Fundamentals of Nanoelectronics

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ECE 453
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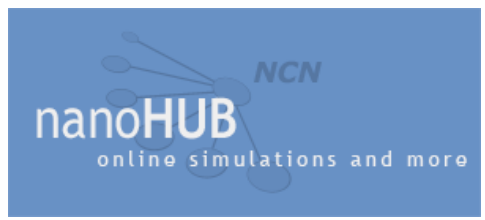
Lecture 21 : Graphene Bandstructure

Ref. Chapter 6.1

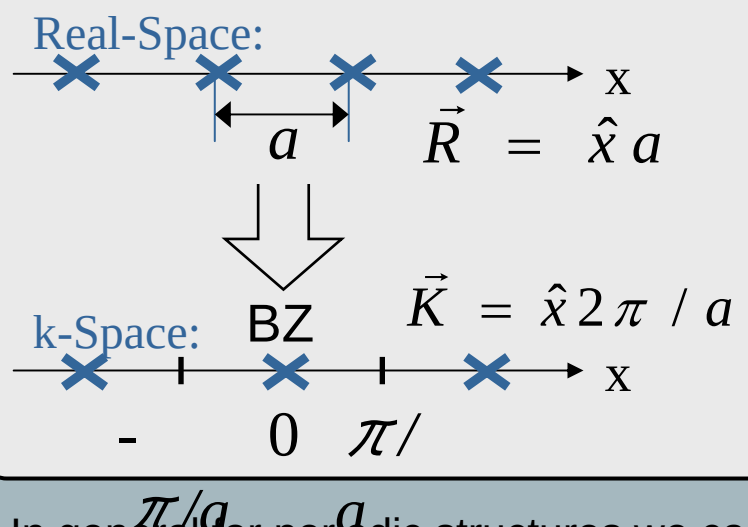
Network for Computational Nanotechnology



Review of Reciprocal Lattice

00:05

• In the last class we learned how to construct the reciprocal lattice.
• For 1D w have:



• In general for periodic structures we can write 3 basis vectors such that any point in the lattice can be written as a linear combination of them with the condition that the coefficients must be integers.

$$\vec{R} = m\,\vec{a}_1 + n\,\vec{a}_2 + p\,\vec{a}_3$$

• Similarly any point in the reciprocal lattice can be written as:

$$\vec{K} = M\vec{A}_1 + N\vec{A}_2 + P\vec{A}_3$$

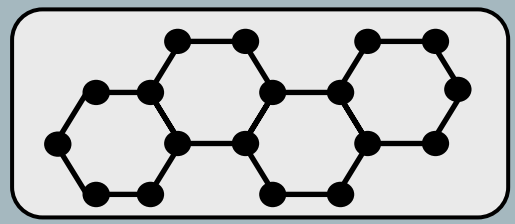
• How are the vectors “A” related to vectors “a”? The defining condition is:

$$\vec{A}_j \cdot \vec{a}_i = 2\pi\delta_{ij} \quad \begin{cases} \delta_{ij} = 0 \text{ for } i \neq j \\ \delta_{ij} = 1 \text{ for } i = j \end{cases}$$

• The significance of reciprocal lattice vectors “A” is that points in k space which are apart from each other by an integer multiple of “Ai’s”, give is the same wavefunction solution.

Graphene

06:50



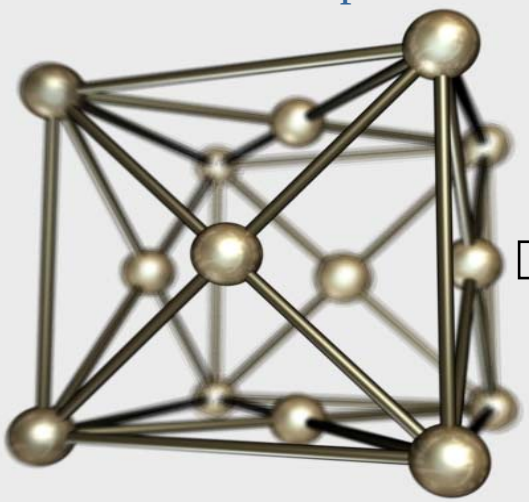
Graphene is made up of carbon atoms bonded in a hexagonal 2D plane.
Graphite is 3D structure that is made up of weakly coupled Graphene sheets.
This is of particular importance because carbon nanotubes are made up of a Graphene sheet that is rolled up like cylinder. Carbon nanotubes themselves are of interest because people believe they can make all kinds of Nano devices with them.

Reciprocal Lattice in 3D

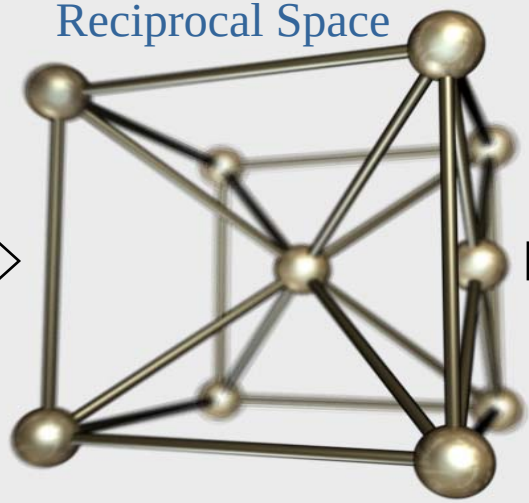
08:03

• Semiconductors of interest to us have what is called a diamond structure. The diamond structure is composed of to interpenetrating FCC lattices the following way: Imagine two FCC lattices such that each atom of each lattice is on top of the corresponding atom of the other lattice. You should only be seeing 1 FCC lattice as of now. Then fix one lattice and move the other one in the direction of the body diagonal of the fixed one by ¼ of the body diagonal. Now you've yourself a diamond lattice. If the two FCC lattices are made up of two different types of atoms, the structure is then called a Zinchblend lattice.
• To visualize the reciprocal lattice **focus only on one FCC lattice** in the diamond structure.

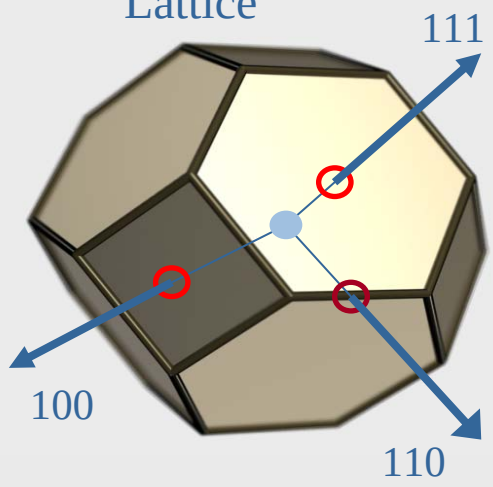
FCC in Real Space



BCC in Reciprocal Space



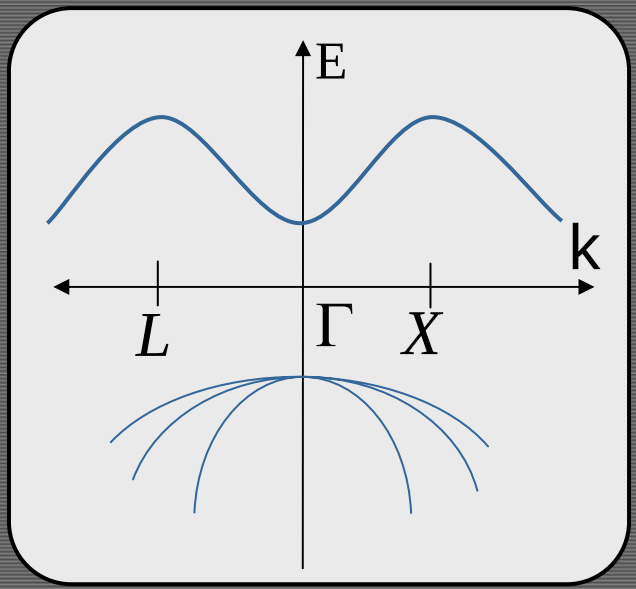
Brillouin Zone in Reciprocal Lattice



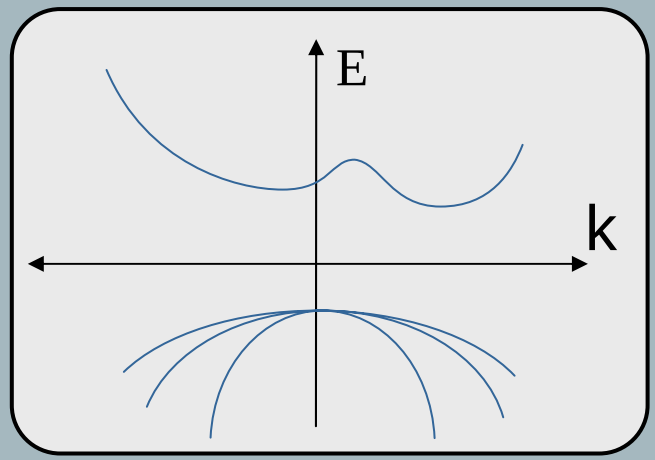
E-k Diagrams for 3D Reciprocal Lattices

11:16

• Since the reciprocal space is now 3 dimensional, to draw the E-k diagram we have choose particular directions and draw E-k diagram along those directions:



• Some useful information:
• The top of the valence band usually occurs at the Gamma point (k=0). The bottom of conduction band however does not always lie at k=0. For example consider Silicon:



• If both conduction band minimum and the valence band maximum lie at the same value of k, the material is called a direction bandgap semiconductor. Other wise the material is indirect like Si.

Parabolic Approximation

• Usually, it is necessary to derive an expression for $E(k_x, k_y, k_z)$ about the conduction points of a bulk solid

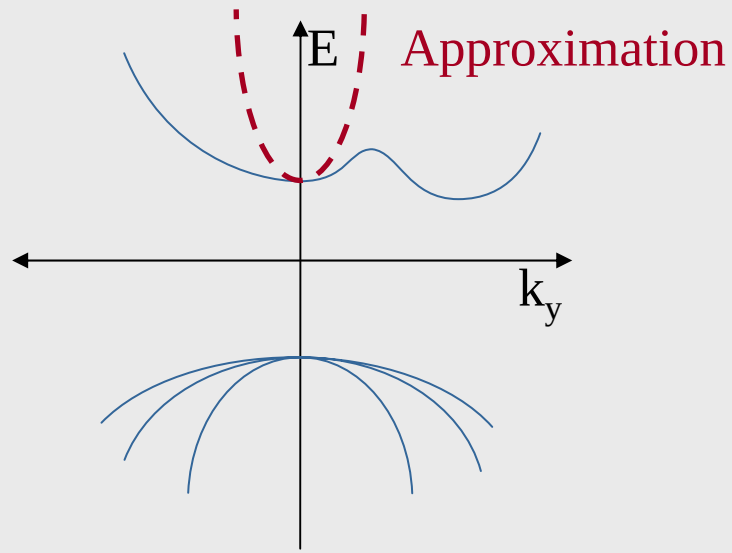
• For silicon, use the parabolic approximation

$$E = E_c + \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2 (k_x^{\,2} + k_y^{\,2} + k_z^{\,2})}{2m^*}$$

where m* is the effective mass.

• For nanotubes we can derive a similar parabolic expression via a Taylor series expansion that approximates the subbands near the conduction valleys

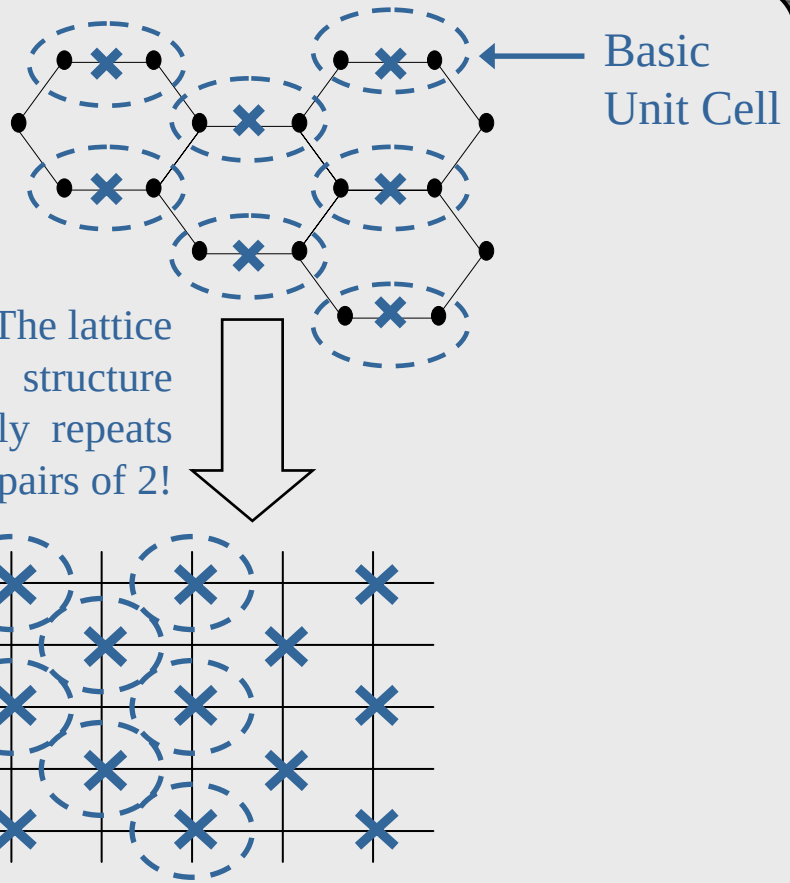
Silicon Parabolic Conduction Band Approximation



E-k Relation for Graphene

21:15

• Let's get back to Graphene. First identify the basic unit cell

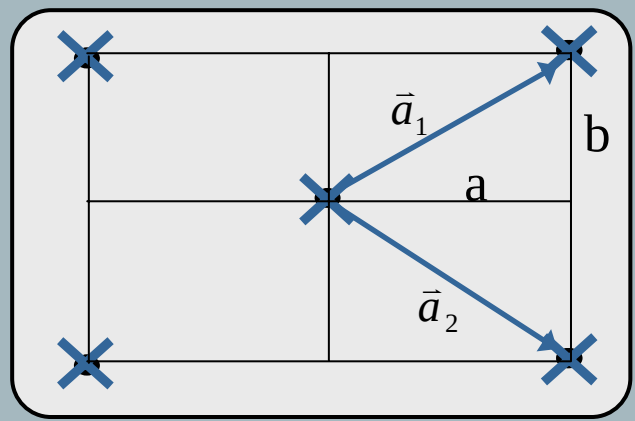


• Remember the general result of principle of bandstructure:

$$E\{\phi_0\} = [h(\vec{k})]\{\phi_0\}$$

$$[h(\vec{k})] = \sum_m [H_{nm}] e^{i\vec{k}\bullet(\vec{d}_m - \vec{d}_n)}$$

• To write h(k) consider one unit cell an its nearest neighbors. Figure shows that there will be 5 terms in the summation for h(k).



Graphene E-k Diagram

23:45

• Remember the general result of principle of bandstructure:

$$E\{\phi_0\} = [h(\vec{k})]\{\phi_0\}$$

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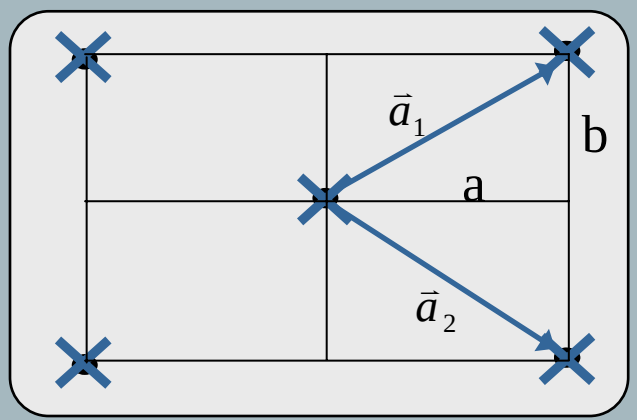


• Writing the summation terms and adding them up we get:

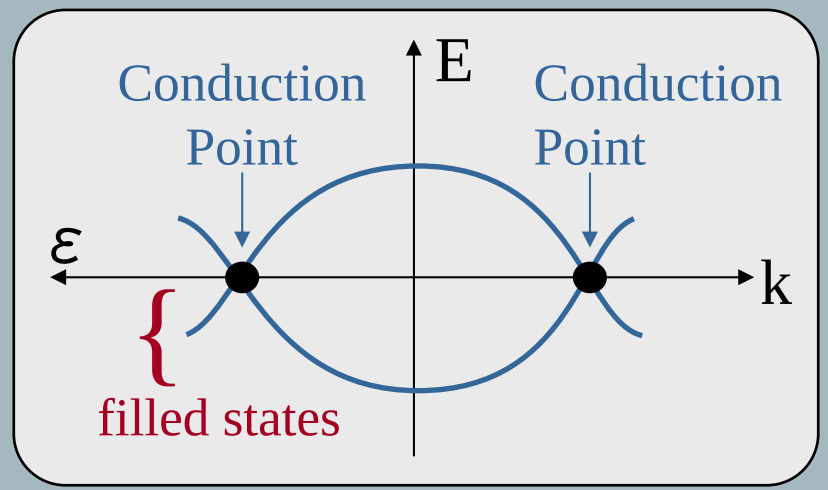
$$h(\vec{k}) = \begin{bmatrix} \varepsilon & h_0^* \\ h_0 & \varepsilon \end{bmatrix}$$

• Where

$$h_0 = t\left(1 + e^{i\vec{k}\cdot\vec{a}_1} + e^{i\vec{k}\cdot\vec{a}_2}\right)$$

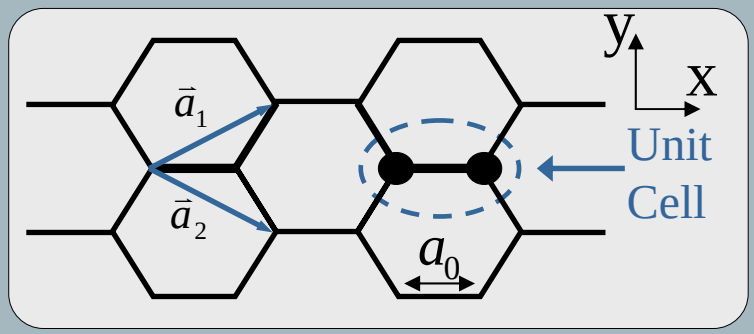
• The eigenvalues of this matrix are given by:

$$E(\vec{k}) = \varepsilon \pm |h_0(\vec{k})|$$



Magnitude of h(k)

- Next we like to locate the conduction points in the 2 dimensional k space:



$$\vec{a}_1 = a\hat{x} + b\hat{y} = \tfrac{3}{2} a_0 \hat{x} + \tfrac{\sqrt{3}}{2} a_0 \hat{y}$$

$$\vec{a}_2 = a\hat{x} - b\hat{y} = \tfrac{3}{2} a_0 \hat{x} - \tfrac{\sqrt{3}}{2} a_0 \hat{y}$$

$$\vec{k} = k_x \hat{x} + k_y \hat{y}$$

$$h_0 = t\left(1 + e^{i\vec{k}\cdot\vec{a}_1} + e^{i\vec{k}\cdot\vec{a}_2}\right) = t\left(1 + e^{i\left(k_x a + k_y b\right)} + e^{i\left(k_x a - k_y b\right)}\right) = t\left(1 + 2e^{ik_x a}\cos k_y b\right)$$

- To find the conduction points we need to set |h(k)|=0. So we need to find |h(k)|:

$$\therefore \left|h_0\right|^2 = h_0 h_0^* = t^2\left(1 + 4\cos k_x a \cos k_y b + 4\cos^2 k_y b\right)$$

so,

$$\left|h_0(\vec{k})\right| = t\sqrt{1 + 4\cos k_x a \cos k_y b + 4\cos^2 k_y b}$$

Conduction Valleys

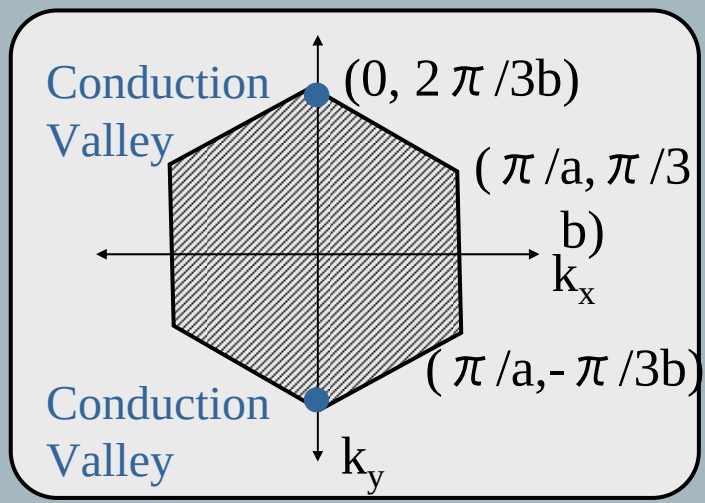
- Now let $\left|h_0(\vec{k})\right| = t\sqrt{1+4\cos k_x a \cos k_y b + 4\cos^2 k_y b} = 0$

- Let kxa=0 and investigate h(k) as a function of ky.

$$h_0 = t\left(1+2\cos k_y b\right) \text{ for } k_x = 0 \Rightarrow k_y b = \frac{2\pi}{3} \text{ to get } h_0(k) = 0$$

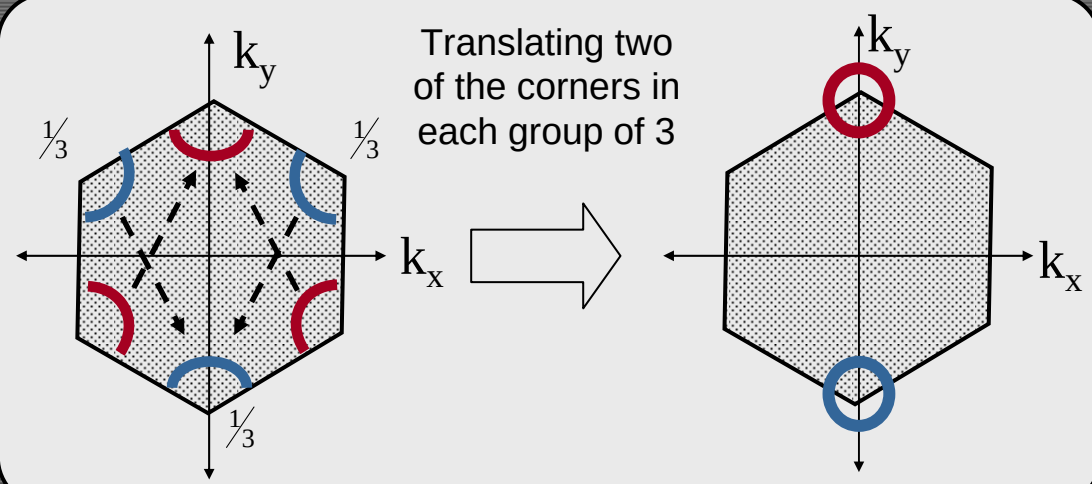
- Let kxa=pi and investigate h(k) as a function of ky.

$$h_0 = t\left(1-2\cos k_y b\right) \text{ for } k_x = \pi \Rightarrow k_y b = \frac{\pi}{3} \text{ to get } h_0(k) = 0$$



Two Full Valleys

• The six Brillouin valleys really only give 2 independent valleys, e.g. in each group of 3 that are in the picture two of the valleys are away form the other by a reciprocal lattice unit vector; hence represent the same state. One can think that each corner in the 1st Brillouin zone contributes 1/3rd.1/3 x 6 = 2(left figure). Alternatively we can translate two of the corners in each group to get the full valleys on the right.



• Dispersion relation along ky.

$$h_0 = t\left(1 + 2\cos k_y b\right) \text{ for } k_x = 0$$

$$E = \varepsilon \pm \left| h_0(\vec{k}) \right|$$