Fundamentals of Solid State Physics

Optical Properties

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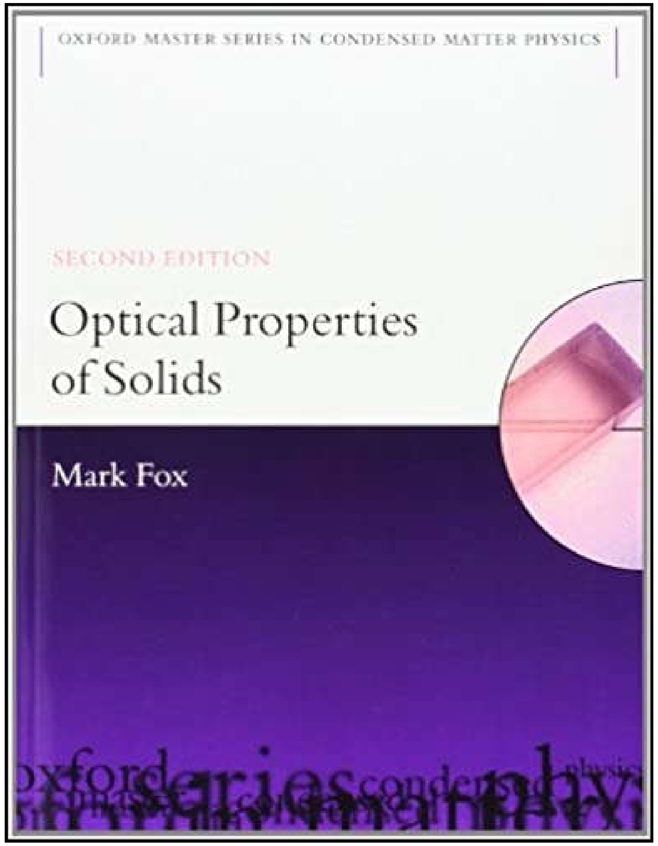
Further Reading

- **Fox, Chapter 1, 2, 7**



Optical Properties of Materials

Metal

SiO_2

Silicon

- Crystal Structures
  - polycrystalline, amorphous, single crystalline
- Electronics
  - conductor, insulator, semiconductor
- Optics (in the visible range)
  - reflective, transparent, absorbing

Fundamentals of Solid State Physics

Optical Processes

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Optical Processes

- Review: Maxwell's Equations

- Reflection, Transmission, Absorption, ...

- Optical propagation in multi-layers
  - Transfer Matrix Method

Electrodynamics

- **Maxwell's Equations**

$$\nabla \cdot \mathbf{D} = \rho_V$$
$$\nabla \cdot \mathbf{B} = 0$$
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$
$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$

$$\oint_s \mathbf{D} \cdot d\mathbf{A} = \int_v \rho \cdot dV$$
$$\oint_s \mathbf{B} \cdot d\mathbf{A} = 0$$
$$\oint_l \mathbf{E} \cdot d\mathbf{l} = -\int_s \frac{\partial \mathbf{B}}{\partial t} \cdot d\mathbf{A}$$
$$\oint_l \mathbf{H} \cdot d\mathbf{l} = \int_s \mathbf{J} \cdot d\mathbf{A} + \int_s \frac{\partial \mathbf{D}}{\partial t} \cdot d\mathbf{A}$$

http://www.maxwells-equations.com/

Electrodynamics

- **Maxwell's Equations**

$$\nabla \cdot \mathbf{D} = \rho_V$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$

Constitutive Relations
本构关系

$$\mathbf{B} = \mu_0 \mu_r \mathbf{H}$$

$$\mathbf{D} = \varepsilon_0 \varepsilon_r \mathbf{E}$$

$\varepsilon_0\ \varepsilon_r$ - **Permittivity (dielectric constant)**

ε_r **= 1 for vacuum**

ε_0 **= 8.85*10^{-12} F/m**

$\mu_0\mu_r$ - **Permeability**

μ_r **= 1 for vacuum**

μ_0 **= 4π*10^{-7} H/m**

Electrodynamics

- **Maxwell's Equations**

$$\nabla \cdot \mathbf{D} = \rho_V$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$

Constitutive Relations
本构关系

$$\mathbf{B} = \mu_0 \mu_r \mathbf{H}$$

$$\mathbf{D} = \varepsilon_0 \varepsilon_r \mathbf{E}$$

For most non-magnetic materials (no magnetic field), $\mu_r = 1$

Optical properties of materials is determined by ε_r

Electrodynamics

- In vacuum
  - $\rho_V = 0$, $\mathbf{J} = 0$
  - $\mu_r = 1$, $\varepsilon_r = 1$

$$\nabla \cdot \mathbf{D} = \rho_V$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$

→

$$\nabla^2 \mathbf{E} = \mu_0 \varepsilon_0 \frac{\partial^2 \mathbf{E}}{\partial t^2}$$

$$\mathbf{E}(x,t) = \mathbf{E}_0 e^{i(kx-\omega t)}$$

Plane Wave

$$k = \frac{2\pi}{\lambda}$$

wavevector

$$\omega = \frac{2\pi}{T}$$

angular frequency

Electrodynamics

- **In vacuum**
  - $\rho_V = 0$, $\mathbf{J} = 0$
  - $\mu_r = 1$, $\varepsilon_r = 1$

$$\nabla \cdot \mathbf{D} = \rho_V$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$

→

$$\nabla^2 \mathbf{E} = \mu_0 \varepsilon_0 \frac{\partial^2 \mathbf{E}}{\partial t^2}$$

$$\mathbf{E}(x,t) = \mathbf{E}_0 e^{i(kx - \omega t)}$$

Plane Wave

$$c = \frac{\omega}{k} = \frac{1}{\sqrt{\mu_0 \varepsilon_0}} = 3 \times 10^8 \text{ m/s}$$

light speed in vacuum

Electrodynamics

- In a dielectric medium
  - ρ_V = 0, J = 0
  - μ_r = 1, $\varepsilon_r \neq$ 1

$$\nabla \cdot \mathbf{D} = \rho_V$$
$$\nabla \cdot \mathbf{B} = 0$$
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$
$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$

→

$$\nabla^2 \mathbf{E} = \mu_0 \varepsilon_0 \varepsilon_r \frac{\partial^2 \mathbf{E}}{\partial t^2}$$

$$\mathbf{E}(x,t) = \mathbf{E}_0 e^{i(kx-\omega t)}$$ **Plane Wave**

$$v = \frac{\omega}{k} = \frac{c}{\sqrt{\varepsilon_r}} = \frac{c}{n}$$

$$\varepsilon_r = n^2$$

light speed in a material

n **- refractive index (折射率)**

Electrodynamics

- **In a dielectric medium**
  - $\rho_V = 0$, **J** = 0
  - $\mu_r = 1$, $\varepsilon_r \neq 1$

$$\mathbf{E}(x,t) = \mathbf{E}_0 e^{i(kx-\omega t)}$$

Plane Wave

$$k = \frac{2\pi}{\lambda'} = \frac{2\pi}{\lambda_0} n$$

λ' - wavelength in the medium
λ_0 - wavelength in vacuum
Frequency ω does not change

Complex Form of ε_r and n

$$\tilde{\varepsilon}_r = \tilde{n}^2$$

$$\tilde{\varepsilon}_r = \varepsilon_1 + i\varepsilon_2$$

$$\tilde{n} = n + i\kappa$$

$$\rightarrow \begin{cases} \varepsilon_1 = n^2 - \kappa^2 \\ \varepsilon_2 = 2n\kappa \end{cases}$$

ε_r and *n* depend on optical frequency / wavelength

Complex Form of ε_r and n

$$\begin{cases} n = \dfrac{1}{\sqrt{2}}\left(\varepsilon_1 + \sqrt{\varepsilon_1{}^2 + \varepsilon_2{}^2}\right)^{1/2} \\ \kappa = \dfrac{1}{\sqrt{2}}\left(-\varepsilon_1 + \sqrt{\varepsilon_1{}^2 + \varepsilon_2{}^2}\right)^{1/2} \end{cases}$$

when ε_1 >> ε_2 (or n >> κ), weakly absorbing

$$\rightarrow \begin{cases} n \approx \sqrt{\varepsilon_1} \\ \kappa \approx \dfrac{\varepsilon_2}{2n} \end{cases}$$

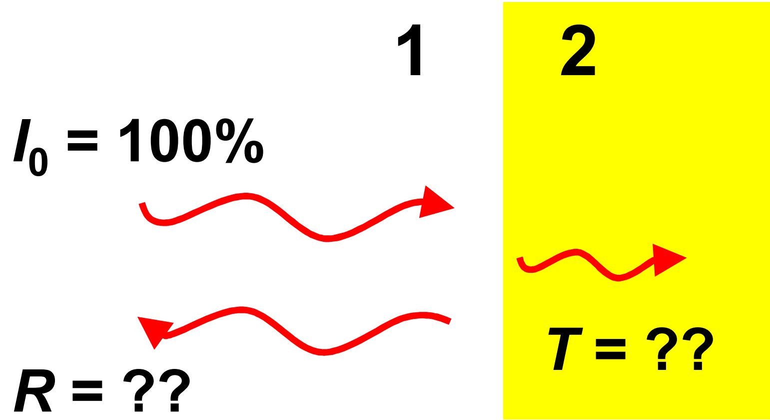
Reflection 反射

Incident wave

$$\mathbf{E}(x,t) = \mathbf{E}_0 e^{i(kx-\omega t)}$$

Intensity

$$I \propto |\mathbf{E}|^2$$



Reflective wave

$$\mathbf{E}_R(x,t) = \mathbf{E}_R e^{i(-kx-\omega t)}$$

Reflectivity 反射率

based on boundary conditions of Maxwell's Equations

$$R = \left|\frac{\mathbf{E}_R}{\mathbf{E}_0}\right|^2 = \left|\frac{\tilde{n}_2 - \tilde{n}_1}{\tilde{n}_2 + \tilde{n}_1}\right|^2$$

If medium 1 is air ($\tilde{n}_1$ = 1)

$$R = \left|\frac{\tilde{n}_2 - 1}{\tilde{n}_2 + 1}\right|^2 = \frac{(n-1)^2 + \kappa^2}{(n+1)^2 + \kappa^2}$$

for normal incidence ($\theta = 0$)

Transmission 透射率

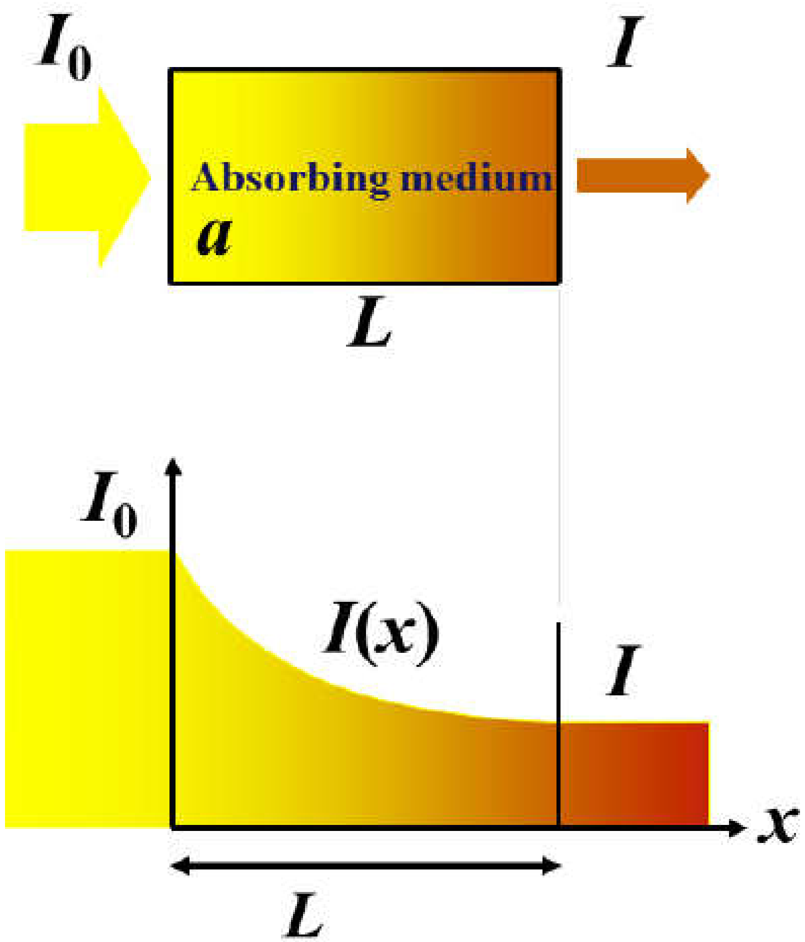
$$T = 1 - R$$

Absorption 吸收

Incident wave

$$\mathbf{E}(x,t)=\mathbf{E}_0 e^{i(kx-\omega t)}$$

Intensity $I \propto |\mathbf{E}|^2$



After traveling a distance *L*

$$\begin{aligned}\mathbf{E}_T(x,t) &= \mathbf{E}_0 e^{i(kx-\omega t)} e^{ikL} \\ &= \mathbf{E}_0 e^{i(kx-\omega t)} e^{i2\pi\tilde{n}/\lambda * L} \\ &= \mathbf{E}_0 e^{i(kx-\omega t)} e^{i2\pi n/\lambda * L} e^{-2\pi\kappa/\lambda * L}\end{aligned}$$

Lambert Beer's Law $I = I_0 e^{-\alpha L}$

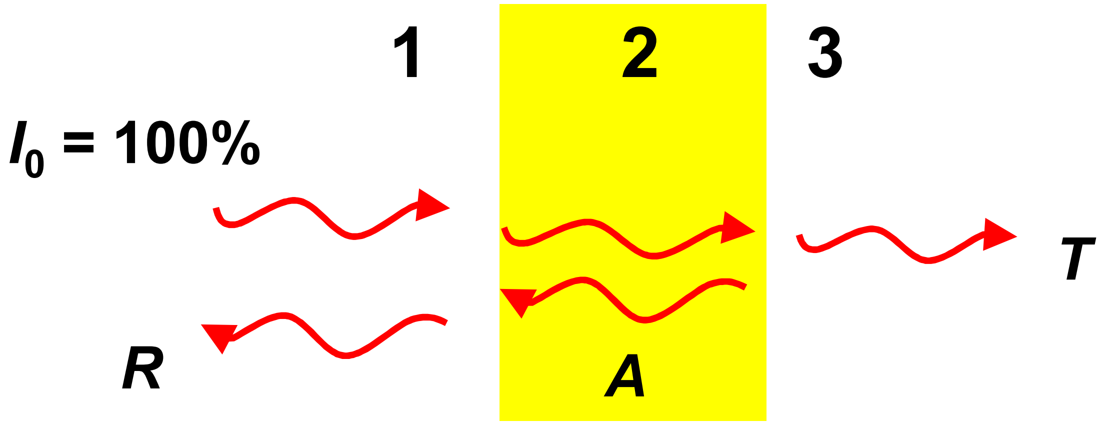
$\alpha = \dfrac{4\pi\kappa}{\lambda}$ **absorption coefficient (unit: /m)**

Transmission 透射

Reflection *R* 反射

Absorption *A* 吸收

Transmission *T* 透射



$$R + A + T = 1$$

Example: Silicon

- **At λ = 600 nm, for Si, $\tilde{n}$ = 3.94 + i*0.025, calculate**
  - **Reflection *R* at the air/Si interface**
  - **Absorption coefficient α at 600 nm**
  - **Absorption by a Si film with thickness *L* = 0.01 mm**

Example: Silicon

- **At λ = 600 nm, for Si, $\tilde{n}$ = 3.94 + i*0.025, calculate**
  - **Reflection *R* at the air/Si interface**
  - **Absorption coefficient α at 600 nm**
  - **Absorption by a Si film with thickness *L* = 0.01 mm**

$$R = \frac{(n-1)^2 + \kappa^2}{(n+1)^2 + \kappa^2} = 35.4\%$$

$$\alpha = \frac{4\pi\kappa}{\lambda} = 5.24 * 10^5 /\mathrm{m}$$

$$A = 1 - e^{-\alpha L} = 99.5\%$$

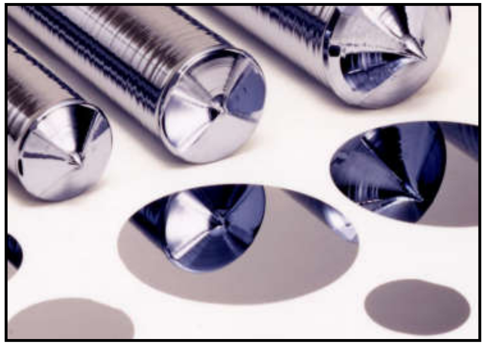
Example: Silicon

- Silicon is a very good absorber at λ = 600 nm
- It can be used to make solar cells and cameras
- Surface reflection is very strong
- It needs an anti-reflective coating ARC (减反膜)

$$R=\frac{(n-1)^2+\kappa^2}{(n+1)^2+\kappa^2}=35.4\%$$

$$\alpha=\frac{4\pi\kappa}{\lambda}=5.24*10^5/\mathrm{m}$$

$$A=1-e^{-\alpha L}=99.5\%$$



bare Si wafer

Si solar cell with ARC

Example: Silver

- At λ = 600 nm, for Ag, $\tilde{n}$ = 0.12 + i*3.66, calculate
  - Reflection R at the air/Ag interface
  - Absorption coefficient α at 600 nm
  - Absorption by a Ag film with thickness L = 100 nm

Example: Silver

- **At λ = 600 nm, for Ag, *ñ* = 0.12 + i*3.66, calculate**
  - **Reflection *R* at the air/Ag interface**
  - **Absorption coefficient α at 600 nm**
  - **Absorption by a Ag film with thickness *L* = 100 nm**

$$R = \frac{(n-1)^2 + \kappa^2}{(n+1)^2 + \kappa^2} = 96.7\%$$

$$\alpha = \frac{4\pi\kappa}{\lambda} = 7.67 * 10^7 /\mathrm{m}$$

$$A = 1 - e^{-\alpha L} = 99.95\%$$

Example: Silver

- **Ag is a very good mirror at visible wavelengths**
- **Light can only propagate in Ag at a very small depth**

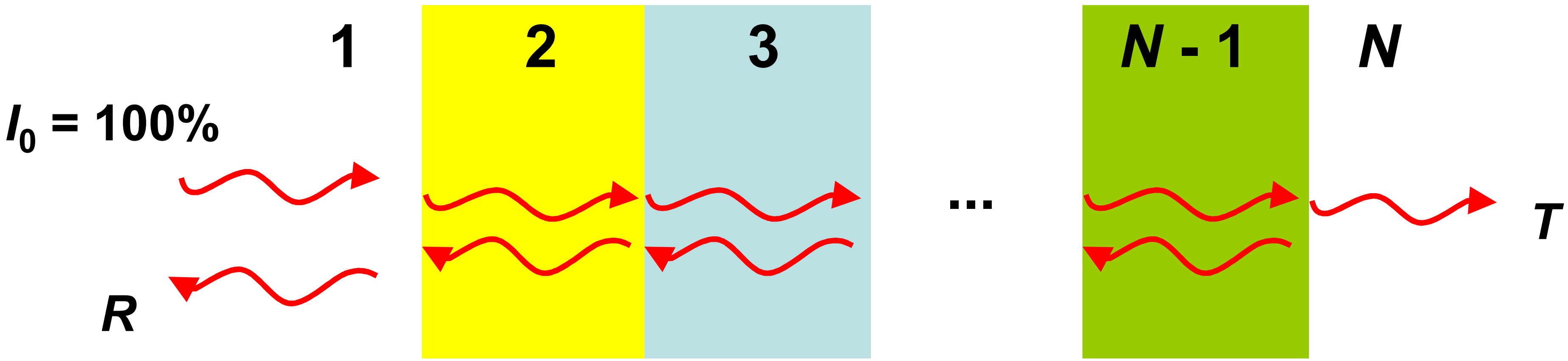
$$R = \frac{(n-1)^2 + \kappa^2}{(n+1)^2 + \kappa^2} = 96.7\%$$

$$\alpha = \frac{4\pi\kappa}{\lambda} = 7.67 * 10^7 /\mathrm{m}$$

$$A = 1 - e^{-\alpha L} = 99.95\%$$

mirror reflection

Multilayer Optical Structures



Solution based on the boundary conditions of Maxwell's Equations

calculated by *Transfer Matrix Method*
Lecture Note 5.2

Example: Anti-Reflective Coating (ARC)

At λ = 600 nm, no ARC

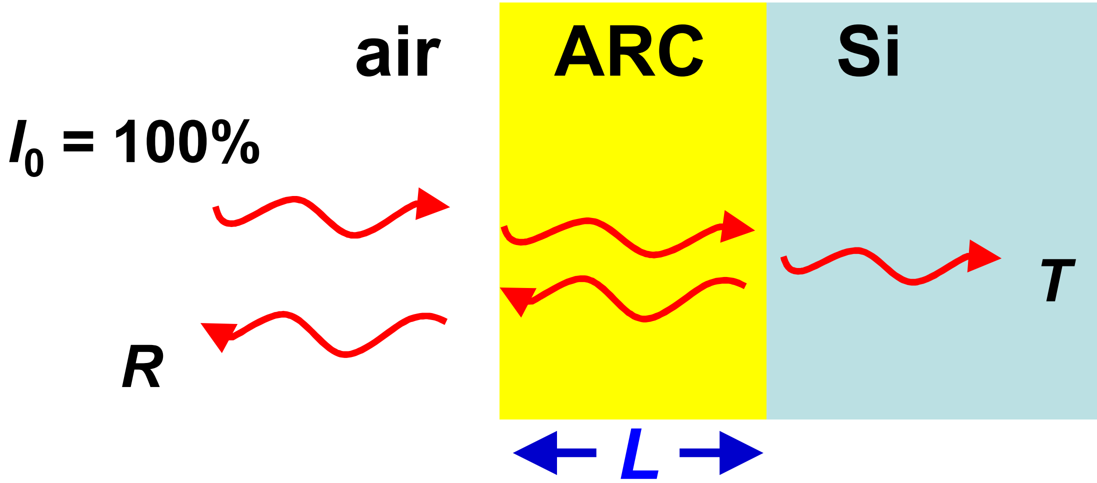
$$R(\text{air/Si}) = 35.4\%$$

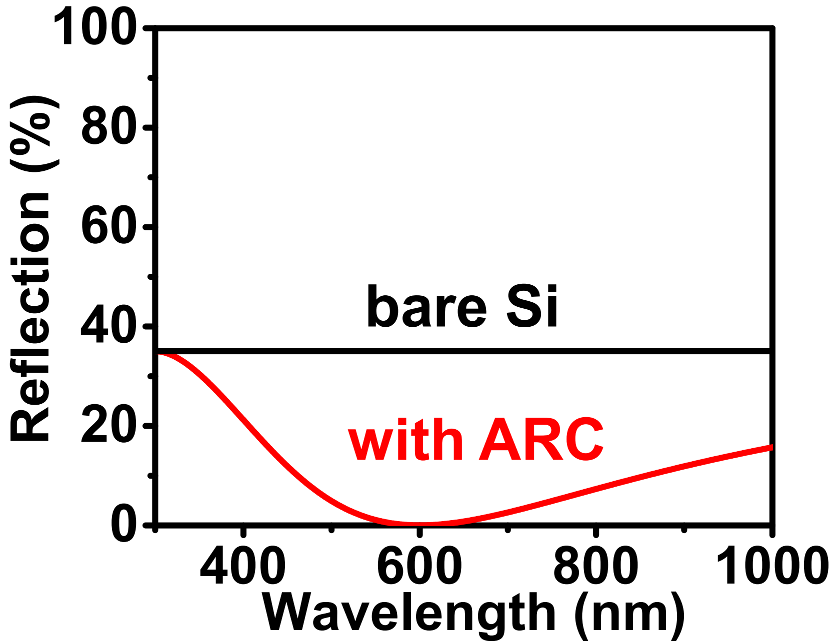
Design an ARC

$$n = \sqrt{n(\text{air}) * n(\text{Si})} = 1.98$$

$$L = \frac{\lambda}{4n} = 75 \text{ nm}$$

$$R(\lambda = 600 \text{ nm}) = 0$$





Homework 9.1

Example: ARC for Si

At λ = 600 nm, no ARC

$$R(\text{air/Si}) = 35.4\%$$

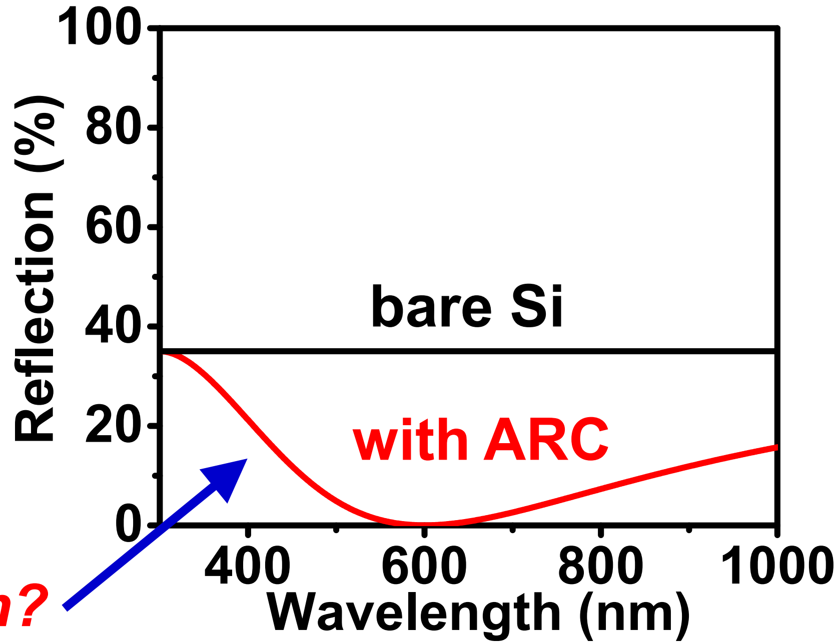
Design an ARC

$$n = \sqrt{n(\text{air}) * n(\text{Si})} = 1.98$$

$$L = \frac{\lambda}{4n} = 75 \text{ nm}$$

$$R(\lambda = 600 \text{ nm}) = 0$$

A Si solar cell with ARC looks blue



Q: How to further reduce the reflection?

Example: ARC for Glass

For glass

$$n = 1.45$$

At λ = 600 nm, no ARC

$$R(\text{air/glass}) = 3.4\%$$

Design an ARC

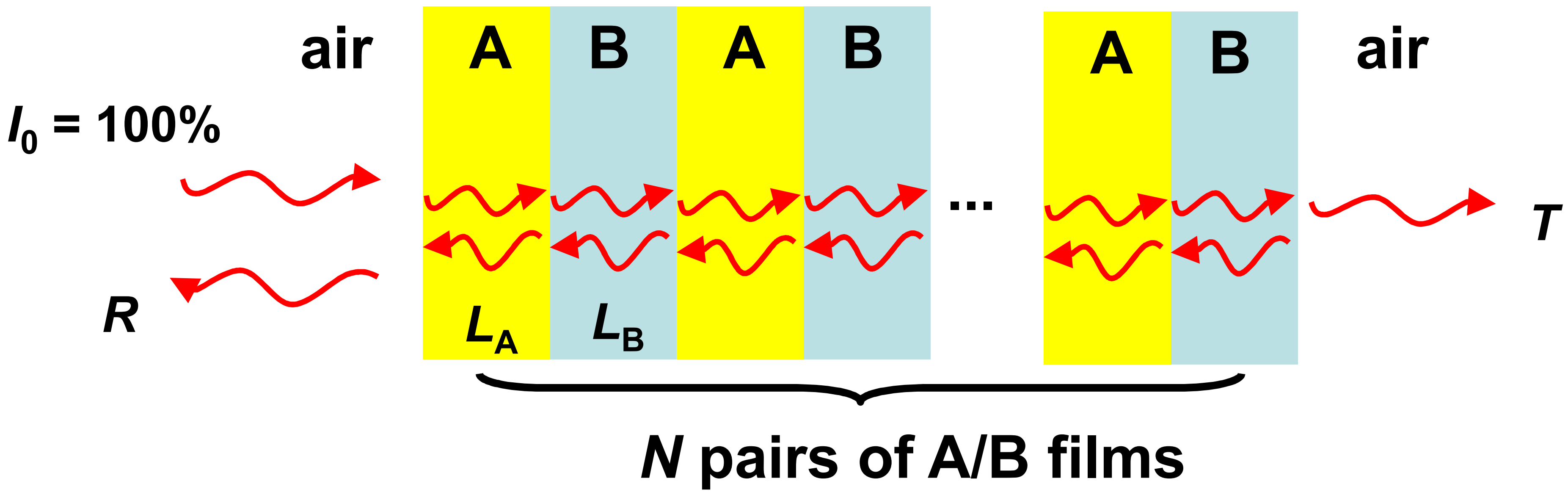
$$n = \sqrt{n(\text{air}) * n(\text{glass})} = 1.2$$

$$\text{thickness} = \frac{\lambda}{4n} = 125 \text{ nm}$$

without ARC

with ARC

Example: Bragg Reflector



If we choose

$$L_A = \frac{\lambda}{4n_A}$$

$$L_B = \frac{\lambda}{4n_B}$$

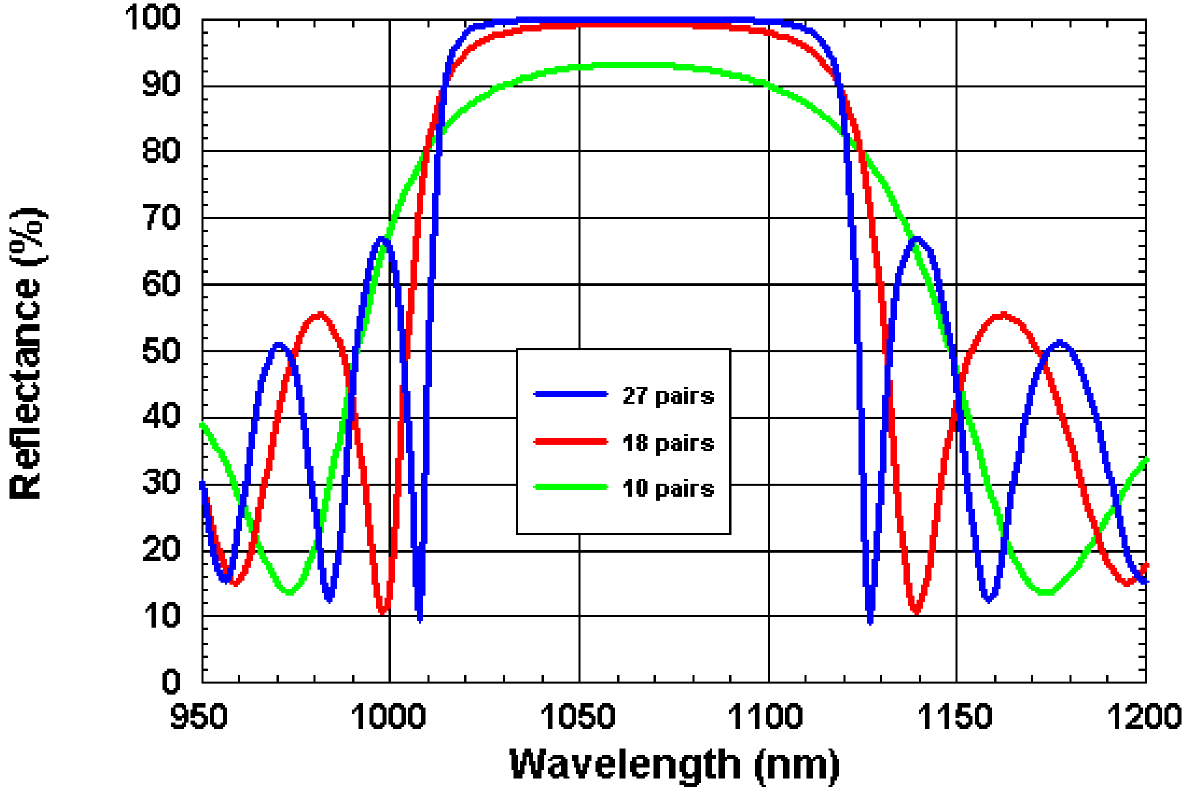
Project 3

$$R = \left(\frac{n_A{}^{2N} - n_B{}^{2N}}{n_A{}^{2N} + n_B{}^{2N}} \right)^2$$

If $n_A \neq n_B$, when $N \to +\infty$

$R \to 100\%$

Example: Bragg Reflector



A perfect mirror (Bragg mirror) (better than silver)

1D photonic crystal (光子晶体)

Project 2

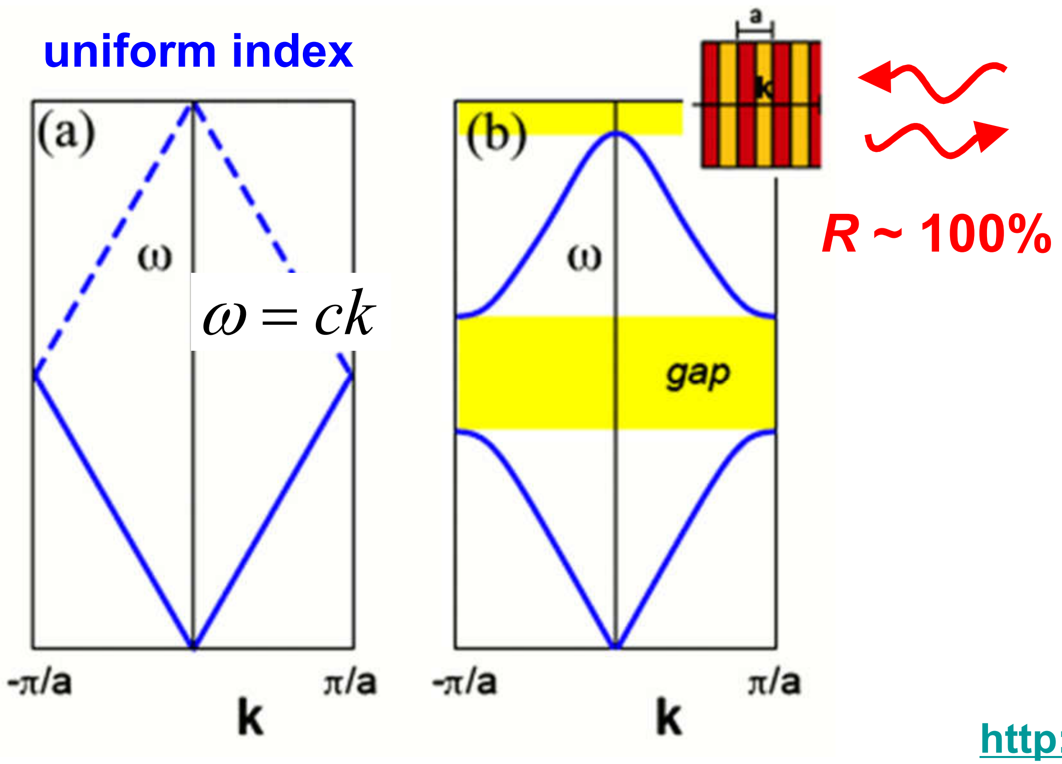
$$R = \left(\frac{n_A^{2N} - n_B^{2N}}{n_A^{2N} + n_B^{2N}} \right)^2$$

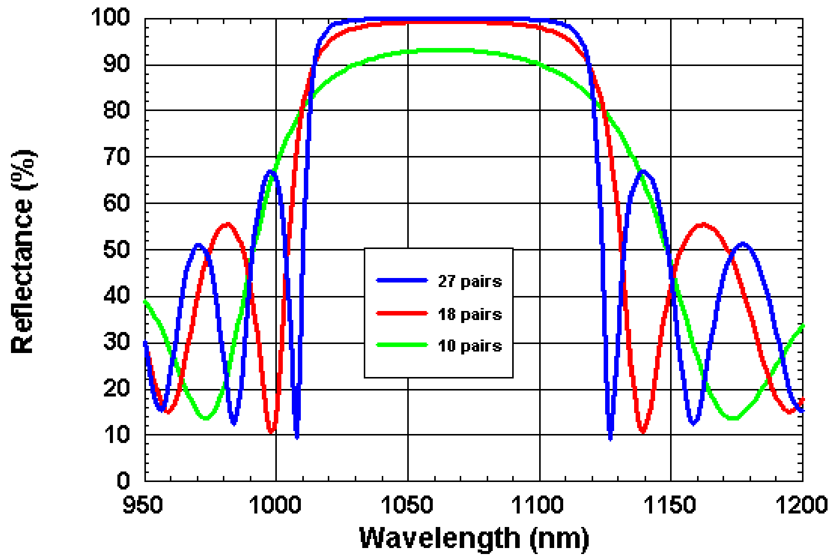
If $n_A \neq n_B$, when $N \to +\infty$

$R \to 100\%$

Photonic Crystals (光子晶体)

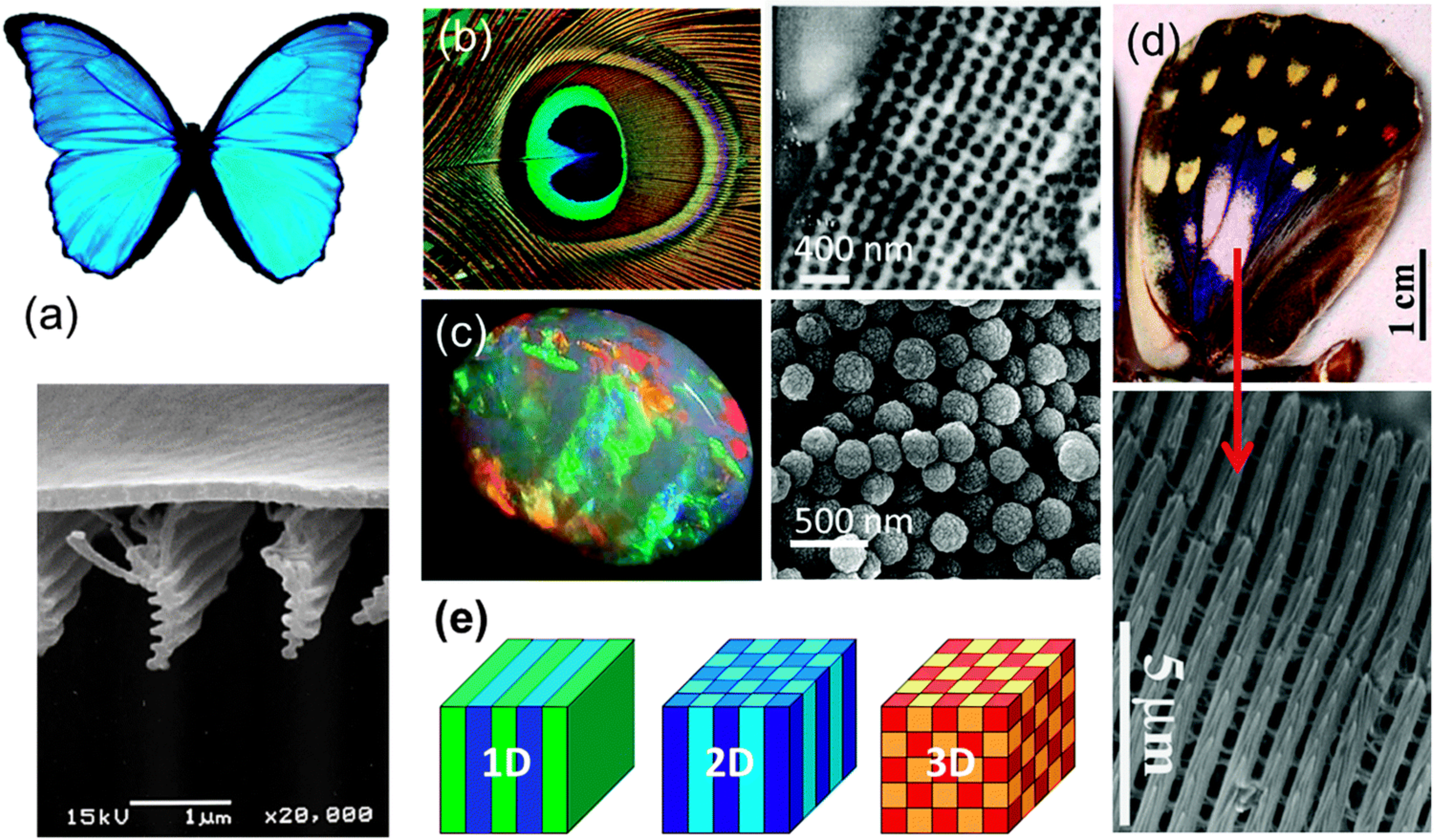
- **Periodically structured optical media**
  - **Forming photonic band gaps**
  - **no light can pass through (~100% reflection)**
  - **color created by structure, not material absorption**





http://large.stanford.edu/courses/2007/ap273/dai1/

Photonic Crystals in Nature



E. Armstrong and C. O'Dwyer, *J. Mater. Chem. C* **3,** 6109 (2015)

Thank you for your attention