P1  20 points Find the primitive vectors of the real \((a_1\) and \(a_2)\) and reciprocal \((b_1\) and \(b_2)\) lattices for graphene, as well as positions of the \(K\) and \(K'\) points [see Fig. 3]. Use the carbon-carbon distance \(a \approx 0.142\) nm as the "yardstick". Notice that \(b_1\) and \(b_2\) connect the centers of the adjacent hexagons in the reciprocal space.

**Solution**

\[
a_1 = \left( a \cos \frac{\pi}{3} + a, a \sin \frac{\pi}{3} \right) = a \left( \frac{3}{3}, \frac{\sqrt{3}}{2} \right) \quad (1)
\]

\[
a_2 = a \left( \frac{3}{3}, -\frac{\sqrt{3}}{2} \right) \quad (2)
\]

The reciprocal lattice vectors are defined by the condition \(a \cdot b = 2\pi \delta_{ij}\), which gives

\[
a_{1x} b_{1x} + a_{1y} b_{1y} = 2\pi
\]

\[
a_{2x} b_{1x} + a_{2y} b_{1y} = 0
\]

or

\[
\frac{3}{2} b_{1x} + \frac{\sqrt{3}}{2} b_{1y} = \frac{2\pi}{a}
\]

\[
\frac{3}{2} b_{1x} - \frac{\sqrt{3}}{2} b_{1y} = 0
\]

which gives

\[
b_1 = \frac{2\pi}{a} \left( \frac{1}{3}, \frac{1}{\sqrt{3}} \right) \quad (5)
\]

By symmetry,

\[
b_2 = \frac{2\pi}{a} \left( \frac{1}{3}, -\frac{1}{\sqrt{3}} \right).
\]

Notice that \(b_1 - b_2 = (0, 4\pi/a\sqrt{3})\) is along the \(y\)-axis. The distance between the \(K\) and \(K'\) points is \(1/3\) of \(|b_1 - b_2|\): \(|KK'| = 4\pi/a3\sqrt{3}\). Therefore, \(K_x = b_{1x} = 2\pi/3a\) and \(K_y = |KK'|/2 = 2\pi/a3\sqrt{3}\), so that \(K = (2\pi/3a)(1, 1/\sqrt{3})\). By symmetry, \(K' = (2\pi/3a)(1, -1/\sqrt{3})\).

P2  20 points A common building block of high \(T_c\) superconductors are copper oxide layers.
A possible choice of the primitive cell. The cell contains 1 Cu atom and 2 O atoms

![Diagram of a CuO2 unit cell]

FIG. 1: Unit cells for a flat (2D) CuO2 plane and for a real (3D) CuO2 sheet.

- Sketch the Bravais lattice, identify the basis, and define the primitive unit cell for a 2D CuO2 plane, as shown in Fig. 4.
- In a parent compound of high $T_c$ superconductors (LaCuO4), the oxygen atoms are displaced above and below the plane in an alternating fashion, as shown in Fig. 5. Identify the primitive unit cell for this case.

Solution

Since the spheres centered at atoms in the basal plane touch each other, $a = 2R$, where $R$ is the radius of the sphere. A sphere centered at point $A$ must touch the one centered at point $O$, therefore, $|OA| = 2R$. If $A'$ is the projection of $A$ onto the basal plane, the distance $|OA'|$ is equal to $(a/2)/\cos(30^\circ) = a/\sqrt{3}$. From the rectangular triangle $OAA'$, $c/2 = |AA'|/2 = \sqrt{|OA|^2 - |OA'|^2}$. Therefore, $c/a = 2\sqrt{2}/3 = \sqrt{8}/3$.

- Sodium transforms from the body-centered cubic (bcc) to $hcp$ phase at $T = 23$ K. Assuming that the number density remains fixed and also that the $c/a$ ratio remains ideal, find the $hcp$ lattice spacing $a$ given that the lattice spacing in the $bcc$ phase is $a' = 4.23\text{Å}$.
Solution A bcc lattice can be viewed as a simple cubic lattice with 2 atoms per unit cell. Therefore, the number density in the bcc phase $n_{bcc} = 2/(a')^3$. The hcp unit cell of volume $(\sqrt{3}/2)a^2c$ also contains 2 atoms, thus $n_{hcp} = 4/\sqrt{3}a^2c$. For an ideal hcp lattice, $c = \sqrt{8}a/3$ and $n_{hcp} = 4/\sqrt{8}a^3$. Equating $n_{bcc}$ and $n_{hcp}$, we obtain $a = a'/2^{1/6} = 3.77\text{Å}$.

P4 20 points Find the volumes of the primitive unit cells of the bcc and fcc cubic lattices. Solution For a bcc lattice, the primitive lattice vectors can be chosen as

$$a_1 = \frac{a}{2}(\hat{y} + \hat{z} - \hat{x})$$

$$a_2 = \frac{a}{2}(\hat{x} + \hat{z} - \hat{y})$$

$$a_3 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$

The volume of the primitive cell

$$V = |a_1 \times (a_2 \times a_2)|.$$  \hspace{1cm} (7)

Simple vector calculus gives $a_1 \times a_2 = (a^2/2)(\hat{y} + \hat{z})$, and $V = a^3/2$.  \hspace{1cm} (8)
P5 20 points Consider an "imperfect crystal", where the nth atom (for all n) is displaced from its ideal position, $R_n$, by a random vector $S_n$. We are interested in a diffraction peak around the reciprocal lattice vector $G$. Assume that the displacements at all sites are small: $|S_n| \ll a$, where $a$ is the lattice spacing. Find the intensity of the diffraction peak.

Hint: Assume that all the three components of $S$ are distributed according to the Gaussian law with zero average $P(S_i) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp(-S_i^2/2\sigma^2)$, where $i = x, y, z$.

Solution The intensity of the scattered wave is proportional to the mod squared of the structure factor averaged over random displacements of atoms

$$I \propto \left| \sum_n \exp(iG \cdot R_n) \exp(iG \cdot S_n) \right|^2$$

$$= \sum_{n,n'} \langle \exp(iGS_n) \exp(iGS_{n'}) \rangle,$$  \hspace{1cm} (10)

where $S_n$ is the projection of $S_m$ onto $G$. Assuming that displacements of different atoms are independent and obey Gaussian distributions with dispersions $S_0$, we obtain

$$\langle \exp(iGS_n) \rangle = \frac{1}{\sqrt{2\pi S_0}} \int_{-\infty}^{\infty} dS_n \exp(-S^2/2S_0^2 + iGS_n)$$

$$= \frac{1}{\sqrt{2\pi S_0}} \int dS_n \exp \left( -\frac{1}{2S_0^2} \left( S_n^2 - 2iS_0^2GS_n \right) \right)$$

$$= \frac{1}{\sqrt{2\pi S_0}} \int dS_n \exp \left( -\frac{1}{2S_0^2} \left( (S_n - iS_0^2G)^2 + S_0^4G^2 \right) \right)$$

$$= \frac{1}{\sqrt{2\pi S_0^2}} \int dz \exp \left( -\frac{z^2}{2S_0^2} \right) \exp(-S_0^2G^2/2)$$

$$= \exp(-S_0^2G^2/2).$$ \hspace{1cm} (11)

Therefore, the intensity of the Bragg peak in the direction of $G$ is attenuated by the factor $\exp(-G^2S_0^2)$. This factor is known as the “Debye-Waller factor”.

$\text{fcc lattice:}$

$$a_1 = \frac{a}{2}(\hat{y} + \hat{z})$$

$$a_2 = \frac{a}{2}(\hat{x} + \hat{z})$$

$$a_3 = \frac{a}{2}(\hat{x} + \hat{y})$$  \hspace{1cm} (9)

$$V = a^3/4.$$
FIG. 3: Graphene lattice in real (left) and reciprocal (right) spaces.
FIG. 4: Flat (2D) CuO$_2$ plane.
FIG. 5: 2D projection of a real (3D) CuO$_2$ sheet.