



# Semiconductor Physics

## Part 1

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# Course Overview

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1. Energy Bandgap
2. Effective Mass
3. Doping
4. Mobility, Scattering, and Relaxation
5. Boltzmann Statistics
6. Recombination
7. Drift-Diffusion Equations

## **Ref:**

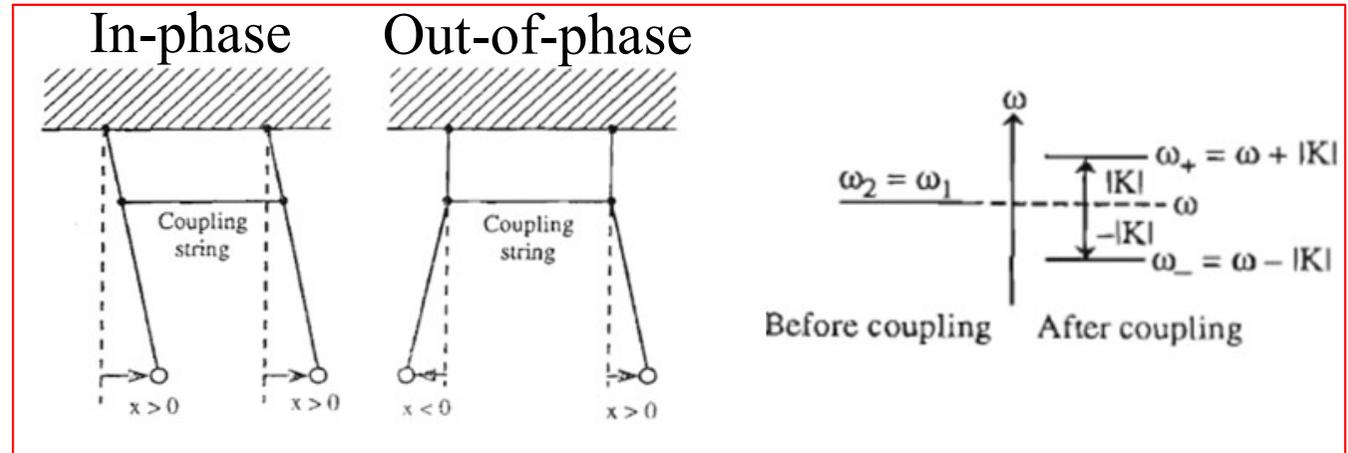
Enke Liu, Semiconductor Physics, Chapter 1-5;

Shun Lien Chuang, Physics of Photonic Devices, Chapter 2.

# 1. Energy Bandgap (1)

## Coupled Mode Theory

$$\begin{cases} \frac{da_1}{dt} = j\omega_1 a_1 + jk_{12} a_2 \\ \frac{da_2}{dt} = j\omega_2 a_2 + jk_{21} a_1 \end{cases}$$

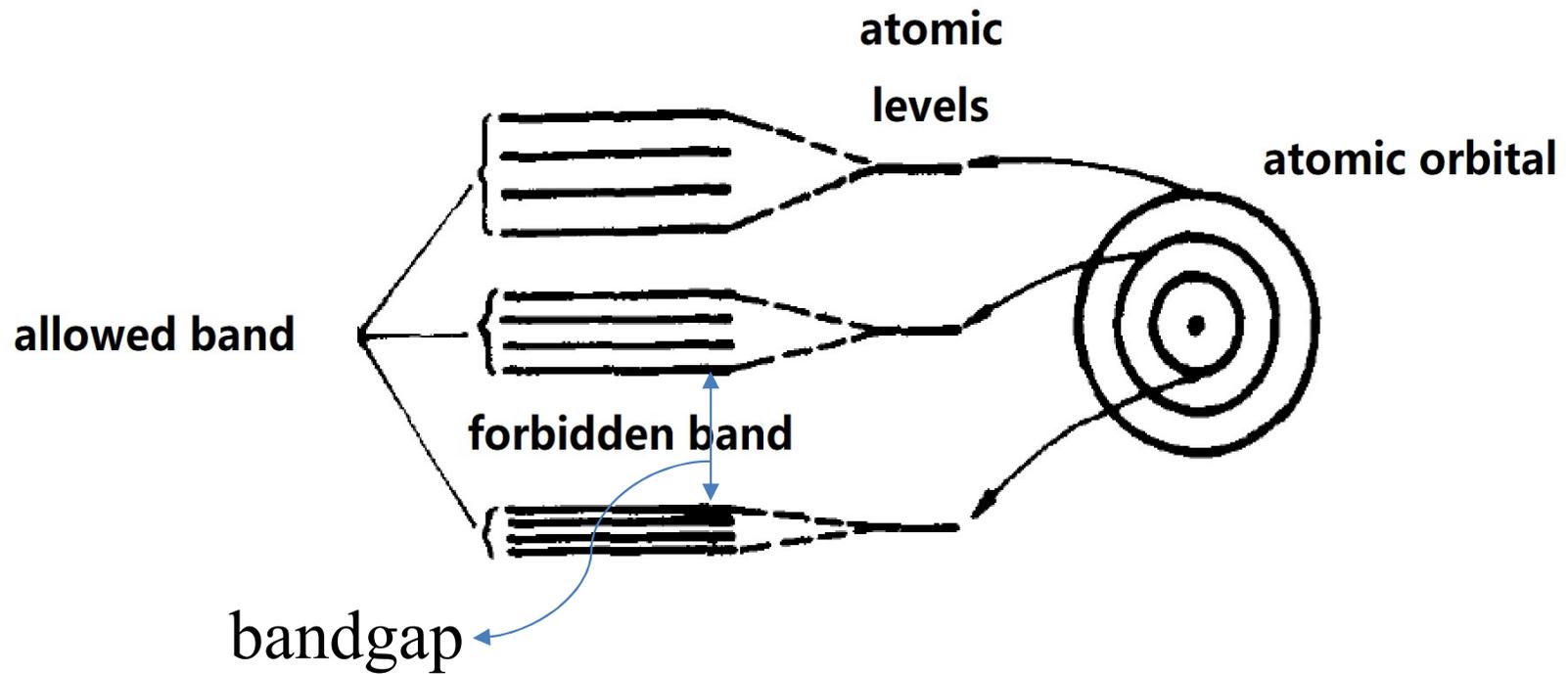
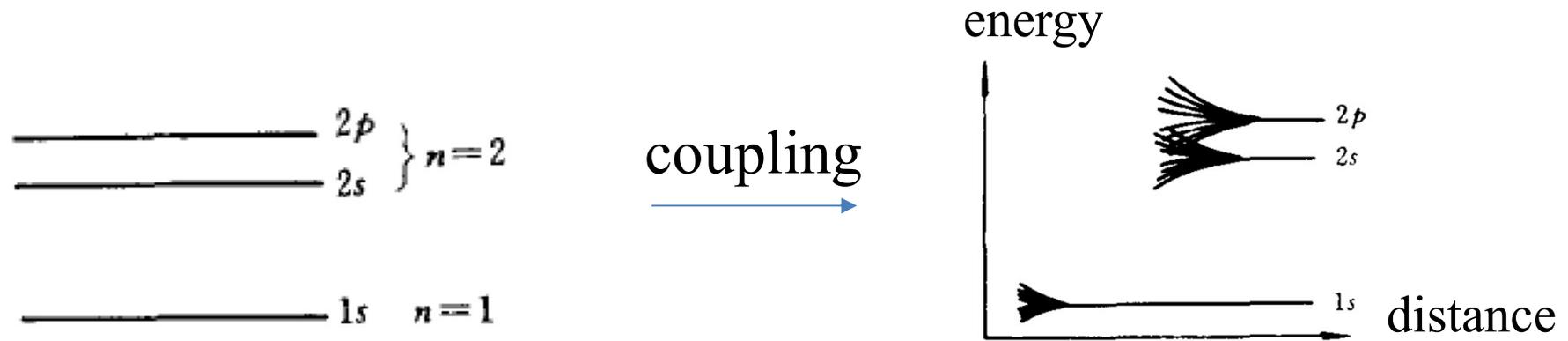


$$\frac{d}{dt} \left( |a_1|^2 + |a_2|^2 \right) = 0 \quad \xrightarrow{\text{energy conservation}} \quad k_{12} = k_{21}^*$$

$$\begin{cases} j\omega \tilde{a}_1 = j\omega_1 \tilde{a}_1 + jk_{12} \tilde{a}_2 \\ j\omega \tilde{a}_2 = j\omega_2 \tilde{a}_2 + jk_{12}^* \tilde{a}_1 \end{cases} \quad \longrightarrow \quad \omega_{\pm} = \frac{\omega_1 + \omega_2}{2} \pm \sqrt{\left( \frac{\omega_1 - \omega_2}{2} \right)^2 + |k_{12}|^2}$$

coupling induces the split of resonant frequency !

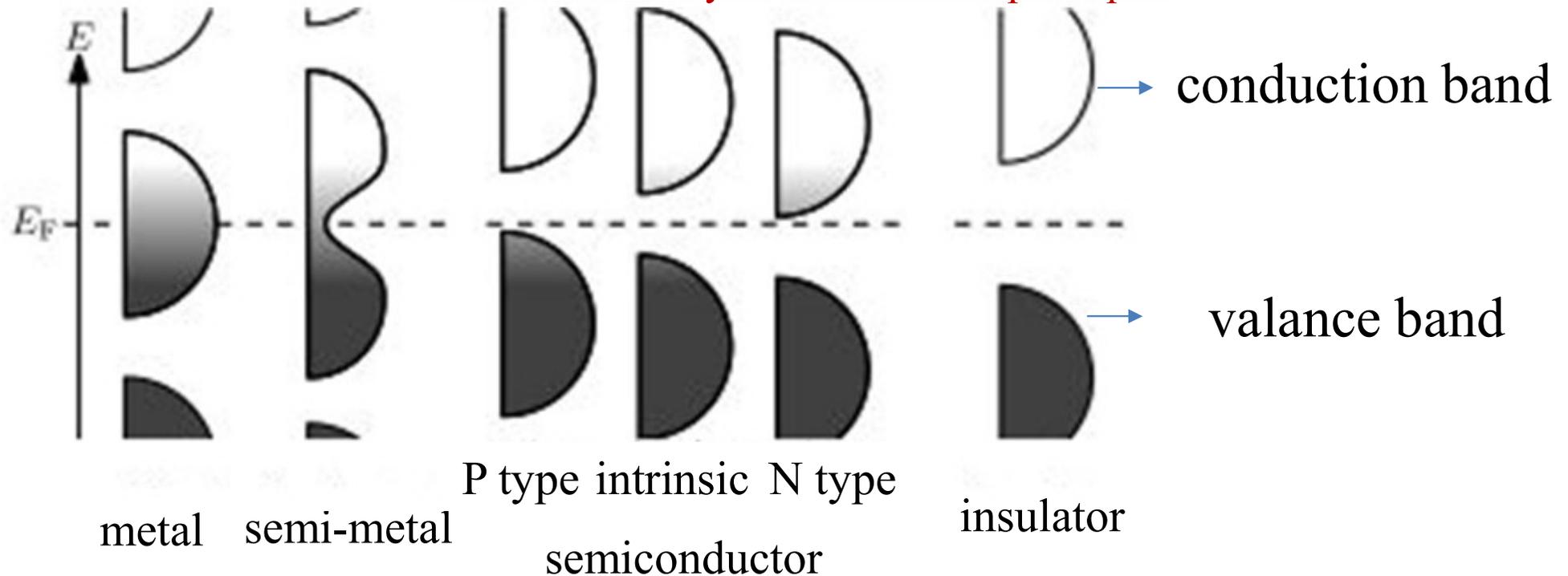
# 1. Energy Bandgap (2)



There is no electronic state within bandgap

# 1. Energy Bandgap (3) *What's the fundamental difference between photon and electron?*

Electrons satisfy Pauli exclusion principle.

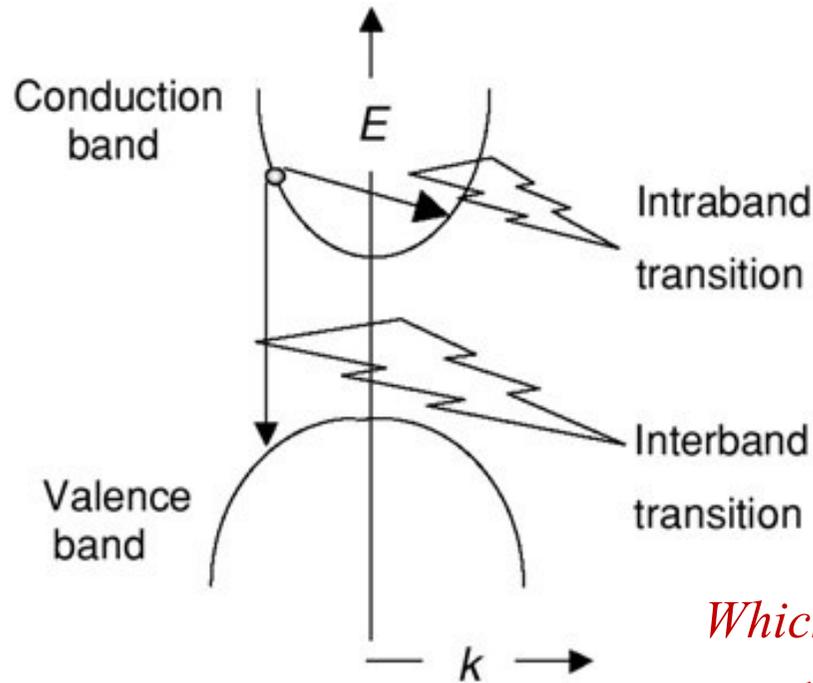


Fermi level: If there is an electronic state at the Fermi level, then this state will have a 50% chance of being occupied. Below the Fermi level, the occupation probability becomes larger and larger. At  $T=0$ , electronic states are fully occupied below the Fermi level.

Metals have a partially filled conduction band. A semimetal has a small overlap between the bottom of the conduction band and the top of the valence band. In insulators and semiconductors, the filled valence band is separated from an empty conduction band by a band gap. For insulators, the magnitude of the band gap is larger.

# 1. Energy Bandgap (4)

## Electronic transitions between valance and conduction bands



1. Intraband transition is the transition between levels within the conduction band. It is caused by electron-electron (electron screening effect) or electron-phonon interaction, and mainly responsible for the real part of permittivity.

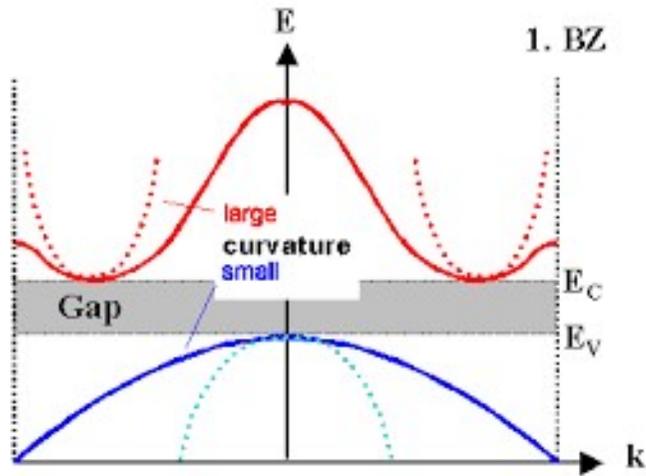
*Which transition is responsible for surface plasmonic effect ?*

Intraband transition is responsible for negative permittivity.

2. Interband transition is the transition between conduction and valence bands. It generates electron-hole pairs, and mainly responsible for the imaginary part of permittivity (lossy term).

3. If electron density is increased or Fermi level is arisen, the interband transition will be forbidden if excitation (photon) energy is low.

## 2. Effective Mass (1)



$$E(k) = E(k_0) + \left. \frac{dE}{dk} \right|_{k=k_0} k + \frac{1}{2} \left. \frac{d^2E}{dk^2} \right|_{k=k_0} k^2 + \dots$$

*Which material has zero effective mass ?*

Graphene with the Dirac-cone band structure

The effective mass is a quantity that is used to simplify band structures by modeling the behavior of a free particle with that mass.

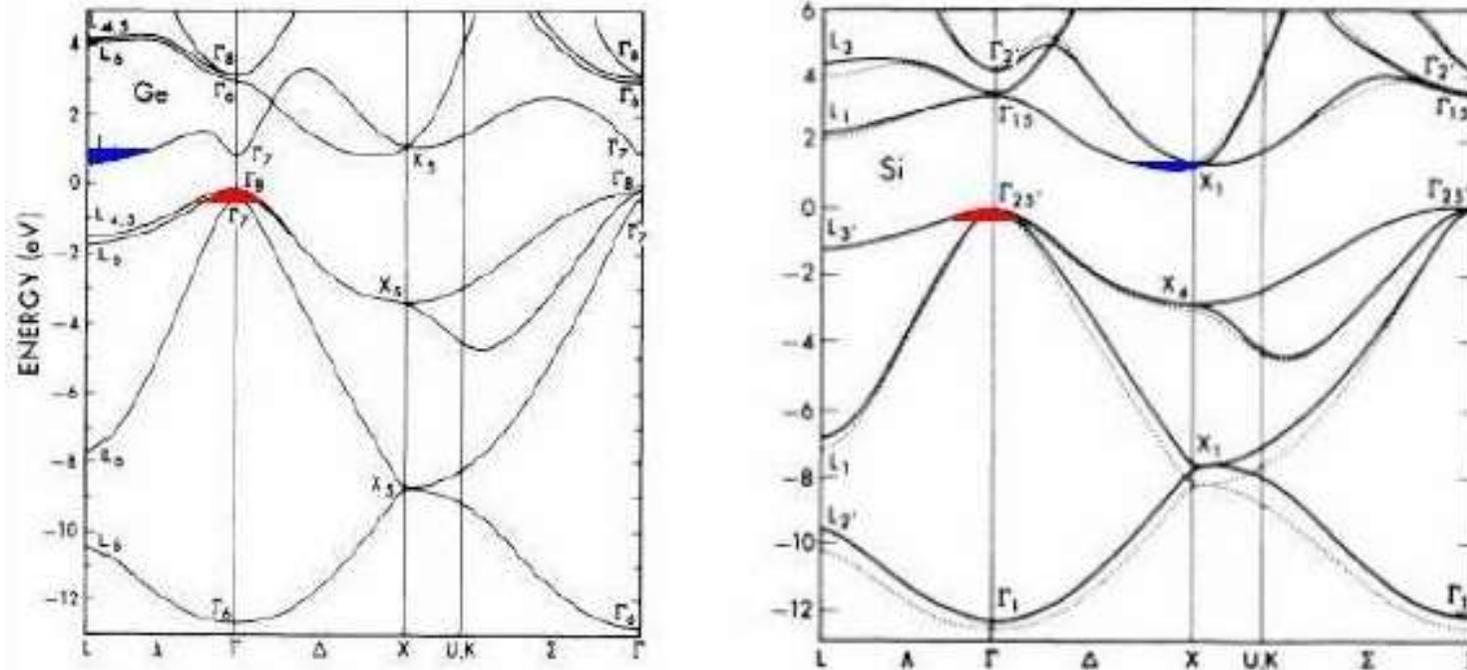
At the highest energies of the valence band and the lowest energies of the conduction band, the band structure  $E(\mathbf{k})$  can be locally approximated as

$$E(\mathbf{k}) = E_0 + \frac{\hbar^2}{2m^*} \mathbf{k}^2 \quad \frac{1}{m^*} = \frac{1}{\hbar^2} \left. \frac{d^2E}{dk^2} \right|_{k=k_0}$$

where  $E(\mathbf{k})$  is the energy of an electron at wavevector  $\mathbf{k}$  in that band,  $E_0$  is a constant giving the edge of energy of that band, and  $m^*$  is a constant (effective mass). electrons or holes placed in these bands behave as free electrons except with a different mass.

## 2. Effective Mass (2)

Band structures of germanium and silicon are complex!



The top of valance band (red) and the bottom of conduction band (blue) are not aligned. In other words, Si and Ge have **indirect bandgap**. Thus, phonon absorption is significant during electronic transition due to momentum conservation.

Newton equation of an electron in semiconductor with the effective mass

$$m_n^* \frac{d\mathbf{v}}{dt} = -(q\mathbf{E} + q\mathbf{v} \times \mathbf{B})$$

### 3. Doping (1)

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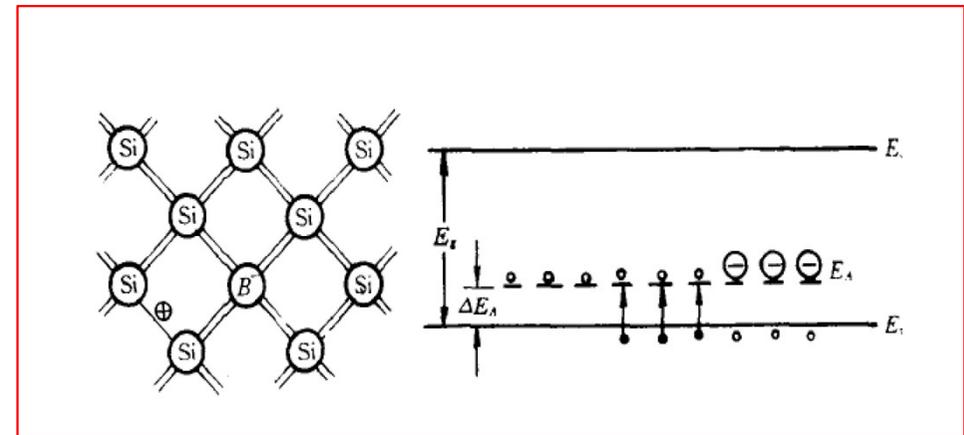
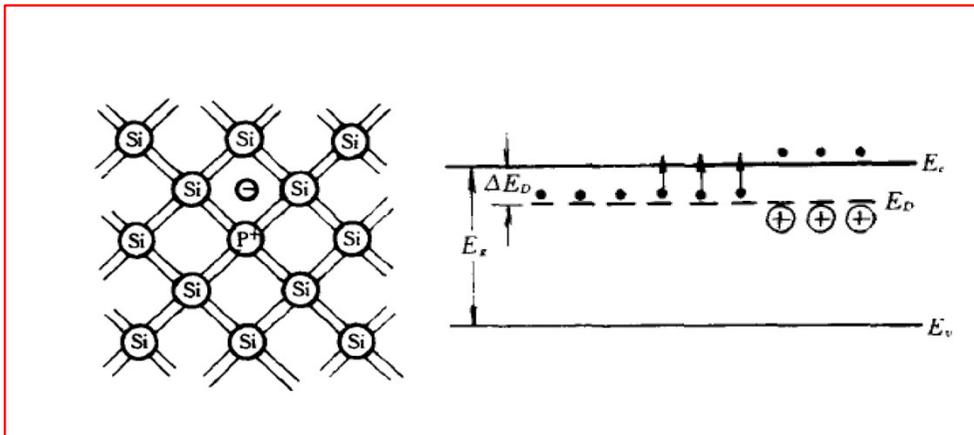
Doping is the intentional introduction of impurities into an intrinsic semiconductor for the purpose of modulating its electrical, optical and structural properties.

Small numbers of dopant atoms can change the ability of a semiconductor to conduct electricity.

When on the order of one dopant atom is added per 100 million atoms, the doping is said to be low or light.

When many more dopant atoms are added, on the order of one per ten thousand atoms, the doping is referred to as high or heavy. This is often shown as  $n+$  for n-type doping or  $p+$  for p-type doping.

### 3. Doping (2)



By doping pure silicon with Group V elements such as phosphorus, extra valence electrons are added that become unbonded from individual atoms and allow the compound to be an electrically conductive n-type semiconductor.

Doping with Group III elements, which are missing the fourth valence electron, creates "broken bonds" (holes) in the silicon lattice that are free to move. The result is an electrically conductive p-type semiconductor.

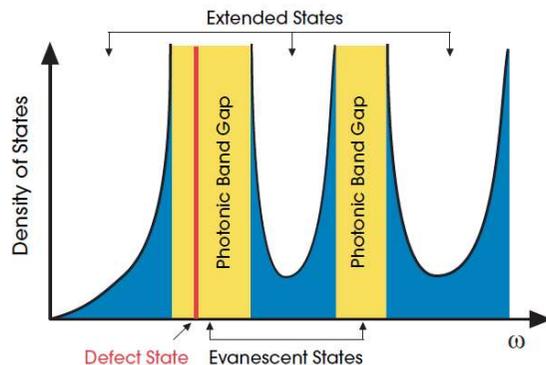
In this context, a Group V element is said to behave as an electron donor, and a group III element as an acceptor.

### 3. Doping (3)

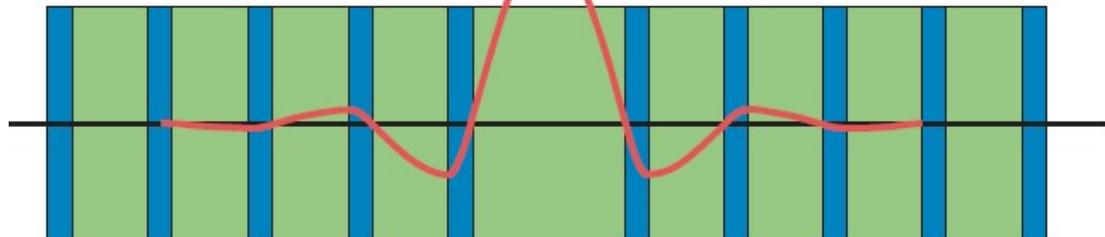
## Analogy between solid crystals and photonic crystals (optional)

	Quantum mechanics	Electrodynamics
Field	$\Psi(\mathbf{r}, t) = \Psi(\mathbf{r})e^{-i\frac{Et}{\hbar}}$	$\mathbf{H}(\mathbf{r}, t) = \mathbf{H}(\mathbf{r})e^{-i\omega t}$
Eigenvalue problem	$\mathcal{H}\Psi = E\Psi$	$\Theta\mathbf{H} = \left(\frac{\omega}{c}\right)^2\mathbf{H}$
Hermitian operator	$\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})$	$\Theta = \nabla \times \frac{1}{\epsilon(\mathbf{r})} \nabla \times$

Electrons in solid crystals	Photons in photonic crystals
Wave-like behavior $\psi(\mathbf{r}, t)$ in periodic potential of lattice	Field $\mathbf{H}(\mathbf{r}, t)$ in periodic dielectric functions
Electronic band structure	Photonic band structure
Electronic Doping/Impurity	Photonic Defect

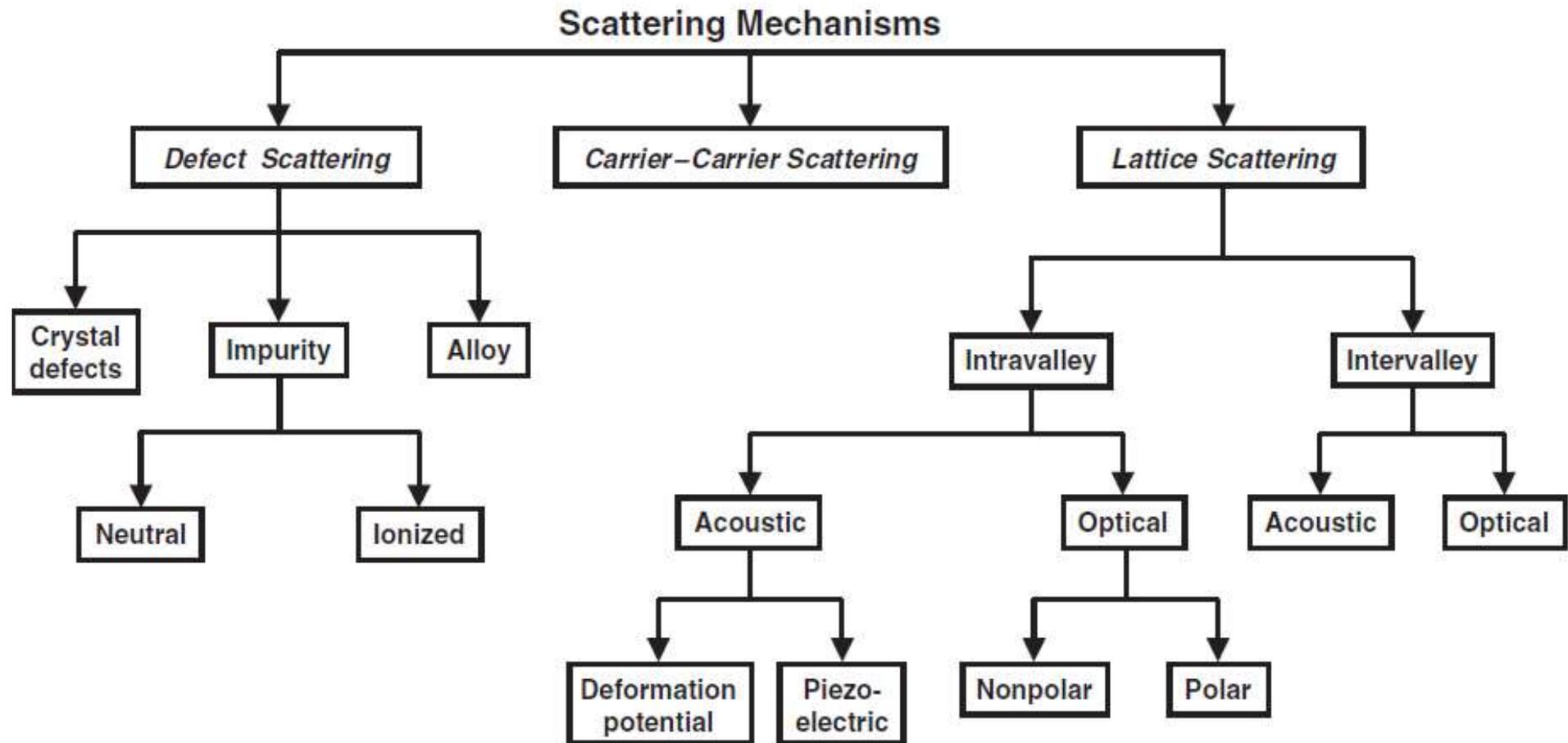


defect state in photonic crystals



## 4. Scattering

Scattering is complex



## 4. Relaxation and Characteristic Length (Optional)

Characteristic length is essential to both electron and photon systems!

	$L \ll l_{e-ph}$			$L \sim l_{e-ph}$	$L \gg l_{e-ph}$
	$L < \lambda$	$L < l_{e-e}$	$L \gg l_{e-e}$		
Transport regime	Quantum	Ballistic	Fluid	Fluid	Diffusive
Scattering	Rare	Rare	e-e (many), e-ph (few)		Many
Model:					
Drift-diffusion					
Hydrodynamic		Quantum hydrodynamic			
Monte Carlo					
Schrodinger/Green's					
Functions	Wave				
Applications	Nanowires, superlattices	Ballistic transistor	Current IC's	Current IC's	Older IC's

*What is the characteristic length of electronic system?*

$l_{e-ph} \gg l_{e-e} \gg \lambda$  (e-e: electron-electron elastic; e-ph: electron-optical phonon inelastic)

**Space:** Fermi wavelength ( $\lambda$ ), mean free path ( $l_{e-e}$ ) and phase coherence length ( $l_{e-ph}$ )

**Time:** momentum relaxation time ( $\tau_{e-e}$ ) and energy (phase) relaxation time ( $\tau_{e-ph}$ )

## 4. Mobility, Scattering, and Relaxation (1)

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Scattering probability  $P$

$$\frac{dN(t)}{dt} = -PN(t)$$

the number of free electrons at  $t$

initial number of electrons

$$N(t) = N_0 e^{-Pt}$$

Number of scattered electrons between  $t \sim t+dt$

$$PN_0 e^{-Pt} dt$$

Mean free time or relaxation time : time between successive scattering

$$\tau = \frac{1}{N_0} \int_0^{\infty} PN_0 e^{-Pt} t dt = \frac{1}{P}$$

## 4. Mobility, Scattering, and Relaxation (2)

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Newton's law

$$m_n \frac{\bar{\mathbf{v}}_n}{\tau_n} = -q\mathbf{E}, \quad m_p \frac{\bar{\mathbf{v}}_p}{\tau_p} = q\mathbf{E} \quad \bar{\mathbf{v}}: \text{mean drift velocity}$$

Mobility

$$\mu_n = \left| \frac{\bar{\mathbf{v}}_n}{\mathbf{E}} \right| = \frac{q\tau_n}{m_n}, \quad \mu_p = \left| \frac{\bar{\mathbf{v}}_p}{\mathbf{E}} \right| = \frac{q\tau_p}{m_p}$$

Conductivity

$$\mathbf{J}_n = -\rho_n \bar{\mathbf{v}}_n = -qn\bar{\mathbf{v}}_n = qn\mu_n \mathbf{E}$$

$$\mathbf{J}_p = \rho_p \bar{\mathbf{v}}_p = qp\bar{\mathbf{v}}_p = qp\mu_p \mathbf{E}$$

$$\sigma_n = qn\mu_n, \quad \sigma_p = qp\mu_p$$

## 5. Boltzmann Statistics (1)

### Boltzmann law of exponential atmosphere

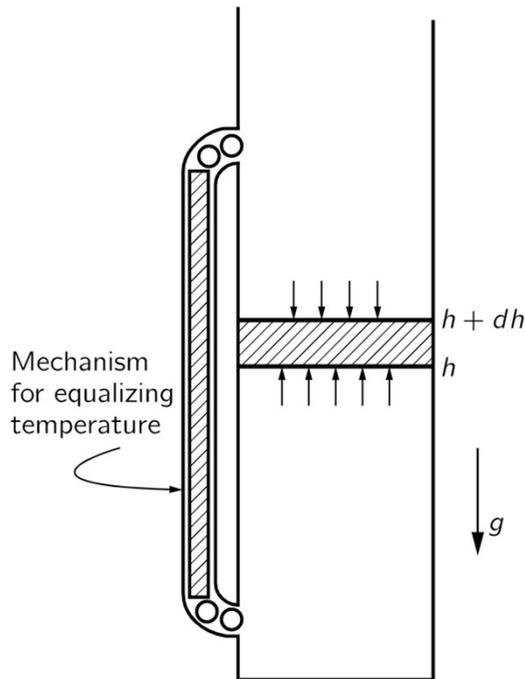
If the temperature is the same at all heights, and  $N$  is the total number of molecules in a volume  $V$  of gas at pressure  $P$ , then we know  $PV=Nk_B T$ . (Density  $n=N/V$ )

The force from below must exceed the force from above by the weight of gas in the section between  $h$  and  $h+dh$

$$P(h + dh) - P(h) = dP = k_B T dn = -mgndh$$

$$\frac{dn}{dh} = \frac{-mg}{k_B T} n$$

$$n = n_0 \exp\left(\frac{-mgh}{k_B T}\right) = n_0 \exp\left(\frac{-P_E}{k_B T}\right)$$



If the energies of the set of molecular states are called,  $E_0, E_1, E_2, \dots$ , then in thermal equilibrium, the probability of finding a molecule in the particular state of having energy  $E_i$  is proportional to  $\exp(-E_i/k_B T)$ .

## 5. Boltzmann Statistics (2)

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### thermal equilibrium

Two physical systems are in thermal equilibrium if there is no net flow of thermal energy between them when they are connected by a path permeable to heat. A system is said to be in thermal equilibrium with itself if the temperature within the system is spatially uniform and temporally constant.

### thermal equilibrium in semiconductor

Electrons and holes in semiconductor have a unified Fermi level. The generation and recombination processes are statistically balanced. External bias and light illumination will break the thermal equilibrium and thus electrons and holes have different local Fermi levels under the nonequilibrium state.

## 5. Boltzmann Statistics (3)

*When does the Boltzmann statistics break down?*

very low temperature or very high doping scenario !

### Carrier concentration in thermal equilibrium

$$n_0 = N_c \exp\left(-\frac{E_c - E_F}{k_B T}\right)$$

$$p_0 = N_v \exp\left(\frac{E_v - E_F}{k_B T}\right)$$

$$n_0 p_0 = N_c N_v \exp\left(-\frac{E_g}{k_B T}\right) = n_i^2 \quad N_c = 2 \left(\frac{m_n^* k_B T}{2\pi\hbar^2}\right)^{3/2} \quad N_v = 2 \left(\frac{m_p^* k_B T}{2\pi\hbar^2}\right)^{3/2}$$

$E_F$ : unified Fermi level for both electrons and holes

$N_c$ : effective density of states for conduction band

$N_v$ : effective density of states for valance band

$n_0$ : electron density in conduction band

$p_0$ : hole density in valance band

$n_i$ : intrinsic carrier density (without doping and defects)

## 5. Boltzmann Statistics (4)

### Carrier concentration in thermal non-equilibrium

$$n = N_c \exp\left(-\frac{E_c - E_{Fn}}{k_B T}\right)$$

$$p = N_v \exp\left(\frac{E_v - E_{Fp}}{k_B T}\right)$$

$$np = n_0 p_0 \exp\left(\frac{E_{Fn} - E_{Fp}}{k_B T}\right) = n_i^2 \exp\left(\frac{E_{Fn} - E_{Fp}}{k_B T}\right)$$

$E_{Fn}$ : quasi-Fermi level of electrons

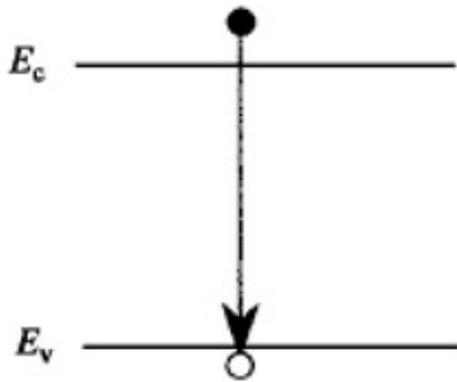
$E_{Fp}$ : quasi-Fermi level of holes

1. Fast thermal induced transitions at conduction band or valence band (but not in between) result in the local equilibrium of carrier concentration at each band.
2. Larger  $E_{Fn} - E_{Fp}$ , which suggests larger external bias voltage, more nonequilibrium carriers ( $\Delta n = n - n_0$ ,  $\Delta p = p - p_0$ ) are generated.

## 6. Recombination (1)

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### Band to band (bimolecular) recombination



The net recombination rate

$$R = B(np - n_0p_0)$$

$B$ : bimolecular recombination coefficient

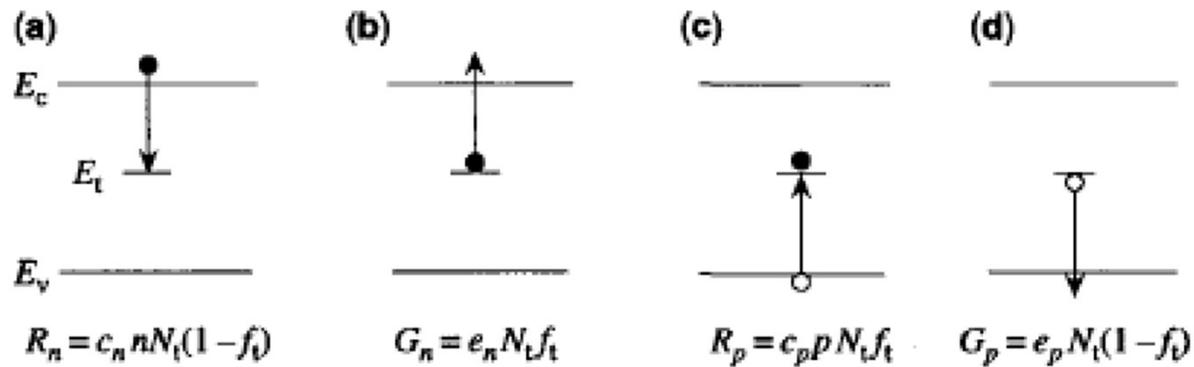
At thermal equilibrium,  $R=0$ , generation (absorption) and recombination (emission) are statically balanced. It is the essential physics of black-body radiation.

At thermal nonequilibrium,  $n \gg n_0$ ,  $p \gg p_0$ ,  $R \approx Bnp$

Radiative recombination is the band-to-band recombination.

## 6. Recombination (2)

### Nonradiative Shockley-Read-Hall (SRH) recombination



(a) electron capture; (b) electron emission; (c) hole capture; (d) hole emission

electron capture: The recombination rate for electrons is proportional to the density of electrons  $n$ , and the concentration of the traps  $N_t$ , multiplied by the probability that the trap is empty ( $1 - f_t$ ),  $R_n = c_n n N_t (1 - f_t)$ , where  $c_n$  is the capture coefficient for the electrons.

electron emission: The generation rate of the electrons due to this process is  $G_n = e_n N_t f_t$ , where  $e_n$  is the emission coefficient and  $N_t f_t$  is the density of the traps that are occupied by the electrons.

hole capture and hole emission:  $R_p = c_p p N_t f_t$  and  $G_p = e_p N_t (1 - f_t)$

## 6. Recombination (3)

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At thermal equilibrium, we have the detailed balancing  $G_n = R_n$  and  $G_p = R_p$

$$\frac{e_n}{c_n} = n_1, \quad \frac{e_p}{c_p} = p_1, \quad n_1 p_1 = n_0 p_0 = n_i^2$$

At thermal nonequilibrium, we have stable condition  $R_n - G_n = R_p - G_p$

$$R = R_n - G_n = R_p - G_p = \frac{np - n_i^2}{\tau_p(n + n_1) + \tau_n(p + p_1)}$$

$$\tau_p = \frac{1}{c_p N_t}, \quad \tau_n = \frac{1}{c_n N_t}$$

## 6. Recombination (4)

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For minority electron,  $p \gg n$

$$R_n - G_n \approx \frac{n}{\tau_n}$$

For minority hole,  $n \gg p$

$$R_p - G_p \approx \frac{p}{\tau_p}$$

SRH recombination can be seen as the monomolecular recombination.

## 6. Recombination (5)

*What is the application of impact ionization?*

Nonradiative Auger recombination **Avalanche diode for single photon detection !**

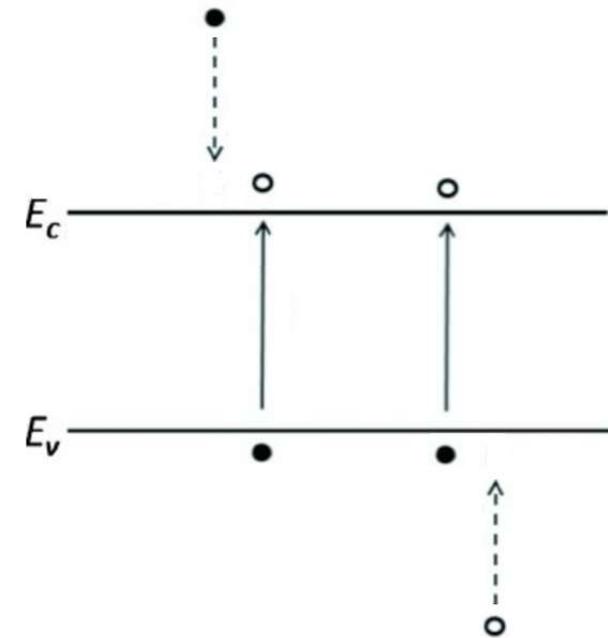
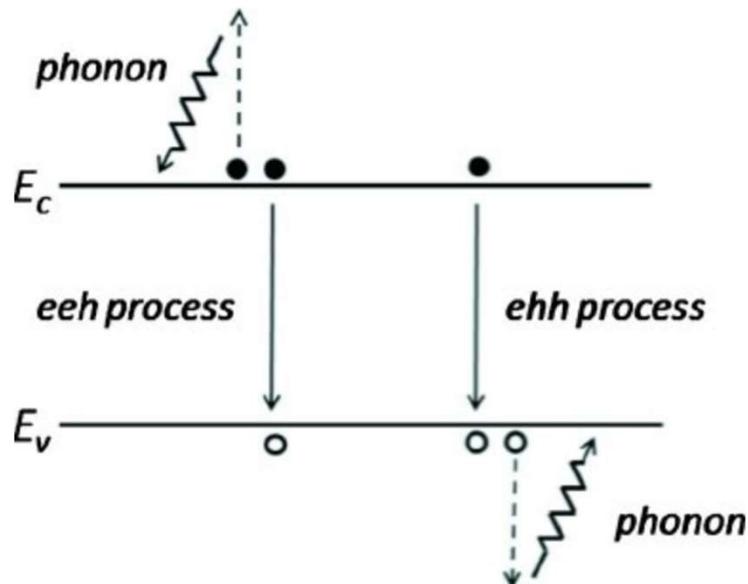


Fig. 1. band-to-band Auger recombination  
left: n-type; right: p-type

Fig. 2. band-to-band Auger generation  
(impact ionization): reverse process of Fig. 1

Band-to-band Auger recombination: An electron in the conduction band recombines with a hole in the valence band and releases its energy to a nearby electron or hole. The excited electron or hole will always relax and produce heat (phonon energy).

Impact ionization: one highly-energetic electron (hole) from the conduction (valance) band transfers its energy to a valance-band electron for generating one e-h pair.

## 6. Recombination (6)

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For Auger recombination,

$$R_{ee} = \gamma_e n^2 p, \quad R_{hh} = \gamma_h np^2$$
$$R_{ee0} = \gamma_e n_0^2 p_0, \quad R_{hh0} = \gamma_h n_0 p_0^2$$

For Auger generation,

$$G_{ee} = g_e n, \quad G_{hh} = g_h p$$
$$G_{ee0} = g_e n_0, \quad G_{hh0} = g_h p_0$$

At thermal equilibrium,

$$G_{ee0} = R_{ee0}, \quad G_{hh0} = R_{hh0}$$

At thermal nonequilibrium,

$$R = (R_{ee} + R_{hh}) - (G_{ee} + G_{hh})$$
$$= (\gamma_e n + \gamma_h p)(np - n_i^2)$$

## 6. Recombination (7)

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### More about recombination

1. Recombination can occur in bulk or at surface.
2. Recombination can be direct (through valance band and conduction band) or indirect (through recombination centers).
3. Energy released from recombination will convert to photon energy, phonon energy, or excite other carriers.
4. Non-radiative recombination is always the dominant electric loss mechanism for state-of-the-art optoelectronic devices.

# 7. Drift-Diffusion Equations (1)

thermal  
nonequilibrium



$$n = n_i \exp\left(-\frac{E_i - E_{Fn}}{k_B T}\right) = n_i \exp\left(q \frac{(\phi - \phi_n)}{k_B T}\right)$$

$$p = n_i \exp\left(\frac{E_i - E_{Fp}}{k_B T}\right) = n_i \exp\left(-q \frac{(\phi - \phi_p)}{k_B T}\right)$$

quasi-Fermi  
(chemical) potential



$$\phi_n = \phi - \frac{k_B T}{q} \log\left(\frac{n}{n_i}\right)$$

$$\phi_p = \phi + \frac{k_B T}{q} \log\left(\frac{p}{n_i}\right)$$

$$\nabla n_i = 0$$

electron current  
hole current



$$J_n = -q\mu_n n \nabla \phi_n = q\mu_n n \mathbf{E} + qD_n \nabla n$$

$$J_p = -q\mu_p p \nabla \phi_p = q\mu_p p \mathbf{E} - qD_p \nabla p$$

$$\mathbf{E} = -\nabla \phi$$

Einstein relation



$$D_n = \mu_n \frac{k_B T}{q}, \quad D_p = \mu_p \frac{k_B T}{q}$$

## 7. Drift-Diffusion Equations (2)

Semiconductor equations (unknowns  $n$ ,  $p$ ,  $\varphi$ )

$$\nabla \cdot (\epsilon \nabla \varphi) = -q(p - n + N_D^+ - N_A^-)$$

**Poisson**

$N_D, N_A$ : doping density  
 $\epsilon$ : dielectric constant (DC)

$$\begin{cases} \frac{dp}{dt} = -\frac{\nabla \cdot \mathbf{J}_p}{q} + G - R \\ \frac{dn}{dt} = \frac{\nabla \cdot \mathbf{J}_n}{q} + G - R \end{cases}$$

**Current continuity**

$R$ : net recombination rate  
 $G$ : generation rate by light  
 $\mathbf{J}_n$ : electron current  
 $\mathbf{J}_p$ : hole current

$$\begin{cases} \mathbf{J}_n = q\mu_n n \mathbf{E}_n + qD_n \nabla n \\ \mathbf{J}_p = q\mu_p p \mathbf{E}_p - qD_p \nabla p \end{cases}$$

**Drift-diffusion**

$D_n, D_p$ : diffusion coefficients  
 $\mu_n, \mu_p$ : mobility  
 $\mathbf{E}_n, \mathbf{E}_p$ : electrostatic fields

$$\mathbf{E}_n = -\nabla \psi_n \quad \psi_n = \varphi + \chi / q + (k_B T / q) \ln(N_c)$$

$$\mathbf{E}_p = -\nabla \psi_p \quad \psi_p = \varphi + \chi / q + E_g / q - (k_B T / q) \ln(N_v)$$

**E-field is complex!**

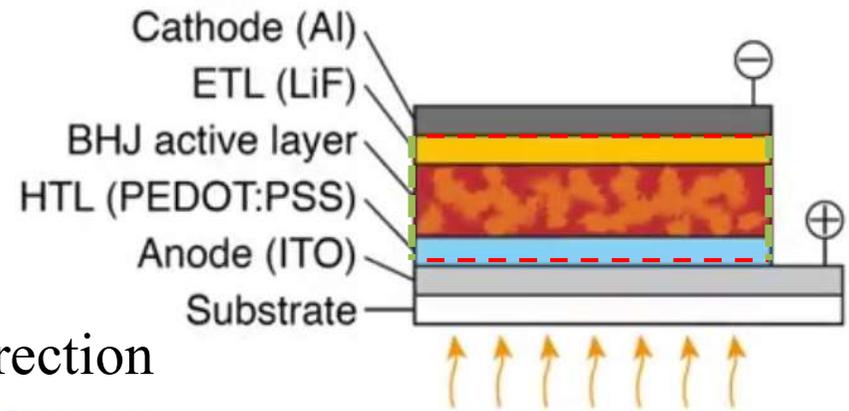
$\chi$ : electron affinity,  $E_g$ : bandgap  
 $N_c, N_v$ : effective DOS

# 7. Drift-Diffusion Equations (3) — Boundary Conditions (Optional)

Non-electrode boundaries (green line)

$$\frac{\partial \varphi}{\partial \hat{n}} = 0, \quad \frac{\partial n}{\partial \hat{n}} = 0, \quad \frac{\partial p}{\partial \hat{n}} = 0$$

normal direction



Electrode boundaries (red line)

$$\varphi_a = V_a - \frac{W_a}{q}, \quad \varphi_c = V_c - \frac{W_c}{q}$$

$V_a, V_c$ : external bias for anode and cathode  
 $W_a, W_c$ : work functions for anode and cathode

anode

$$J_{na} = qS_{na}(n - n_0), \quad J_{pa} = qS_{pa}(p - p_0)$$

$$p_0 = N_v \exp\left(\frac{-\Phi_p}{k_B T}\right), \quad n_0 = N_c \exp\left(\frac{-E_g + \Phi_p}{k_B T}\right)$$

$S_{na}$ : surface recombination velocity for electrons  
 $S_{pa}$ : surface recombination velocity for holes  
 $\Phi_p$ : injection barrier for holes

cathode

$$J_{nc} = qS_{nc}(n - n_0), \quad J_{pc} = qS_{pc}(p - p_0)$$

$$n_0 = N_c \exp\left(\frac{-\Phi_n}{k_B T}\right), \quad p_0 = N_v \exp\left(\frac{-E_g + \Phi_n}{k_B T}\right)$$

$S_{nc}$ : surface recombination velocity for electrons  
 $S_{pc}$ : surface recombination velocity for holes  
 $\Phi_n$ : injection barrier for electrons