# Fundamentals of Nanoelectronics

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ECE 453
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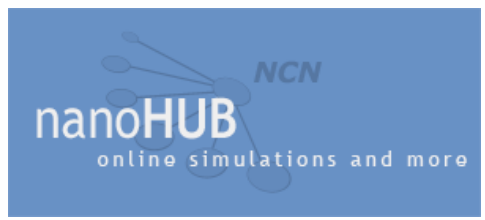
## Lecture 20: Reciprocal Lattice

Ref. Chapter 5.2

*Network for Computational Nanotechnology*



# Dispersion Relation Quantized k States

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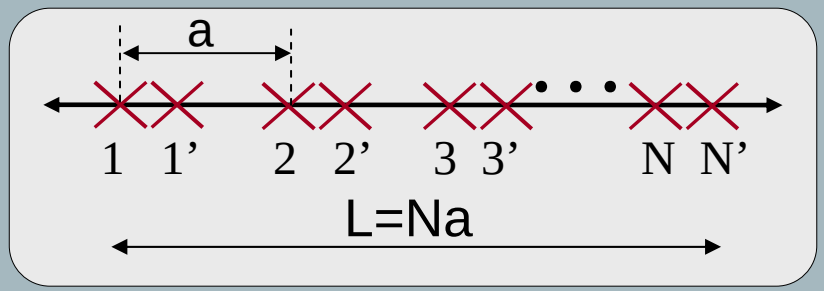
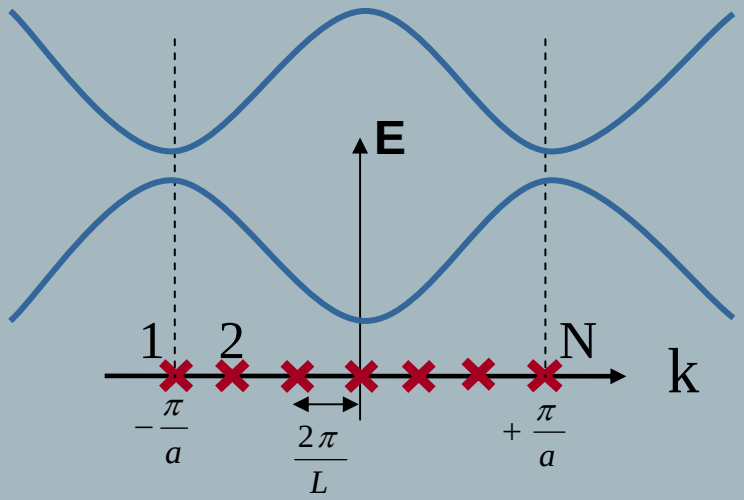
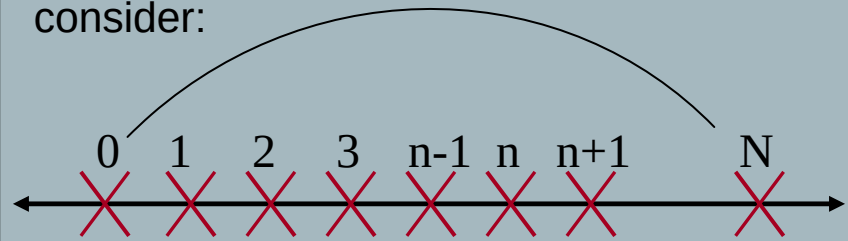
- Given any periodic structure we've discussed how to calculate the E-k relationship. For example consider a 1D dimerized solid with two orbitals per unit cell




- The number of allowed values of k can be found as: $\frac{2\pi / a}{2\pi / L} = \frac{L}{a} = N$
- Notice that the spacing between the k states comes from the imposition of periodic boundary conditions. To see this consider:




$$e^{inka} = e^{i(n+N)ka} \Rightarrow$$

$$e^{iNka} = 1 = e^{i2\pi(\text{integer})} \Rightarrow$$

$$Nka = 2\pi\nu \quad \nu : \text{integer} \Rightarrow$$

$$\boxed{k = \frac{2\pi}{Na}\nu}$$

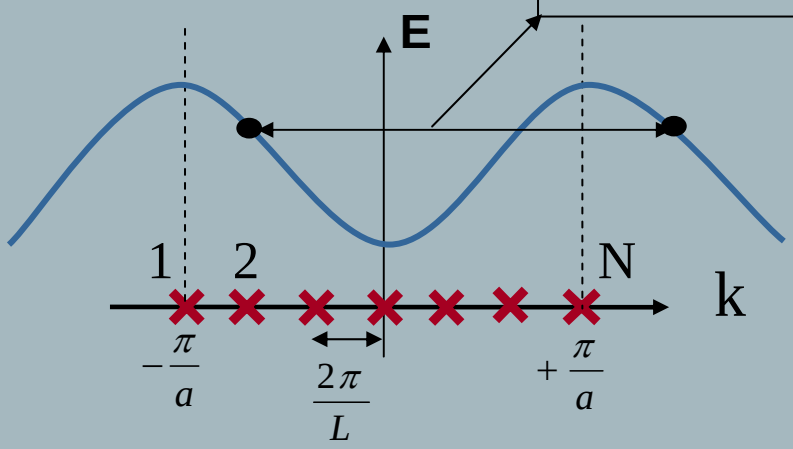
# Brillouin Zone



• To see why the k values are bounded between –pi/a and pi/a consider the simple dispersion relation of 1D solid:

$$E = \varepsilon + 2t\cos ka$$

The two k states give us the same wavefunction




• The point is that if you take any value of k within the range and add 2pi/a to it, you will not get a new independent wavefunction.
• To see this consider the solution…

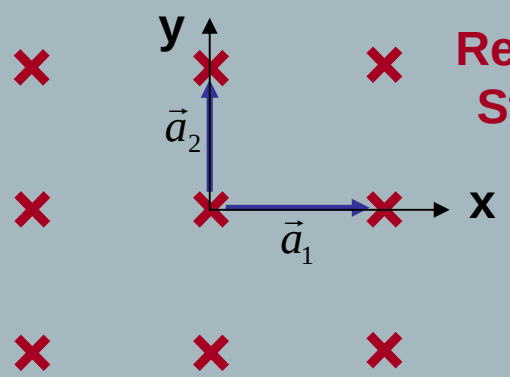
$$(1)\ \psi_n = \psi_0 e^{ikna}$$

$$(2)\ \psi_n = \psi_0 e^{ikna} e^{i2\pi n} = \psi_0 e^{ikna}$$

• You can clearly see that 1 and 2 are the same. This is why we do not need to consider any k values outside of the range –pi/a →2pi/a. The point is that corresponding to any point outside the range there is a point within the range which is an integer multiple of 2pi/a from it. It is the same story for all of them. Add this amount to k and you will get the same answer.
• This symmetric interval around k=0 states that gives us a complete set of k values is called the first Brillouin zone.

# Reciprocal Lattice in 2D






**Real Space Structure**

• Any point in the real space can be written as: $\vec{r} = m\underbrace{\hat{x}a}_{\vec{a}_1} + n\underbrace{\hat{y}a}_{\vec{a}_2}$

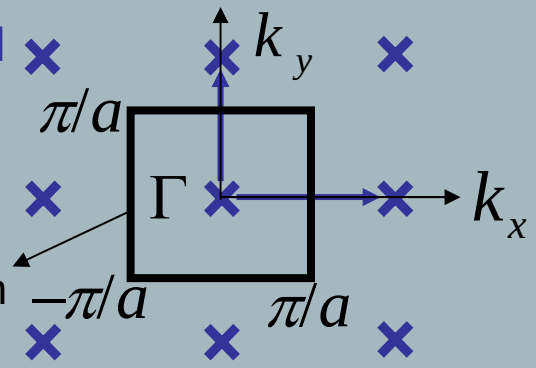
Where the general solution is: $\psi(\vec{r}) = \psi_0 e^{i\vec{k}\cdot\vec{r}}$

To construct the reciprocal lattice we need to find a vector K such that:

$$e^{i(\vec{k}+\vec{K})\cdot\vec{r}} = e^{i\vec{k}\cdot\vec{r}} \Rightarrow$$

the $e^{i\vec{K}\cdot\vec{r}} = 1 \Rightarrow \vec{K}\cdot\vec{r} = (2\pi)\upsilon$

**Reciprocal Lattice**




• Any point in the reciprocal lattice can be written as: $\vec{K} = M\vec{A}_1 + N\vec{A}_2$

• To find K the general procedure is to find the vectors A1 and A2 that satisfy:

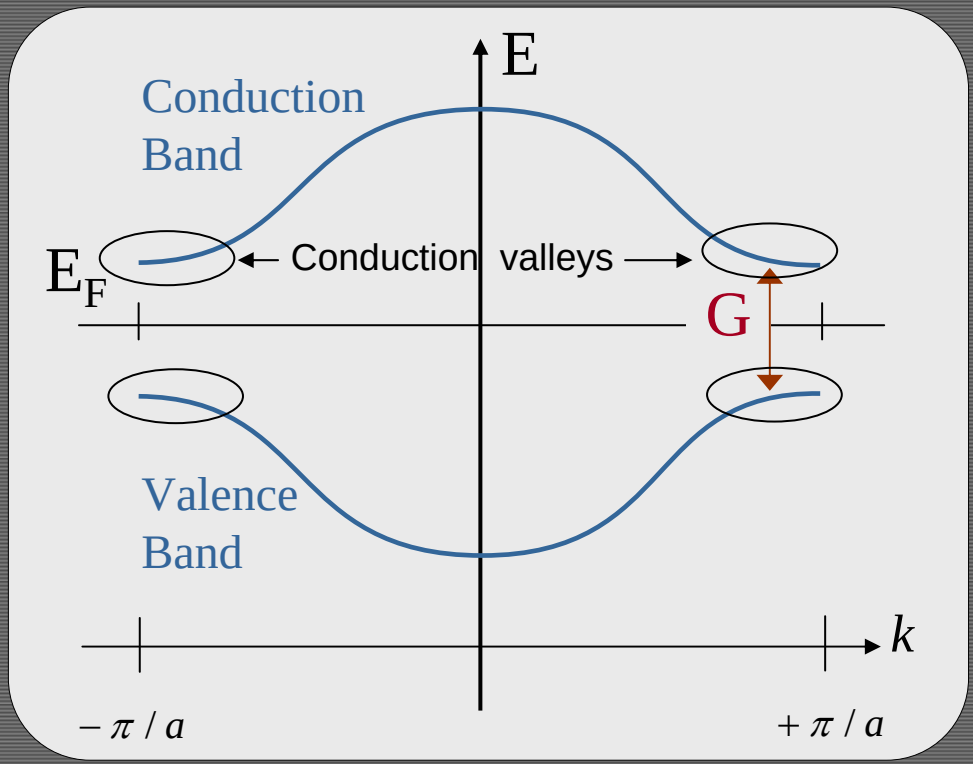
$$\vec{a}_1\cdot\vec{A}_1 = \vec{a}_2\cdot\vec{A}_2 = 2\pi \qquad \vec{a}_1\cdot\vec{A}_2 = \vec{a}_2\cdot\vec{A}_1 = 0 \Rightarrow \begin{cases} \vec{A}_1 = \hat{x}(2\pi/a) \\ \vec{A}_2 = \hat{y}(2\pi/a) \end{cases}$$

• We can now check to see if we have right answer:

$$\vec{K}\cdot\vec{r} = (m\hat{x}a + n\hat{y}a)\cdot(\hat{x}\frac{2\pi}{a} + \hat{y}\frac{2\pi}{a}) = 2\pi(Mm + Nn)$$

# E-k Diagram and Conduction






• We are studying this course to understand the electrical properties of semiconductors. Looking at this E-k diagram, you can see that the chemical potential lies in the gap between the bands. Ordinary there is no conduction. But if we move the levels relative to Ef via applying a voltage we get conduction.

# FCC Lattice to BCC Reciprocal Lattice

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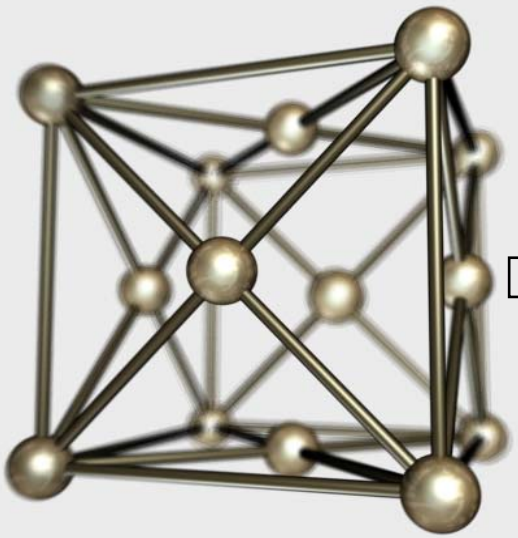
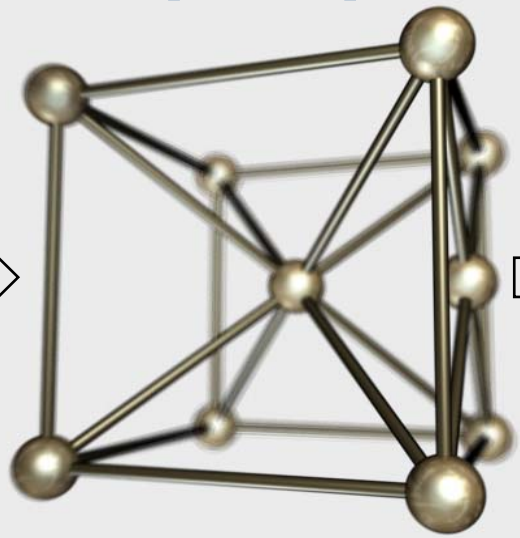
FCC in Real Space



BCC in Reciprocal Space



Brillouin Zone in Reciprocal Lattice