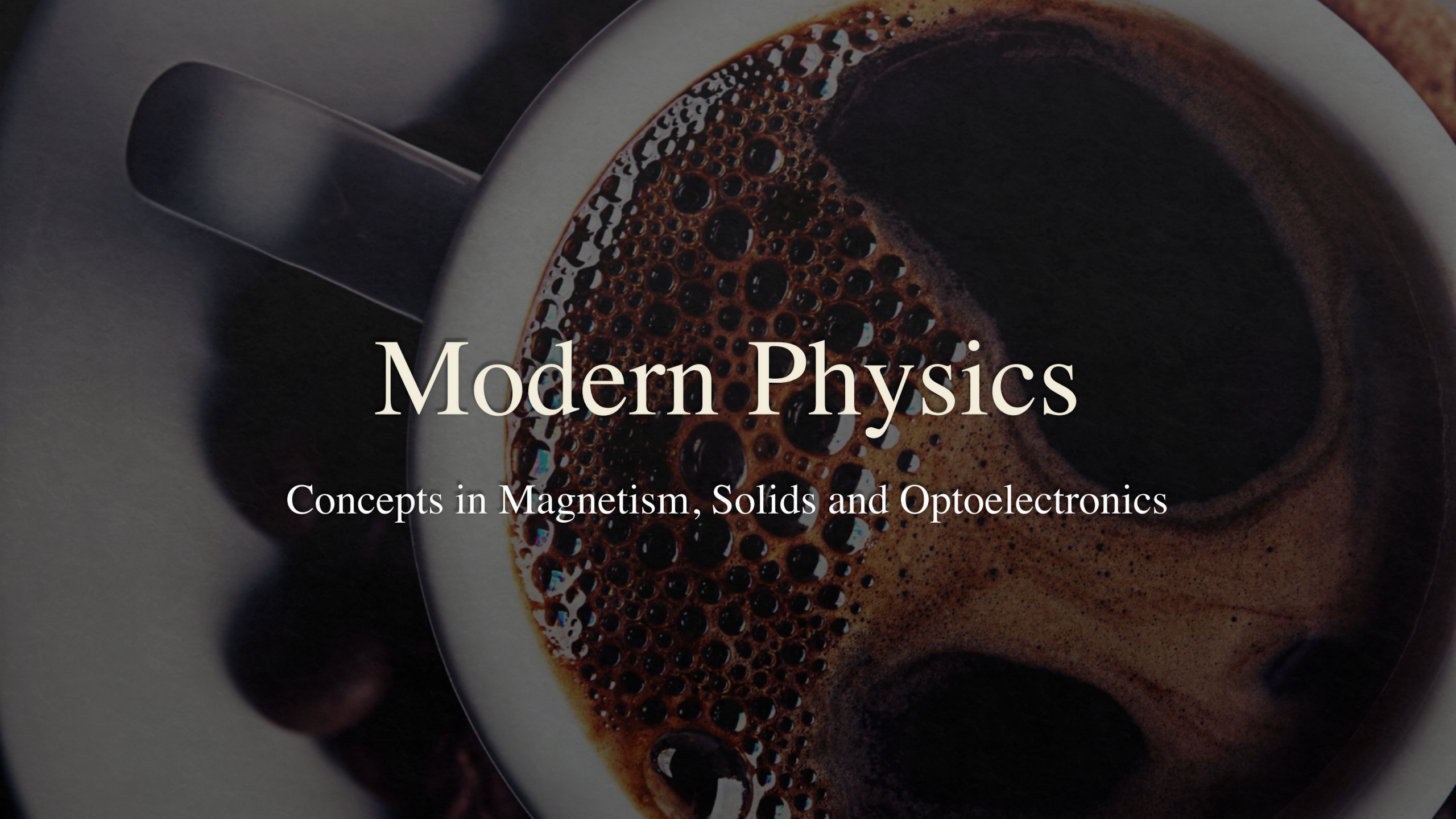


Modern Physics

Concepts in Magnetism, Solids and Optoelectronics

Concepts

01

MAGNETISM

02

SOLIDS

03

OPTOELECTRONICS

Electromagnetic Waves

- The Maxwell's Equations and some examples

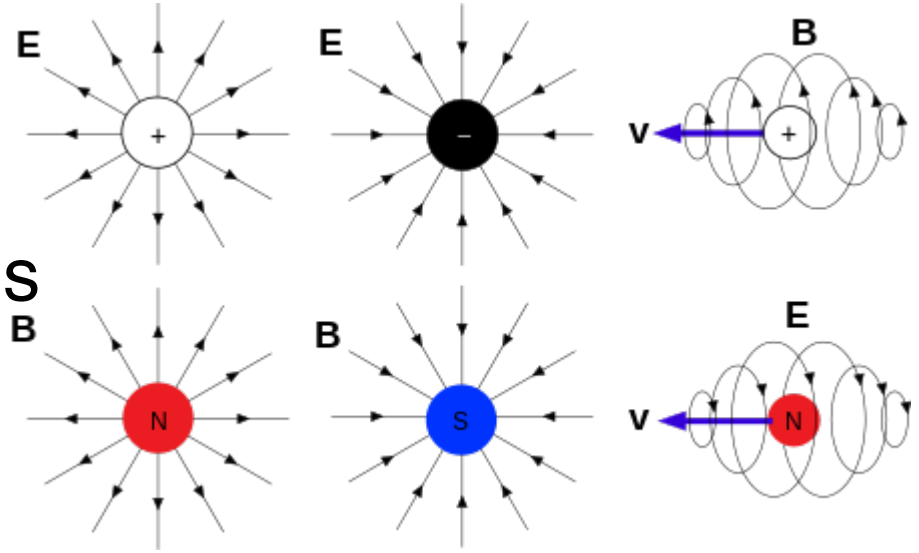
$$\nabla \bullet E = \frac{\rho}{\epsilon_0} \qquad \nabla \bullet D = \rho$$

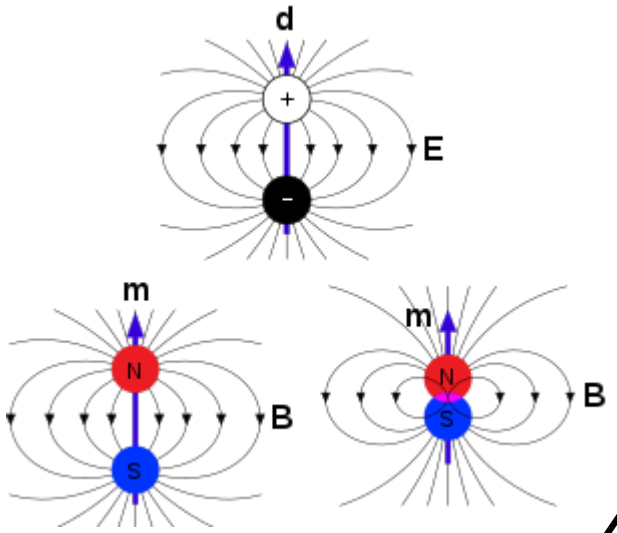
$$\nabla \bullet B = 0 \qquad \nabla \bullet B = \rho_m$$

$$\nabla \times E = -\frac{\partial B}{\partial t} \qquad \nabla \times E = -\frac{\partial B}{\partial t} + j_m$$

$$\nabla \times B = \mu_0 j + \frac{1}{c^2}\frac{\partial E}{\partial t} \qquad \nabla \times H = j + \frac{\partial D}{\partial t}$$

Describing magnetic monopoles





Magnetism

Material equations

$$j = \sigma E$$ Units A

$$D = \epsilon_0 \epsilon E$$ Units V/m

$$B = \mu_0 \mu H = \mu_0 (H + M)$$ Units A/m

$$M = \sum_{Volume} m_i = lim_{I \to \infty; F \to 0} (IA)$$

$$M = (\mu - 1) H = \chi H$$

Based on the value of the moment or susceptibility, material magnetic properties are classified as

Diamagnetic $\chi < 0$

Paramagnetic $\chi > 0$

Ferrimagnetic or Ferromagnetic $\chi(H) \gg 1$

Ultimately, it is a mechanical torque from the induction B on the moment m that generates the magnetic behavior

Magnetism

The magnetic susceptibility of materials

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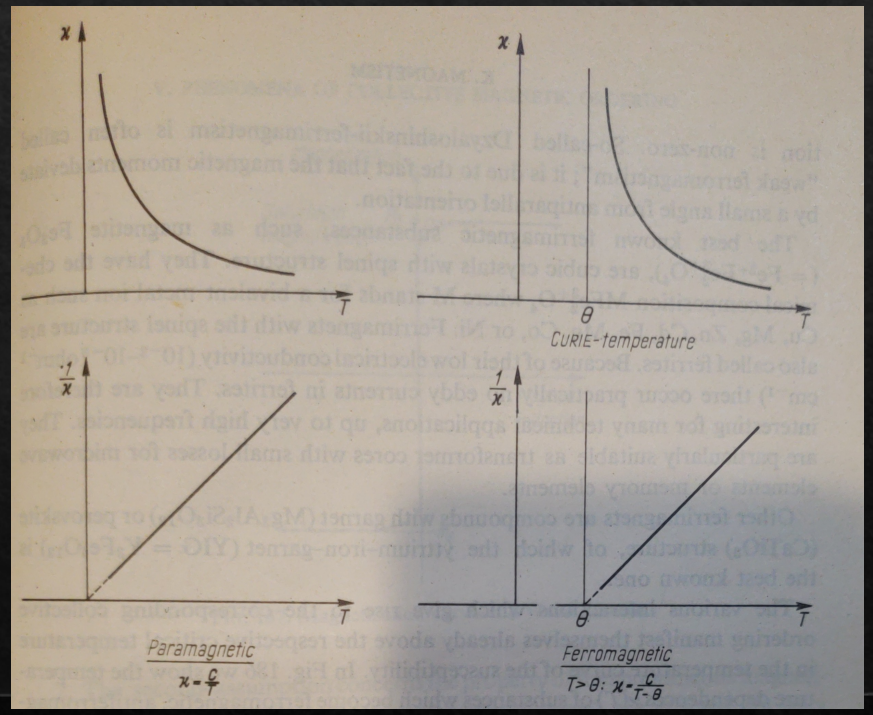
As a function of temperature, the magnetic materials exhibit the following behaviors:



from Kittel's Solid State Physics

Magnetism

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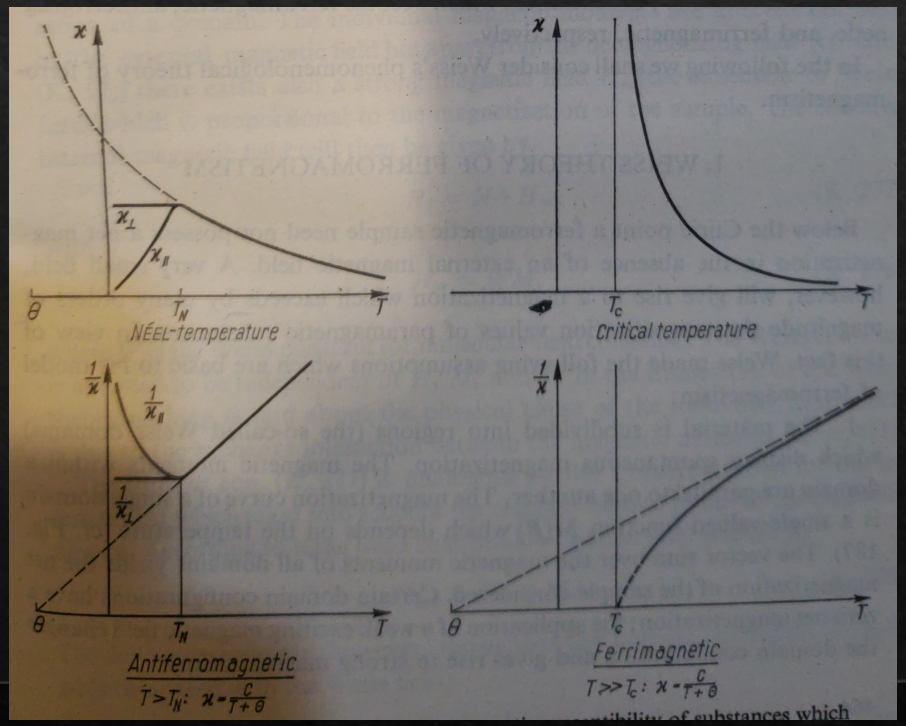
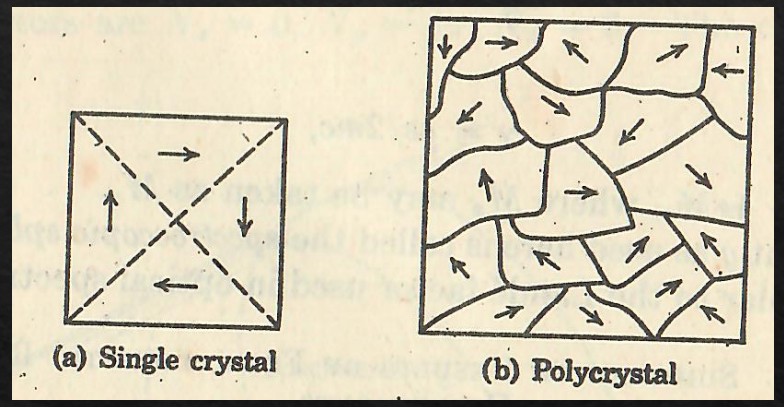


Permanent Magnets

Magnetic Domains



Kittel Solid State Physics

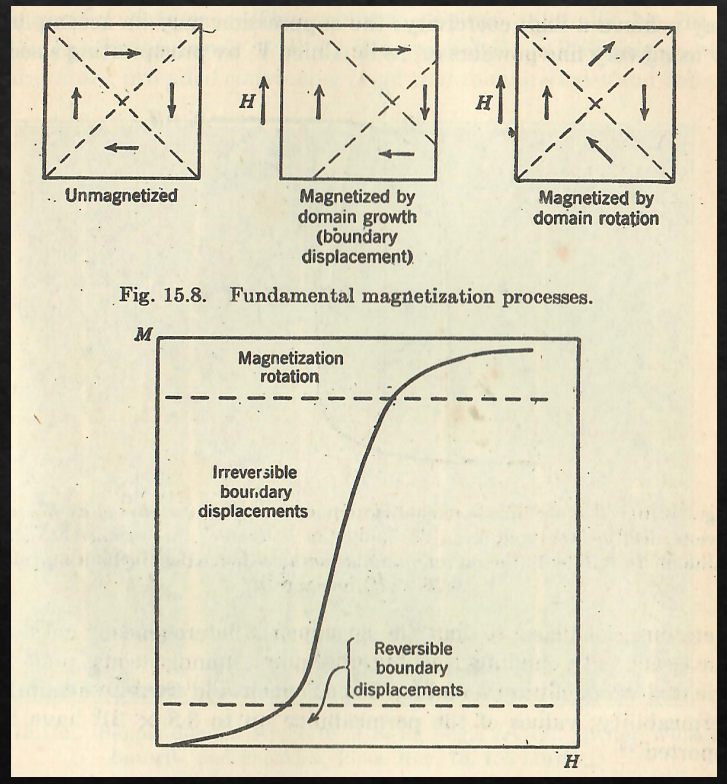


Fig. 15.8. Fundamental magnetization processes.

Permanent Magnets

± Ferromagnetic materials exhibit a distinctive magnetization response

Saturation flux density depends on the saturation magnetization M_s.

$$B_s = 4\pi M_s$$

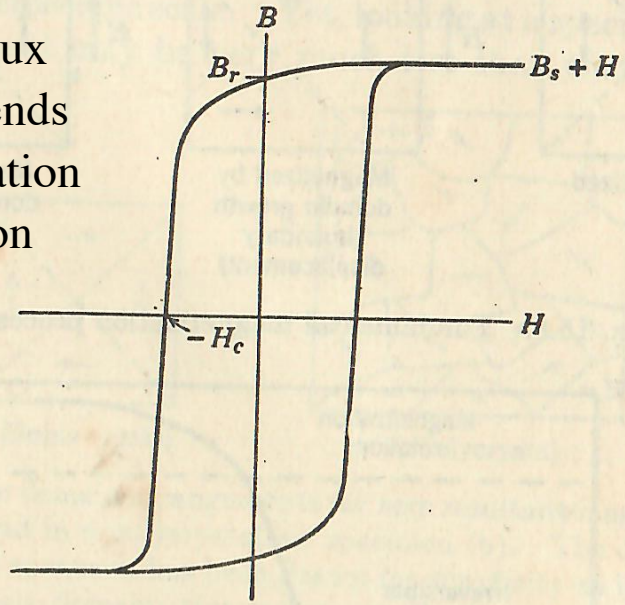


Fig. 15.10. The technical magnetization curve. The *coercive force* H_c is the reverse field necessary to bring the induction B to zero; the *remanence* B_r is the value of B at $H = 0$; the *saturation induction* B_s is defined as the limiting value of $(B - H)$ for large H.

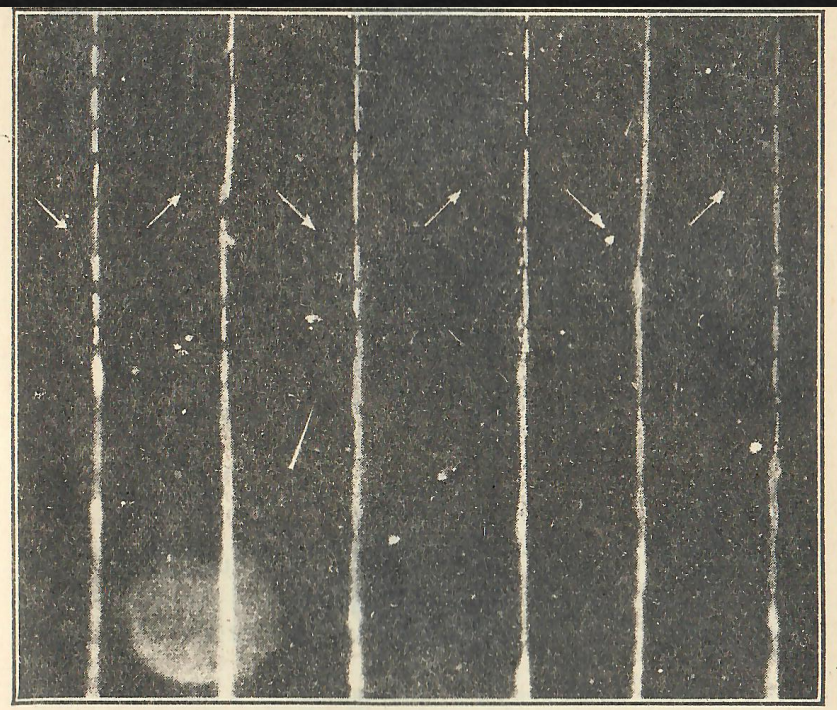
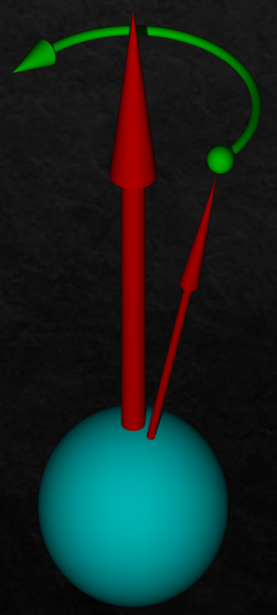
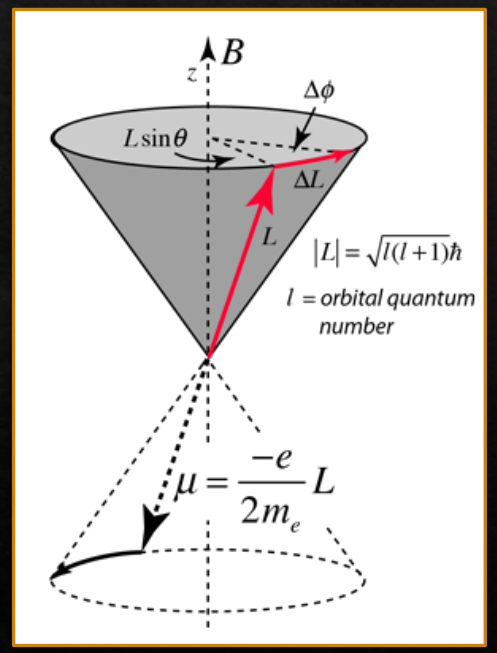


Fig. 15.11a. Simple domain structure in Si-Fe single crystal. [After Williams, Bozorth, and Shockley, Phys. Rev. **75**, 155 (1949).]

Diamagnets

± We consider the "Larmor" precession of electrons about a (external, applied or otherwise) magnetic field -> analysis from the cyclotron frequency (recall Lorentz force)





$$\omega_L = -eH/2mc$$

$$\chi = M/H = \mu/H = \frac{-Ze^2}{4mc^2}Nr^2$$

If we work out the electron distribution in r (for material of interest), then the susceptibility can be understood!

Diamagnets

- Given this understanding, the molar diamagnetic susceptibilities of ions, and also molecules, in crystals can be experimentally extracted.

	Experimental values in 10^{-6} cm^3/mole	Theoretical Values
He	-1.9	-1.9
Ne	-7.2	-8.6
Xe	-43	
F-	-9.4	-17
Cl-	-24.2	-41.3
Na+	-6.1	-5.6
K+	-14.6	-17.4
Mg2+	-4.3	-4.2
Ca2+	-10.7	-13.1

Paramagnets

- The Langevin paramagnet model is a medium of N atoms per unit volume each bearing a magnetic moment μ. Then the interaction energy or potential is $V = -\mu \cdot H$.
- In this case

$$M = -\mu \cdot B = -\mu B cos\theta = \int_0^2 \pi 2\pi sin\theta cos\theta e^{\mu B cos\theta/kT} d\theta / \int_0^\pi 2\pi sin\theta e^{\mu B cos\theta/kT} d\theta = N\mu L(a) \approx N\mu^2 H/3kT$$

- Thus, $\chi = M/H = N\mu^2/3kT = C/T$

Quantum Theory of Magnetism

- So far we describe materials using a macroscopic moment, μ. In paramagnets if an external field is applied then a Zeeman energy splitting is induced in the energy levels.
- This modifies $M = \frac{Ng\mu_B}{2} tanh(g\mu_B H/2kT) \approx N(g\mu_B)^2 H/4kT$, with $g = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$ and Bohr magneton $\mu_B = e/2mc = -0.927 * 10^{-20} erg/oersted$. This is because there are two levels separated by the external field.

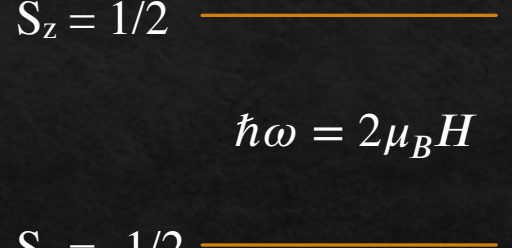
$S_z = 1/2$

$\hbar\omega = 2\mu_B H$

$S_z = -1/2$

Quantum Theory of Magnetism

- So far we describe materials using a macroscopic moment, μ. In paramagnets if an external field is applied from internal mechanisms, such as with atomic doping or substitution, then anenergy splitting is also induced in the energy levels.
- This modifies $M = NgJ\mu_B B_J(x)$, with Brillouin function $B_J(x) = \frac{2J+1}{2J} ctnh(\frac{x(2J+1)}{2J}) - \frac{1}{2J} ctnh(\frac{x}{2J})$ and $\chi \approx NJ(J+1)g^2\mu_B^2/3kT$.
- This method could be used to probe, for example, the insertion of rare earth ions in matrix.



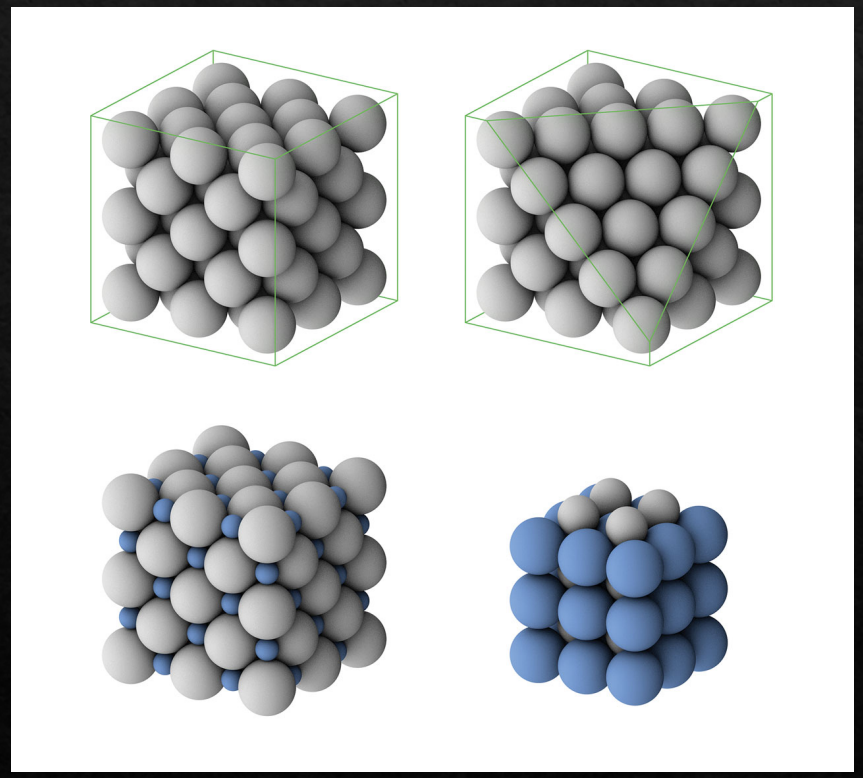
Ferromagnets

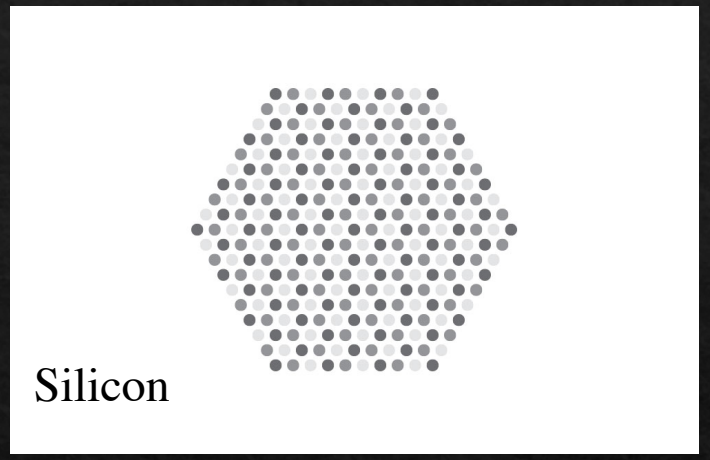
- Can be empirically understood from Curie-Weiss law, with the applied (whether internal or external) field $H_E = \lambda M \approx kT_c / gS\mu_B$ so that $\chi = \dfrac{C}{T - C\lambda} = \dfrac{C}{T - T_c}$
- Quantum mechanically we must consider taking a paramagnet and adding an additional energy term, the exchange integral J to account for electron-electron "exchanges." This term depends on spin, orbit, lattice energies.

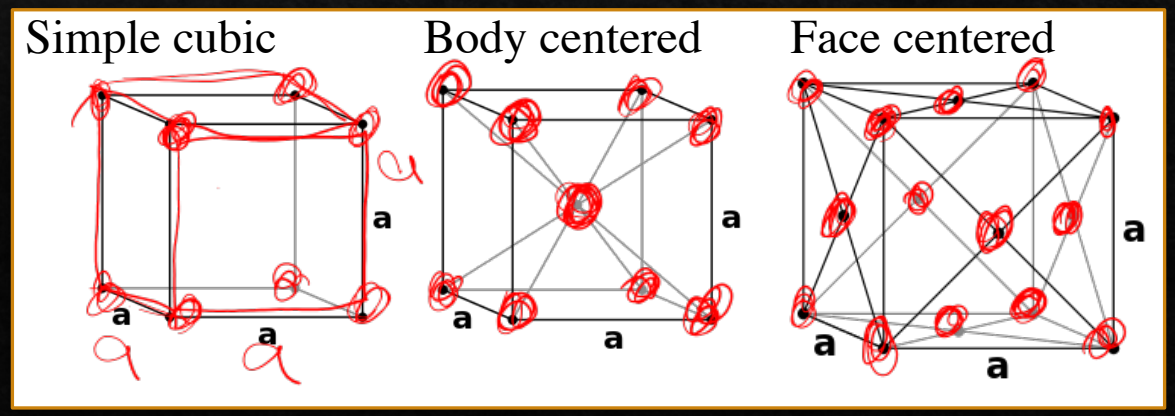
	C ($deg^{-3/2}$)	J (spin waves)
Iron	3.5*10-6	205k (S=1)
Nickel	8.6*10-6	230k (S=1/2)

Crystal Structure

± For example, the NaCl and CsCl structures, cubic.



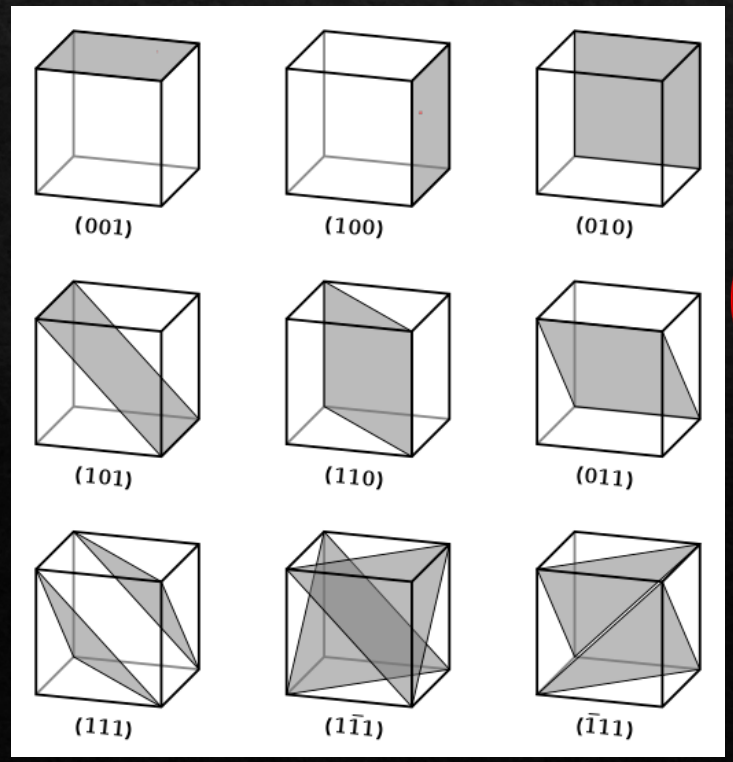




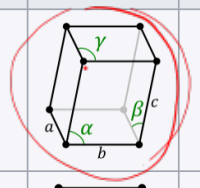
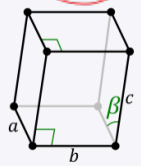
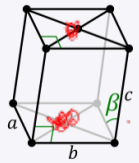
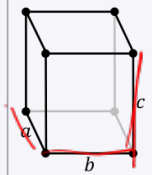
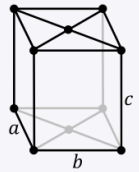
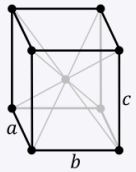
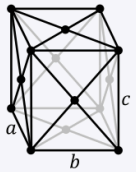
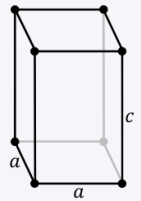
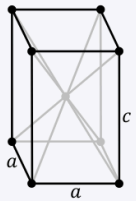
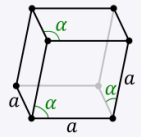
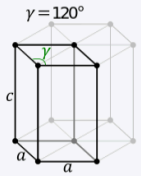
https://www.beautifulchemistry.net/crystal-structure
https://en.wikipedia.org/wiki/Crystal_structure

Crystal Structure

- Various types of known lattices
- Miller index planes



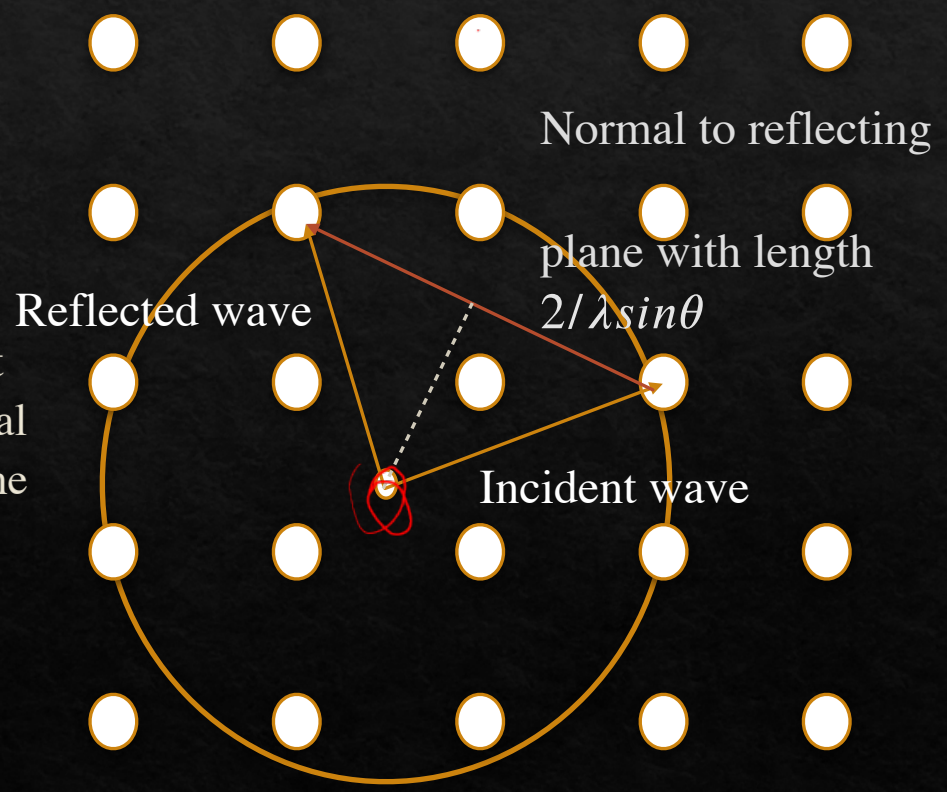
$$d = \frac{2\pi}{|g_{lmn}|}$$

Crystal family	Lattice system	Schönflies	14 Bravais lattices			
			Primitive	Base-centered	Body-centered	Face-centered
triclinic		C_i				
monoclinic		C_{2h}				
orthorhombic		D_{2h}				
tetragonal		D_{4h}				
hexagonal	rhombohedral	D_{3d}				
	hexagonal	D_{6h}				

https://en.wikipedia.org/wiki/Crystal_structure

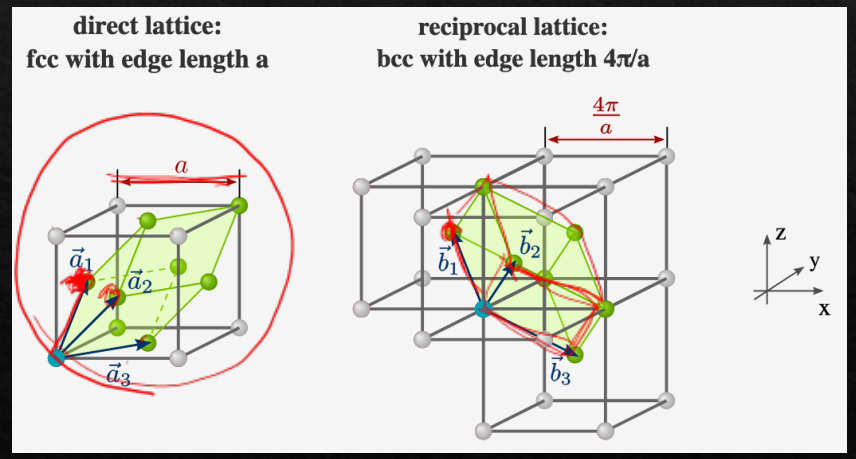
The Reciprocal Lattice

- A way to describe the lattice. For example, a, b, c are primitive translations of the crystal lattice.
- $a^* \cdot a = b^* \cdot b = c^* \cdot c = 1$ and $a^* \cdot b = a^* \cdot c = b^* \cdot c = b^* \cdot a = c^* \cdot a = 0$
- $a^* = \dfrac{b \times c}{a \cdot b \times c}, b^* = \dfrac{c \times a}{a \cdot b \times c}, c^* = \dfrac{a \times b}{a \cdot b \times c},$
- From this construction, the vector $r^*(hkl)$ from the origin to the point (h,k,l) of the reciprocal lattice is normal to the (hkl) plane of the crystal lattice. The length of the vector $r^*(hkl)$ is equal to the reciprocal of the spacing of the planes (hkl) of the crystal lattice.
- $d(hkl) = n \cdot a/h = r^* \cdot a/h|r^*| = 1/|r^*|$



The Reciprocal Lattice

- The Bragg condition can then be generally written as $(k+G)^2 = k^2$ or $2k \cdot G + G^2 = 0$ where G is 2π times the vector from the origin to a lattice point in the reciprocal lattice, and k is the propagation vector (of magnitude $2\pi/\lambda$).
- An important example is one of the face centered cubic lattice with reciprocal lattaice equal to the body centered cubic lattice.
- $\vec{a}_1 = \frac{a}{2} \cdot (\hat{y} + \hat{z}), \vec{a}_2 = \frac{a}{2} \cdot (\hat{x} + \hat{z}), \vec{a}_3 = \frac{a}{2} \cdot (\hat{x} + \hat{y})$
- $\vec{b}_1 = \frac{8\pi}{a^3} \cdot \vec{a}_2 \times \vec{a}_3 = \frac{4\pi}{a} \cdot \frac{1}{2}(-\hat{x} + \hat{y} + \hat{z}), \vec{b}_2 = \frac{8\pi}{a^3} \cdot \vec{a}_3 \times \vec{a}_1 = \frac{4\pi}{a} \cdot \frac{1}{2}(\hat{x} - \hat{y} + \hat{z}), \vec{b}_3 = \frac{8\pi}{a^3} \cdot \vec{a}_1 \times \vec{a}_2 = \frac{4\pi}{a} \cdot \frac{1}{2}(\hat{x} + \hat{y} - \hat{z})$



https://www.physics-in-a-nutshell.com/article/15/the-reciprocal-lattice

Point Groups

Mathematically are matrices that satisfy y = M x

And is described as a group of geometric symmetries that keep at least one point fixed.

For example the rotation matrices in our spin discussion of the Stern-Gerlach experiment with $\mu = 1$.

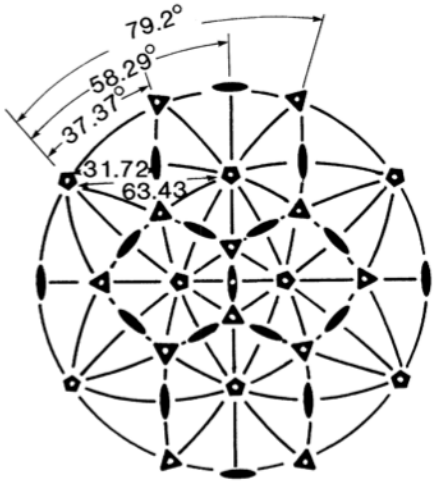


FIG. 1. Stereographic projection of the symmetry elements of the icosahedral group $m\bar{3}\bar{5}$.

https://en.wikipedia.org/wiki/Point_group

Calcite image from Aldoaldoz

Quasicrystals

Quasicrystals [From the Website]. In 1982, D. Shechtman observed a diffraction pattern that he hardly believed when he was using electron diffraction to study a fast quenched Al-Mn alloy (above image). The spots were as clear as the diffraction spots from crystals, but what confused him was the decagonal symmetry, which was impossible for crystals. Shechtman immediately realized that this pattern should imply a totally new solid structure, ordered but not periodic, and which was why it still generated clear diffraction patterns. Shechtman published the result in 1984. Scientist named this type of material "quasicrystals" and realized its similarity to Penrose pattern (p100). The discovery of quasicrystals triggered intense debates in academia. Many scientists, including L. Pauling, the two-time Nobel Laureate, denied its existence. He criticized that "No quasicrystals but only quasi-scientists." However, more and more quasicrystals were discovered. In 1992, the International Union of Crystallography revised the definition of crystals and included the quasicrystal into the new definition. In 2011, Shechtman received Nobel Prize in chemistry for his contribution in quasicrystals. The establishment of quasicrystal is a typical example of a new idea challenging old ideas in the history of science. [Figure reference: Shechtman, D. et al. *Phys. Rev. Lett.* **53**, 1951 (1984)]

[Abstract from the PRL Paper] We have observed a metallic solid (Al-14-at.%-Mn) with long-range orientational order, but with icosahedral point group symmetry, which is inconsistent with lattice translations. Its diffraction spots are as sharp as those of crystals but cannot be indexed to any Bravais lattice. The solid is metastable and forms from the melt by a first-order transition.

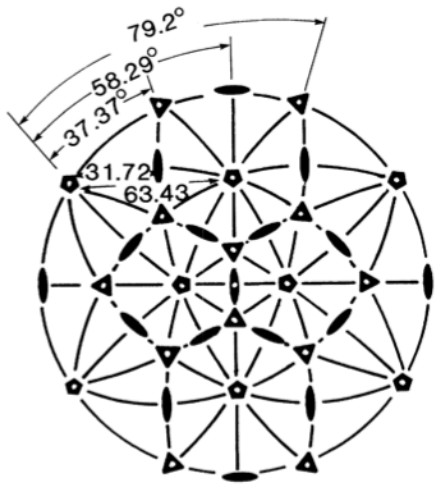


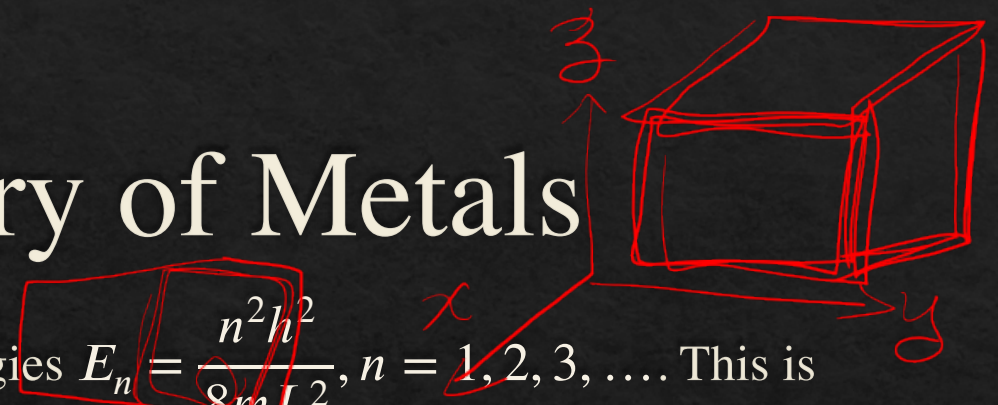
FIG. 1. Stereographic projection of the symmetry elements of the icosahedral group $m\bar{3}\bar{5}$.

https://www.beautifulchemistry.net/crystal-structure

The Band Theory of Solids

- Free electron theory of metals: the assumption is that weakly bound valence electrons of the atoms composing the metal are not bound to particular atoms but move throughout the entire solid. Equivalently, the electron moves throughout the metal in a constant electrostatic potentail.
- At the boundaries of the metal the potential will rise rapidly because of the net electrostatic force acting on an electron at the boundary. Thus, in this model, the electrons in a metal are treated like a gas composed of non-interacting spin-1/2 “fermions” confined to a three-dimensional box.

Free Electron Theory of Metals



- For example: a 1D infinite square well of length l has energies $E_n = \frac{n^2h^2}{8mL^2}, n = 1, 2, 3, \ldots$. This is generalized to a 3D infinite well of side l as $E_n = \left(n_x^2 + n_y^2 + n_z^2\right)E_0,\ E_0 = \frac{h^2}{8ml^2}$. For each n in x, y, z, the possible values are integer numbers and so a different number of states may in fact have the same energy, a situation termed "degenerate".

Energy	Equal-Energy States	Order of Degeneracy
$2E_0$	(1,1,1)	1
$6E_0$	(2,1,1) (1,2,1) (1,1,2)	3
$9E_0$	(2,2,1) (2,1,2) (1,2,2)	3
$11E_0$	(3,1,1) (1,3,1) (1,1,3)	3
$12E_0$	(2,2,2)	1
$14E_0$	(1,2,3) (1,3,2) (2,1,3) (2,3,1) (3,1,2) (3,2,1)	6

Free Electron Theory of Metals

- In a metal or gas molecules in a container, given in a box of length l, where l is made very large, the number of states (and ultimately electrons) is found by taking

$$N = \sqrt{n_x^2 + n_y^2 + n_z^2},\ number\ of\ states\ dS = \frac{1}{8}\left(4\pi N^2 dN\right) = \frac{\pi}{2} N^2 dN \rightarrow N^2 = n_x^2 + n_y^2 + n_z^2 = E\left(\frac{8ml^2}{h^2}\right)\ in\ E\ to\ E + dE.$$

- $$dN = \frac{\left(\frac{8ml^2}{h^2}\right)^{\frac{1}{2}} dE}{2E^{\frac{1}{2}}};\ dS = \frac{\pi}{2} E\left(\frac{8ml^2}{h^2}\right)\left(\frac{8ml^2}{h^2}\right)^{\frac{1}{2}}\left(\frac{dE}{2E^{\frac{1}{2}}}\right) = \frac{2\pi l^3 (2m)^{\frac{3}{2}}}{h^3} E^{\frac{1}{2}}\, dE$$

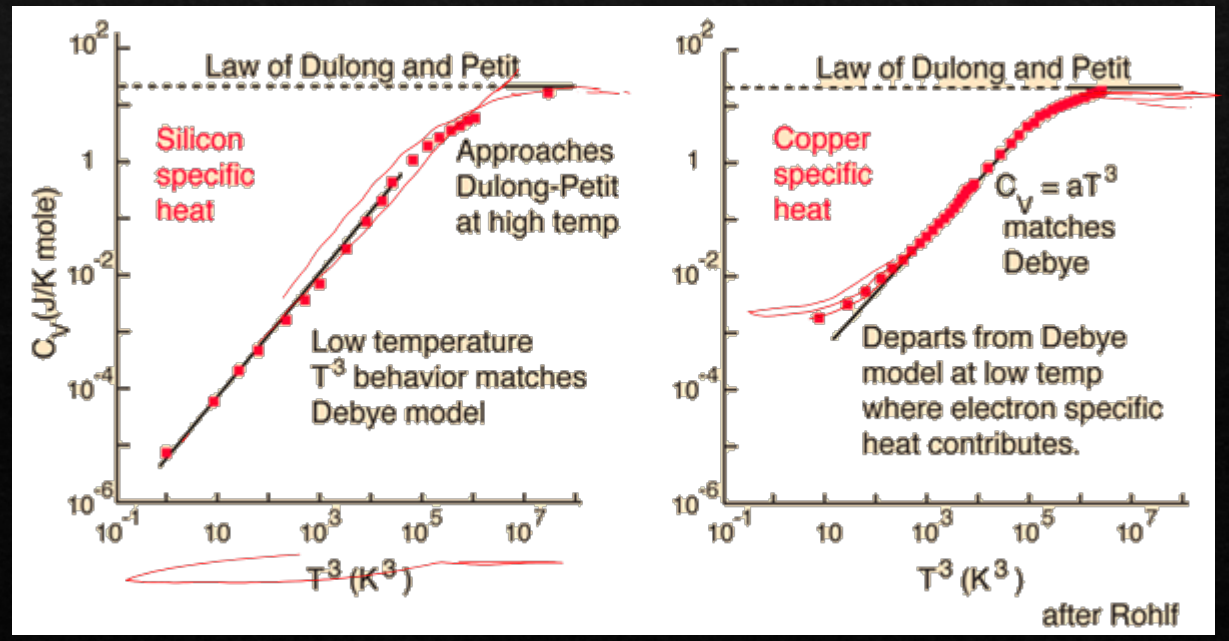
- iF the volume V=l^3, the density of states $g(E) = \frac{2\pi V (2m)^{\frac{3}{2}}}{h^3} E^{\frac{1}{2}}$

Specific Heat of Solids

- The molar specific heat at constant volume of a solid is defined as

$$C_V = \frac{1}{N}\left(\frac{\partial E_T}{\partial T}\right)_V$$

- Classically considering the 3N modes of a crystalline solid, the expected value of $C_V = 3R$, the ideal gas constant.



Examples: Dulong-Petit Law

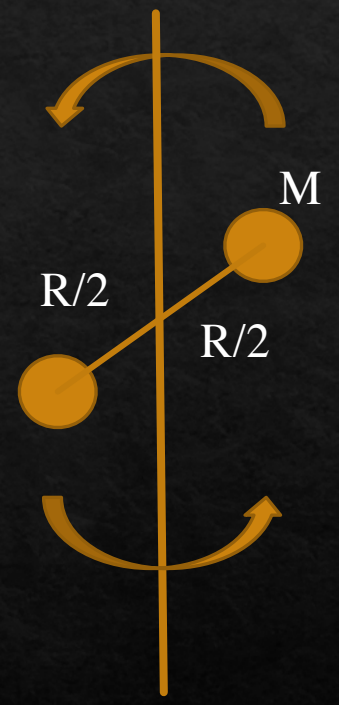
- Imagine a crystal lattice as a system of regularly spaced atoms connected by springs.
- $E = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) + \frac{1}{2}(\kappa_x x^2 + \kappa_y y^2 + \kappa_z z^2)$

- From Equipartition Theorem, $E_{tot} = N_0(6)\left(\frac{kT}{2}\right) = 3N_0kT$.
- The molar specific heat is $C_V = \frac{dE_{tot}}{dT} = 3N_0k = 3R$.
- This expression is known as the Dulong-Petit Law.

Examples: Diatomic Molecule Specific Heat

- The diatomic molecule, free to rotate but not to vibrate.
- Let's find the molar heat capacity of a diatomic gas.
- The energy of one diatomic molecule is $E = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) + \frac{1}{2}I\omega_1^2 + \frac{1}{2}\omega_2^2$.
- The Equipartition Theorem says that effectively each degree of freedom adds ½ kT of energy so that the energy of one mole of gas is $E_{tot} = N_0 n\left(\frac{kT}{2}\right) = \frac{5}{2}N_0 kT$.

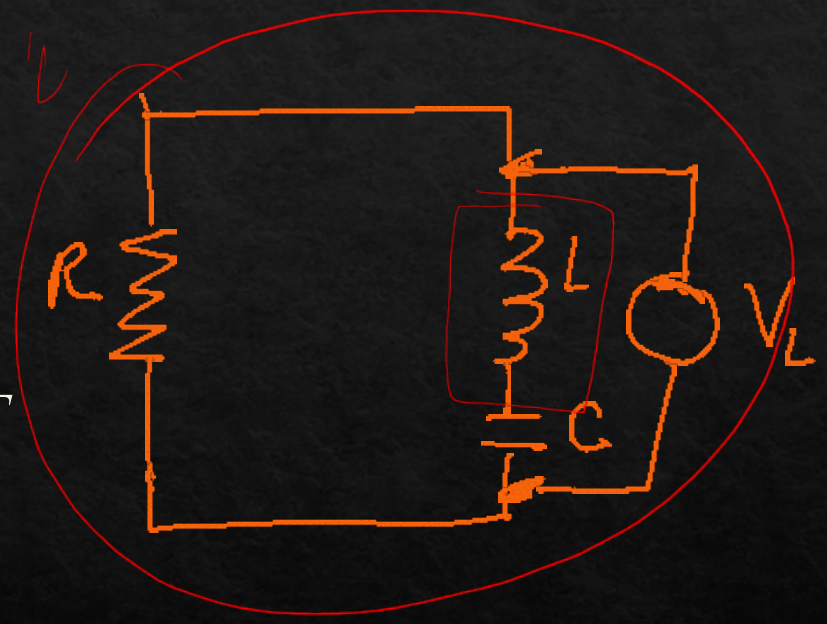
  Then the molar specific heat $C_V = \frac{dE_{tot}}{dT} = \frac{5}{2}N_0 k = \frac{5}{2}R$.



Examples: Induced RMS Voltage in RLC Inductor from Thermal Energy

- Imagine a high-Q RLC circuit at some temperature T.
- The rms value of the induced voltage in the inductor from thermal fluctuations can be estimated with the Equipartition Theorem.
- $E = \int_0^I V_L i dt = \int_0^I L i di = \frac{1}{2} L I^2 \rightarrow E_{avg} = \frac{1}{2} L \left(I^2\right)_{avg} = \frac{1}{2} kT$
- $\omega_0 = \frac{1}{\sqrt{LC}}$ a high quality factor circuit is tuned to resonance, and the voltage across the inductor is

$$V_L = \omega_0 L I \rightarrow V_{L_{avg}}^2 = \omega_0^2 L k T \text{ or } V_L, rms = \omega_0 \sqrt{L k T} = \sqrt{\frac{kT}{C}}$$



Counting Particles: Maxwell-Boltzmann Distribution

- We assume statistically that particles have an "intrinsic probability" gi of occupying the ith cell.
- This probability is a counting $P_n = \frac{N!}{n_{1!}n_2!\ldots n_r!} g_1^{n_1} g_2^{n_2} \ldots g_r^{n_r}$

  with the constraints that $\sum n_i = N \; and \; \sum E_i n_i = E_{tot}$
- This counting formula is rewritten in the following way

  $\frac{\partial F}{\partial n_i} = ln \frac{P_n}{N!} = \sum n_i lng_i - \sum ln\, n_i! = \sum n_i lng_i - \sum n_i ln\, n_i + \sum n_i = \sum n_i lng_i - \sum n_i ln\, n_i - \lambda_1 \left(\sum n_i - N \right) - \lambda_2 (\sum E_i n_i - E_{tot})$

  with objective to maximize the probability → finding that

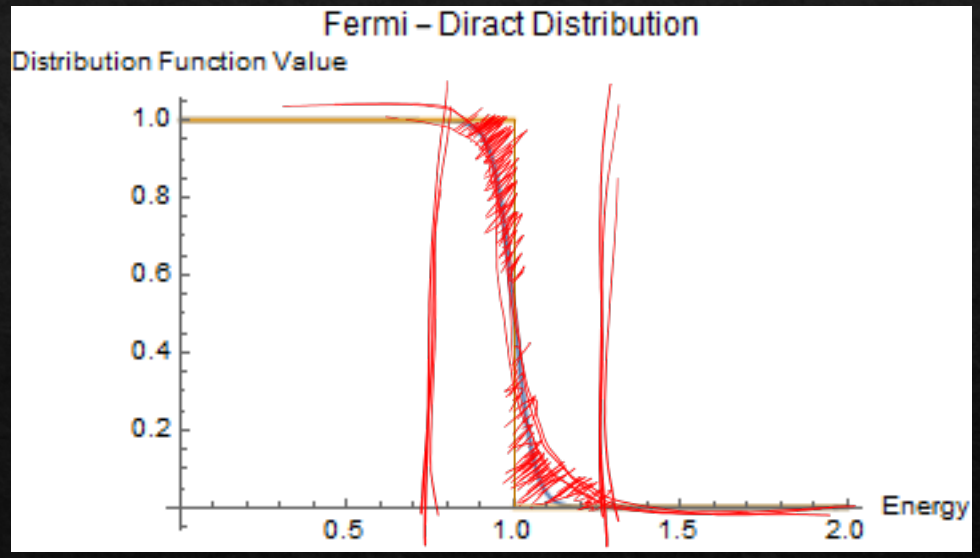
  $n_i = g_i e^{-1-\lambda_1} e^{-\lambda_2 E_i} = A g_i e^{-\beta E_i}$

$\beta = \frac{1}{k_B T}$

Fermi Dirac Distribution Function

$$F_{FD} \approx \frac{1}{\exp\left(\frac{E - E_{f0}}{kT}\right) + 1}$$

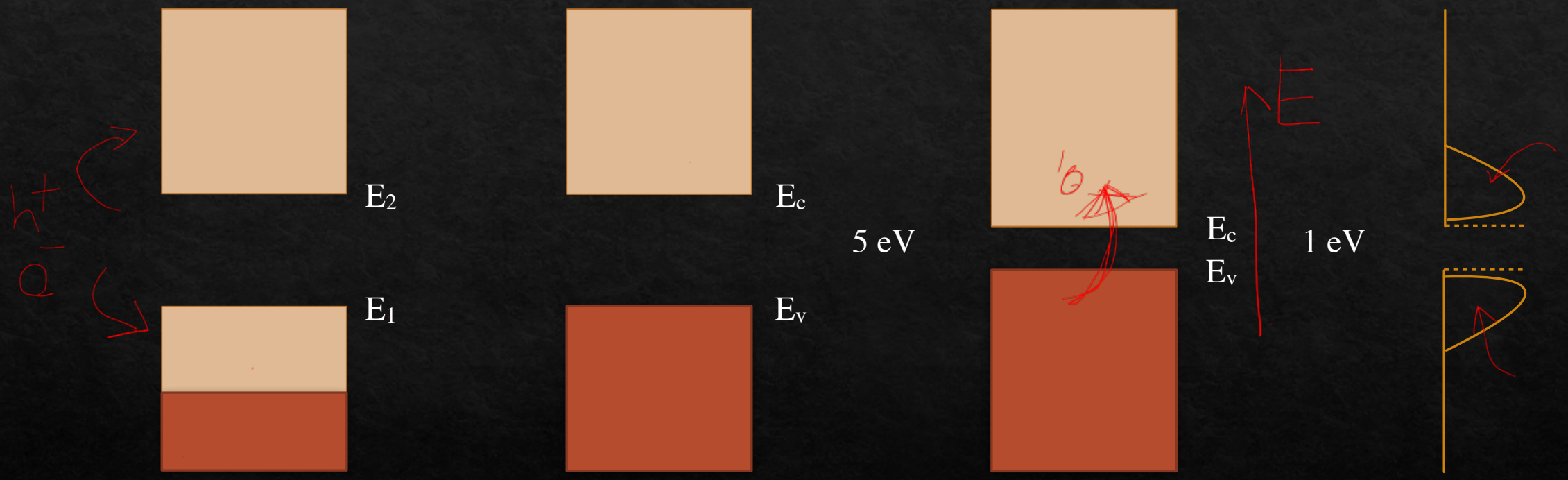
- Blue – T > 0 K
- Orange – T = 0 K.



Total Number N of Fermions and Its Energy

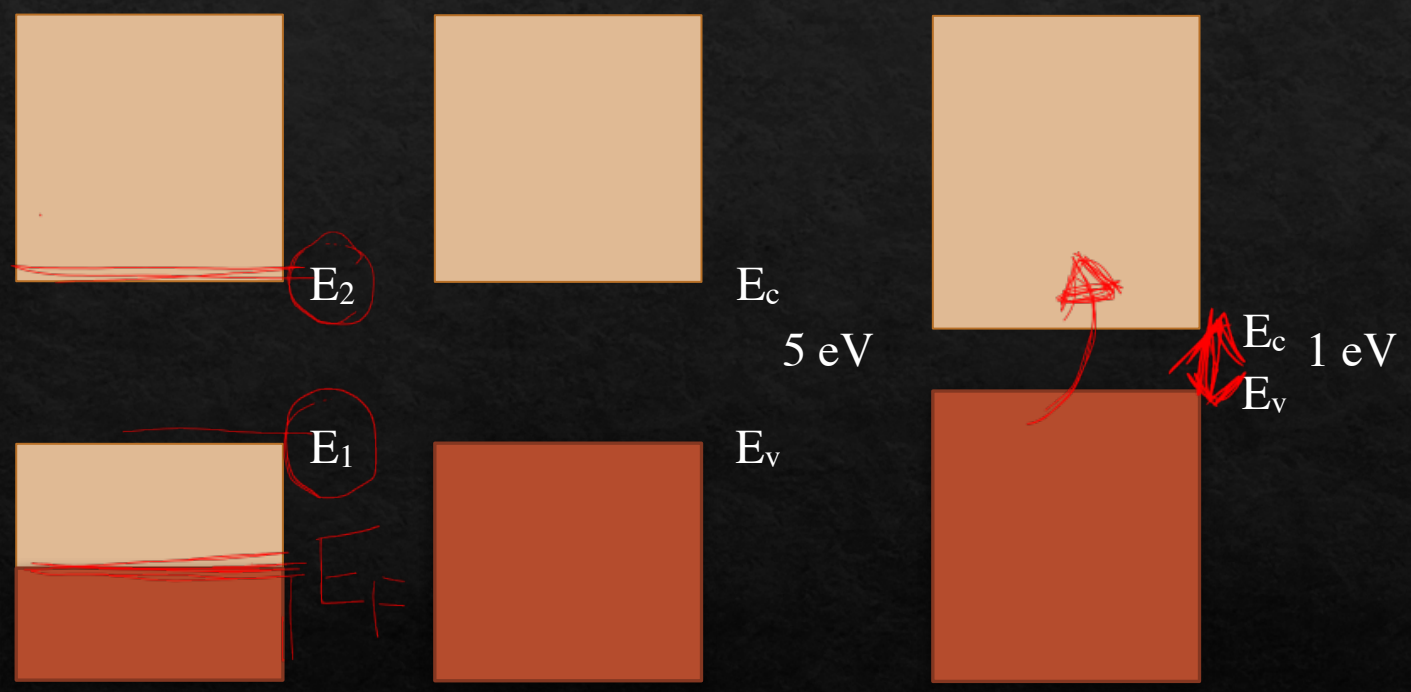
- $$N = 2\int_0^\infty F_{FD} g(E)\,dE = \frac{4\pi V(2m)^{\frac{3}{2}}}{h^3}\int_0^\infty E^{\frac{1}{2}}\,dE\,\frac{1}{\frac{\exp(E-E_f)}{kT}+1} = \frac{4\pi V(2m)^{\frac{3}{2}}}{h^3}\left(\frac{2}{3}E_{f0}^{\frac{3}{2}}\right)$$
- Thus, $E_{f0} = \frac{h^2}{8m}\left(\frac{3N}{\pi V}\right)^{2/3}$
- As the temperature increases, the Fermi energy remains about equal to E_{f0}.

Band Theory of Solids



± Conductors ± Insulators ± Semiconductors

Band Theory of Solids



± Conductors ± Insulators ± Semiconductors

We can estimate the density of carriers, electron and holes.

$$n_e = f_{FD} g(E) dE$$

$$n_h = (1 - f_{FD}) g(E') dE'$$

Optoelectronics

± Recall our discussion of the hydrogen atom and molecule.

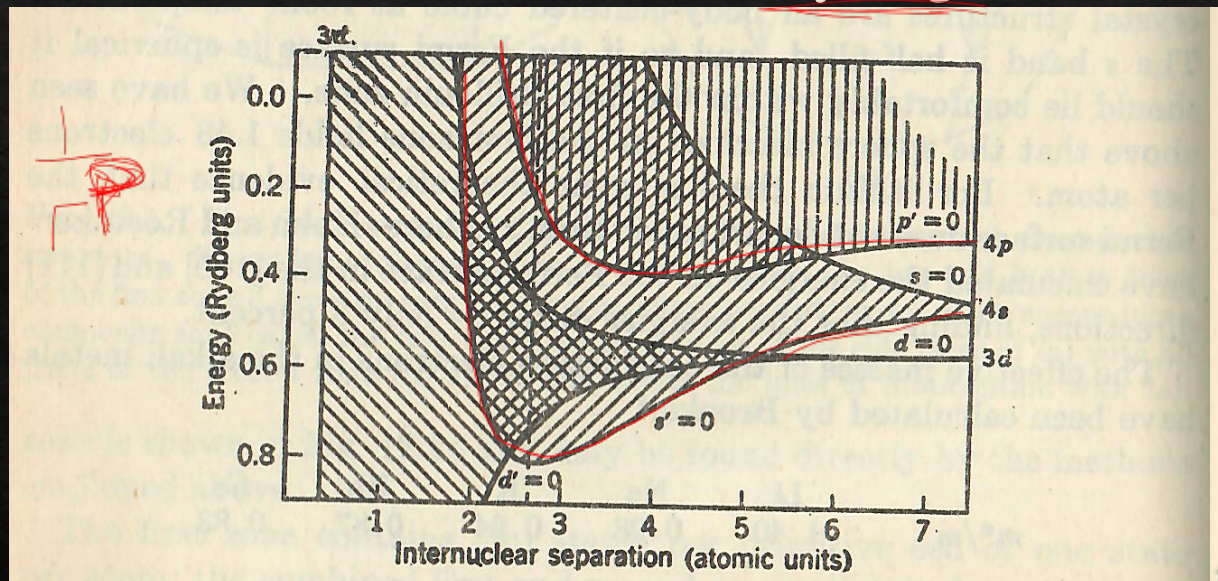


Fig. 12.3. Energy bands in copper as a function of internuclear separation. [After H. M. Krutter, Phys. Rev. 48, 664 (1935).]

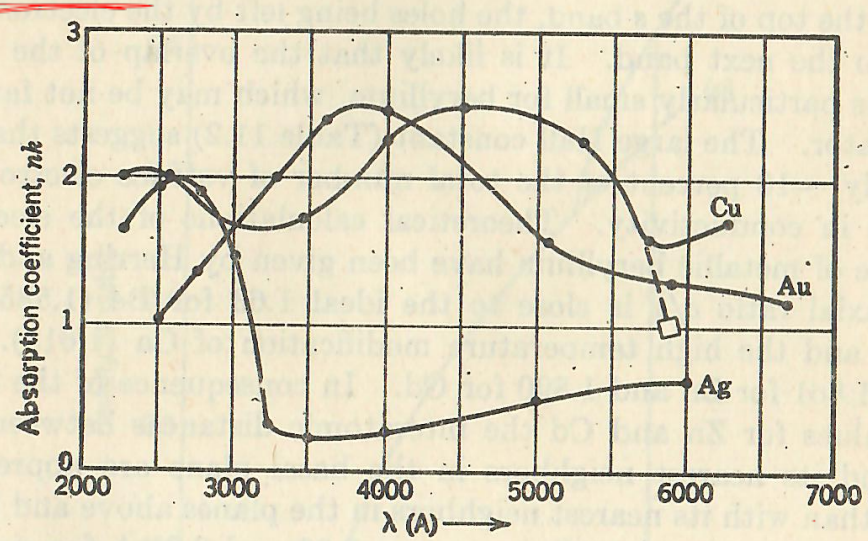


Fig. 12.4. Optical absorption coefficients for copper, silver, and gold. (After Minor and Meier.) The point for copper denoted by a hollow square is from work by Lowery, Bor, and Wilkinson, using a lightly polished surface.

The d band and s band are thought to overlap

The 3d band estimated as 3.46 eV in width and the Fermi surface lying in the 4s band is 3.7 eV, above the 3d band. For free electrons the Fermi surface is estimated at 7.1 eV

Reddish color of Cu comes from strong absorption in the blue-green spectrum, onset at 575 nm with 2.1 eV

	Cu	Ag	Au
m^*/m	1.012	0.992	0.994

PN Junctions

$D = \nabla\phi$

- For rectifiers,

  $$\nabla \cdot D = 4\pi\rho \rightarrow \frac{d^2\phi}{dx^2} = \frac{4\pi Ne}{\epsilon} \rightarrow \phi = \frac{2\pi Ne}{\epsilon}x^2$$

  meaning the thickness is then $D = (\epsilon\phi_0/2\pi eN)^{1/2}$ with the thickness forming a barrier layer that acts as an insulator (creating or allowing the voltage drop across the contact region)

- The net current is

  $$j = 1/4Neve^{-e\phi_0/kT}(e^{eV/kT-1}).$$

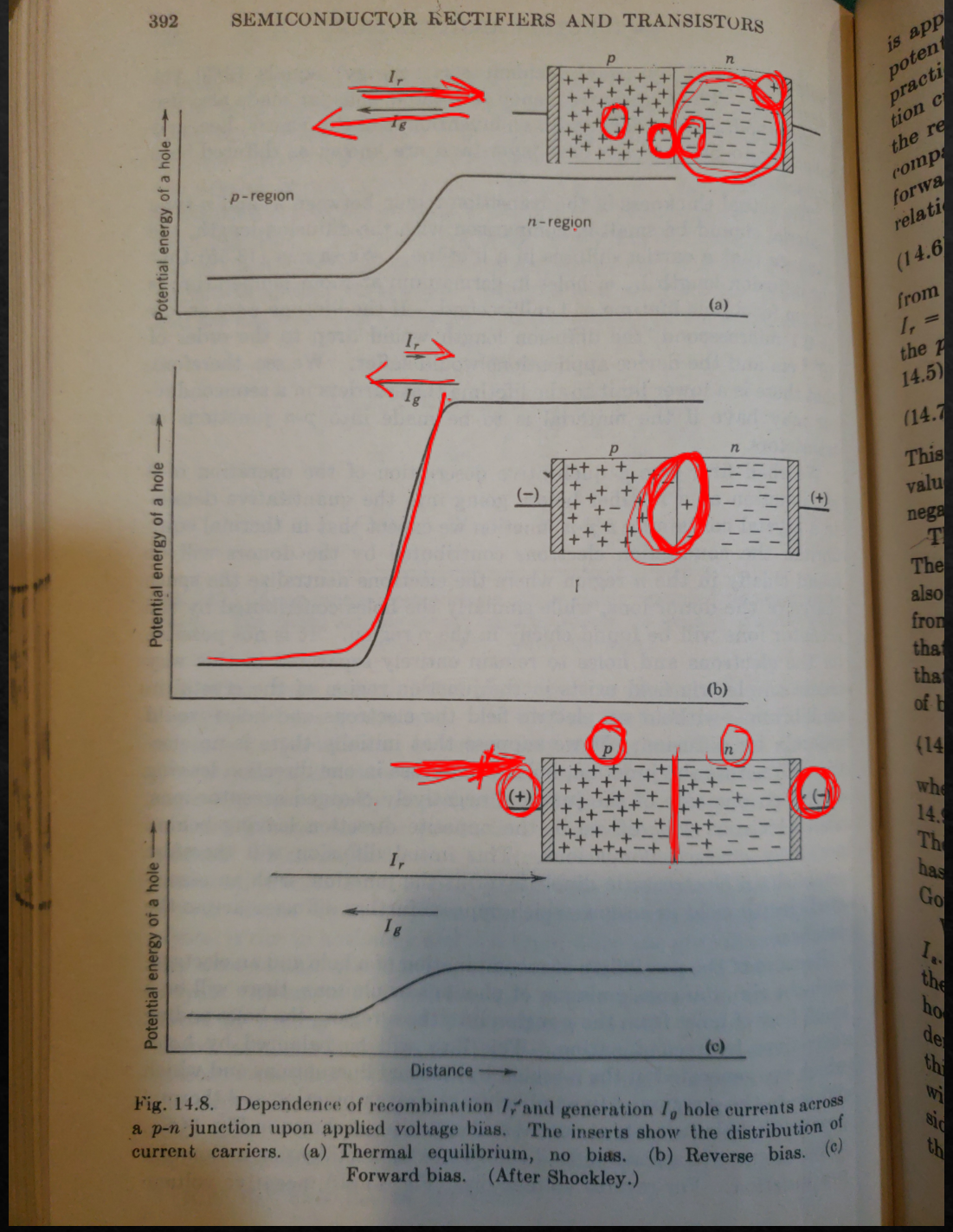
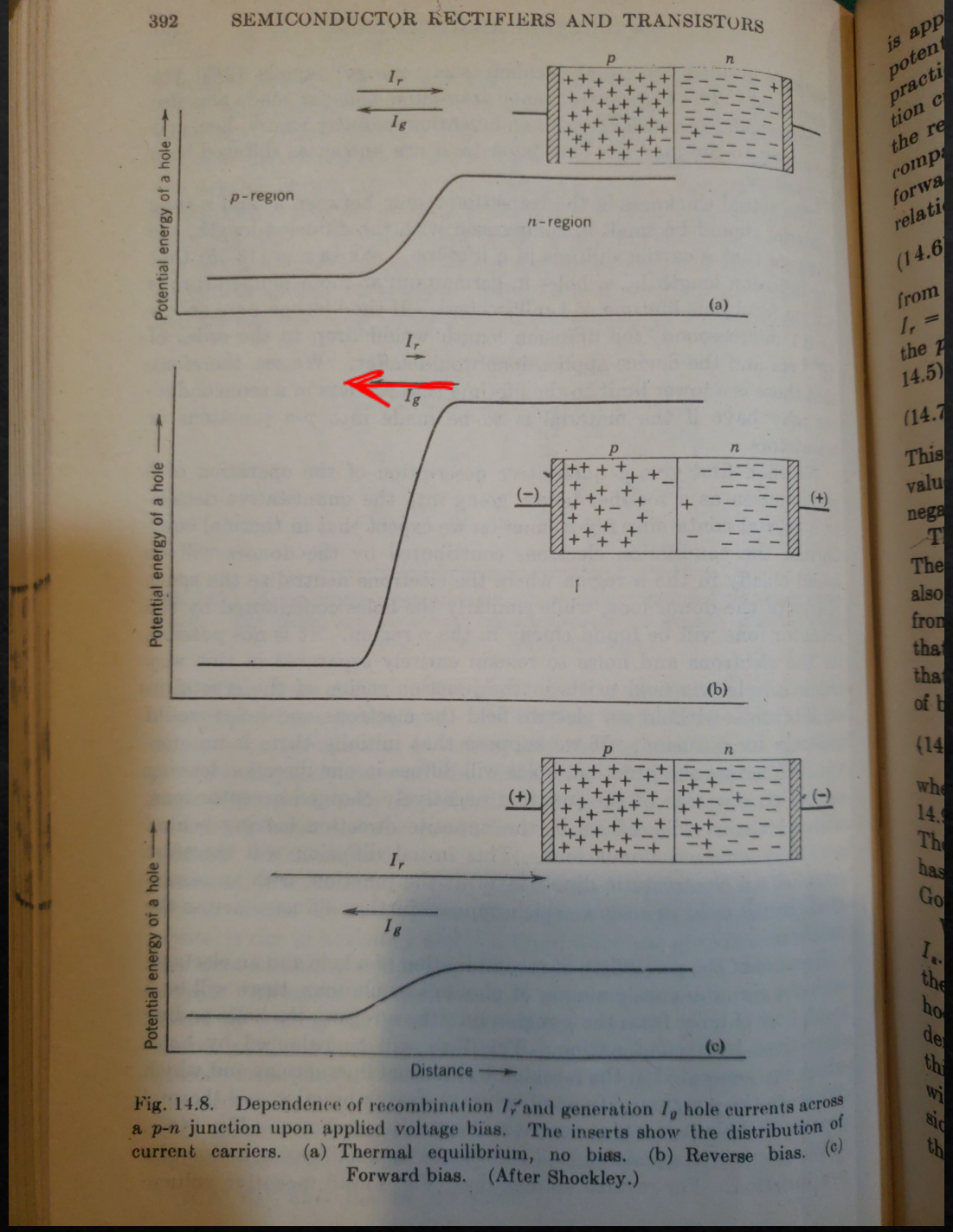


Fig. 14.8. Dependence of recombination I_r and generation I_g hole currents across a p-n junction upon applied voltage bias. The inserts show the distribution of current carriers. (a) Thermal equilibrium, no bias. (b) Reverse bias. (c) Forward bias. (After Shockley.)

PN Junctions

- The net current is
  $j = 1/4 N e \bar{v} e^{-e\phi_0/kT}(e^{eV/kT-1})$.
- In forward bias, recombination current
  $I_r = I_g e^{eV/kT} \rightarrow I_r - I_g = I_g(e^{eV/kT} - 1)$
  depends on generation current.
- The total current
  $I = I_s(e^{eV/kT} - 1) = I_n + I_p = p_n|e|D_p/L_p + n_p|e|D_n/L_n(e^{eV/kT} - 1)$
  .

temperature dependence



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Luminescence

- An example is to consider the sulfide phosphors, ZnS:Ag, ZnS:Cu. Here the activators are Ag and Cu. The ZnS is either a cubic-zincblende (3.64 eV, 3410 Angstrom) or hexagonal-wurtzite (3.7 eV, 3350 Angstrom) structure. From crystalline imperfections the excitation, via interbank transitions, at 3650 Angstrom are possible.

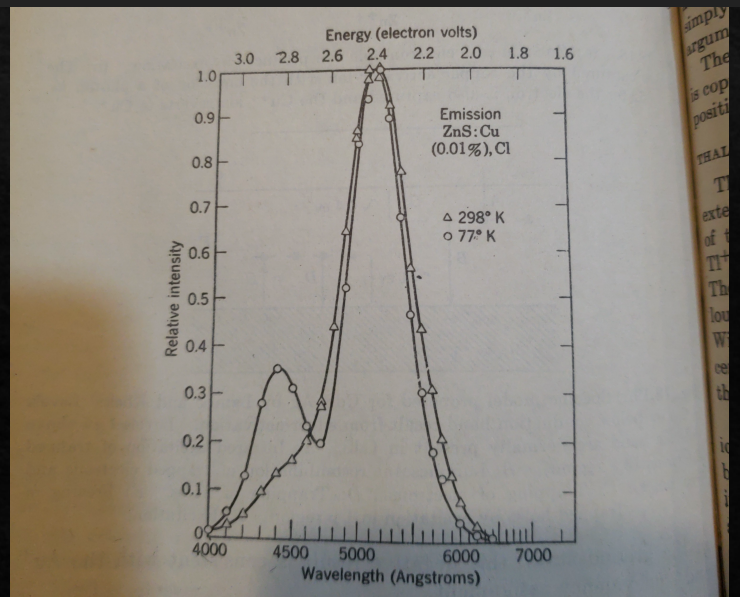


Fig. 18.21. Emission spectrum of ZnS containing chloride and 0.01 percent copper.

https://www.youtube.com/watch?v=_FXukyeNEFQ

Optoelectronics

± Concerned with the optical properties of novel materials, specifically often metal-semiconductor combinations or junctions, such as the following structure:

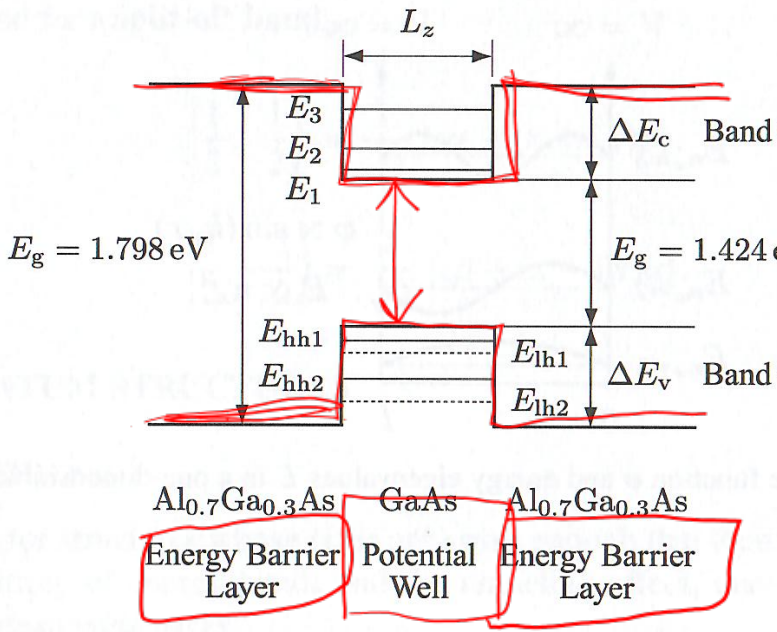


FIGURE 1.5 Quantum well structure.

$$\psi_n(\boldsymbol{k}, \boldsymbol{r}) = \exp(\mathrm{i}\,\boldsymbol{k} \cdot \boldsymbol{r}) u_{n\boldsymbol{k}}(\boldsymbol{r}), \quad u_n(\boldsymbol{k}, \boldsymbol{r}) = u_{n\boldsymbol{k}}(\boldsymbol{r} + \boldsymbol{R}).$$

$$\varphi(x, y, z) = \sqrt{\frac{8}{L^3}} \sin k_x x \cdot \sin k_y y \cdot \sin k_z z.$$

Quantum Wells

- In 1D, 2D, 3D the density of states (density of electrons follows the following structure).

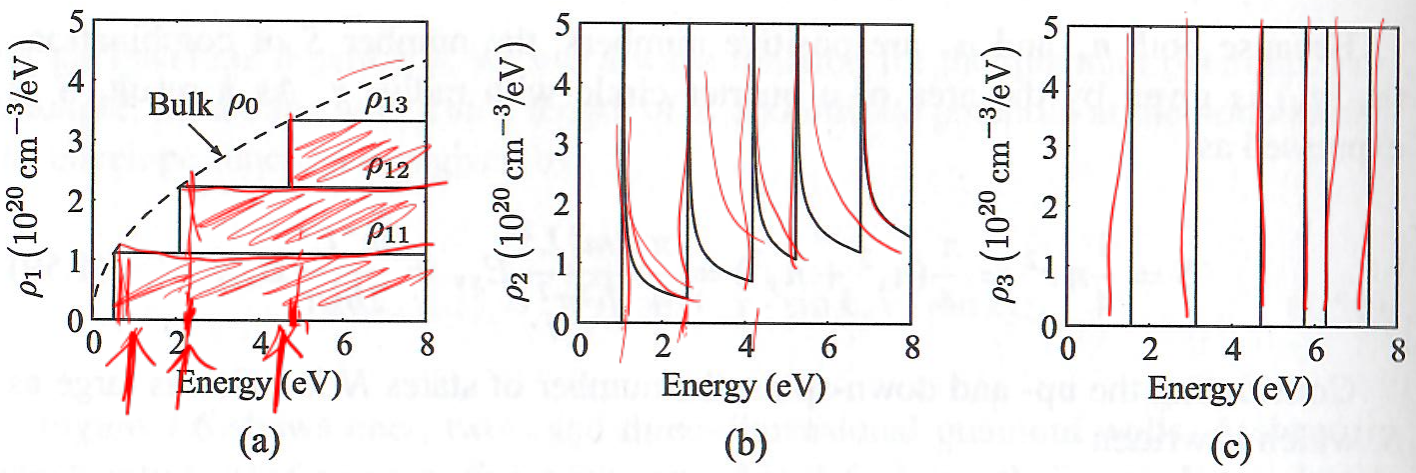
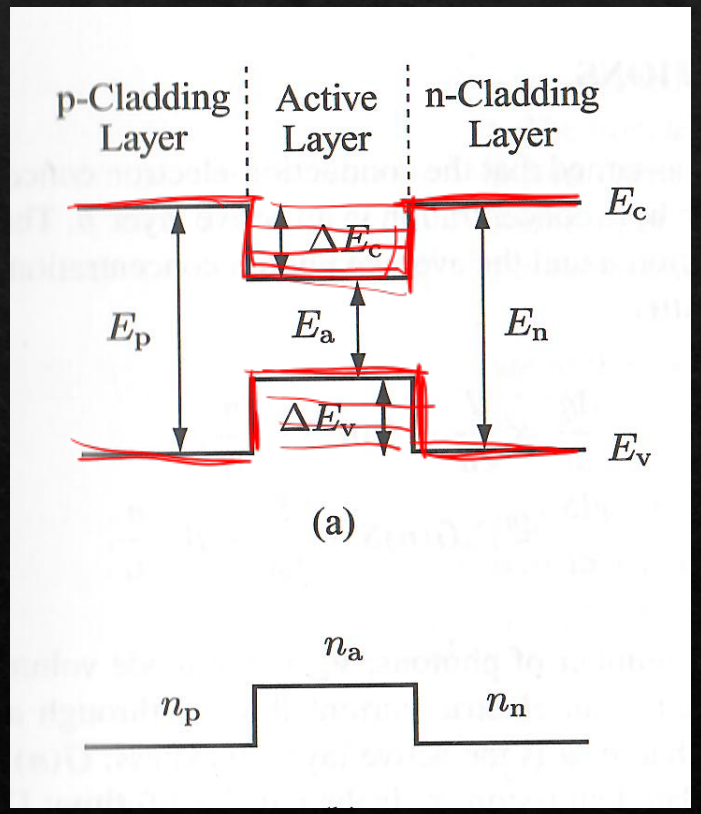


FIGURE 1.7 Density of states for (a) one-, (b) two-, and (c) three-dimensional quantum wells.

- Understanding the electron density and effective mass (what kind of material from the periodic table) is the first step in determining the quantum well behavior, from conduction to optics!

Double Well Heterostructure

bias ↑ or bias →



$$\frac{dn}{dt} = \frac{J}{ed} - G(n)S - \frac{n}{\tau_n},$$

$$\frac{dS}{dt} = \Gamma_a G(n)S - \frac{S}{\tau_{ph}} + \beta_{sp}\frac{n}{\tau_r}.$$

J is the injected current density, d the active thickness, G(n) the amplification rate due to stimulated emission, τ_n the carrier lifetime, Γ_a the optical confinement factor of the active layer, τ_{ph} the photon lifetime, β_{sp} the spontaneous emission coupling factor, and τ_r the radiative recombination lifetime

± Double well and the refractive indices

Double Well Heterostructure

- Current-Voltage Characteristics
- Under forward bias, V > 0, the hole concentration in the n-region is increased, so that the carriers in the n region have a concentration as
- The current as a function of the voltage is then written explicitly

$$S = -\beta_{sp}\frac{n}{\tau_r}\frac{1}{\Gamma_a G(n) - 1/\tau_{ph}},$$

$$I = eV_a\left[G(n)S + \frac{n}{\tau_n}\right].$$

$$np = n_n p_n = n_i^2 \exp\left(\frac{eV}{k_B T}\right)$$

$$I = eV_a\left[-\beta_s\frac{n_i e^{eV/2k_BT}}{\tau_r}\frac{G(n_i e^{eV/2k_BT})}{\Gamma_a G(n_i e^{eV/2k_BT}) - 1/\tau_{ph}} + \frac{n_i e^{eV/2k_BT}}{\tau_n}\right]$$

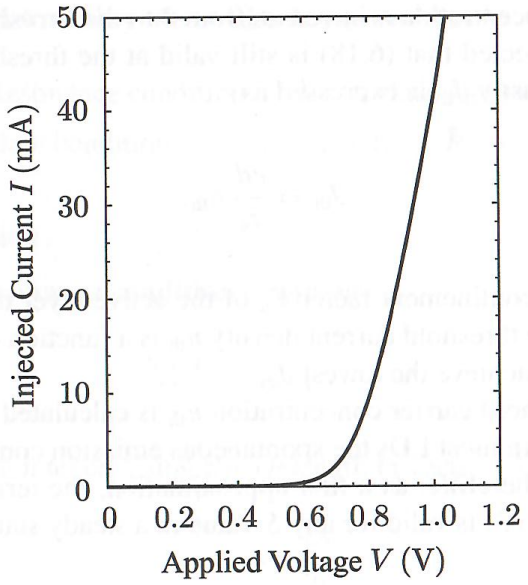


FIGURE 6.4 Current versus voltage (I–V) characteristics.

Conventional light diodes operating at room temperature have electron concentrations 10^{11} /cm^3 with 1 ps photon lifetime, 4 Ω resistance, 3.5 (effective) refractive index. The electron group velocities 10^9 cm/s.