3 Absorção Interbandas

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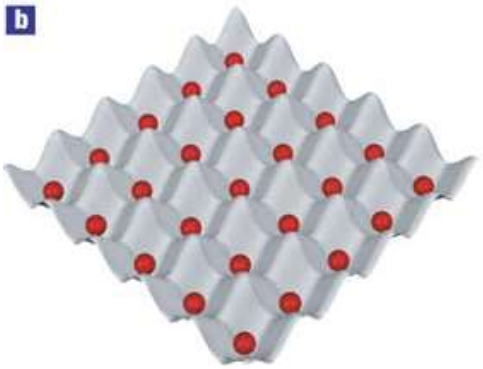
em semicondutores de gap direto

3.4 Absorção na borda da banda
em semicondutores de gap indireto

3 Absorção Interbandas

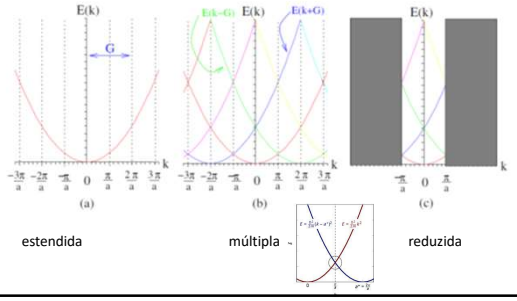
3.0 Teoria de Bandas (Apêndice D)



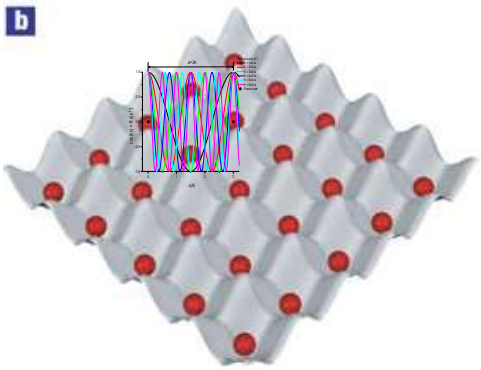
dispersão $E(\vec{k})$

$$E_k = \frac{h^2 k^2}{2m}$$

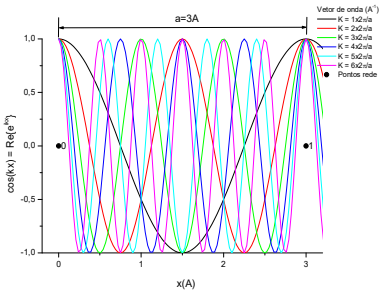
elétron livre



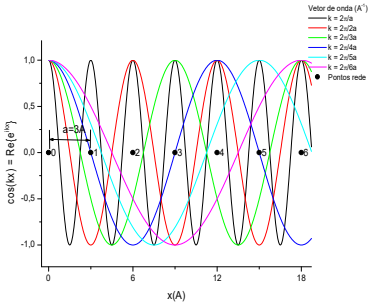
estendida múltipla reduzida



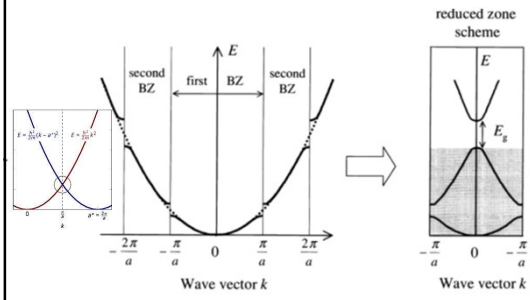
cos(Kx)

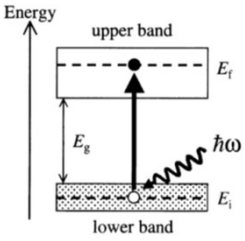


cos(kx)



Modelo Elétrons Quase Livres



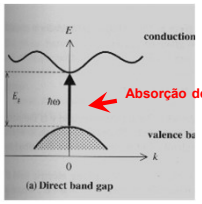


conservação da energia

$$E_f - E_i = \hbar\omega$$

criação de par **elétron - buraco**

3 Absorção Interbandas



Absorção de fóton

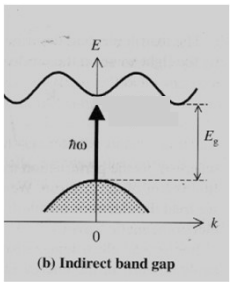
Transições diretas

conservação do momento cristalino:
$\hbar\vec{k}$ - momento linear (elétron livre/fóton)

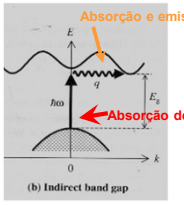
$$\hbar\vec{k_i} - \hbar\vec{k_f} = \hbar\vec{k_{fóton}} \approx \vec{0}$$

⇒ Transições verticais

$$\Rightarrow \vec{k_i} = \vec{k_f}$$



3.1 Transições interbandas



Transições *in*diretas

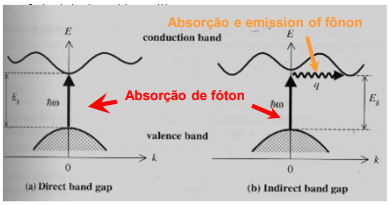
conservação do momento cristalino:

$$\hbar\vec{k}_i - \hbar\vec{k}_f = \hbar\vec{q}_{fônon} \gg \vec{0}$$

⇒ Transições oblíquas

⇒ *necessitam* $\boldsymbol{q}_{fônon}$

3.1 Transições interbandas



3.2 Taxa de transição para absorção direta

coeficiente de absorção $\alpha \propto W_{i->f}$ taxa de transição

$$W_{i\to f} = \frac{2\pi}{h}|M|^2 g(h\omega).$$ **(Regra de Ouro de Fermi)**

Onde
- Elemento de matriz ***M,***
- Densidade de estados $g(\hbar\omega)$.

$$M = \langle f|H'|i\rangle = \int \psi_f^*(\vec{r})H'\psi_i(\vec{r})d^3\vec{r}$$

$$H' = -\vec{p}_e\vec{E}_{foton}$$

Momento de dipolo elétrico $\vec{p}_e = -e\vec{r}$ x campo $\vec{E}_{foton}$

Elemento de Matriz

$$M$$

Hamiltoniana de perturbação

$$H'(\vec{r}) = e\vec{E}_o.\vec{r}.e^{i\vec{k}.\vec{r}}$$

$$\psi_i(\vec{r}) = \frac{1}{\sqrt{V}}u_i(\vec{r})e^{i\vec{k}_i.\vec{r}}$$

$$\psi_f(\vec{r}) = \frac{1}{\sqrt{V}}u_f(\vec{r})e^{i\vec{k}_f.\vec{r}}$$

$$M = \frac{1}{V}\int_{cristal} u_f^*(\vec{r})e^{-i\vec{k}_f.\vec{r}}.(e\vec{E}_o\, e^{i\vec{k}.\vec{r}}.\vec{r})\,.u_i(\vec{r})e^{i\vec{k}_i.\vec{r}}d^3\vec{r}$$

Se o fator de fase na integral não for zero, as diferentes células unitárias estarão fora de fase, e a integral dará zero.

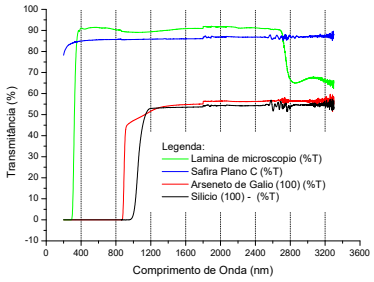
$$M \neq 0$$
$$\Rightarrow$$
$$\hbar\vec{k}_f - \hbar\vec{k}_i = \hbar\vec{k} \quad \textbf{(conservação de momento)}$$

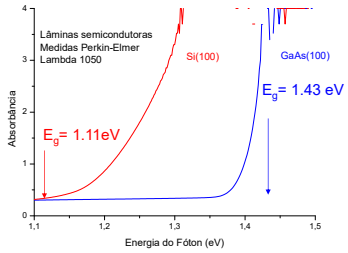
$$\hbar\vec{k} \cong \mathbf{0}$$
$$\hbar\vec{k}_f \cong \hbar\vec{k}_i \quad \textbf{(transições verticais)}$$

Bloch => u_i e u_f - periodicidade da rede

$$|M| \propto \int_{célula\ unit} u_f^*(\vec{r})xu_i(\vec{r})d^3\vec{r}$$

X=> onda polarizada ao longo do eixo x.



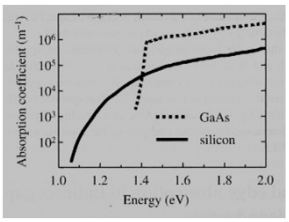


3.4 Absorção nas proximidades das bandas – gap direto x indireto

Coeficiente de absorção :

$$E_f = E_i + \hbar\omega \pm \hbar\Omega,$$
$$\hbar\vec{k}_f = \hbar\vec{k}_i \pm \hbar\vec{q}.$$

$$For \quad indirect, \quad \alpha^i(\hbar\omega) \propto (\hbar\omega - E_g \mp \hbar\Omega)^2.$$
$$For \quad direct, \quad \alpha^d(\hbar\omega) \propto (\hbar\omega - E_g)^{\frac{1}{2}}.$$



Densidade de Estados

$$g(\hbar\omega)$$

densidade conjunta de estados eletrônicos associada com a energia de fóton $\hbar\omega$

Densidade de estados

- Átomos isolados: níveis de energia discretos
- Sólidos: número grande de níveis de energia em um determinado intervalo (densidade de estados).

$$g(E)dE = núm\ de\ estados\ entre\ E\ e\ E + dE$$

$$g(E)dE = 2g(k)dk$$

spin

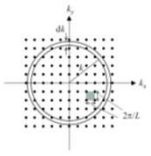
$$g(E) = \frac{2g(k)}{dE/dk} \qquad \text{E.2}$$

$$g(k)dk = \frac{1}{(2\pi)^3}.4\pi k^2 dk \;\therefore\; g(k) = \frac{k^2}{2\pi^2}$$

Número de estados por unidade de volume no espaço k.

De onde se pode deduzir tb que (3.a):

$$(\Delta k)^3 = \frac{(2\pi)^3}{L_x L_y L_z}$$



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

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m^*}$$

$$E.2 \;\rightarrow\; g(E) = \frac{2 \times \frac{k^2}{2\pi^2}}{\frac{\hbar^2 k}{m^*}} = \frac{m^*}{\pi^2 \hbar^2 k} = \frac{m^*}{\pi^2 \hbar^2}\sqrt{\frac{2m^* E}{\hbar^2}} = \frac{1}{2\pi}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E}$$

$$g(k)dk = \frac{1}{2\pi^3}4\pi k^2 dk$$

$$g(k) = \frac{k^2}{2\pi^2}$$

$$g(E) = \frac{2g(k)}{dE/dk}$$

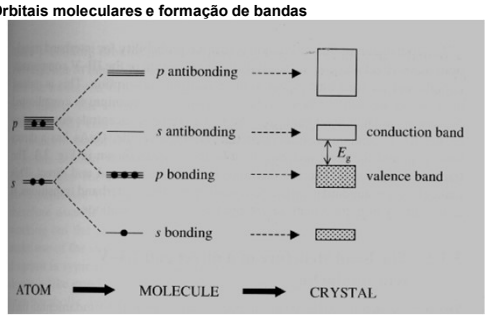
Gradiente da curva de dispersão E-k

$$g(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)E^{1/2}$$

Continuação, Cap.3....

3 Absorção Interbandas

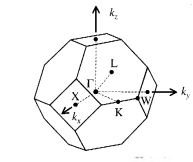
Orbitais moleculares e formação de bandas

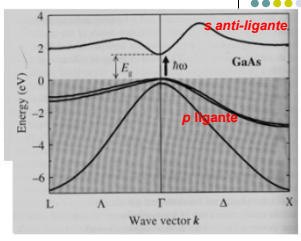


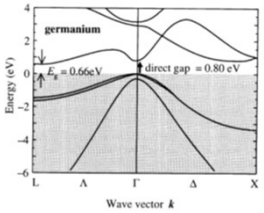
Ge: $4s^2 4p^2$ → $4sp^3$ anti-lig. (s dominante) → banda de condução

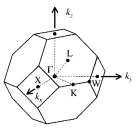
$4sp^3$ ligantes (p dominante) → banda de valência

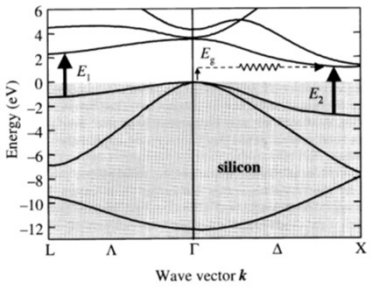
Estrutura de bandas de um semicondutor III-V de gap direto











3.3 Absorção fundamental em semicondutores de gap direto

Regras de seleção (transições de dipolo elétrico):

(1) estados inicial => paridade diferente
(2) Δj = -1, 0 or +1. (momento angular total => muda uma unidade)
(3) $\Delta l = \pm 1$. (momento angular orbital => muda uma unidade)
(4) $\Delta m_s = 0$. (números quânticos de spin => não muda).

Transições permitidas de dipolo elétrico:

altas taxas de transição, tempos radiativos curtos (10^{-9}– 10^{-8} s)– **fluorescência.**

3.3 Absorção fundamental em semicondutores de gap direto

Regras de seleção (transições de dipolo elétrico):

(1) estados inicial => paridade diferente
(2) Δj = -1, 0 or +1. (momento angular total => muda uma unidade)
(3) $\Delta l = \pm 1$. (momento angular orbital => muda uma unidade)
(4) $\Delta m_s = 0$. (números quânticos de spin => não muda).

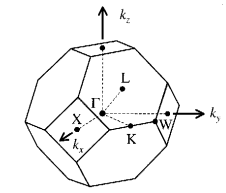
Transições proibidas de dipolo elétrico:

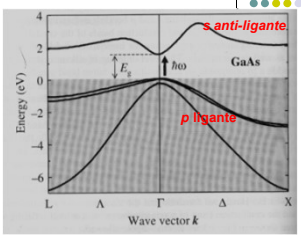
Dipolo magnético ou quadrupolo elétrico:

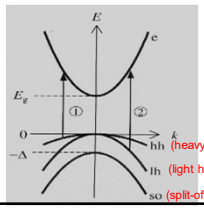
taxas de transição menores e tempos radiativos mais longos (10^{-6} s para acima) – a emissão lenta das transições proibidas de dipolo elétrico são chamadas de **fosforescência.**

3.3 Absorção no limite das bandas em semicondutores de gap direto

Estrutura de bandas de um semicondutor III-V de gap direto





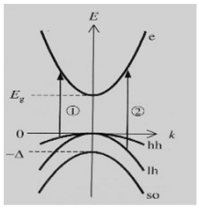


Modelo de 4 bandas

Massas efetivas

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

Relação ***E— k*** nas proximidades de k ~ 0



Elétron

$$E_e(k) = E_g + \frac{\hbar^2 k^2}{2m_e^*}$$

Buraco

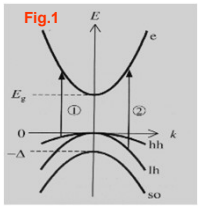
$$E_{hh}(k) = -\frac{\hbar^2 k^2}{2m_{hh}^*}$$

$$E_{lh}(k) = -\frac{\hbar^2 k^2}{2m_{lh}^*}$$

$$E_{so}(k) = -\Delta - \frac{\hbar^2 k^2}{2m_{so}^*}$$

Densidade conjunta de estados

Fig.1



$$g(E) = \frac{2g(k)}{dE/dk} \qquad g(k) = \frac{k^2}{2\pi^2}$$

Conservação de energia em transições envolvendo formação de buracos leves ou buracos pesados

$$\hbar\omega = E_C(k) - E_V(k)$$
$$= E_g + \frac{\hbar^2 k^2}{2m_e^*} + \frac{\hbar^2 k^2}{2m_{hh(lh)}^*}$$
$$= E_g + \frac{\hbar^2 k^2}{2\mu}$$

$$onde \quad \frac{1}{\mu} = \frac{1}{m_e^*} + \frac{1}{m_{hh(lh)}^*}$$

Semicondutor de gap direto

$$g(\hbar\omega) = 0 \qquad para \quad \hbar\omega < E_g,$$
$$g(\hbar\omega) = \frac{1}{2\pi^2}\left(\frac{2\mu}{\hbar}\right)^{\frac{3}{2}}(\hbar\omega - E_g)^{\frac{1}{2}} \qquad para \quad \hbar\omega \geq E_g.$$

3.3.4 The frequency dependence of the band edge absorption

$$\alpha(\hbar\omega) \propto W_{i\to f} = \frac{2\pi}{\hbar}|M|^2 g(\hbar\omega).$$

$$g(\hbar\omega) = 0 \qquad for \quad \hbar\omega < E_g,$$

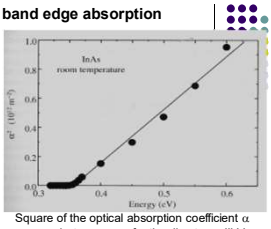
$$g(\hbar\omega) = \frac{1}{2\pi^2}\left(\frac{2\mu}{\hbar}\right)^{\frac{3}{2}}(\hbar\omega - E_g)^{\frac{1}{2}} \qquad for \quad \hbar\omega \geq E_g.$$

$$For \quad \hbar\omega < E_g, \quad \alpha(\hbar\omega) = 0.$$

$$For \quad \hbar\omega > E_g, \quad \alpha(\hbar\omega) \propto (\hbar\omega - E_g)^{\frac{1}{2}}.$$

Frequency dependence approximately obeyed

- The coulomb attraction of excitons neglected;
- Impurity or defect states within gap neglected;
- The parabolic band approximation only valid near k = 0.



Square of the optical absorption coefficient α versus photon energy for the direct gap III-V semiconductor InAs at room temperature. The band gap can be deduced to be 0.35 eV by extrapolating the absorption to zero.

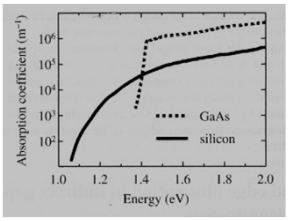
3.4 Band edge absorption in indirect gap semiconductor

Absorption coefficient :

$$E_f = E_i + \hbar\omega \pm \hbar\Omega,$$
$$\hbar\vec{k}_f = \hbar\vec{k}_i \pm \hbar\vec{q}.$$

$$For \quad indirect, \quad \alpha^i(\hbar\omega) \propto (\hbar\omega - E_g \mp \hbar\Omega)^2.$$

$$For \quad direct, \quad \alpha^d(\hbar\omega) \propto (\hbar\omega - E_g)^{\frac{1}{2}}.$$



$$\alpha^2 \propto (\hbar\omega - E_g^{dir}), \quad where \quad E_g^{dir} = 0.8eV$$

3.3.5 Efeito Franz-Keldysh

Dois efeitos principais devidos à aplicação de um campo elétrico externo *E*:

$$para \quad \hbar\omega < E_g, \quad \alpha(\hbar\omega) \propto \left(-\frac{4\sqrt{2m_e^*}}{3|e|\hbar E}(E_g - \hbar\omega)^{3/2} \right)$$

$$para \quad \hbar\omega > E_g, \quad \alpha(\hbar\omega) \quad \rightarrow oscilações$$

Consequências do efeito F-K

Efeito eletro-óptico:

O campo elétrico modula as constants ópticas (n,κ).

Eletro-refletância:

A refletividade pode mudar devido a modulações nas constants ópticas (n,κ).

3.3.4 The frequency dependence of the band edge absorption

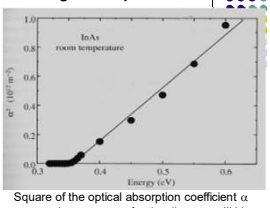
$$\alpha(\hbar\omega) \propto W_{i\to f} = \frac{2\pi}{\hbar}|M|^2 g(\hbar\omega).$$

$$g(\hbar\omega) = 0 \qquad for \ \hbar\omega < E_g,$$

$$g(\hbar\omega) = \frac{1}{2\pi^2}\left(\frac{2\mu}{\hbar}\right)^{\frac{3}{2}}(\hbar\omega - E_g)^{\frac{1}{2}} \qquad for \ \hbar\omega \geq E_g.$$

$$For \ \hbar\omega < E_g, \ \alpha(\hbar\omega) = 0.$$

$$For \ \hbar\omega > E_g, \ \alpha(\hbar\omega) \propto (\hbar\omega - E_g)^{\frac{1}{2}}.$$



Square of the optical absorption coefficient α versus photon energy for the direct gap III-V semiconductor InAs at room temperature. The band gap can be deduced to be 0.35 eV by extrapolating the absorption to zero.

Frequency dependence approximately obeyed

- The coulomb attraction of excitons neglected;
- Impurity or defect states within gap neglected;
- The parabolic band approximation only valid near k = 0.

3.3.5 The Franz-Keldysh effect

Two main effects on band edge absorption by application of an external electric field *E*:

$$For \ \hbar\omega < E_g, \ \alpha(\hbar\omega) \propto \left(-\frac{4\sqrt{2m_e^*}}{3|e|\hbar E}(E_g - \hbar\omega)^{3/2} \right)$$

$$For \ \hbar\omega > E_g, \ \alpha(\hbar\omega) \ oscillations$$

Electro-optic effect:

The electric field modulated optical constants (n,κ). (K-K relationship).

Electroreflectance:

The reflectivity can be changed due to modulated optical constants (n,κ).

3.3.6 Band edge absorption in a magnetic field

The electrons in magnetic field:

$$\omega_c = \frac{eB}{m_0} \qquad \text{(cyclotron frequency)}$$

The quantized energy (**Landau levels**):

$$E_n = (n+\frac{1}{2})\hbar\omega_C \qquad (n = 0,1,2\cdots)$$

The energies electrons and holes within the bands are given by:

$$E_n(k_z) = (n+\frac{1}{2})\frac{ehB_z}{m^*} + \frac{\hbar^2 k_z^2}{2m^*}$$

Quantized motion in the (x, y) plane, free motion in the z direction. *E*=0 at the top of the valence band:

$$E_n^e(k_z) = E_g + (n+\frac{1}{2})\frac{ehB_z}{m_e^*} + \frac{\hbar^2 k_z^2}{2m_e^*}$$

$$E_n^h(k_z) = -(n'+\frac{1}{2})\frac{ehB_z}{m_h^*} - \frac{\hbar^2 k'^2_z}{2m_h^*}$$

The interband transition creates an electron in the conduction band and a hole in valence band

Selection rule: $n = n', \quad k_z = k'_z$. (the momentum is negligible)

The transition energy:

$$\hbar\omega = E_n^e(k_z) - E_n^h(k_z)$$

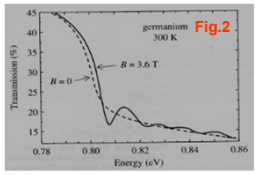
$$= E_g + (n+\frac{1}{2})\frac{ehB_z}{\mu} + \frac{\hbar^2 k_z^2}{2\mu}$$

The absorption spectrum with k_z=0 given by:

$$\hbar\omega = E_g + (n+\frac{1}{2})\frac{ehB_z}{\mu}; \qquad n = 0,1,2\cdots.$$

Two consequences:

1. **The absorption edge shifts by $heB_z/2\mu$;**
2. **Equally spaced peaks in the spectrum.**



Transmission spectrum of germanium of germanium for B=0 and B=3.6T at 300 K. The electron effective mass can be determined from the energies of minima.

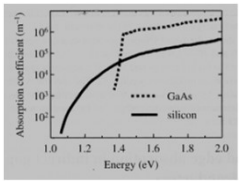
3.4 Band edge absorption in indirect gap semiconductor

The indirect transition involve both photons and phonons ($\hbar\omega$, $\hbar\mathbf{q}$):

$$E_f = E_i + \hbar\omega \pm \hbar\Omega,$$

$$\hbar\vec{k}_f = \hbar\vec{k}_i \pm \hbar\vec{q}.$$

This is a second-order process, the transition rate is much smaller than for direct absorption.



Comparison of the absorption coefficient of GaAs and Silicon near their band edges. GaAs has a direct band gap at 1.42 eV, while silicon has an indirect gap at 1.12 eV. The absorption rises much faster with frequency in a direct gap material, and exceeds the indirect material.

Absorption coefficient of indirect band gap:

$$For \ indirect, \ \alpha^i(\hbar\omega) \propto (\hbar\omega - E_g \mp \hbar\Omega)^2.$$

$$For \ direct, \quad \alpha^d(\hbar\omega) \propto (\hbar\omega - E_g)^{\frac{1}{2}}.$$

The differences:

1. Threshold;
2. Frequency dependence.

The differences provide a way to determine whether the band gap is direct or not.

(接下页) As *T* decrease, phonons decrease gradually. At very low *T*, no phonons excited with enough energy. Thus at the lowest *T*, the indirect absorption edge is determined by phonon emission rather than phonon absorption;

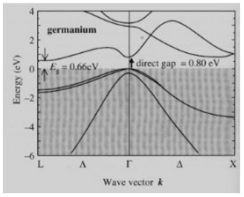
5. The direct absorption dominates over the indirect processes once $\hbar\omega$ > 0,8eV,

$$\alpha^2 \propto (\hbar\omega - E_g^{dir}), \quad where \quad E_g^{dir} = 0.8eV$$

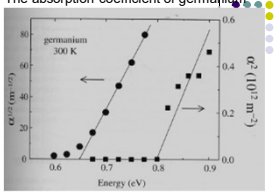
is the band gap for the transition at the Γ

3.4 Band edge absorption in indirect gap semiconductor

Band structure of germanium.



The absorption coefficient of germanium



1. The lowest conduction band minimum occurs at the L point (**k**=π/a(1,1,1), not at Γ (*k*=0);
2. Indirect gap=0.66eV, direct gap (Γ)= 0.8eV;

Table 3.1 Phonon energies for germanium at the L point where $\mathbf{q} = \frac{\pi}{a}(1,1,1)$, a being the unit cell size. After [6].

Mode	$\hbar\Omega$ (eV)
Longitudinal acoustic (LA)	0.027
Transverse acoustic (TA)	0.008
Longitudinal optic (LO)	0.030
Transverse optic (TO)	0.035

1. $\sqrt{\alpha}$ vs $h\omega$ close to the band gap at 0.66 eV ;
2. The straight line extrapolates back to 0.65 eV, which indicates that a phonon(TA)of energy ~ 0.01 eV has been absorbed and **q** (phonon) **= k(**electron**)** at L-point of the Brillouin zone;
3. A tail down to 0.6 eV, this is caused by absorption of the higher frequency and also multi-phonons absorption;
4. The temperature dependence of the absorption edge:

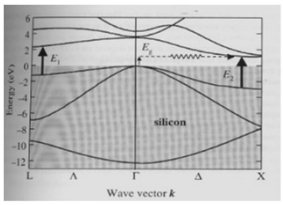
$$f_{BE}(E) = \frac{1}{\exp(E/k_BT) - 1}$$

Bose-Einstein Formula

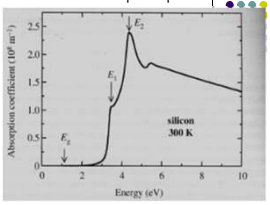
(接上页)

3.5 Interband absorption above the band edge

The band structure of silicon



Th e interband absorption spectrum of silicon



E_g is indirect and occurs at 1.1 eV;

E_1 and E_2 are the separation of the bands at the L and X points, where the conduction and valence are approximately parallel along the (111) and (100).

E_1 = 3.5 eV is the minimum direct separation, and corresponds to the sharp increase in absorption at E_1, and E_2 correspond to the absorption maximum at 4.3 eV. Absorption at these energies is very high due to the **Van Hove singularities** in the joint density of states (band are parallel. E for direct transition does not depend on k, dE/dk =0, g(E) diverges (critical point)

1. The optical properties at the band edge determine the emission spectra;

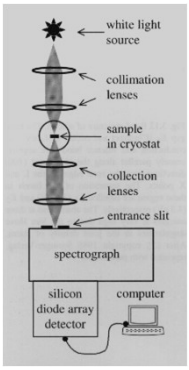
   For indirect, $\alpha^i(\hbar\omega) \propto (\hbar\omega - E_g \mp \hbar\Omega)^2$.

   For direct, $\alpha^d(\hbar\omega) \propto (\hbar\omega - E_g)^{\frac{1}{2}}$.

2. The spectrum can be worked out by *dE/dk* from the full band structure.

$$g(E) = \frac{2g(k)}{dE/dk}$$

3.6 Measurement of absorption spectra



The measurement of absorption coefficient:

1. Measure transmission coefficient;

$$I(z) = I_0 e^{-\alpha z}$$

2. Measure reflectivity spectra R ($h\omega$)

$$R = \left|\frac{\tilde{n}-1}{\tilde{n}+1}\right|^2 = \frac{(n-1)^2+\kappa^2}{(n+1)^2+\kappa^2}.$$

$$\alpha = \frac{2\cdot\kappa\cdot\omega}{c} = \frac{4\pi\cdot\kappa}{\lambda}$$

Self-consistent fitting of the reflectivity spectra using the Kramers-Kronig formula.

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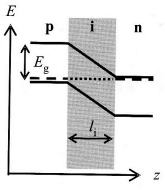
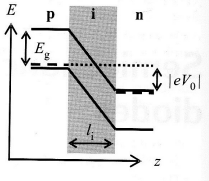


(a) $V_0 = 0$

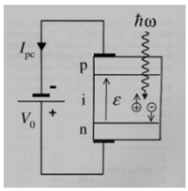


(b) Reverse bias V_0 applied

3.7 Semiconductor photodectors

The operating principles:

Light with photon energy greater than the band gap is absorbed in the semiconductor, and this create free electrons in the conduction band and free hole in the valence band. The presence of the light can therefore be detected either by measuring a change in resistance of the sample or by measuring an electrical current in an external circuit.



The p-i-n photodiode is operated in reverse bias with a positive voltage V_o applied to the n-region. This generates of a strong DC electric field E across the i-region. Absorption of photons in the i-region creates free electron – and hole ⊕ that are attracted to the n-region and p-regions respectively then flow into the circuit by the field, generating the **photocurrent I_{pc}**

3.7.1 Photodiodes

$$I(z) = I_0 e^{-\alpha z}$$

The fraction of light absorbed in a length l :

$$I^{ab} = I_0(1-e^{-\alpha(\omega)l})$$

Photocurrent I_{pc}

$$I_{pc} = e\eta\frac{P}{\hbar\omega}(1-e^{-\alpha(\omega)l}).$$

η: quantum efficiency,

$P/\hbar\omega$: the flux of photons per unit time

$$\therefore responsivity = \frac{I_{pc}}{P} = \frac{\eta e}{\hbar\omega}(1-e^{-\alpha(\omega)l}) \quad (A/W)$$

If $\eta \approx (1-e^{-\alpha l}) \approx 1$

$$responsivity \approx \frac{I_{pc}}{P} \approx \frac{e}{\hbar\omega}.$$

3.7 Semiconductor photdectors

Table Common semiconductor photodetectors. E_g: band gap, T: operating temperature, λ_{max}: maximum wavelength that can be detected. The band gap of alloy semiconductors such as InGaAs and HgCdTe can be varied by altering the composition. The compositions listed here correspond to typical values used in detectors.

Semiconductor	E_g (eV)	T (K)	λ_{max} (μm)
Si	1.1	300	1.1
$In_{0.53}Ga_{0.47}As$	0.75	300	1.65
Ge	0.66	300	1.9
Ge	0.73	77	1.7
InAs	0.42	77	3.0
InSb	0.23	77	5.2
$Hg_{0.8}Cd_{0.2}Te$	0.09	77	14

3.7.2 Photoconductive devices

The device relies on the change of the conductivity of material when illuminated by light. The conductivity increase due to the generation of free carriers after absorption of photons by interband transitions.

Compared with photodiodes, the detectors are simpler, but tend to have slow response times.

3.7.3 Photovoltaic devices (solar cell)

The device generates a photovoltage when irradiated by light. This in turn can be used to generate electrical power in an external power.