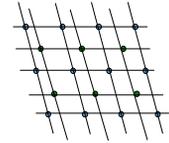
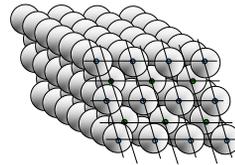


## Sólidos Redes Direta e Recíproca

### Simplificação: reticulado cristalino

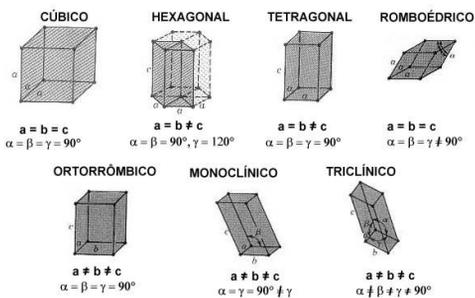


Sólido cristalino no qual os átomos são representados por esferas rígidas.

Reticulado cristalino.

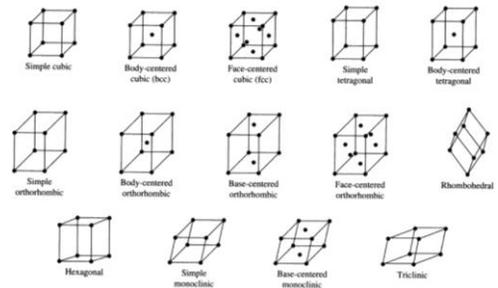
### Sistemas cristalinos

Existem somente sete diferentes combinações dos parâmetros de rede. Cada uma dessas combinações constitui um sistema cristalino.



### Reticulados de Bravais

Qualquer reticulado cristalino pode ser descrito por um dos 14 reticulados de Bravais.



## Espaço recíproco / Rede Recíproca

Espaço recíproco => vetores de onda  $\mathbf{k}$

Rede recíproca => arranjo periódico  $\mathbf{K}$

(parte algébrica - escrita no quadro) ... => quadro

## Primitive Lattice Vectors: BCC Lattice

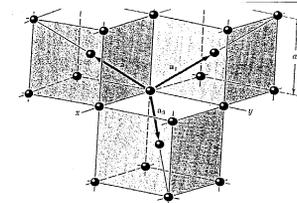


Figure 12 Primitive basis vectors of the body-centered cubic lattice.

## Rede Recíproca

- Definição de Rede Recíproca
- Zonas de Brillouin

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

## First Brillouin Zone: Two Dimensional Oblique Lattice

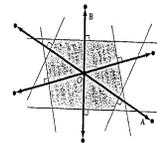


Figure 10 Construction of the first Brillouin zone for an oblique lattice in two dimensions. We first draw a number of vectors from  $O$  to nearby points in the reciprocal lattice. Next we construct lines perpendicular to these vectors at their midpoints. The smallest enclosed area is the first Brillouin zone.

### First Brillouin Zone: BCC

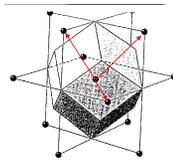


Figure 13 First Brillouin zone of the body-centered cubic lattice. The figure is a regular rhombicuboctahedron.

### Primitive Lattice Vectors: FCC

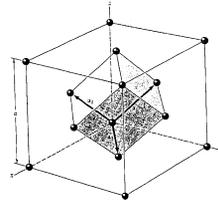


Figure 14 Primitive basis vectors of the face-centered cubic lattice.

### Brillouin Zones: FCC

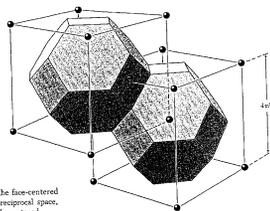
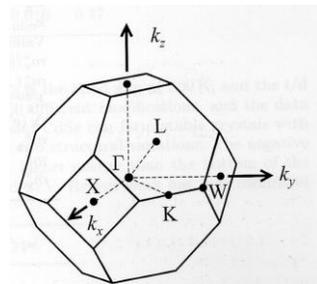
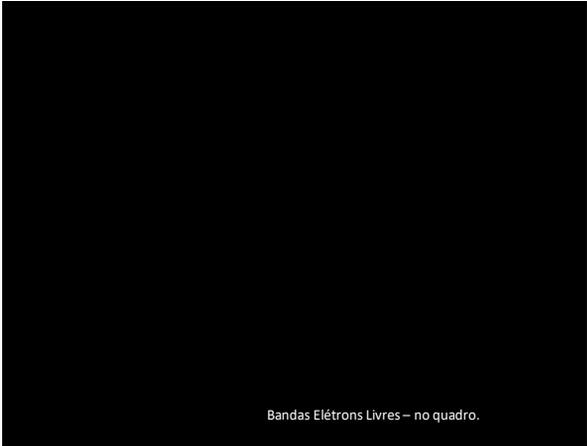


Figure 15 Brillouin zones of the face-centered cubic lattice. The cells are in reciprocal space, and the reciprocal lattice is body-centered.

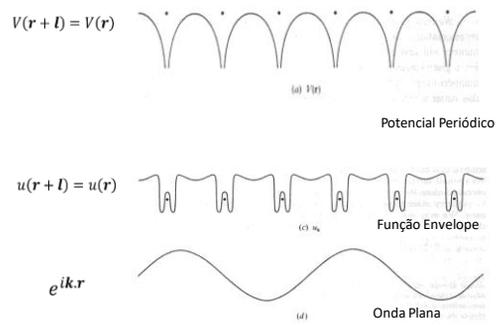
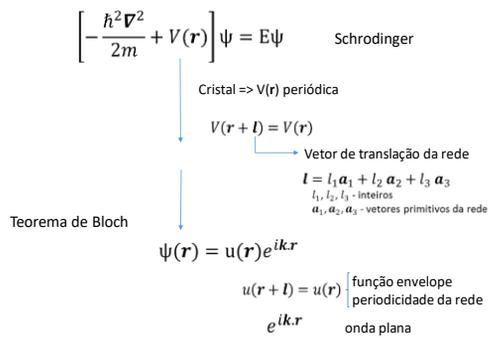


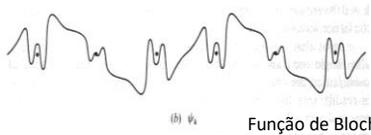
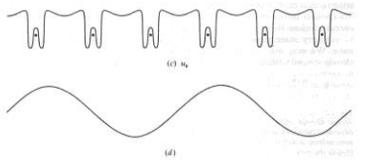
Primeira zona de Brillouin de uma rede direta FCC (é célula de Wigner-Seitz de um arranjo BCC na rede recíproca).



# Resumo Teoria de Bandas

Bandas Elétrons Livres – no quadro.





Função de Bloch

$$\psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r})e^{i\vec{k}\cdot\vec{r}}$$

$$\left[ -\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) \right] \psi = E\psi \quad \text{Schrodinger}$$

$$\psi_{\vec{k}}(\vec{r}) \leftrightarrow E_{\vec{k}}$$

dispersão  $E(\vec{k})$

Espaço  $\mathbf{k} \Rightarrow$  espaço recíproco  
espaço de vetores de onda

$$\psi(\mathbf{r}) = u(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \quad \psi_{\vec{k}}(\vec{r}) \leftrightarrow E_{\vec{k}}$$

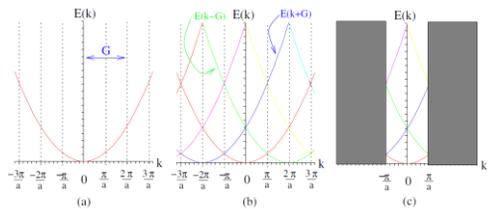
Exemplo + simples: Diagrama de bandas elétron livre

elétron livre

$$u(\mathbf{r}) = u_0 \Rightarrow E_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}$$

dispersão  $E(\vec{k})$

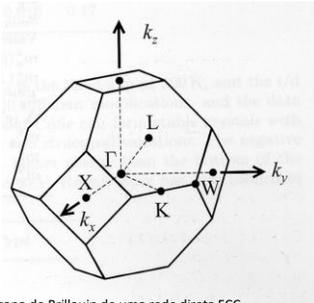
$$E_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m} \quad \text{elétron livre}$$



estendida

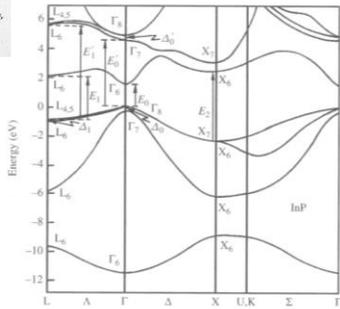
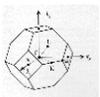
múltipla

reduzida



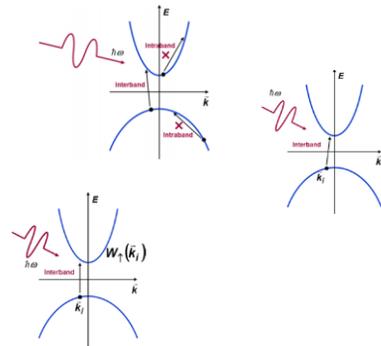
Primeira zona de Brillouin de uma rede direta FCC (é célula de Wigner-Seitz de um arranjo BCC na rede recíproca).

## Bandas de Energia Reais e Transições Ópticas



[Adachi]

Rana - Cornell



## Exercícios

- E1) Mostre que os vetores da rede recíproca de uma rede FCC constituem uma rede BCC.
- E2) Mostre que os vetores da rede recíproca de uma rede BCC constituem uma rede FCC.
- E3) Problemas da lista...

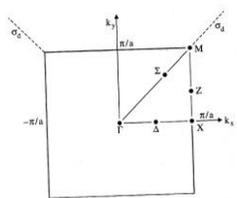


Fig. 2.2 A plan view of the Brillouin zone of a square lattice, with some points of high symmetry labelled.

Singleton. Ex. 2.2