Empty Lattice Approximation

by Dr. Colton, Physics 581 (last updated: Fall 2020)

1) Actual Band Structures

From Yu and Cardona, *Fundamentals of Semiconductors*, 1 st edition (Springer, New York, 1996).

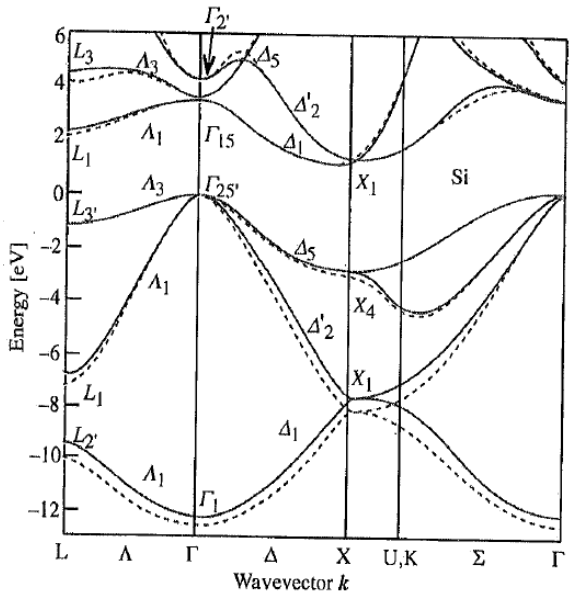


Fig 2.10. Electronic band structure of Si calculated by the pseudopotential technique. The solid and the dotted lines represent calculations with a nonlocal and a local pseudopotential, respectively. [Ref.: M.L. Cohen and J. Chelikowsky, *Electronic Structure and Optical Properties of Semiconductors*, 2nd edition, Springer Ser. Solid-State Sci., Vol.75 (Springer, Berlin, 1989).]

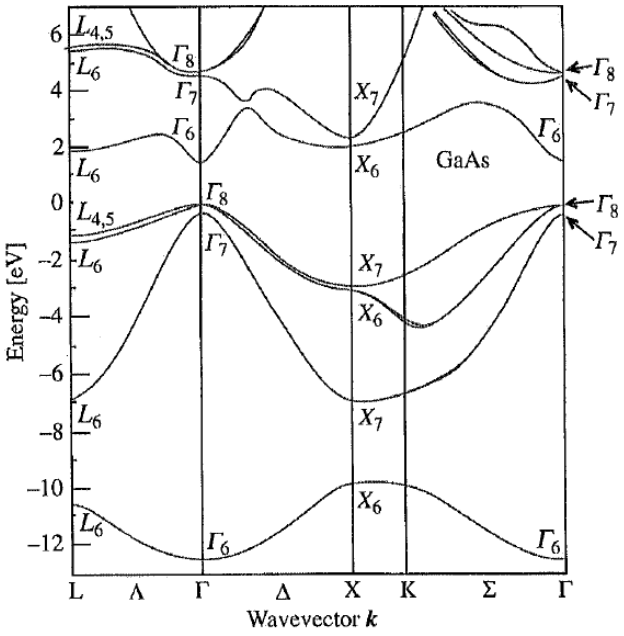


Fig. 2.14. Electronic band structure of GaAs calculated by the pseudopotential technique. [Ref.: Cohen and Chelikowsky, 1989.]

2) Empty Lattice Approximation (also from Yu and Cardona)

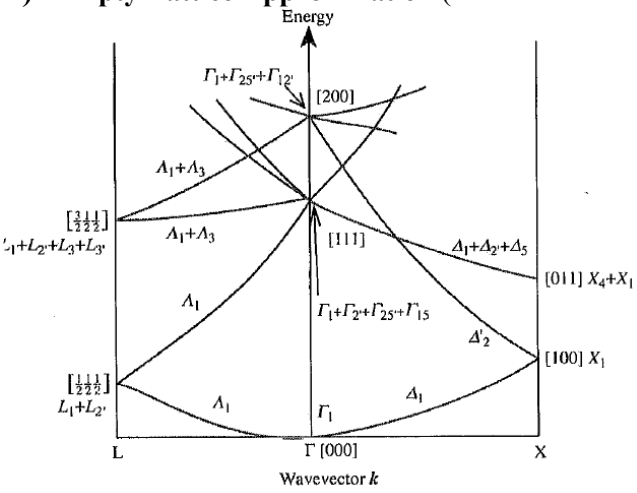


Fig. 2.9. Band structure of nearly free electrons for a diamond-type crystal in the reduced zone scheme. The numbers in *square brackets* denote corresponding reciprocal lattice vectors in the extended zone scheme in units of $(2\pi/a)$, a being the size of the unit cube.

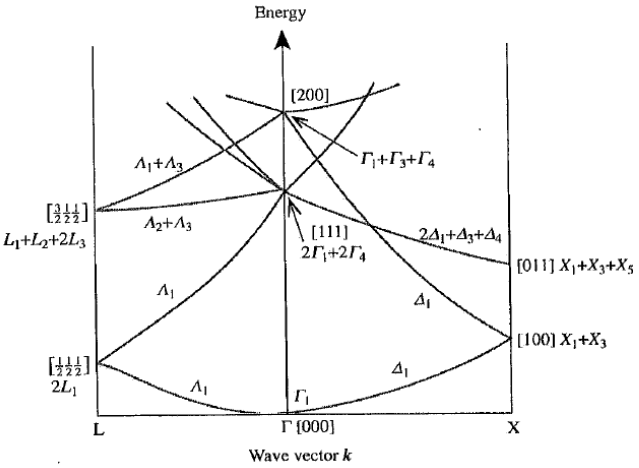
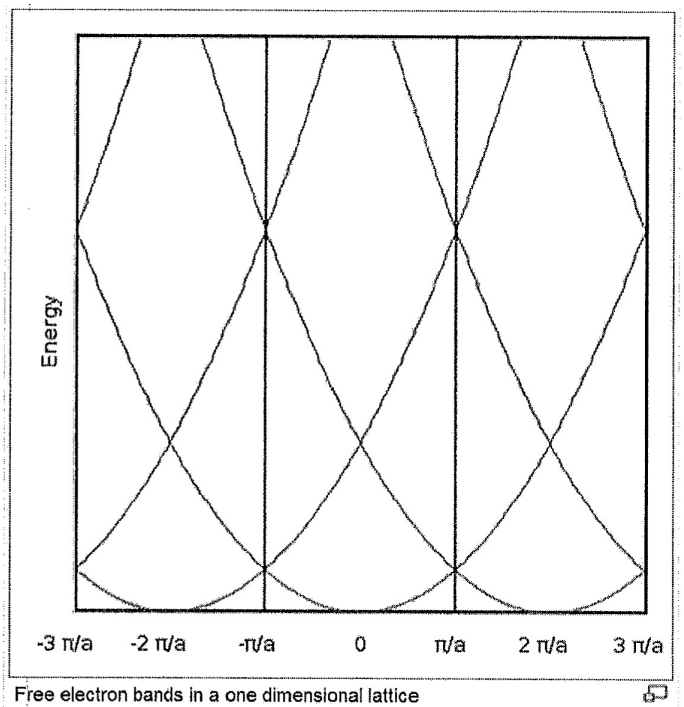


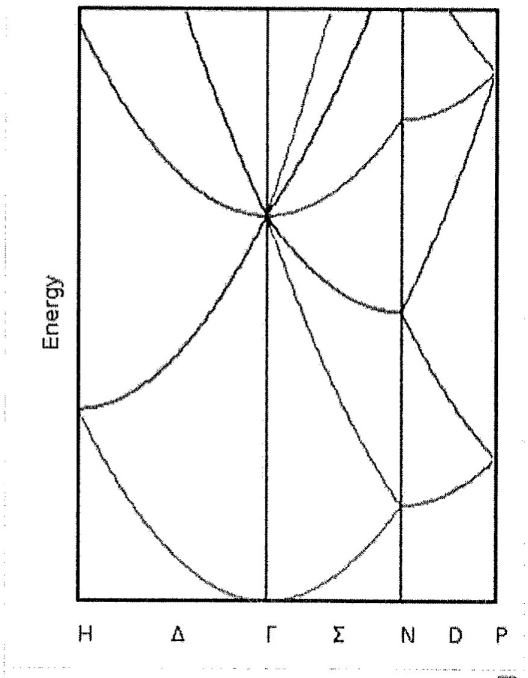
Fig 2.8. Band structure of nearly free electrons in a zinc-blende-type crystal in the reduced zone scheme.

3) Empty Lattice Approximation

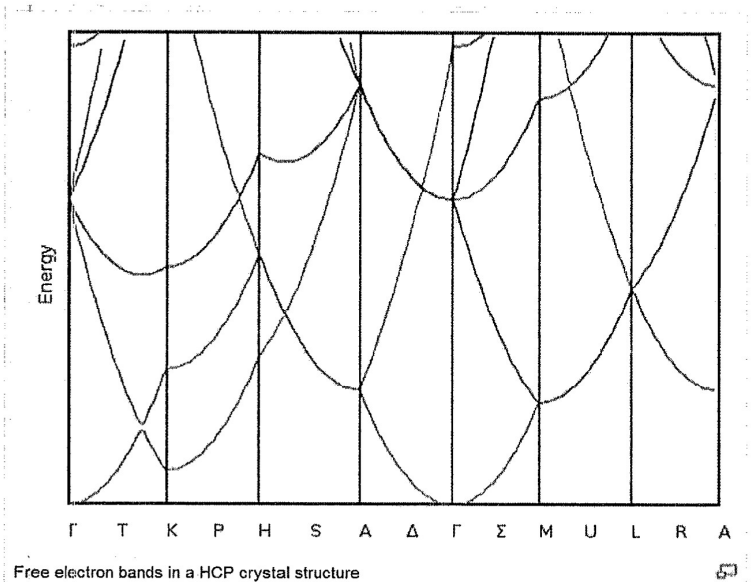
From Wikipedia, https://en.wikipedia.org/wiki/Empty_lattice_approximation



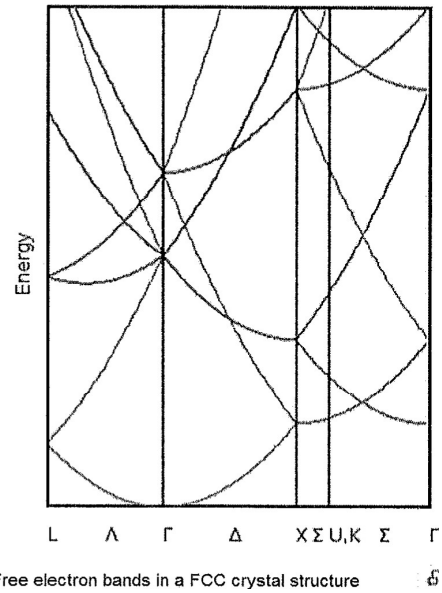
Free electron bands in a one dimensional lattice



Free electron bands in a BCC crystal structure



Free electron bands in a HCP crystal structure



Free electron bands in a FCC crystal structure

4) Calculating the Empty Lattice Approximation – Example, Simple Cubic, [100] direction

$\epsilon(\vec{k},\vec{G}) = \frac{\hbar^2}{2m}\left(\vec{k}+\vec{G}\right)^2$ Where $\vec{k}$ is in the first B.Z and $\vec{G}$ is any reciprocal lattice vector.

(1) $\vec{k}$ is in the [100] direction for this problem $\rightarrow \vec{k} = (k,0,0)$

(2) Simple Cubic Lattice

$\rightarrow \vec{G} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3 \quad (h,k,\ell) \in \mathbb{Z}$ (this k is not the wavevector!)

and

$\vec{b}_1 = \frac{2\pi}{a}(1,0,0)$

$\vec{b}_2 = \frac{2\pi}{a}(0,1,0)$

$\vec{b}_3 = \frac{2\pi}{a}(0,0,1)$

$\Longrightarrow \vec{G} = \frac{2\pi}{a}(h,k,\ell)$

$$(k+G)^2 = \left(k_x+G_x, k_y+G_y, k_z+G_z\right)\cdot\left(k_x+G_x, k_y+G_y, k_z+G_z\right)$$
$$= (k_x+G_x)^2 + \left(k_y+G_y\right)^2 + (k_z+G_z)^2$$
$$= (k+2\pi h/a)^2 + (0+2\pi k/a)^2 + (0+2\pi\ell/a)^2$$

Define x to go from 0 to 1 first BZ in the [100] direction,

$$x = \frac{k}{k_{max}} = \frac{k}{\pi/a} \rightarrow k = \frac{\pi}{a}x$$

$$E = \frac{\hbar^2}{2m}\left[\left(\frac{\pi}{a}x + \frac{2\pi}{a}h\right)^2 + \left(\frac{2\pi}{a}k\right)^2 + \left(\frac{2\pi}{a}\ell\right)^2\right]$$

$$= \frac{\hbar^2}{2m}\frac{\pi^2}{a^2}[(x+2h)^2 + 4k^2 + 4\ell^2]$$

Define a reference energy, $E_{\text{ref}} = E(x=1,(h,k,\ell)=0) = \frac{\hbar^2}{2m}\frac{\pi^2}{a^2}$

y axis $= \frac{E}{E_{\text{ref}}} = (x+2h)^2 + 4k^2 + 4\ell^2$

Plots for variations combinations of (h,k,l) up to $\frac{E}{E_{\text{ref}}} = 7$

(picking the h,k,l numbers for the plots can be challenging. I did it with trial and error, and by thinking about the equation. For example, the plots with (011), (011), (011), and (011) will all be the same.)

In[1]:=
```
e[x_, h_, k_, l_] = (x + 2 h)^2 + 4 k^2 + 4 l^2
```

Out[1]=
$$4\,k^2 + 4\,l^2 + (2\,h + x)^2$$

In[2]:=
```
Plot[{e[x, 0, 0, 0], e[x, 1, 0, 0], e[x, -1, 0, 0], e[x, 0, 1, 0],
  e[x, 1, 1, 0], e[x, -1, 1, 0], e[x, 0, 1, 1]}, {x, -1, 1}, PlotRange → {0, 9}]
```

Out[2]=