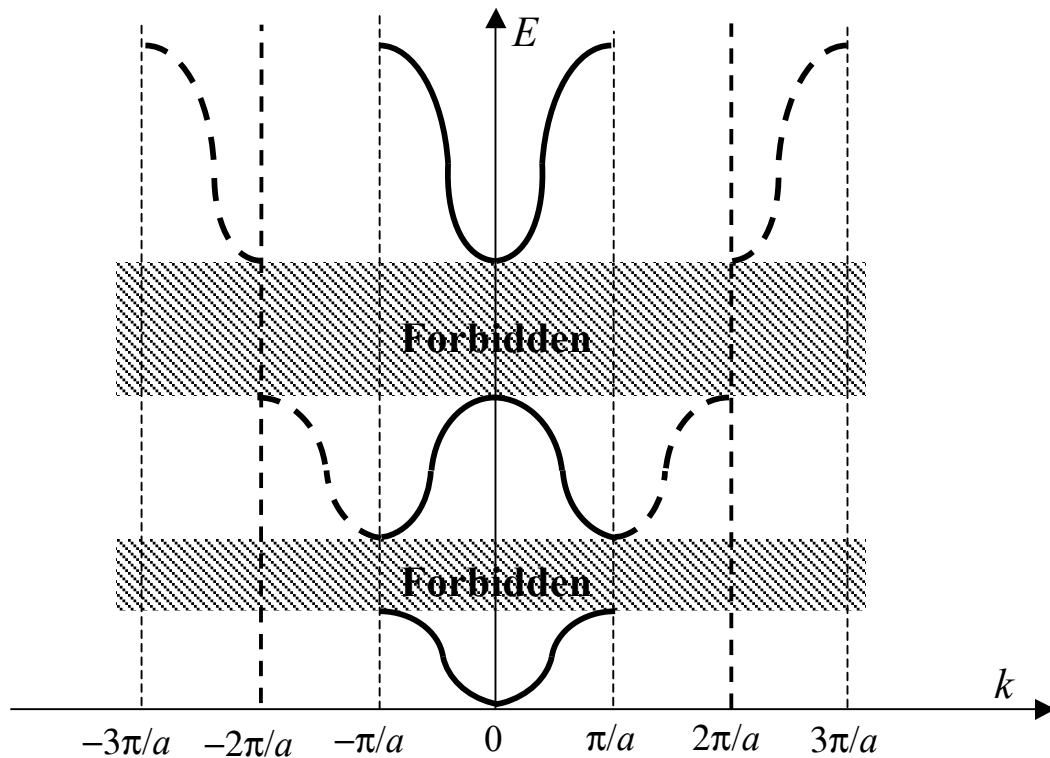


K-space diagram

The k-space diagram is the relation of particle energy E versus the momentum (wave number) k . This relation has to satisfy the Kronig-Penney mathematic model:

$$M \frac{\sin(\alpha a)}{\alpha a} + \cos(\alpha a) = \cos(ka)$$

Where, $M \equiv \frac{mV_0ba}{\hbar^2}$, $\alpha = \frac{\sqrt{2mE}}{\hbar}$



Direct bandgap

In order to satisfy the Kronig-Penney model, the k-E diagram is not continuous, which determines the allowed bands and forbidden bands. Physically, this is due to the

interference within the crystal lattice structures (constructive or destructive).

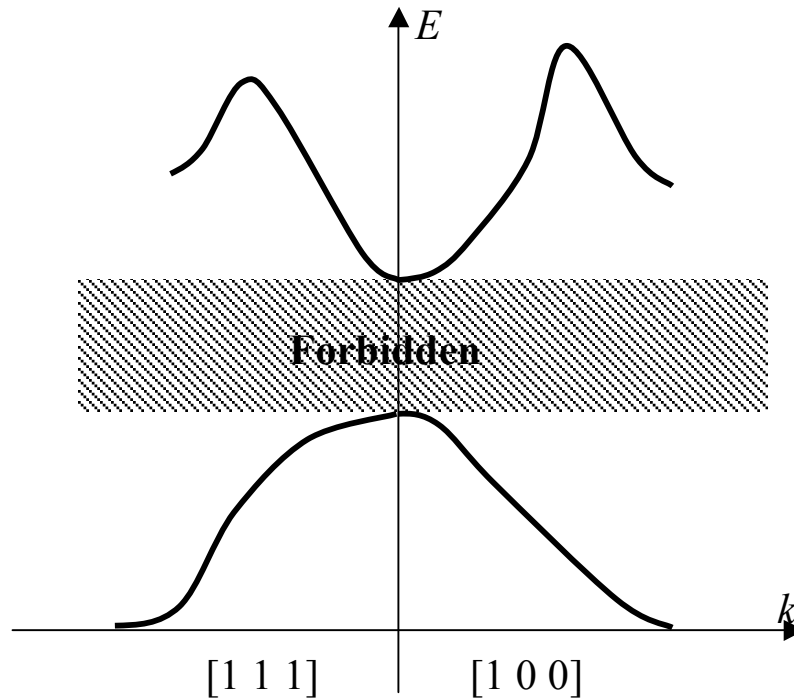
Due to the repetitive nature of the wave number k (the period is $2\pi/a$ in this case) in terms of the interference effect, the k -space diagram can be rearranged to concentrate near the region of $k = 0$.

The lattice constant a is a critical parameter to determine the band structure: when a increases, interference effect becomes weaker and forbidden band shrinks. On the other hand, if a decreases, the atom density increases, the interference becomes stronger and the forbidden band may become widened.

In **3-dimensional** structures, distance between atoms (lattice constant) may be different for different directions. Therefore, the wave number k is a "wave vector", \mathbf{k} . Its orientation indicates the direction in which a particular particle moves.

A complete description of k -space program must be presented in a 4-dimensional plot (\mathbf{k} vector is 3-dimensional, and energy E is the 4th dimension). But obviously a 4-dimensional plot is not possible.

A simple way is to plot the k -space diagrams separately for different directions represented by Miller indices, such as $[1\ 1\ 0]$, $[1\ 1\ 1]$.



Direct and indirect bandgaps:

For the equation

$$M \frac{\sin(\alpha a)}{\alpha a} + \cos(\alpha a) = \cos(ka)$$

Take d/dk at each side

$$\left\{ M \frac{\alpha a^2 \cos(\alpha a) - a \sin(\alpha a)}{(\alpha a)^2} + a \sin(\alpha a) \right\} \frac{1}{\hbar} \sqrt{\frac{m}{2E}} \frac{dE}{dk} = -a \sin(ka)$$

at $k=0$, the right hand side $-a \sin(ka) = 0$, therefore,

we must have $dE/dk = 0$ at $k = 0$. This means that there is always a saddle point at $k = 0$ (either a maximum or a minimum).

Direct semiconductor (direct bandgap):

At $k = 0$, there is a valence band maximum and a conduction band minimum. In this case, energy transition between the bottom of the conduction band and the top of the valence band does not require momentum change.

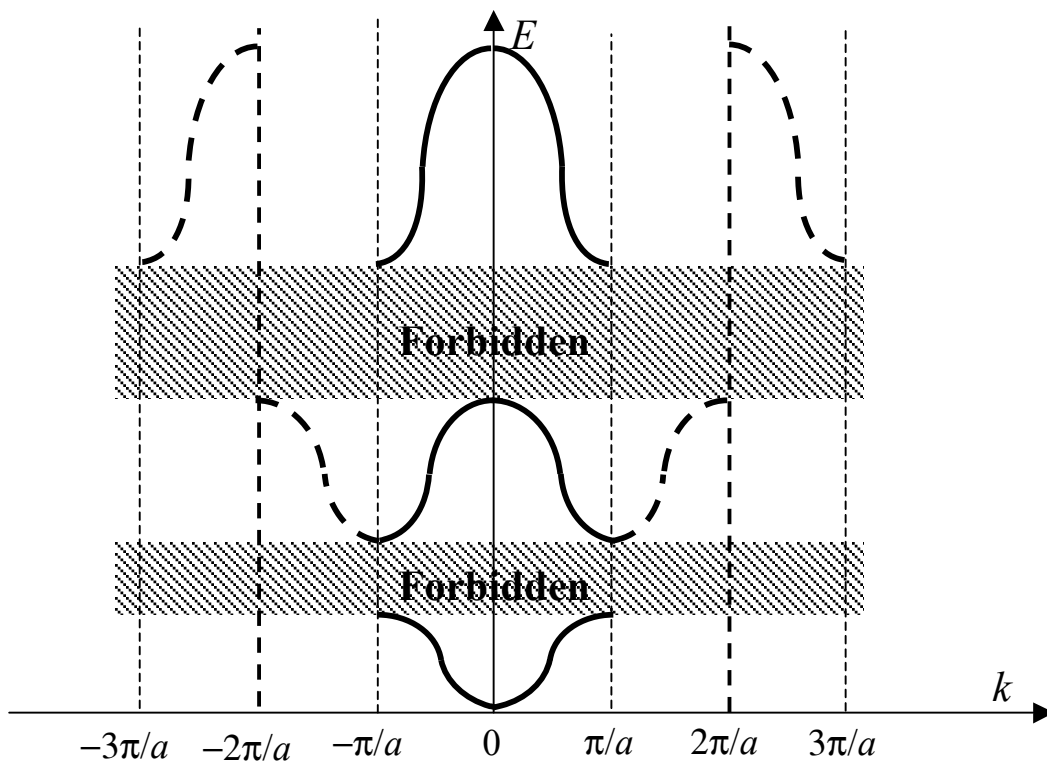
Significance: in a direct semiconductor, a photon with energy $h\nu = E_g$ can excite an electron from the top of the valence band to the bottom of the conduction band. Or vice versa, an electron jumps down from the bottom of the conduction band to the top of the valence band can generate a photon with energy $h\nu = E_g$.

Indirect semiconductor (indirect bandgap):

The top of the valence band and the bottom of the conduction are not aligned at $k = 0$. In this case, energy transition between the bottom of the conduction band and the top of the valence band requires momentum change.

Significance: in an indirect semiconductor, a photon with energy $h\nu = E_g$ cannot excite an electron from the top of the valence band to the bottom of the conduction band, an extra momentum change is required for this transition.

Indirect semiconductor such as silicon cannot be used to make semiconductor lasers and LEDs.



Indirect bandgap