second Nearest

Figure 4: Simple cubic Bravais lattice nearest and second nearest neighbours

Solution

An arrangement of simple cubic Bravais lattices are depicted in Figure 4. Consider the nearest neighbors to the red point in Figure 4(a). 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:

$$\begin{aligned} r_1 &= a\hat{x} \\ r_2 &= -a\hat{x} \\ r_3 &= a\hat{y} \\ r_4 &= -a\hat{y} \\ r_5 &= a\hat{z} \\ r_6 &= -a\hat{z} \end{aligned}$$

Now consider the second nearest neighbors to the red point in Figure 4(b). 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:

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

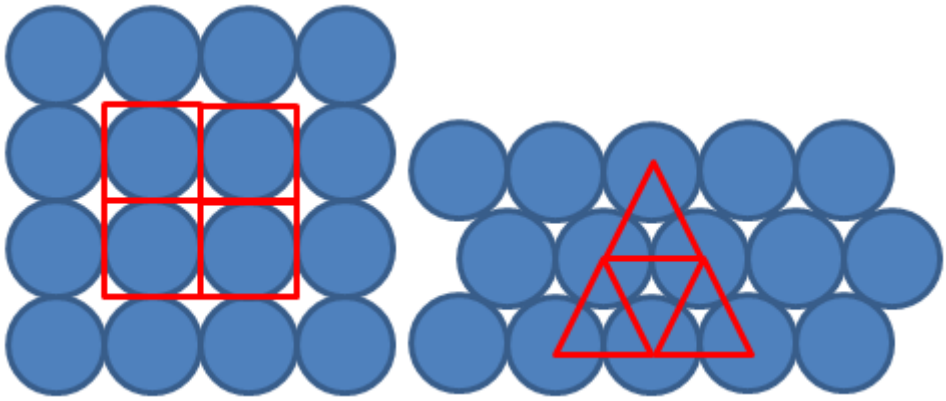
3

Problem

Packing fraction in two dimensions: A two-dimensional crystal is constructed by packing circles. The ratio between the area occupied by the circles and the total area is referred as the packing fraction in two dimensions. Find the packing fraction for a two-dimensional square Bravais lattice.

Repeat the same calculation for a two-dimensional triangular lattice. Which one of the two is more closely packed?

Solution



(a) Square (b) Triangle

Figure 5: 2D Lattice Packing Fraction

First, consider the packing fraction for the 2D square Bravais lattice shown in Figure 5(a). 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:

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

Now consider the packing fraction for the 2D triangular Bravais lattice shown in Figure 5(b). 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:

$$\text{triangular lattice packing fraction} = \frac{\text{circle area}}{\text{unit area}} = \frac{\frac{1}{2}\pi\frac{a^2}{4}}{\frac{\sqrt{3}a^2}{4}} = \frac{\pi}{2\sqrt{3}} \tag{4}$$

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

4

Problem

Show that the angle between two planes (or two directions) is

$$\cos(\theta) = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\sqrt{h_2^2 + k_2^2 + l_2^2}}$$

$[h_i, k_i, l_i]$ are the miller indices of the two planes, where $i = 1, 2$

Solution

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

$$a_1 x + b_1 y + c_1 z = d_1 \tag{5}$$

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:

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \frac{d_1 - b_1 t - c_1 r}{a_1} \\ t \\ r \end{bmatrix} = \begin{bmatrix} \frac{d_1}{a_1} \\ 0 \\ 0 \end{bmatrix} + t \begin{bmatrix} -\frac{b_1}{a_1} \\ 1 \\ 0 \end{bmatrix} + r \begin{bmatrix} -\frac{c_1}{a_1} \\ 0 \\ 1 \end{bmatrix} \tag{6}$$

The last two column vectors are independent and span the plane shifted from the orgin 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 nullspace of the basis vectors.

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

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

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

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

$$r \begin{bmatrix} a_1 \\ b_1 \\ c_1 \end{bmatrix} \tag{7}$$

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

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

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

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

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 (5). 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
   $x = d_1/a_1$, $y = d_1/b_1$, $z = d_1/c_1$
2. Invert the intercepts
   $x^{-1} = a_1/d_1$,$y^{-1} = b_1/d_1$,$z^{-1} = c_1/d_1$

3. Find the smallest possible set of whole numbers (multiply by d_1)
   $h = d_1 x^{-1} = a_1$,$h = d_1 y^{-1} = b_1$,$h = d_1 z^{-1} = c_1$

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

$$\cos(\theta) = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\sqrt{h_2^2 + k_2^2 + l_2^2}} \tag{8}$$

5

Problem

For silicon (Fig. 1.5a in ASF), answer the following questions:

a. How many Si atoms per sq. cm are there on a (100) plane?

b. How many on a (110) and (111) plane?

Solution

a

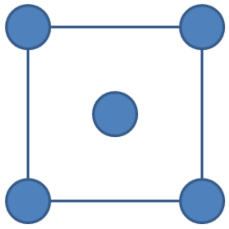


Figure 6: (100) plane for Silicon

Figure 6 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.

$$\frac{\text{atoms}}{\text{cm}^2} = 6.781 \times 10^{14} \tag{9}$$

b

Figure 7 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 $a * \sqrt{2}a = \sqrt{2}a^2$. 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.

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

Figure 8 represents the 2D cross-section of the (111) plane of a Si unit cell. As shown there are a total of

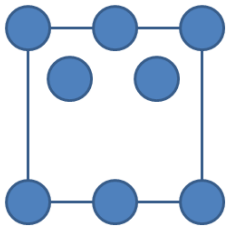


Figure 7: (110) plane for Silicon

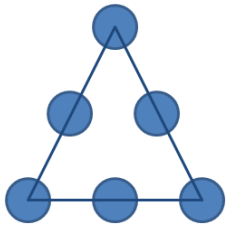


Figure 8: (111) plane for Silicon

$3(1/6)+3(1/2)=2$ atoms for an area of $\sqrt{3}(\sqrt{2}a)^2/4=\sqrt{3}a/2$. These values come from the 3 atoms on the 3 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.

$$\frac{\text{atoms}}{\text{cm}^2}=\frac{2}{\sqrt{3}a^2/2}=7.830\times10^{14} \tag{11}$$

6

Problem

The density of BCC iron is 8,000 kg/m^3. Determine the lattice constant of the cubic unit cell.

Solution

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:

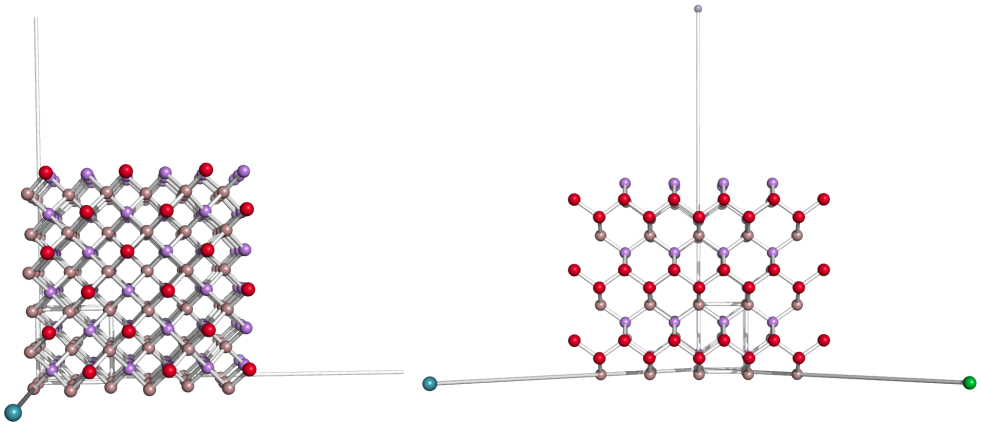
$$\begin{aligned}\frac{(2)(9.273\times10^{-26}\text{kg})}{a^3}&=8000\frac{\text{kg}}{\text{m}^3}\\ \frac{(2)(9.273\times10^{-26}\text{kg})}{8000\frac{\text{kg}}{\text{m}^3}}&=a^3\\ 2.318\times10^{-29}\text{m}^3&=a^3\\ a&=2.851\text{Å}\end{aligned} \tag{12}$$

7

Problem

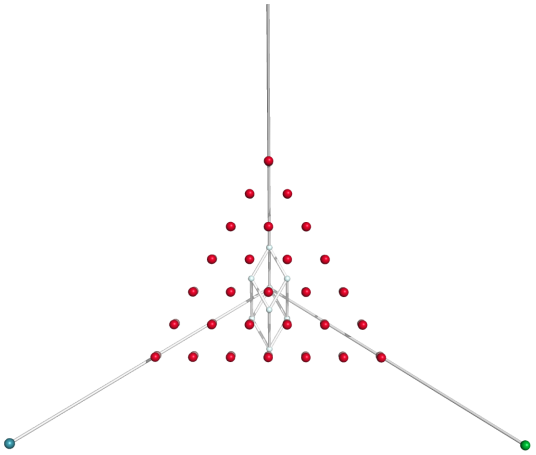
Visualize a zinc blende crystal system from three different directions [100], [110], [111] taken from three different crystal cuts. Utilize the Crystal Viewer Tool in ABACUS on nanoHUB. The tool can be found at: https://nanohub.org/tools/abacus (you will need a free nanoHUB login)

Solution



(a) GaAs Zinc Blende in [100] direction

(b) GaAs Zinc Blende in [110] direction



(c) GaAs Zinc Blende in [111] direction