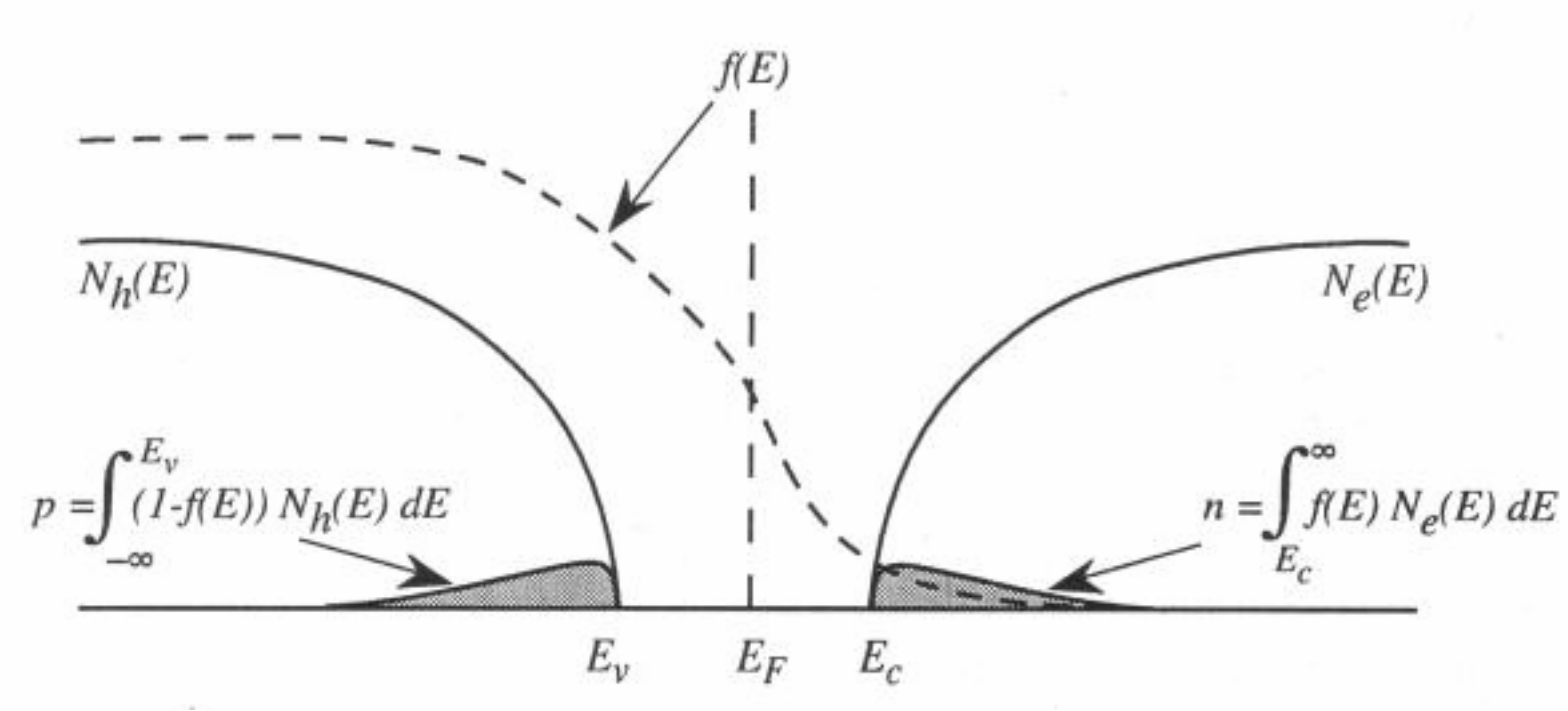
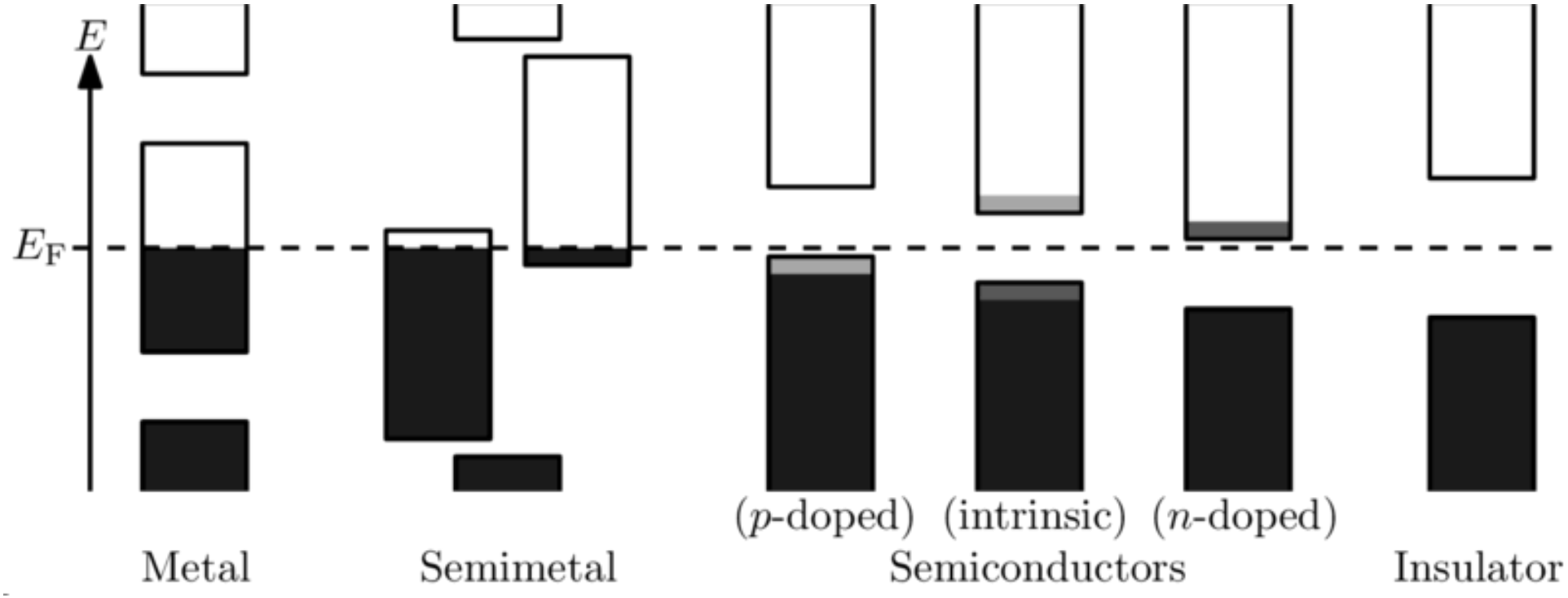
PH575 Spring 2019

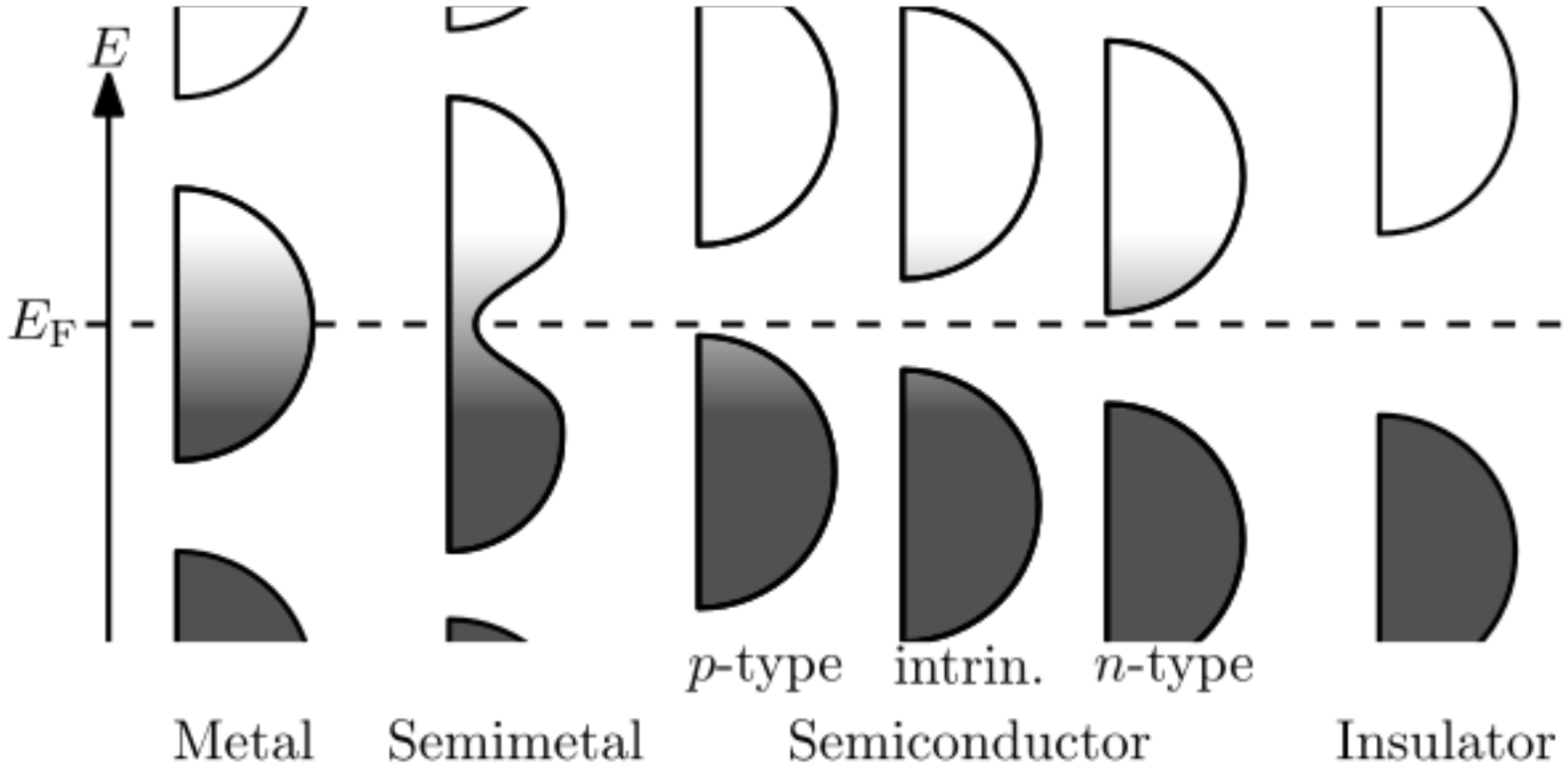
Lecture #19
Semiconductors: electrical properties: Kittel Ch. 8 pp. 205-214; Ch. 20





Simplified diagram of the filling of electronic band structure in various types of material, relative to the Fermi level E_F (materials are shown in equilibrium with each other). Degenerate semiconductors are missing from the picture. They are heavily doped semiconductors where E_F moves inside the band.

http://en.wikipedia.org/wiki/File:Band_filling_diagram_by_Nanite.png



Density of states version of the previous slide.

http://en.wikipedia.org/wiki/Semimetal

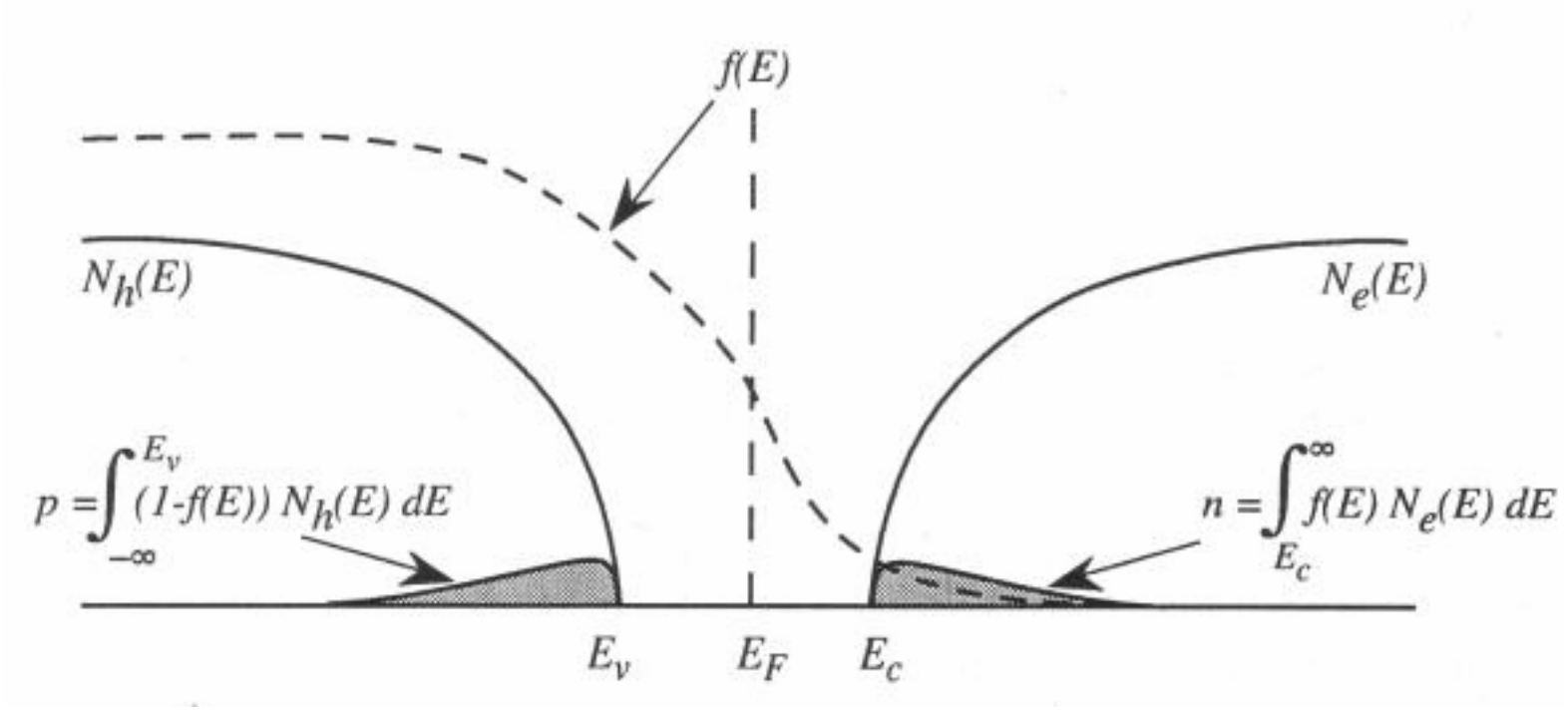


Figure VI-2-3: A schematic of the density of states. For an **intrinsic semiconductor** the Fermi energy is in the middle of the band gap and $n = p$.

http://kottan-labs.bgsu.edu/teaching/workshop2001/chapter6.htm

Sample carrier concentration calculation: ELECTRONS
Near band minimum in semiconductors, band is often free-electron-like ($E \approx k^2$; DoS(E) $\approx E^{1/2}$), but mass (m_e) is different from f.e. mass (m_0), and may be anisotropic.

$$n_e (= n) = \int_{E_c}^{\infty} D_c(E) f(E) dE$$

$$= \int_{E_c}^{\infty} \frac{1}{2\pi^2} \left(\frac{2m_e}{\hbar^2} \right)^{3/2} (E - E_C)^{1/2} \frac{1}{e^{(E-\mu)/k_B T} + 1} dE$$

$$\approx 2 \left(\frac{m_e k_B T}{2\pi\hbar^2} \right)^{3/2} e^{(\mu - E_C)/k_B T}$$

Most semiconductors: $E_g >> k_B T$ (0.026 eV at RT), and provided Fermi level is several $k_B T$ away from bottom of CB. Called **non-degenerate semiconductor.**
Here $E-\mu > 0$

Sample carrier concentration calculation: HOLES

Similar to electrons but m_h, $f_h(E) \rightarrow 1-f_e(E)$, E_V.

$$n_h (= p) = \int_{-\infty}^{E_V} D_V(E) f_h(E)\, dE$$

$$= \int_{E_V}^{\infty} \frac{1}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2} (E - E_v)^{1/2} \left\{1 - \frac{1}{e^{(E-\mu)/k_B T} + 1}\right\} dE$$

$$= \int_{E_V}^{\infty} \frac{1}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2} (E - E_v)^{1/2} \left\{\frac{e^{(E-\mu)/k_B T} + 1 - 1}{e^{(E-\mu)/k_B T} + 1}\right\} dE$$

$$\approx 2\left(\frac{m_h k_B T}{2\pi\hbar^2}\right)^{3/2} e^{(E_V - \mu)/k_B T}$$

Most semiconductors: $E_g >> k_B T$ (0.026 eV at RT), and provided Fermi level is several $k_B T$ away from top of VB. Called **non-degenerate semiconductor**.

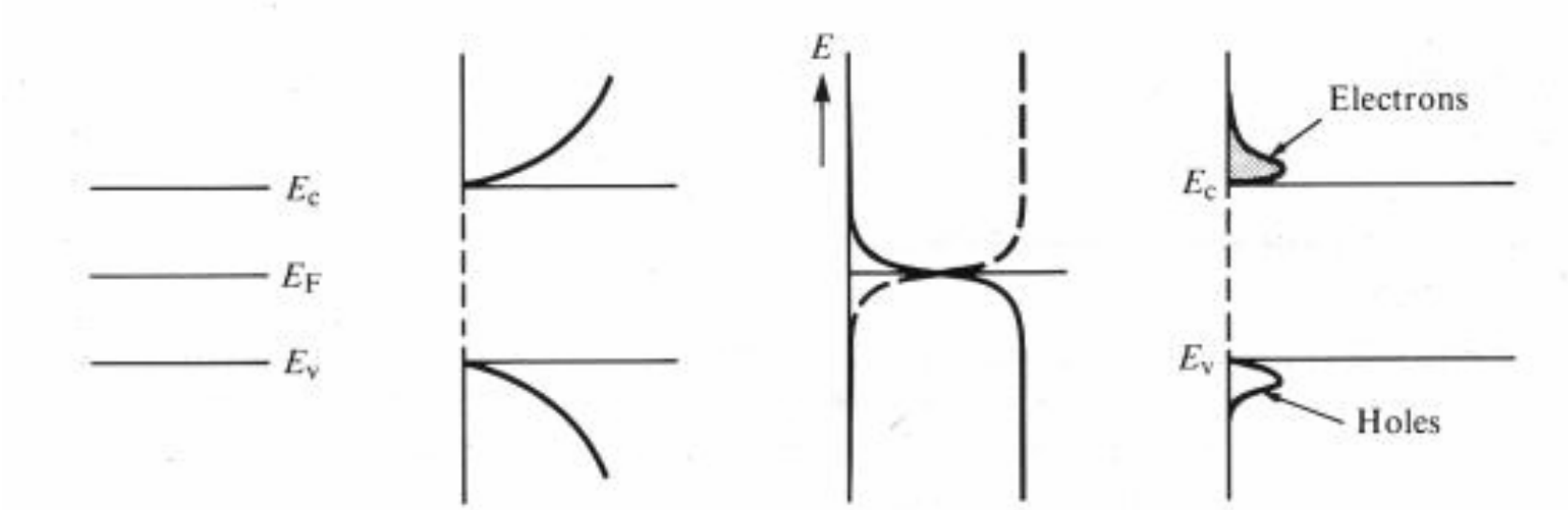
Here $E-\mu < 0$

Law of mass action:
The product of *n* and *p* is independent of the position of the chemical potential (Fermi level).

$$np = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 \left(m_e m_h\right)^{3/2} e^{-E_G/k_B T}$$

Intrinsic semiconductor (no extra states in gap); μ is close to gap center - only a few conduction electrons; only a few holes.

$$n_i = p_i \approx 5\times 10^9 cm^{-3} \quad \text{(Si)}$$



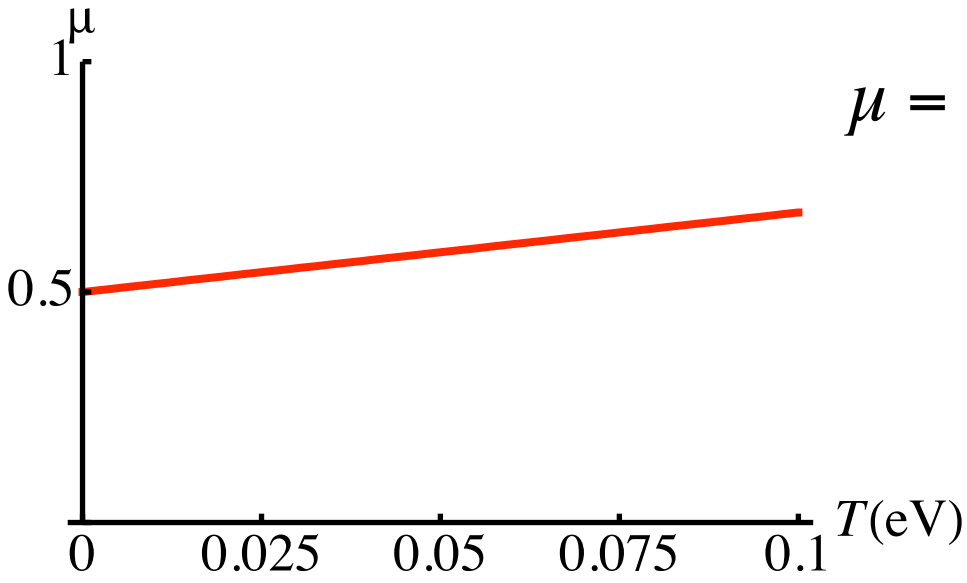
(b) E_F near midgap

Intrinsic semiconductor (no extra states in gap); μ is close to gap center - only a few conduction electrons; only a few holes.

$$n_i = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2}\left(m_e m_h\right)^{3/4} e^{-E_G/2k_B T}$$

$$n_i = 2\left(\frac{m_e k_B T}{2\pi\hbar^2}\right)^{3/2} e^{(\mu - E_C)/k_B T}$$

$$\mu = E_v + \frac{1}{2}E_g + \frac{3}{4}k_B T \ln\left(\frac{m_h}{m_e}\right)$$



Extrinsic (or "natively doped") semiconductor (extra states in gap); μ is close to one or other band edge. Either

- many conduction electrons; only a few holes, or
- many valence band holes; only a few electrons

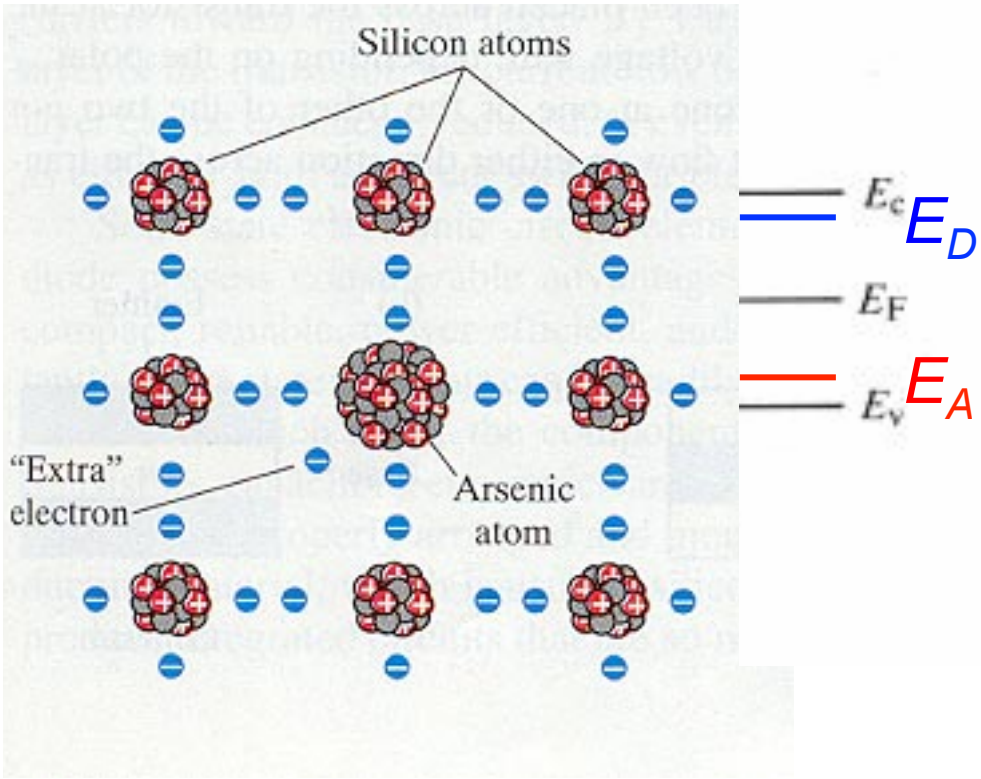
Defects:
Defects produce states that have energies in the regions previously forbidden in the perfect crystal. They determine the Fermi level.
Defects raise the energy of the system, but also increase the entropy, so they are very common.

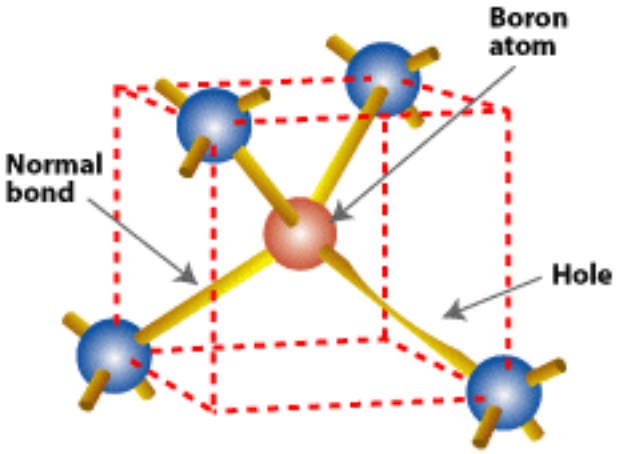
Examples of **point** defects:
Substitutional impurities - Si:As and Si:B (homework problem)

Fermi level depends sensitively on number and type of defect.
Some defects are electrically active; others are not.
Most familiar defects are the "shallow" donor & acceptor defects in common semiconductors. These are electrically active - they result in extrinsic conductivity in semiconductors.

Substitutional Defects:
Si:As and Si:B

As_{Si}





B_{Si}

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

Can control doping by controlled impurities in semiconductor and manipulation of Fermi level. *e.g.* Si:As

$$np = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 \left(m_c m_h\right)^{3/2} e^{-E_G/k_B T}; n >> p$$

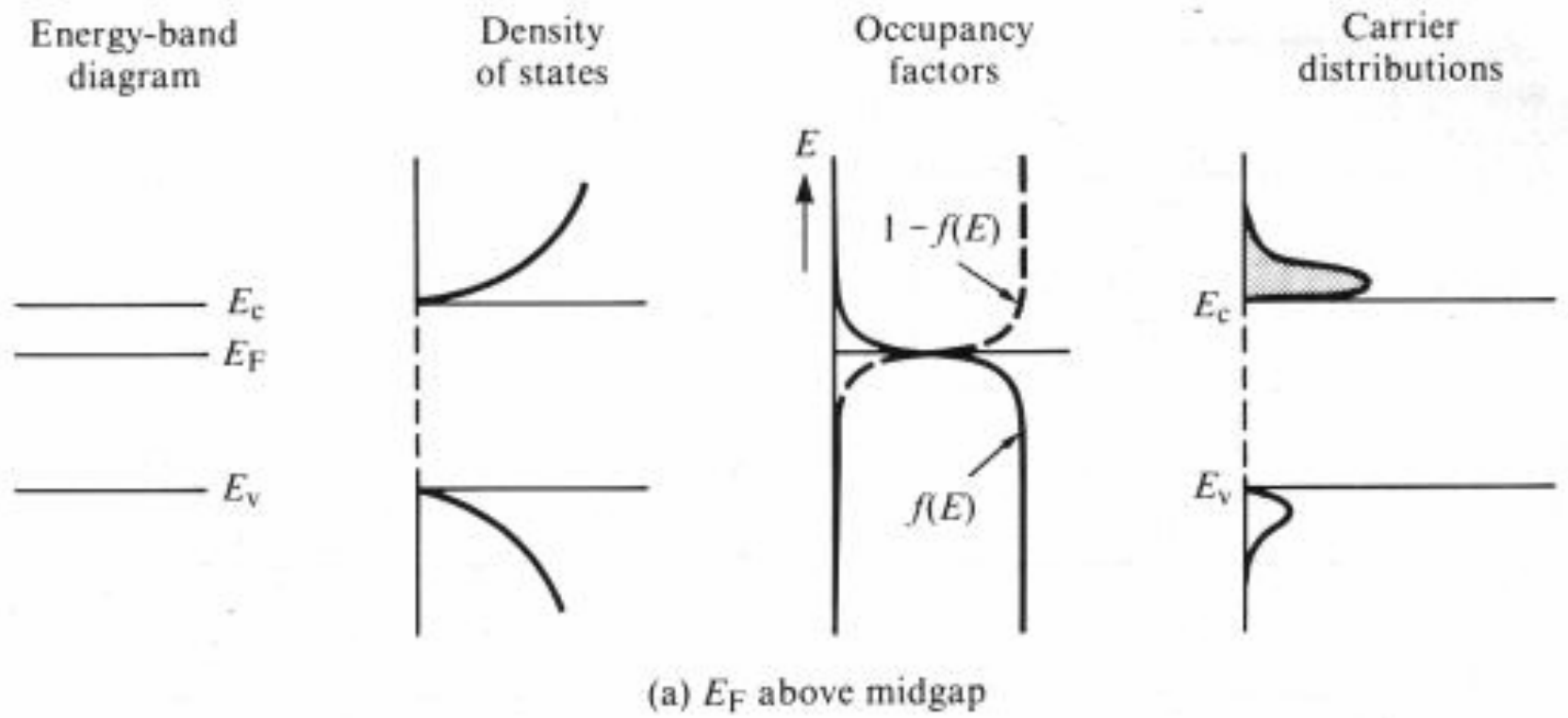


Figure VI-2-4: Carrier distribution if the Fermi level is positioned above midgap (*n*-type semiconductor)

http://kottan-labs.bgsu.edu/teaching/workshop2001/chapter6.htm

Can control doping by controlled impurities in semiconductor and manipulation of Fermi level. *e.g.* Si:B

$$np = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 \left(m_c m_h\right)^{3/2} e^{-E_G/k_B T}; p >> n$$

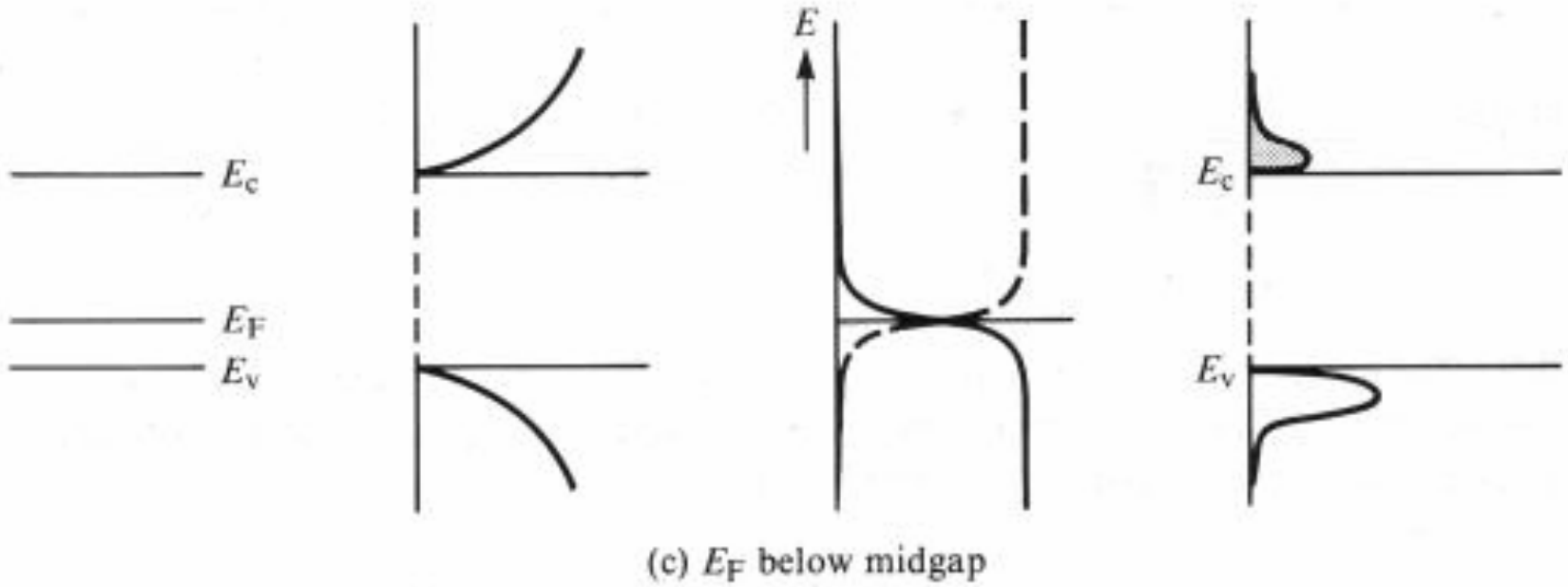
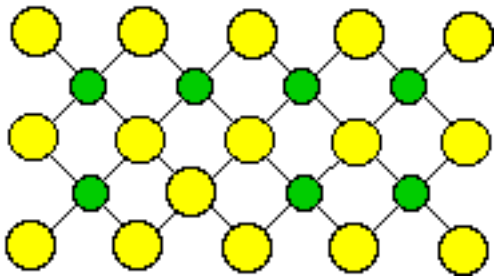


Figure VI-2-4: Carrier distribution if the Fermi level is positioned below midgap (*p*-type semiconductor)

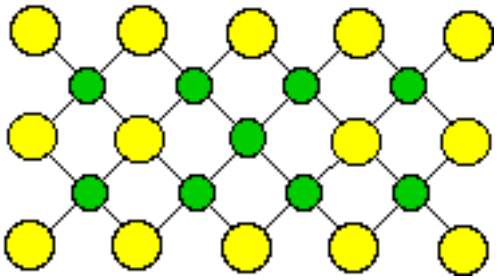
http://kottan-labs.bgsu.edu/teaching/workshop2001/chapter6.htm

Defects:
Defects produce states that have energies in the regions previously forbidden in the perfect crystal. They determine the Fermi level.
Defects raise the energy of the system, but also increase the entropy, so they are very common.

Examples of **point** defects:
Substitutional impurities - Si:As and Si:B (homework problem)
Antisite defects
- *A* on *B* site in *AB* lattice (A_B)
- *B* on *A* site in *AB* lattice (B_A)

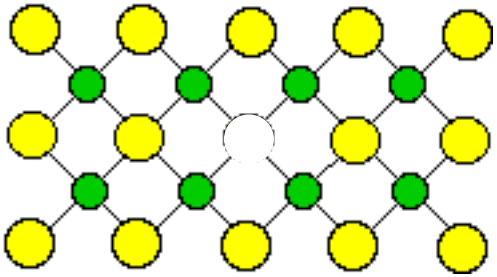


B_A antisite defect

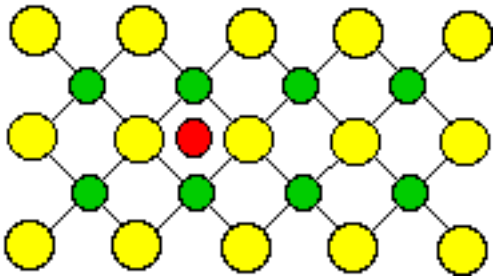


A_B antisite defect

Defects:
Examples of point defects:
Vacancies - a missing atom
Interstitials - atoms occupying interstitial space in a lattice



Vacancy (missing atom)



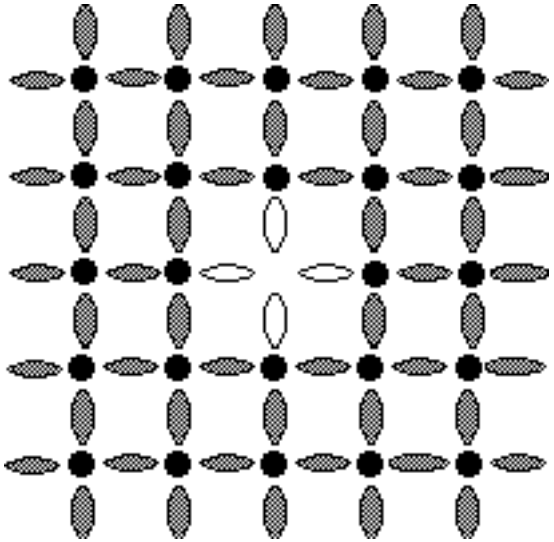
Interstitial defect (Frenkel defect)

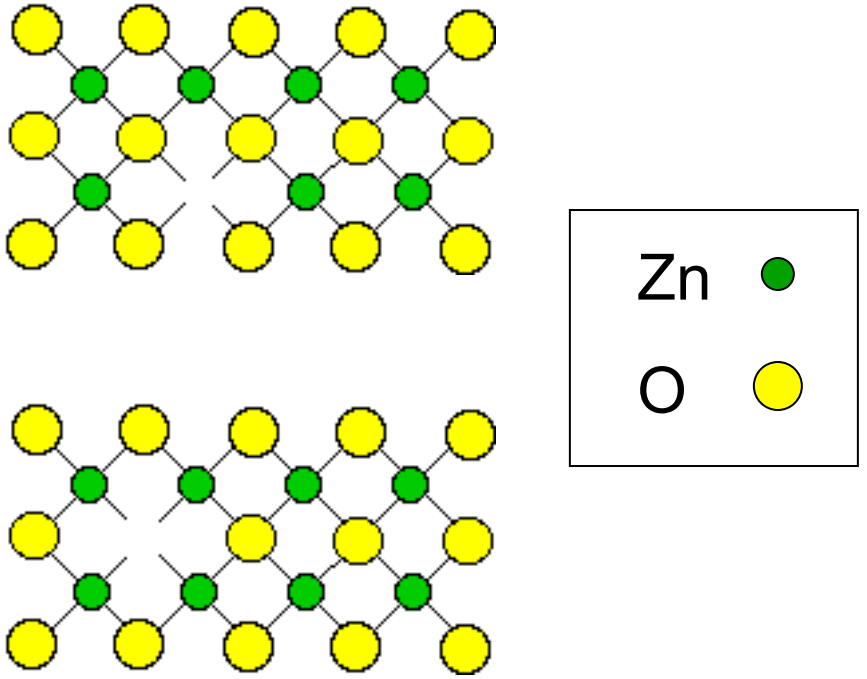
http://python.rice.edu/~arb/Courses/360handouts2.htm

ZnO vacancy example:

ZnO_{1-x} produces *n*-type or *p*-type conductivity? Why?

$Zn_{1-x}O$?





ZnO:Al

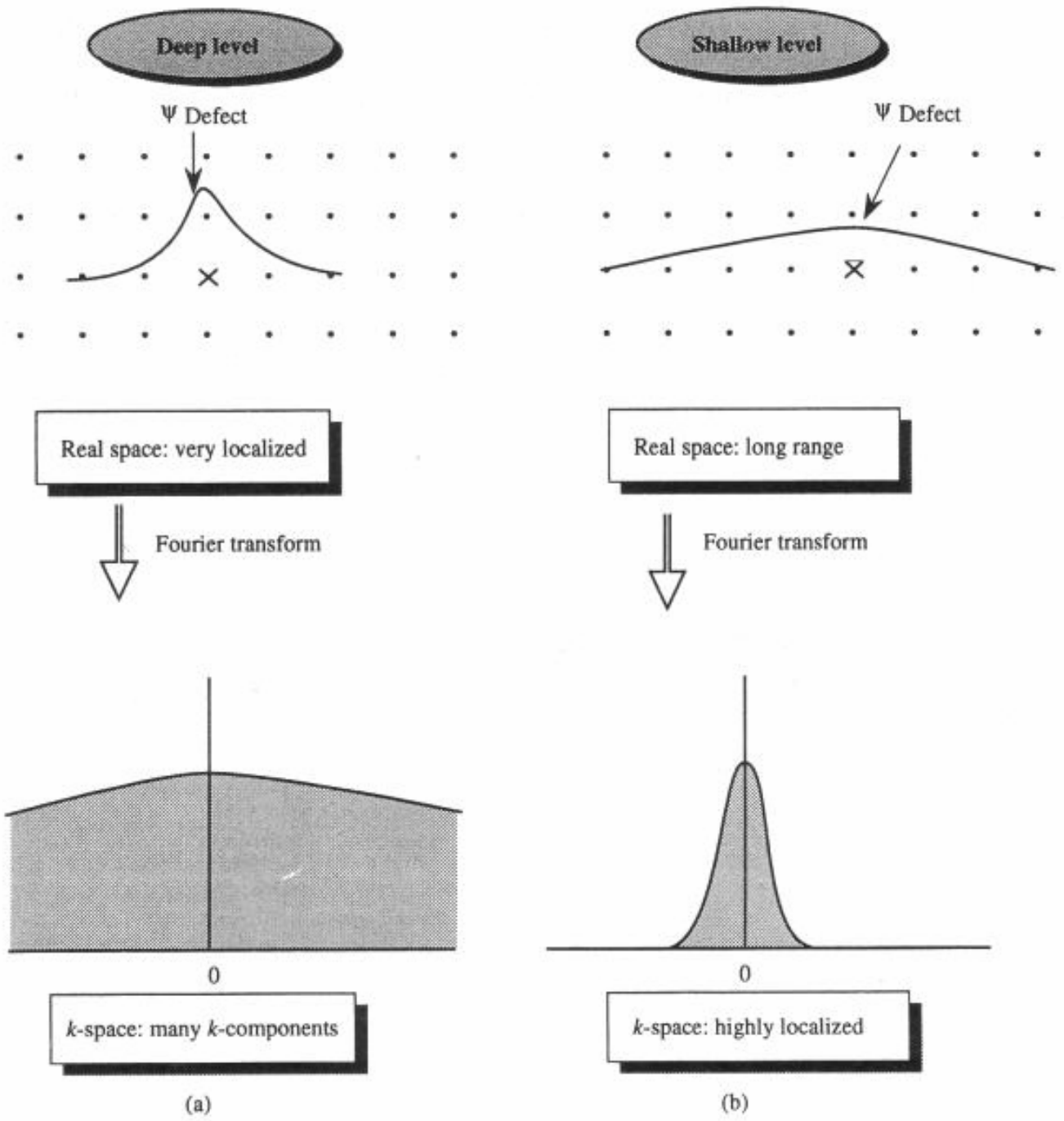
($Zn_{1-x}Al_xO$) is what type of defect?

It produces *n*-type or *p*-type conductivity? Why?

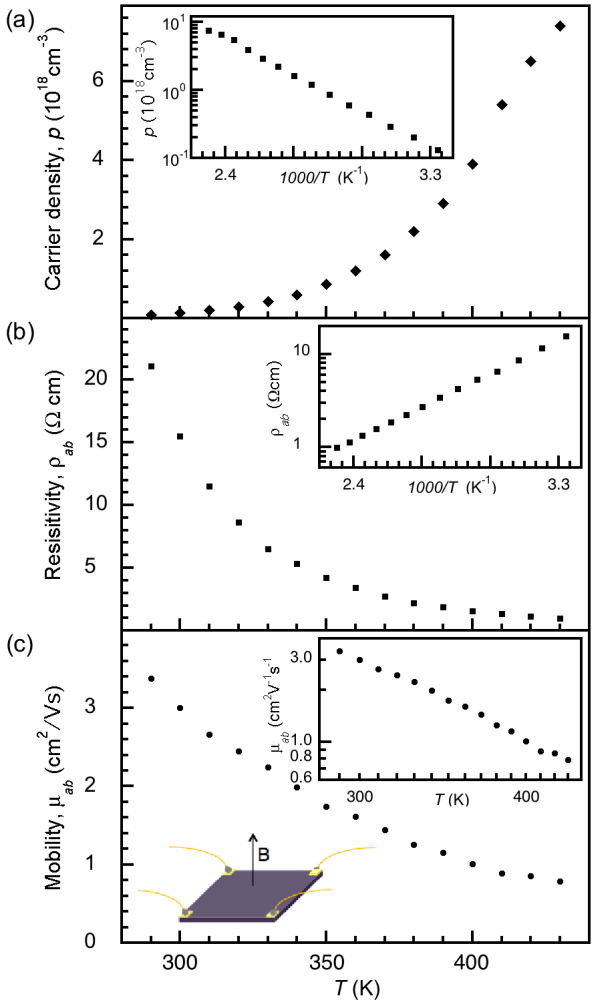
What defect might produce the other type of conductivity?

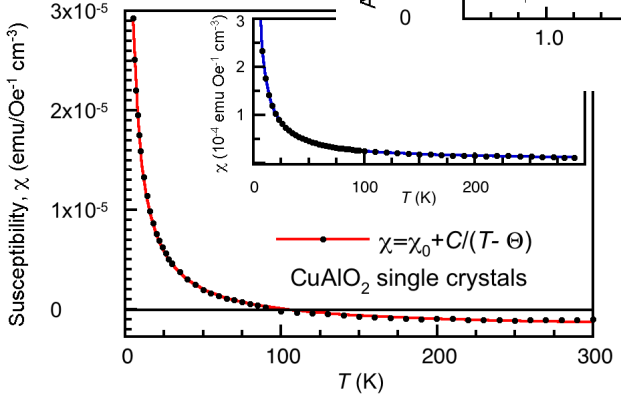
p-ZnO has been a hot topic of research in the past few years.

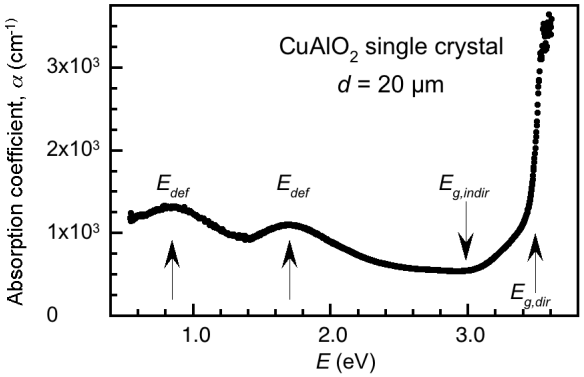
Figure VI-2-7: A schematic of the wave functions associated with
(a) a short range potential, and
(b) a long range potential defect.

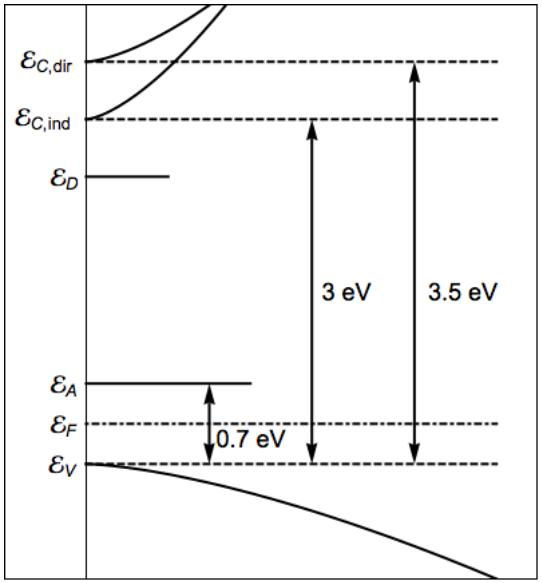


Example: p-type $CuAlO_2$









Extra slides

Other Defects:

Color centers: Heat alkali halide in excess of the metal, creating halide vancancies.

$NaCl + xNa \rightarrow Na_{1+x}^{+} + Cl^{-} + xe^{-}$

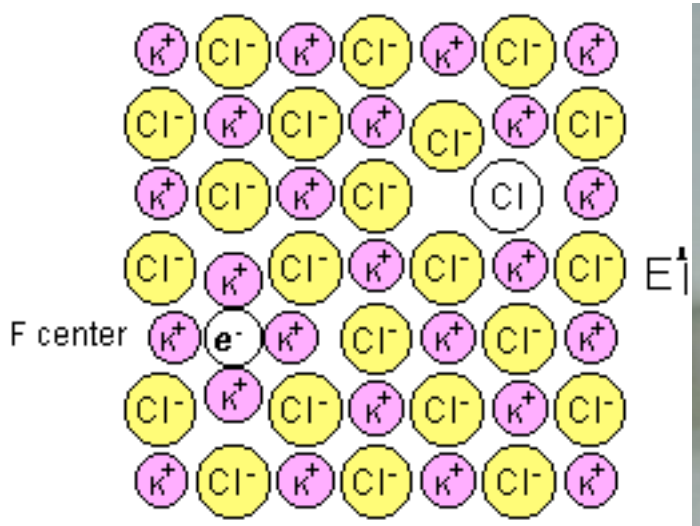
Extra electron bound to V_{Cl}

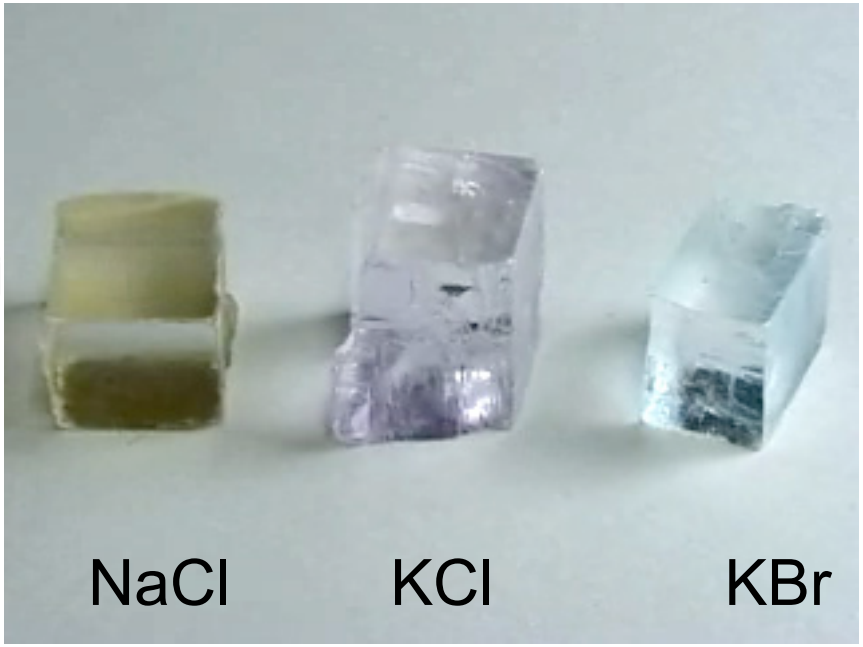
F-center (Kittel Ch. 20, Fig 7) *F* - "farbezentrum".

NaCl becomes yellow; KCl becomes magenta.

http://mrsec.wisc.edu/Edetc/cineplex/Fcenter/index.html

Many other color centers are possible.





http://www.ensta.fr/~muguet/papers/ECCC7/Fcenter.html

Defects: Al_2O_3:Cr (ruby) Cr^{3+} has same valence as Al^{3+}, so it does not produce the same kind of donor/acceptor electrically active defect, but it changes the light absorbing properties markedly!

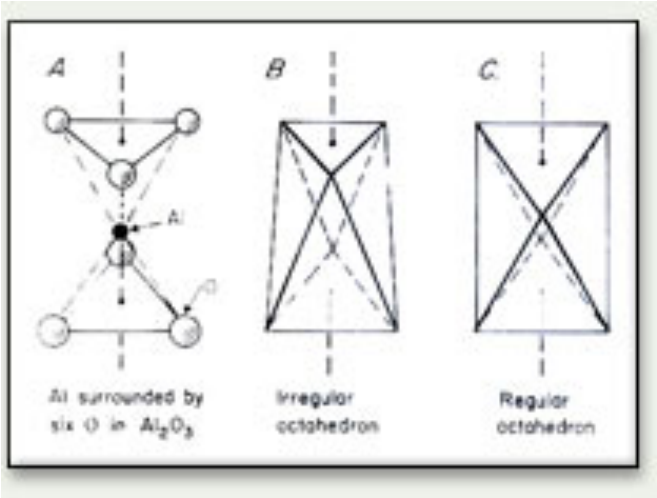
Al_2O_3 (white sapphire or corundum)

Al_2O_3:Cr^{3+} (ruby)

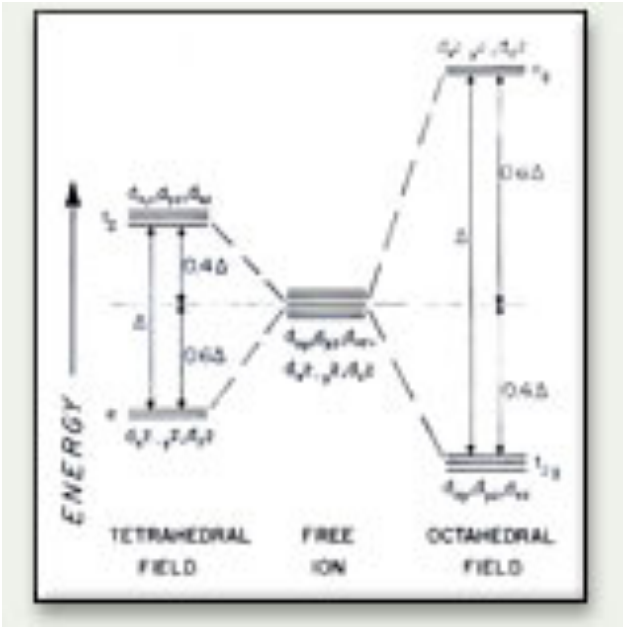
Al_2O_3:Fe^{2+}/Ti^{4+} (blue sapphire)

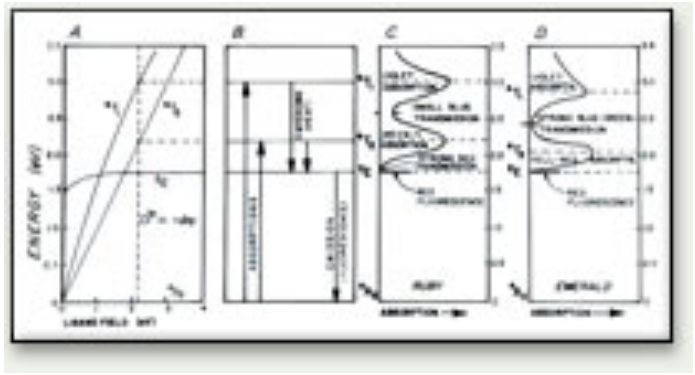
Cr^{3+} in beryl (emerald)

Defects: Many gemstones have color because they have transition metals with unfilled *d* states. These states are split in the ligand field of the (transparent) host. Then, electron transitions can occur and color results. http://webexhibits.org/causesofcolor/index.html

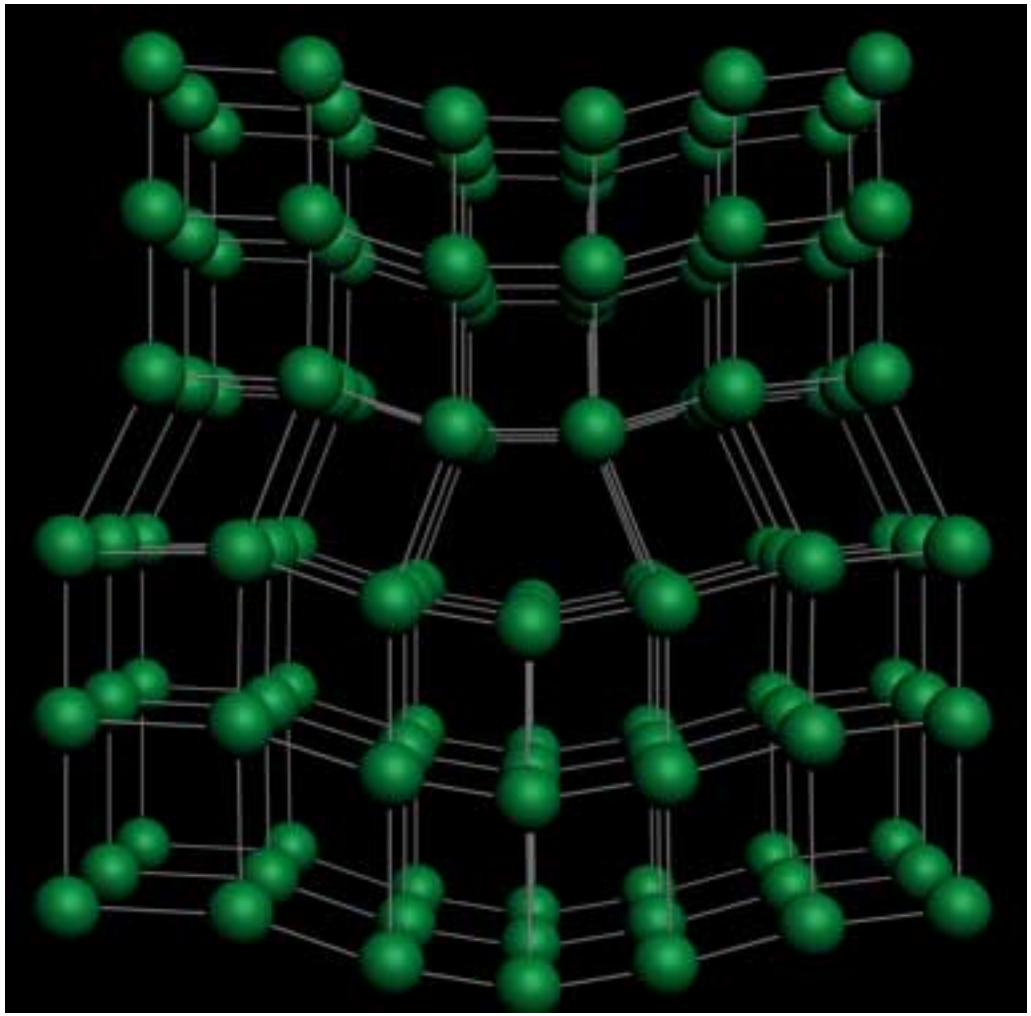


Ruby



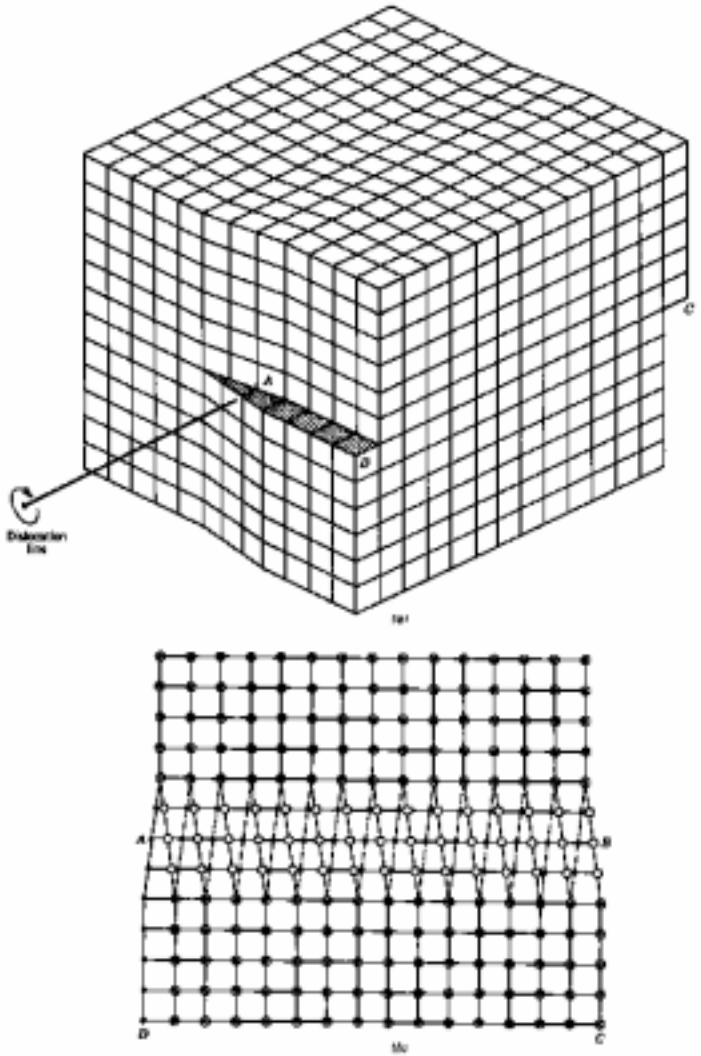


Extended Defects: affect mechanical and elastic properties (where point defects are more important to electrical and optical properties).
Example of extended defects: edge dislocation



http://www.ndt-ed.org/EducationResources/CommunityCollege/Materials/Graphics/EdgeDislocation1.jpg

Defects:
Examples of extended defects: screw dislocation



Screw Dislocation

Screw Dislocation viewed from above

Dislocation along line AB

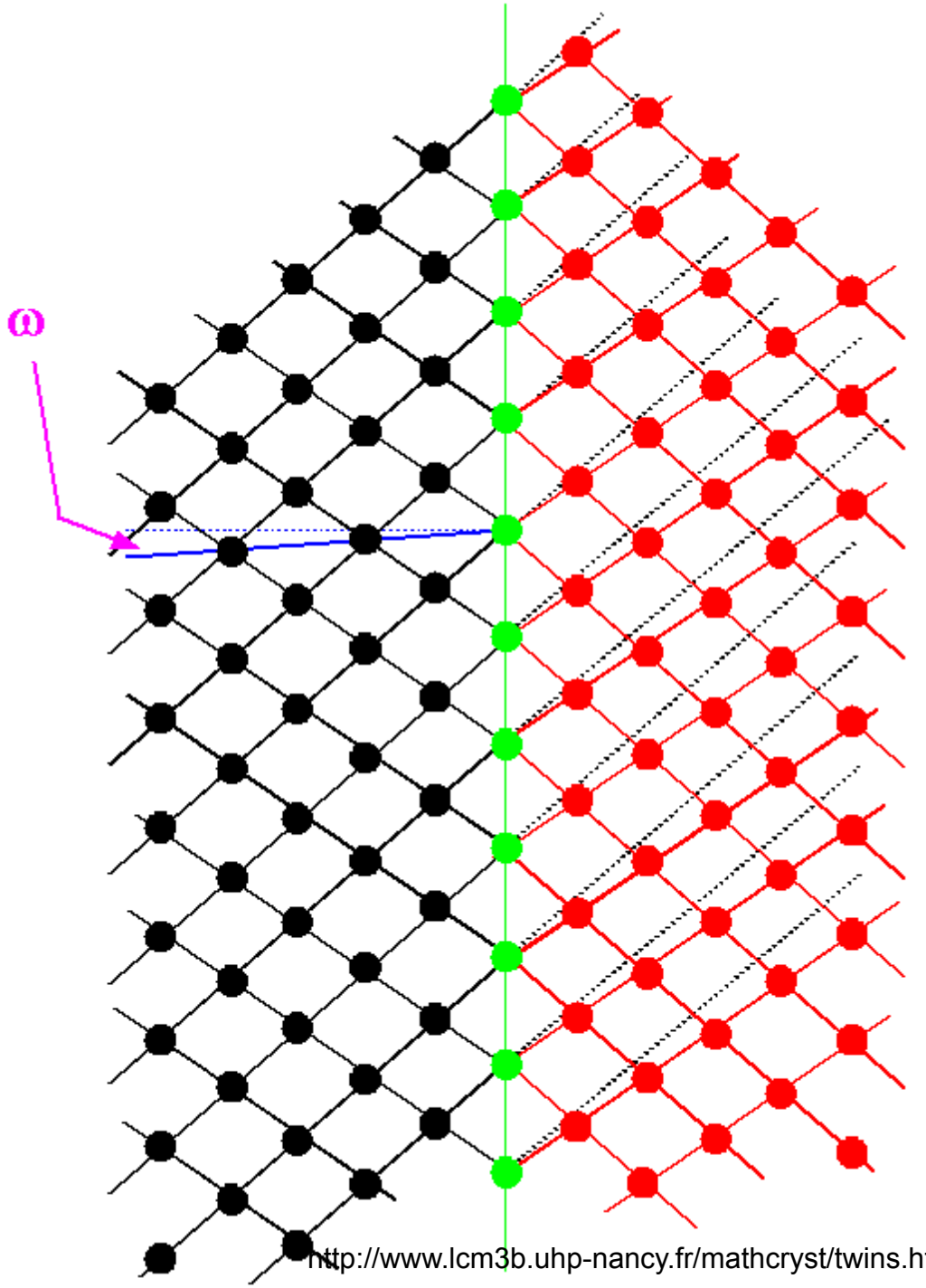
open circles: atoms above slip plane
closed circles: atoms below slip plane

William D. Callister, Jr. Materials Science and Engineering, An Introduction. John Wiley & Sons, Inc. 1985

http://www.engr.ku.edu/~rhale/ae510/lecture2/sld031.htm

Defects:
Examples of extended defects: twinning.

Twinning can destroy the symmetry that is important for manifestation of certain properties.



http://www.lcm3b.uhp-nancy.fr/mathcryst/twins.htm