Schrödinger equation

- Schrödinger equation with a periodic potential has the form
- *U* is a periodic function
- *a, b, c* are the lattice constants

$$-\frac{\hbar^2}{2m}\nabla^2\psi + U\psi = E\psi$$

$$U(x, y+b, z) = U(x, y, z)$$
$$U(x+a, y, z) = U(x, y, z)$$
$$U(x, y, z+c) = U(x, y, z)$$

Bloch functions

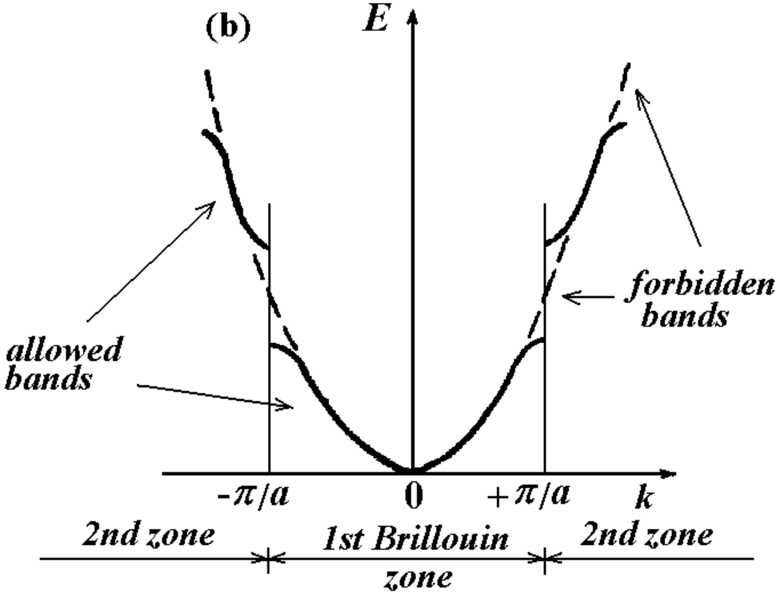
- Felix Bloch proved that the solution of the Schrödinger equation a periodic function

$$\psi_{\mathbf{k}} = u_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{kr}}$$

- $u_{\mathbf{k}}(\mathbf{r})$ is a function having the periodicity of the potential, i.e. periodicity of the lattice.

Band structure

- In the periodic field of a crystal, the dependence of *E* on *k* is also periodic. The bands of quasicontinuously change of energy (allowed bands) depicted by solid lines alternate with the forbidden bands



Band structure

- Each allowed band consists of closely arranged discrete levels which number equals the number of atoms in a crystal. The region of *k* - space in which the energy of an electron in a crystal changes quasicontinuously is called a *Brillouin zone.* There is an interruption in the energy at the boundaries of the zones.

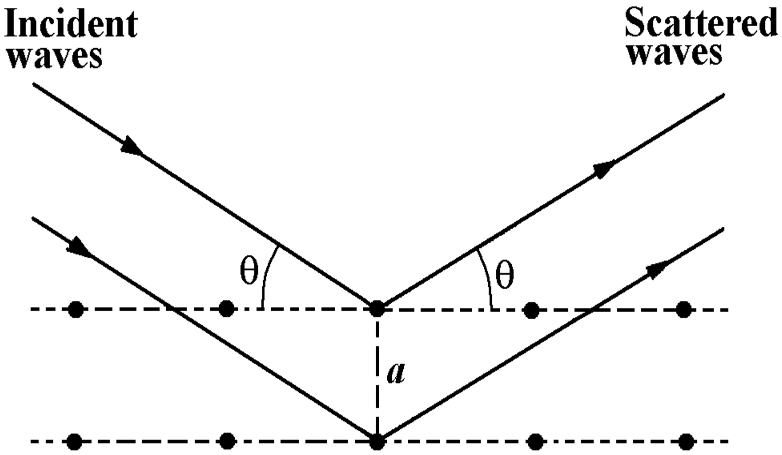
  Previous figure shows the Brillouin zones for a one-dimensional crystal.

motion of an electron

- the lattice affects the motion of an electron only when k is close to $n\pi/a$ and this effect produces energy gaps
- at intermediate values of k, the electrons move freely through the lattice

scattering

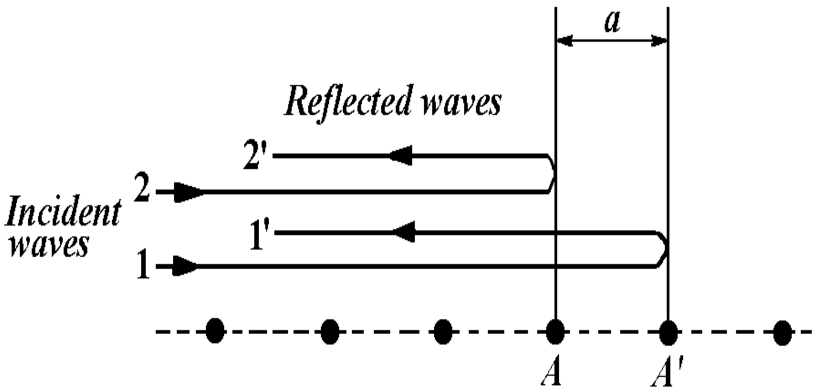
- The motion of electrons in the lattice can be considered as similar to the propagation of an electromagnetic wave in a crystal The scattering of the electromagnetic wave by the atoms in the lattice gives rise to a reinforced scattered wave when Bragg's condition is satisfied



$$2a\sin\theta = n\lambda$$

linear lattice and Bragg's condition

- for normal incidence ($\theta = \pi/2$), and $2a=n\lambda$
- the reflected rays 1' and 2' have a path difference $2a$ and a phase difference $2\pi(2a)/\lambda$



the motion of electrons

- For maximum reinforcement of 1' and 2', this phase difference must be equal to $2\pi n$, resulting in $2a = n\lambda$. Setting $\lambda = 2\pi/k$, we obtain $k = n\pi/a$. Therefore, these values of k are those at which the linear lattice blocks the motion of electrons in a given direction by forcing them to move in the opposite direction

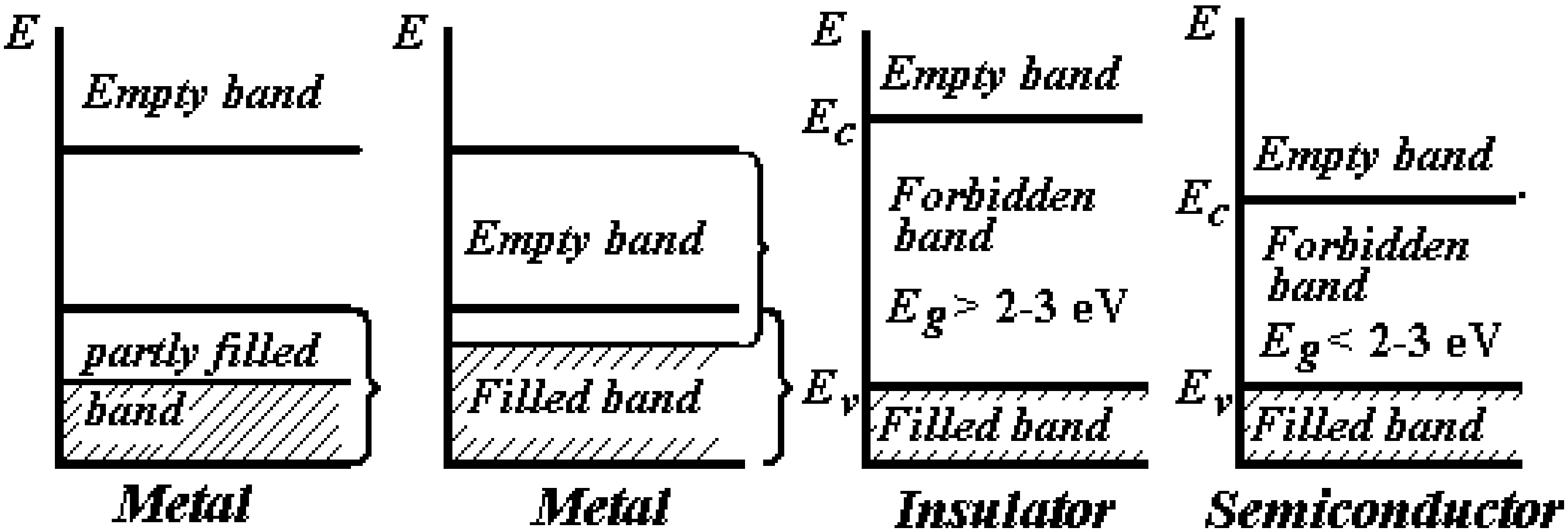
Brillouin zone

- The range of *k* - values between - π/a and $+\pi/a$ constitutes the *first Brillouin zone.* For *k* between $-2\pi/a$ and $-\pi/a$ and between π/a and $2\pi/a$, we have the *second Brillouin zone,* and so on.
- the spectrum of possible values of the energy of valence electrons in a crystal is divided into a number of allowed and forbidden bands

Metals, Dielectrics, Semiconductors

- The existence of energy bands makes it possible to explain the existence of metals, semiconductors, and dielectrics

Metals, Dielectrics, Semiconductors



Metals, Dielectrics, Semiconductors

- Metals and dielectrics differ principally;
- Dielectrics and semiconductors differ only quantitatively
- The type of the filling of energy band depends also on crystalline structure. For example, the Carbon structured as diamond is dielectric. The Carbon structured as graphite is a metal.