PH575 Spring 2019

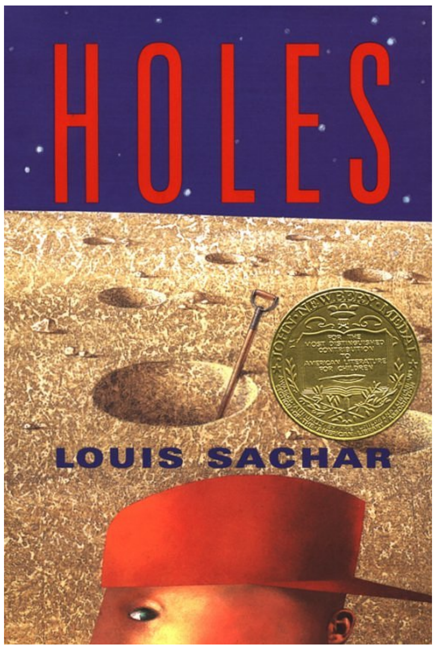
Lecture #10

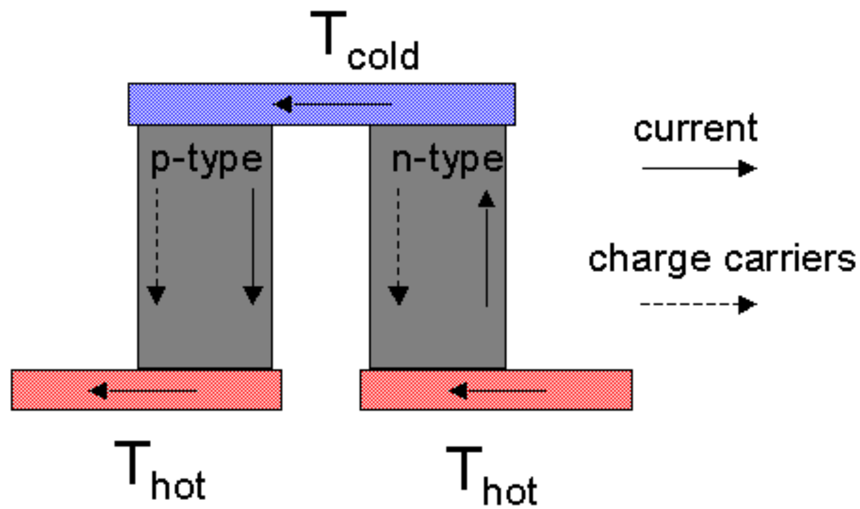
Electrons, Holes; Effective mass

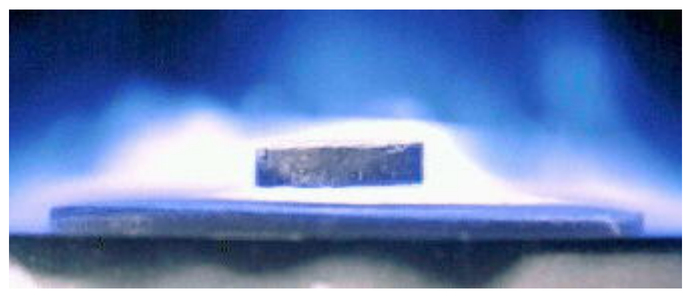
Sutton Ch. 4 pp 80 -> 92;

Kittel Ch 8 pp 194 – 197;

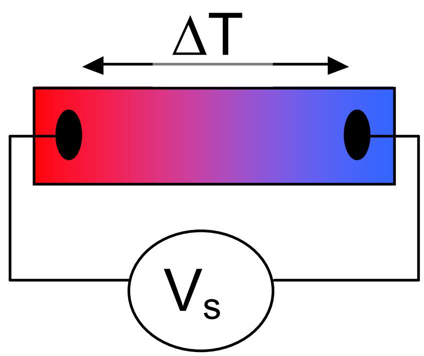
AM p. <-225->

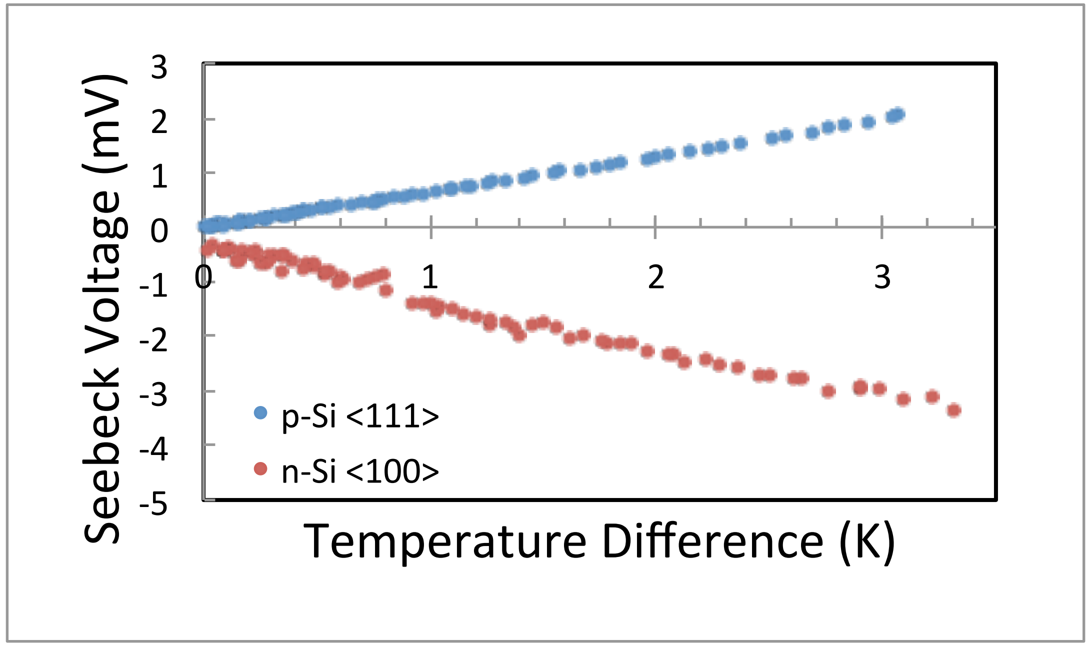






Thermal properties of Si (300K)





- *p*-type <111> Si
- $p = 6.25\times10^{18}$ cm^{-3}
- ρ = 0.014 Ωcm
- S = + 652 μV K^{-1}
- κ = 148 W/mK
- *PF* = 3 x 10^{-3} V^2/K^{2}Wm
- *ZT* = 0.006

- *n*-type <100> Si
- $n = 9.5\times10^{17}$ cm^{-3}
- ρ = 0.021 Ωcm
- S = - 872 μV K^{-1}
- κ = 148 W/mK
- *PF* = 3 x 10^{-3} V^2/K^{2}Wm
- *ZT* = 0.006

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Dispersion relation for a free electron, where *k* is the electron momentum:

$$E(k)=\frac{\hbar^2k^2}{2m}$$

Group velocity

$$\frac{1}{\hbar}\frac{dE(k)}{dk}=\frac{\hbar k}{m}=\frac{p}{m}=v$$

mass

$$\left[\frac{1}{\hbar^2}\frac{d^2E(k)}{dk^2}\right]^{-1}=\left[\frac{d}{dk}\left(\frac{k}{m}\right)\right]^{-1}=m$$

These are generalizable to the periodic solid where, now, *k* is NOT the individual electron momentum, but rather the quantity that appears in the Bloch relation. It is called the CRYSTAL MOMENTUM

$$\boxed{\vec{v}=\frac{1}{\hbar}\nabla_k E(k)}$$

$$\boxed{m^*=\hbar^2\left[\nabla^2{}_k E(k)\right]^{-1}}$$

Problem on hwk

Change in energy on application of electric field:

$$\delta E = q\vec{\varepsilon}\cdot\vec{v}\delta t \quad (\vec{F}\cdot\vec{d})$$

Change in energy with change in *k* on general grounds:

$$\delta E = \nabla_k E\cdot\delta\vec{k}$$

$$\vec{v} = \frac{1}{\hbar}\nabla_k E(k)$$

$$q\vec{\varepsilon}\cdot\vec{v}\delta t = \hbar\vec{v}_k\cdot\delta\vec{k} \Rightarrow q\vec{\varepsilon} = \frac{d(\hbar\vec{k})}{dt}$$

Get an equation of motion just like *F* = *dp/dt* !
hk/2π acts like momentum ….. We call it crystal momentum, because it's not the true electron momentum.

Crystal momentum is what is changed by the external force.
Now define *m** by:

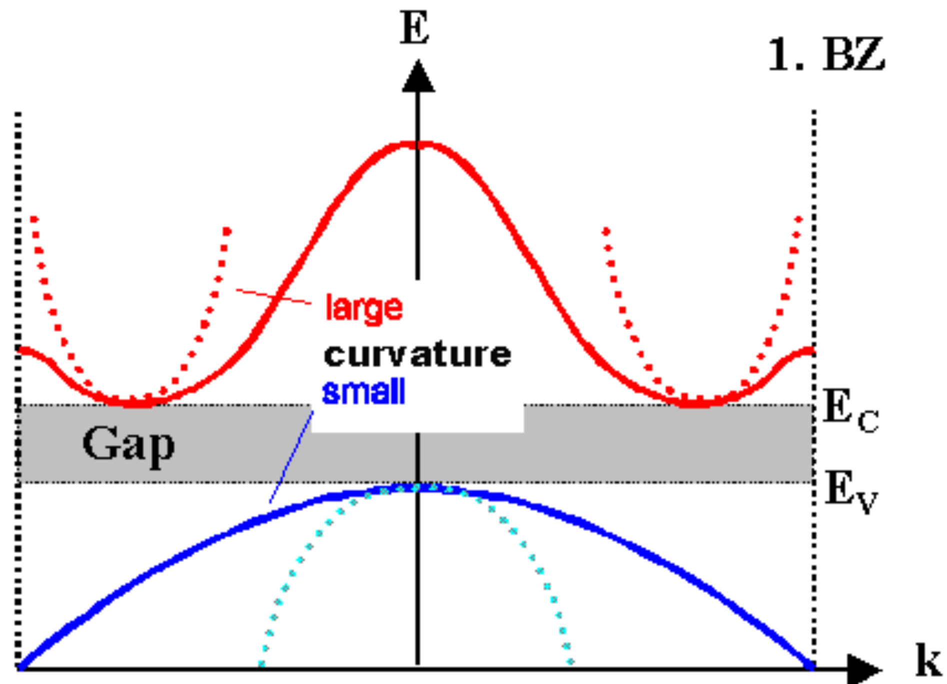
$$\frac{d\left(\hbar\vec{k}\right)}{dt} \equiv m^*\frac{d\vec{v}_k}{dt}$$

$$m^*\frac{d\vec{v}_k}{dk}\frac{dk}{dt} = \frac{m^*}{\hbar^2}\frac{d^2E}{dk^2}\frac{d\left(\hbar\vec{k}\right)}{dt}$$

$$\frac{m^*}{\hbar^2}\frac{d^2E}{dk^2} = 1 \Rightarrow m^* = \frac{\hbar^2}{\dfrac{d^2E}{dk^2}}$$

In 3-d:

$$m^* = \frac{\hbar^2}{\nabla_k^2 E}$$



http://www.tf.uni-kiel.de/matwis/amat/semi en/kap 2/illustr/effective mass.gif

1-dimensional chain (& β<0):

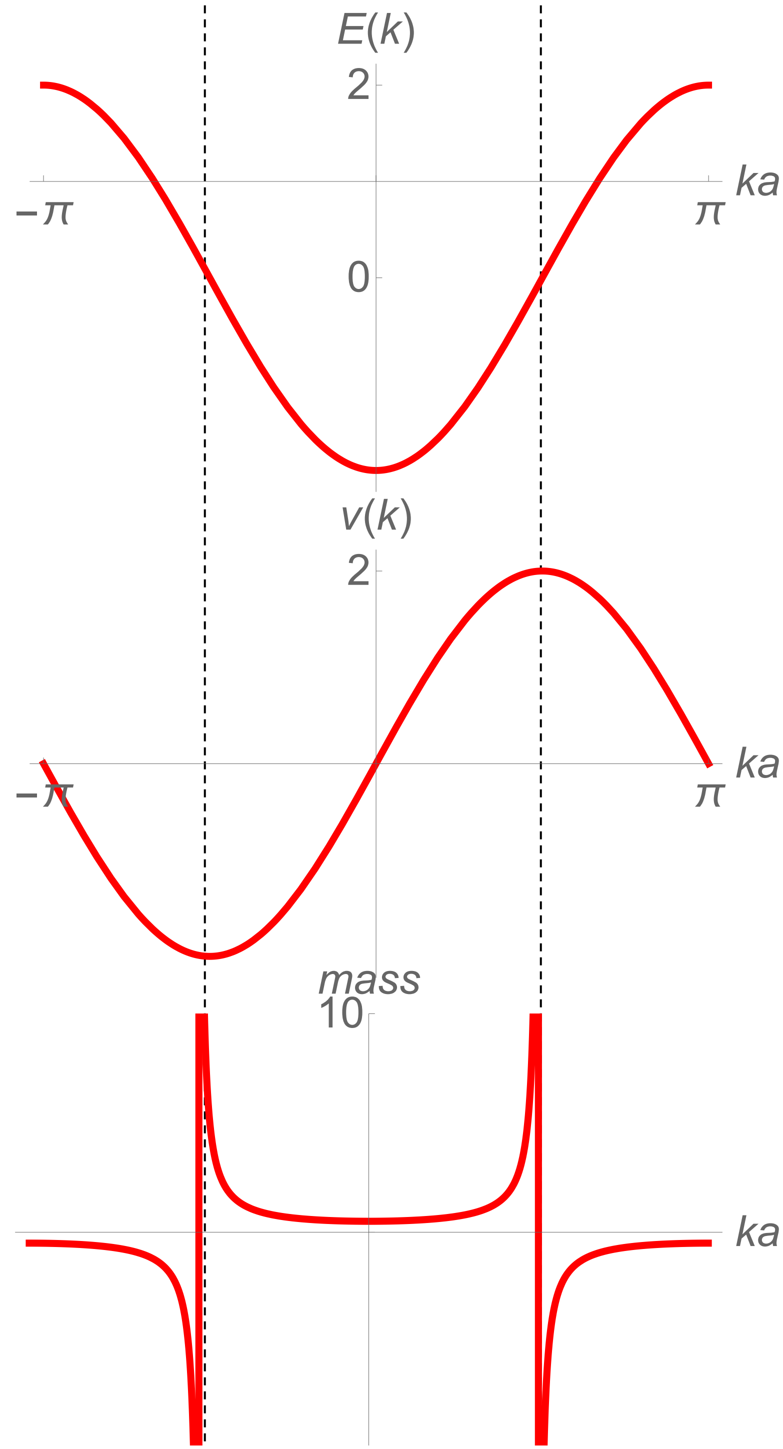
$$E(k) = \alpha + 2\beta\cos(ka)$$

$$\vec{v} = \frac{1}{\hbar}\nabla_k E(k)$$

$$v(k) = -2\beta a\sin(ka)$$

$$m^* = \frac{\hbar^2}{\frac{d^2E}{dk^2}}$$

$$m^* = \frac{-\hbar^2}{2\beta a^2\cos(ka)}$$



Holes

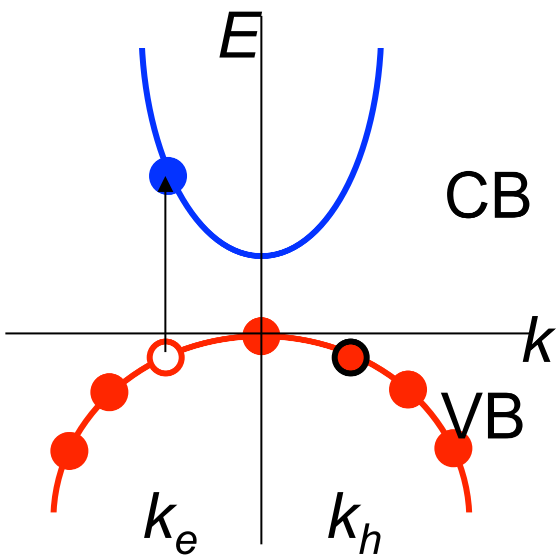
• If one electron in state *k* is missing from an otherwise filled band, all the other ≈ 10^{23} electrons can be described by the concept of a single hole.
What is this hole's momentum, energy, velocity, mass ?

•Momentum:

The hole's momentum is -*k* (in units of *h*/2π); in other words the opposite of the momentum of the missing electron.

$$\boxed{\vec{k}_h = -\vec{k}_e}$$

The completely filled band has zero total momentum (as many states *k* as -*k*). The loss of electron with momentum *k* changes total band momentum to -*k*. This is the momentum of the equivalent hole.



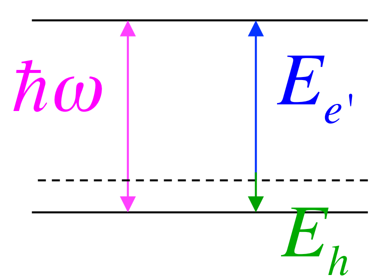
Holes - Energy

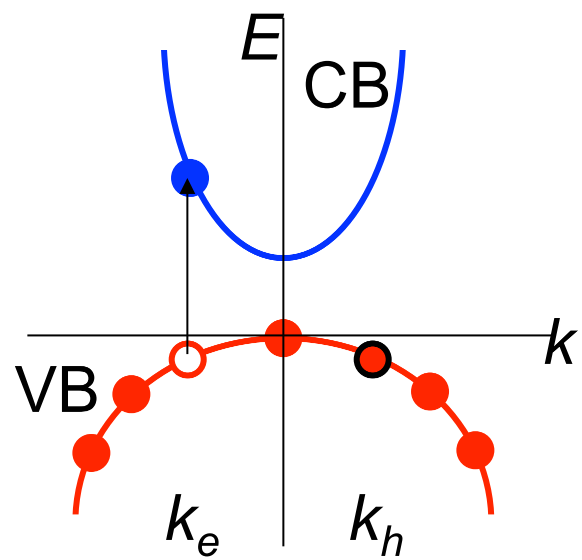
- The energy of the hole is the negative of the energy of the missing electron (E=0 is top of VB).

$$\boxed{E_h\left(\vec{k}_h\right) = -E_e\left(\vec{k}_e\right)}$$

- In order to excite an electron to create an electron-hole pair, energy is added to the system, e.g. optically.

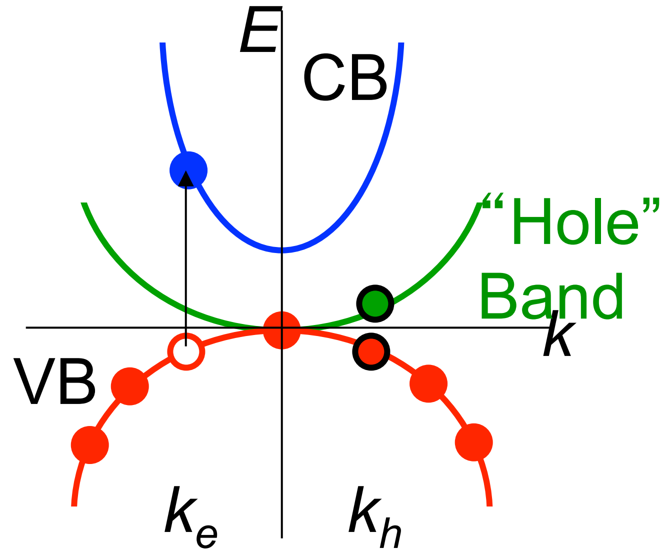
- Of the added energy, $E_{e'}$ is assigned to the electron in the CB, and E_h is assigned to hole in the VB.

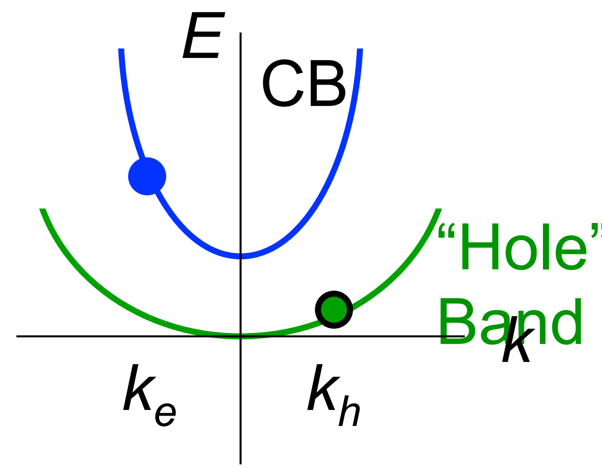




Holes

- These properties can be described by <u>replacing</u> the entire valence band (with many electrons and 1 missing one), by a band with a single particle of momentum k_h=-k_e and energy E = -E_e (where subscript *e* refers to the state of the MISSING electron, not the the state in the CB the electron has gone to (e').
- This is the green band in the picture.



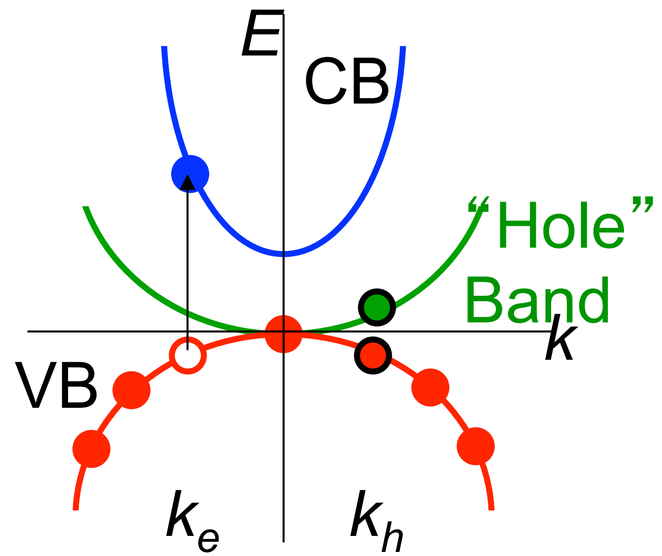


$$\hbar\omega = \underbrace{E_{e'}}_{>0} + \underbrace{E_h}_{>0}$$

Holes - velocity

- The (instantaneous) velocity of the hole is equal to the (instantaneous) velocity of the unoccupied electron state (same slope of $E(k)$.

$$\boxed{v_h\left(\vec{k}_h\right) = v_e\left(\vec{k}_e\right)}$$

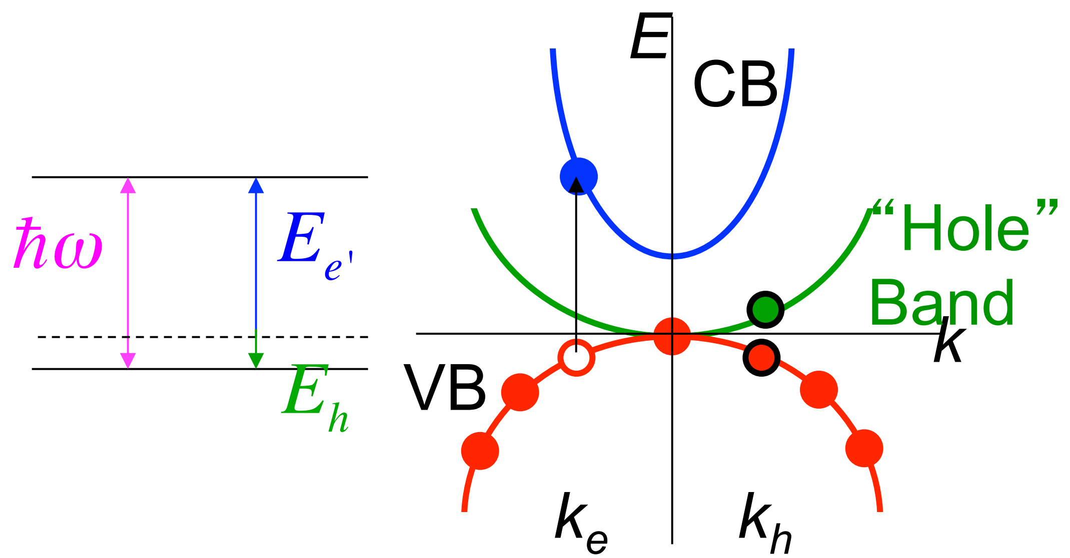


- But note that the the velocity of the excited electron in the CB is **not relevant** here!

Holes

•Effective mass:
The effective mass of the hole is opposite to the effective mass of the missing electron. (Curvature of inverted dispersion relation is opposite).

$$\boxed{m_h\left(\vec{k}_h\right) = -m_e\left(\vec{k}_e\right)}$$



Holes

- Equation of motion:

The equation of motion of the hole state is same as the unoccupied electron state, except with a positive charge!

$$\boxed{\hbar \frac{d\vec{k}_h}{dt} = e\left(\vec{\varepsilon} + \vec{v}_h \times \vec{B}\right)}$$

Electron:

$$\hbar \frac{d\vec{k}_e}{dt} = -e\left(\vec{\varepsilon} + \vec{v}_e \times \vec{B}\right) \qquad \vec{k}_e \rightarrow -\vec{k}_h; \vec{v}_e \rightarrow \vec{v}_h$$

Positive charge is consistent with electric current carried by VB. Current is carried by the unpaired electron (the one whose opposite at k_e is missing):

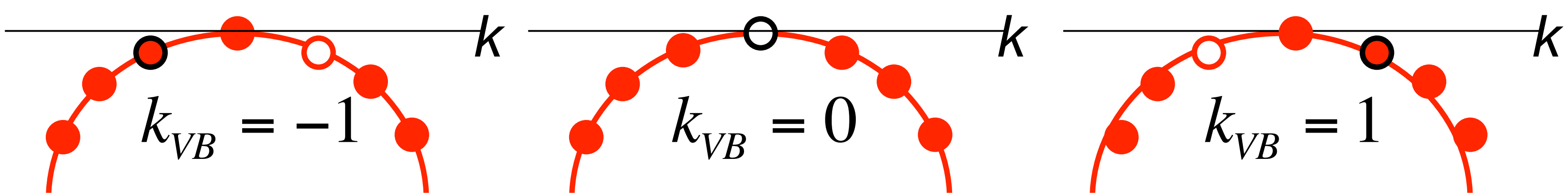
$$\vec{j}_{VB} = -e\vec{v}_e\left(-\vec{k}_e\right) = -e\left[-\vec{v}_e\left(\vec{k}_e\right)\right] = e\vec{v}_e\left(\vec{k}_e\right)$$

Holes

- Electric field in +*x* direction.

$$F = q\varepsilon \begin{cases} < 0 \text{ for -ve charge} \\ > 0 \text{ for +ve charge} \end{cases} \qquad \frac{dk}{dt} = \frac{F}{\hbar} \begin{cases} < 0 \text{ for -ve charge} \\ > 0 \text{ for +ve charge} \end{cases}$$

$\varepsilon \longrightarrow$



$$\frac{dk_{VB}}{dt} > 0$$

Electrons in VB overall behave as +ve charge does. *e* here is +ve #

$$\vec{j}_{VB} = (-e)\vec{v}_e\left(-\vec{k}_e\right) = (-e)\left[-\vec{v}_e\left(\vec{k}_e\right)\right] = e\vec{v}_e\left(\vec{k}_e\right)$$

Holes

- A hole is the description of a nearly full valence band with the absence of an electron: 1 hole ≈ 10^{23}-1 electrons !
- If an electron in state *k* is missing, all other electrons have total momentum -*k*. Thus hole has momentum -*k.*
- If electron with negative charge and negative mass in state *k* is missing, the remaining electrons can be described as a hole with positive charge and positive mass.
- The energy of the hole is the negative of the energy of the electron (rel to top of VB) because it takes more energy to remove an electron deep in the band.
- The velocity of a hole is equal to the velocity of the missing electron in the valence band.
- Within a particular band, we can describe carriers as electrons OR holes, but not both.
- Can use electron description for one band and hole description for a different band, but don't mix descriptions for one band.

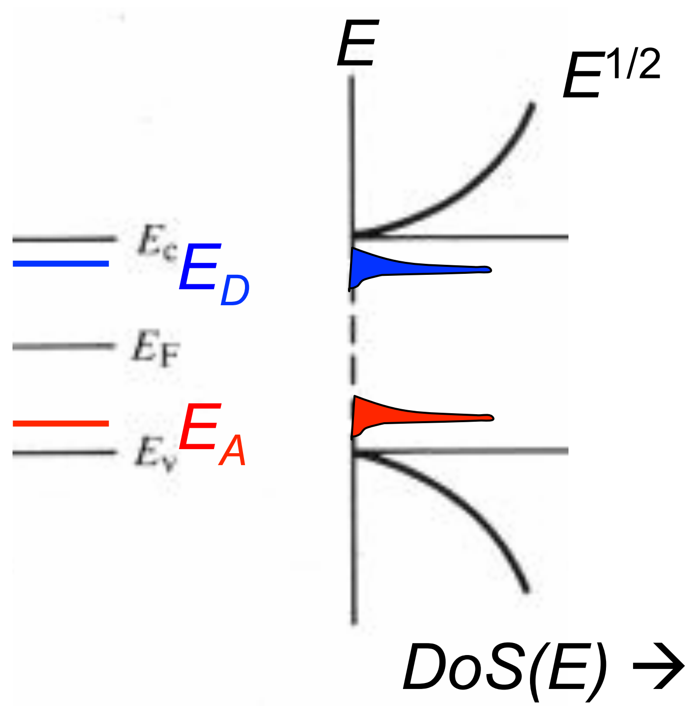
Holes - how do you make them?

- Excite an electron into the conduction band, and then a hole remains in the valence band. In this case, we have 2 mobile charge carriers - both contribute to the current (and the contributions add)
- Add a dopant with one fewer valence electrons than the site onto which it substitutes. This results in a very-low-mobility state in the gap. It is unoccupied at low T, but an electron from the VB can occupy it at finite T, and this electron is effectively immobilized. The remaining hole in the VB is mobile. Si:B is the classic example.
- If you add a dopant with one more valence electron, then what?

Holes - how do you measure them?

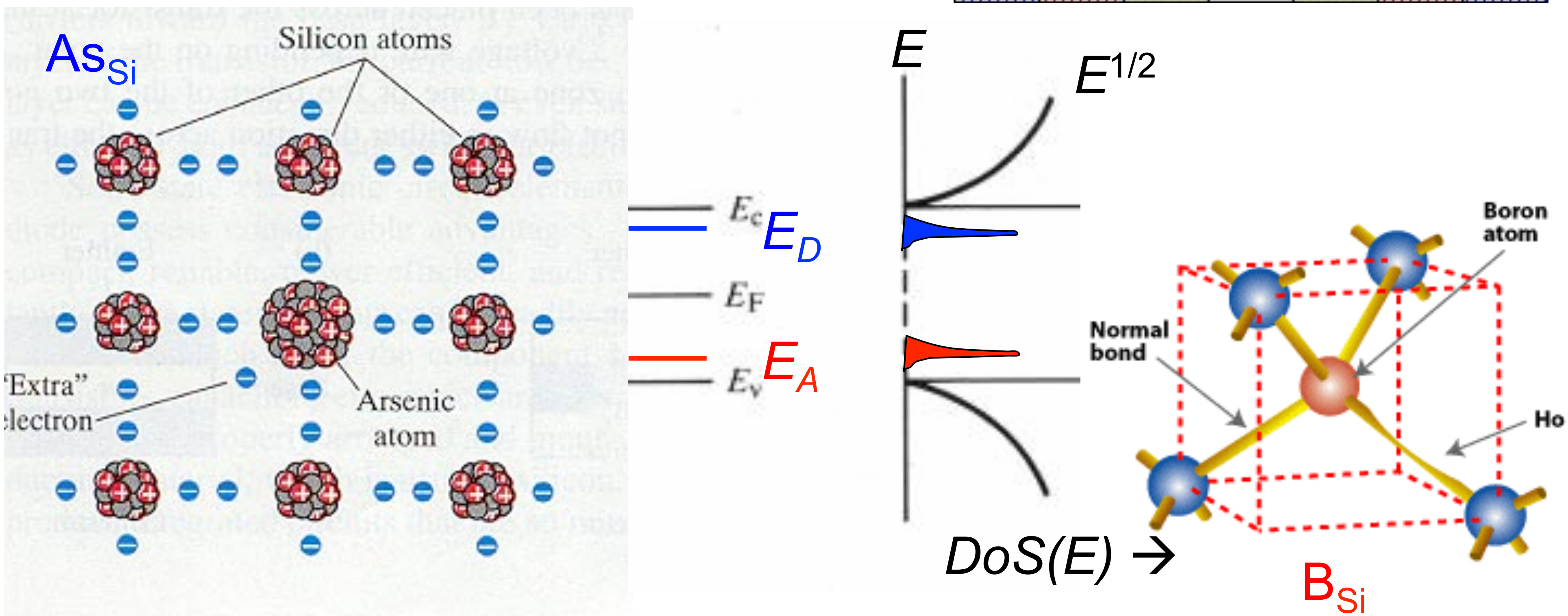
- Are holes “real”? No, not like positrons, but, yes, in a sense. They are a single-particle description of a multi-electron phenomenon.
- Measure the Hall effect in a classic semiconductor - clear evidence.
- Seebeck effect also.

Holes & electrons - how do you represent them?



Substitutional Defects:
Si:As and Si:B

11	12	13	14	15	16	17
		B	C	N	O	F
		Al	Si	P	S	Cl
Cu	Zn	Ga	Ge	As	Se	Br
Ag	Cd	In	Sn	Sb	Te	I
Au	Hg	Tl	Pb	Bi	Po	At



http://www.astro.virginia.edu/class/oconnell/astr511/im/Si-As-doping-JFA.jpg

http://www.eere.energy.gov/solar/images/illust_boron_atom.gif