

PHS6317

NANO-ENGINEERING OF THIN FILMS

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Based on the notes first prepared in 2008 by Stéphane Larouche
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Winter 2024

Bienvenue - Welcome

**POLYTECHNIQUE
MONTRÉAL**





PHS 6317 Nanoengineering of thin films

Course schedule – Winter 2024

12 January	Introduction – Scientific and technological challenges
19	Fabrication methods – Vacuum physics and vapor-phase techniques
26*	Fabrication methods – Plasma processes and process optimization
2 February	Fabrication methods - Plasma-surface interactions and diagnostics
9**	Fabrication methods – Thermal/Plasma spray technologies
16*	Optics of thin films 1, optical characterization, Miniquiz 1 (5%)
23*	Optics of thin films 2, design of optical filters
1*** March	<i>Presentations – Emerging fabrication techniques (30%)</i>
	<i>March 4-8 - Winter/Spring break</i>
15**	Tribomechanical properties of films and coatings
22**	Electrochemical properties – corrosion and tribo-corrosion (<i>filter-20%</i>)
5 April	Passive functional films and coatings, <i>Miniquiz 2 (5%)</i>
12	Active functional films and coatings
16	Life cycle analysis and environmental impact
19***	<i>Presentations – Emerging applications of nanostructured films (40%)</i>

Deadlines:

Project #1 – Fabrication technique:

Choice of the subject: **26 January**

Abstract and references: **9 February**

Report and presentation: **1st March**

Projet #2 – Design of an optical filter:

Choice of the subject: **23 February**

Report: **22 March**

Projet #3 – Application of nanostructured thin films:

Choice of the subject: **16 February**

Abstract and references: **15 March**

Report and presentation: **19 April**



Evaluation

- | | |
|--|-----|
| 1. Project 1: Bibliographic research on an emerging fabrication technique of thin films - Report and presentation | 30% |
| 2. Project 2: Design of an optical filter - Report | 20% |
| 3. Project 3: Bibliographic research on a specific application of the nano- engineering of thin films - Report and presentation | 40% |
| 4. Miniquiz 1 and 2 (@ 5%) | 10% |



Project 2: Design of an optical filter (20%)

Specific requirements:

Deliverables: Report, maximum 8 pages (letter size paper, 2 cm margins, Times New Roman 12 pts).

Structure and contents:

- Introduction – describe the choice of the specific filter and its application
- Optical specifications of the filter: spectral characteristics in T and R , color coordinates, tolerances, etc.
- Methodology of the design: architecture, materials, optimization, etc.
- Discussion of the performance and sensitivity to the fabrication process
- Conclusions

Deadlines

Choice of filter: **February 23**

Report: **March 22**

8A – Thin-film optics - Overview



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Chapter 8A

Page 8A-6

1. Introduction

2. Basics

- Waves
- Maxwell equations and electromagnetic waves
- Admittance
- Irradiance
- Reflection and transmission at an interface
- Reflection and transmission for a thin film
- Matrix approach
- Quarter-waves and half-waves
- Simple filters (antireflective, reflective)
- Oblique incidence



8A – References



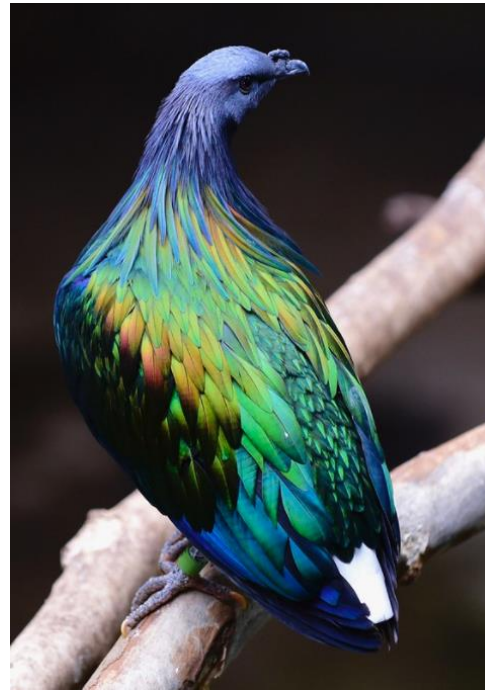
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Chapter 8A

Page 8A-7

- Hugh Angus Macleod, *Thin-Film Optical Filters*, third edition, Institute of Physics Publishing, Bristol, UK, 2001.
 - This book covers practically all aspects of optical filters. Available at the library (QC 373 L5 M34 2001).
- Hugh Angus Macleod, *Thin-Film Optical Filters*, fourth edition, CRC Press, Boca Raton, USA, 2010.
- Max Born and Emil Wolf, *Principles of optics*, seventh edition (extended), Cambridge University Press, Cambridge, UK, 1999.
 - This book covers in much more detail light and matter interactions.
- Larouche, S., & Martinu, L. (2008). *OpenFilters*: open-source software for the design, optimization, and synthesis of optical filter. *Applied Materials & Interfaces*, 47(13), 219–230.
 - Article which covers the software you will be using to design your own filters.

8A - Where do these colors come from?



Wikipedia.org

T. L. Tan, D. Wong and P. Lee, « Iridescence of a shell of mollusk *Haliotis Glabra* » *Opt. Express*, vol. 12, 2004, 4847-4854.

8A – Brief history of optics



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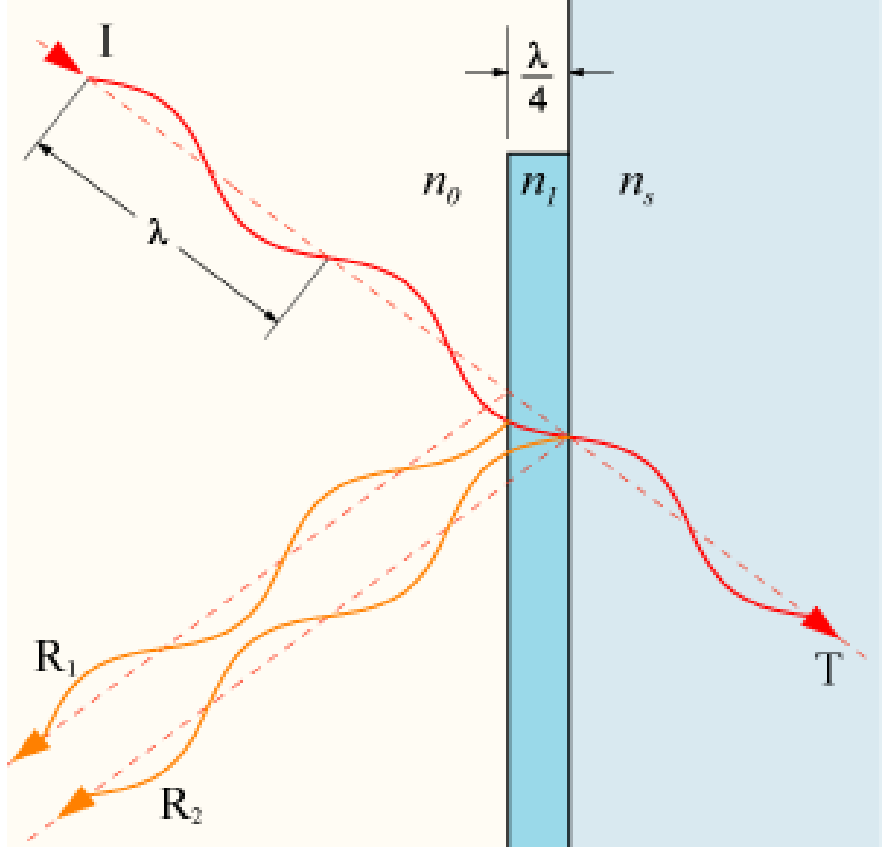
Chapter 8A

Page 8A-9

- Robert Boyle (1663) and Robert Hooke (1665) describe Newton rings (1704).
- 1801: Young explains the interference phenomenon, supported by Fresnel (1816) who also explains diffraction.
- 1816: Fraunhofer fabricates the first antireflective filters by tarnishing glass.
- 1873: Maxwell publishes his famous equations.
- 1891: Taylor and Kollmorgen (1916) propose and develop the use of antireflective filters obtained through tarnishing in optical systems.
- 1913: Langmuir invents the diffusion pump.
- 1934: Bauer, who studies the properties of halides, deposits antireflective coatings.
- 1939: Strong produces antireflective filters using fluorides.
- World War II: the beginning of mass production of MgF_2 antireflective coatings.*
- 1950s: Theoretical developments for filter designing.
- 1970s to present: design and fabrication of highly complex filters (> 1000 layers) using computers and sophisticated coating systems.

**“...antireflection coatings were perfected in the early 1940's, and it was not long before the advantage of "coated optics" was fully recognized. During World War II, Britain, Germany and the U.S. coated most of their military optical equipment with such films. These coatings were considered to be so important that coating machines were installed on U.S. battleships so that the optical elements in range finders could be recoated at sea if necessary.”* Baumeister and Pincus, Scientific American, 1970.

8A - Interference



Wikipedia.org

8A – Antireflective filters



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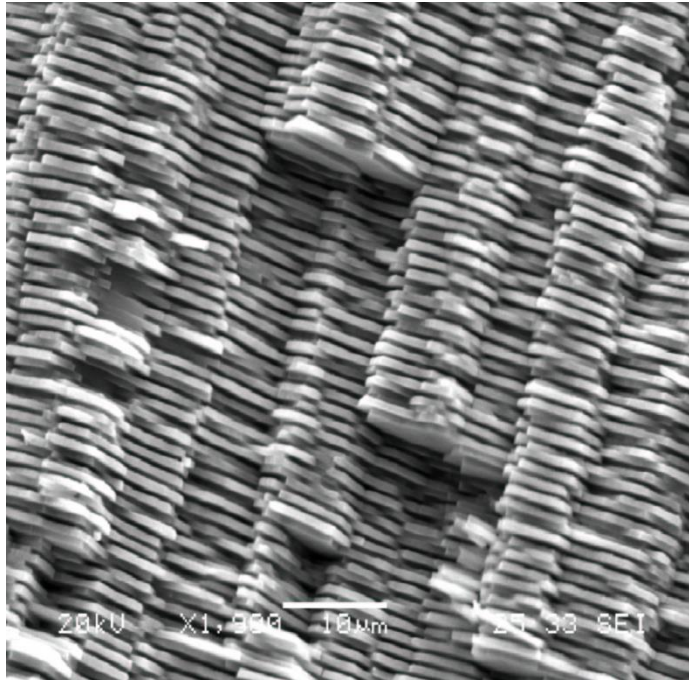
Chapter 8A

Page 8A-11



www.allaboutvision.com

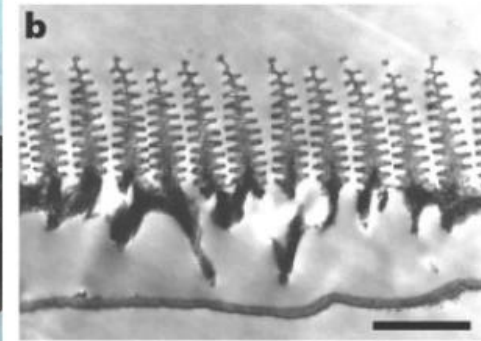
8A - Microstructure



T. L. Tan, D. Wong and P. Lee, «Iridescence of a shell of mollusk *Haliotis Glabra*» *Opt. Express*, vol. 12, 2004, 4847–4854.



Butterfly *Morpho rhetenor*



Pete Vukusic et J. Roy Sambles, «Photonic structures in biology», *Nature*, vol. 424, 2003, 952–855.

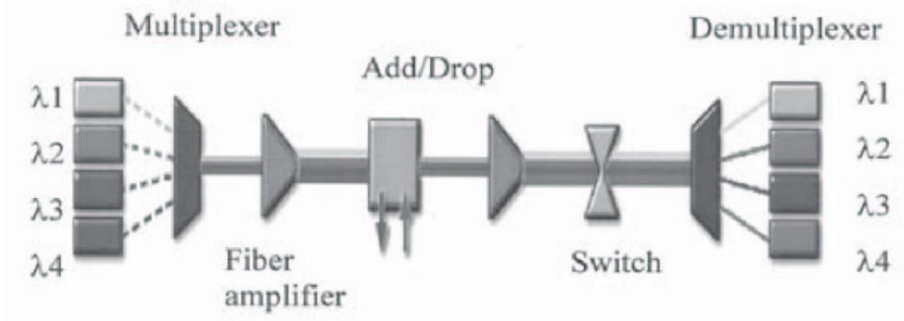


8A - Telecommunications

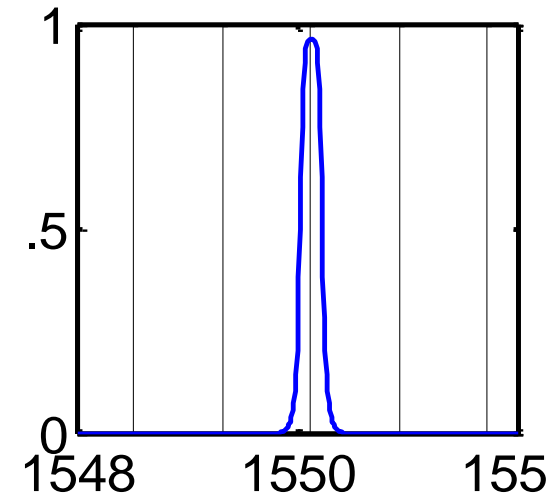
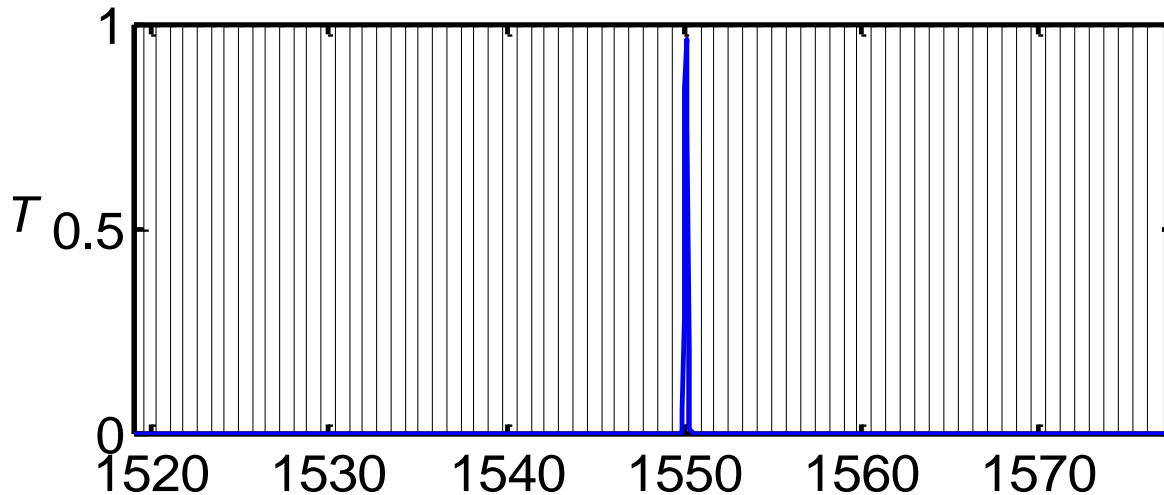


PHS6317 –
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Chapter 8A
Page 8A-13



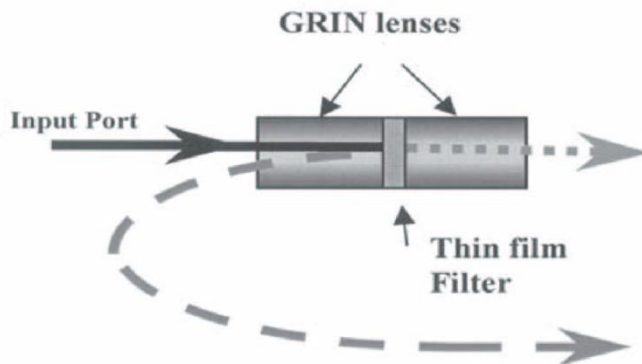
N.A. O'Brien *et al.*, «Recent Advances in Thin Film Interference Filters for Telecommunications», *SVC 44th Annual Tech. Conf. Proc.*, 2001, 255–261.



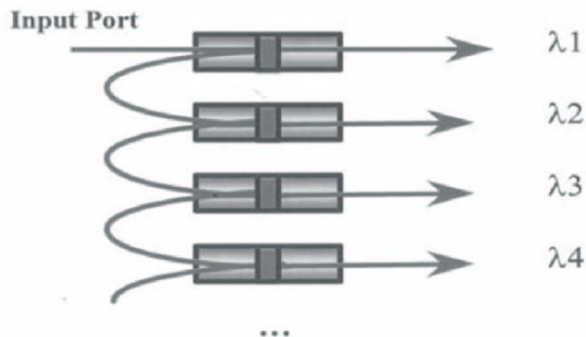


8A - Telecommunications

Graded index optics



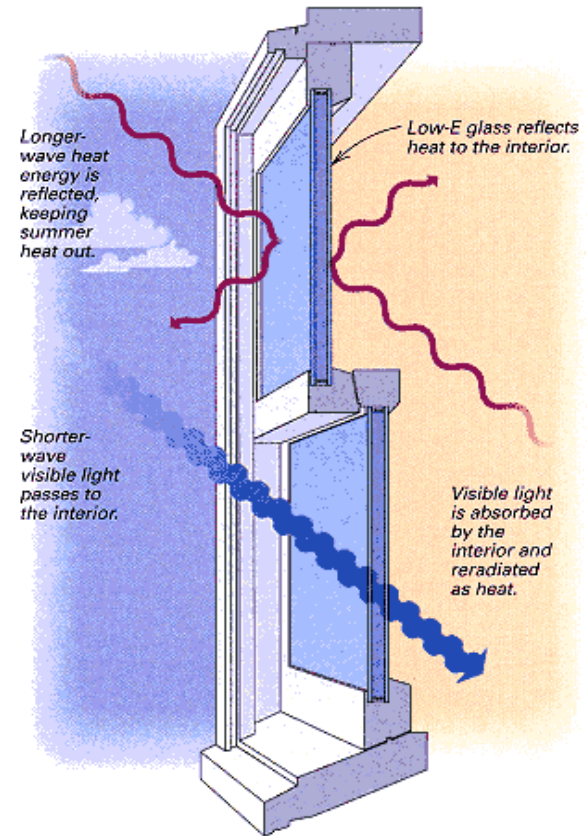
Cascaded structure



VIAVI Solutions (www.viavisolutions.com)

N.A. O'Brien *et al.*, «Recent Advances in Thin Film Interference Filters for telecommunications», *SVC 44th Annual Tech. Conf. Proc.*, 2001, 255–261.

8A – Architectural glass



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Chapter 8A

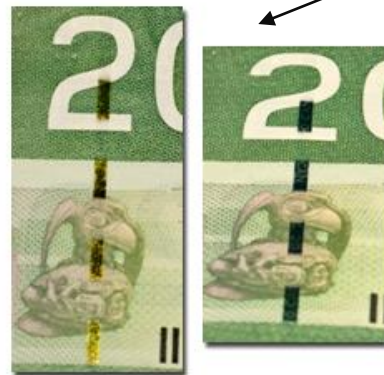
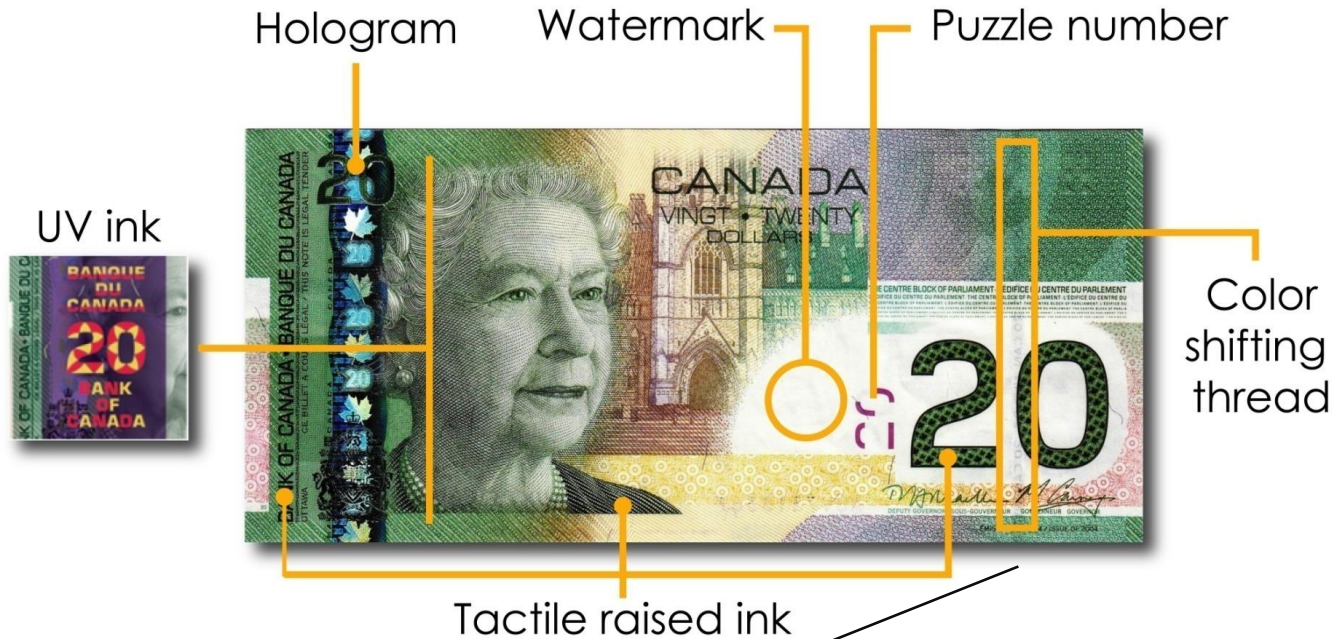
Page 8A-15



Chair partner
of the FCSEL.

Paul Fisette, «Understanding Energy-Efficient Windows», *Fine Homebuilding*, no. 114, 68–73.

8A – Optical security devices



First developed by
J.A. Dobrowolski
for the Bank of Canada

8A – Decorative coatings



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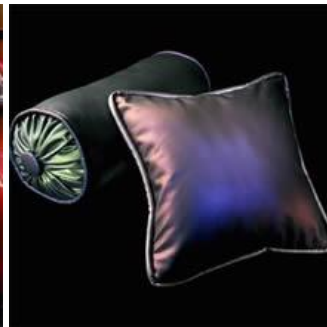
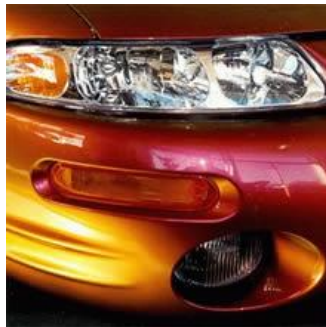
Chapter 8A

Page 8A-17



Lexus Structural Blue

pcimag.com





8A – LIGO

Laser Interferometer Gravitational-wave Observatory



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Chapter 8A

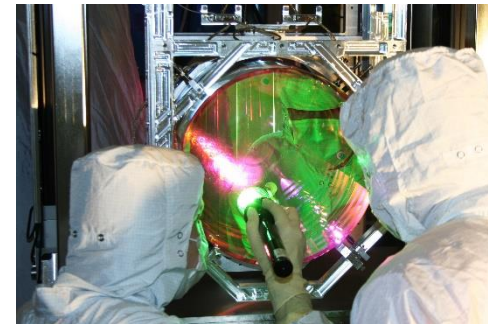
Page 8A-18



LIGO detector in Hanford, Washington Phys.org

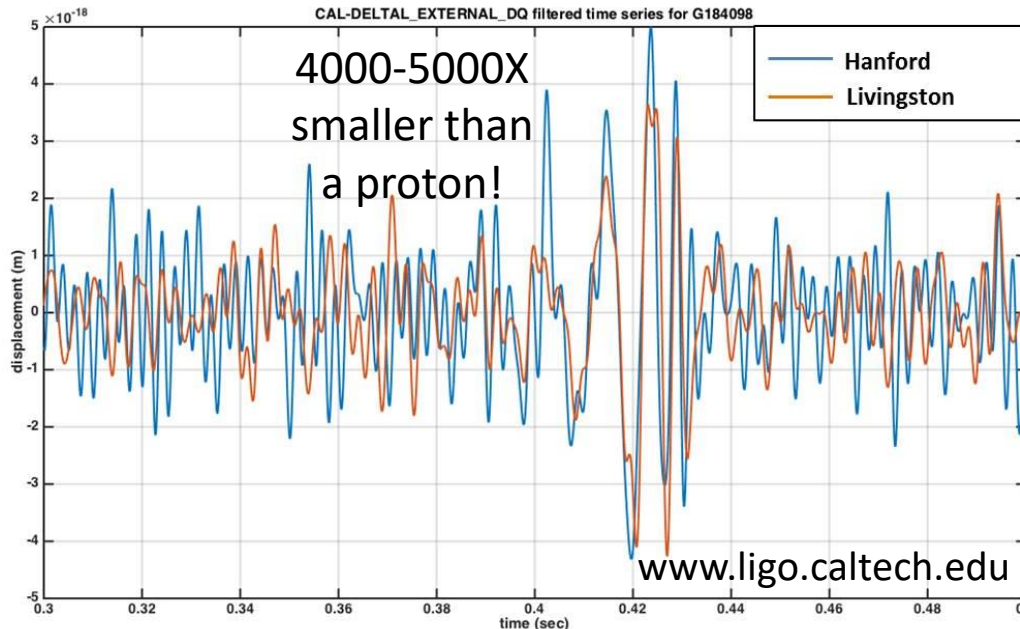
Two arms, each 4 km long!

Huge Michelson interferometer +
Fabry-Perot cavities.



www.ligo.caltech.edu

LIGO dielectric
mirrors
(99.999%
reflection, 0.5
nm roughness,
less than 1 ppm
of losses, etc.)



Gravitational wave from
a binary black hole
merger.

8A –Optical filter market

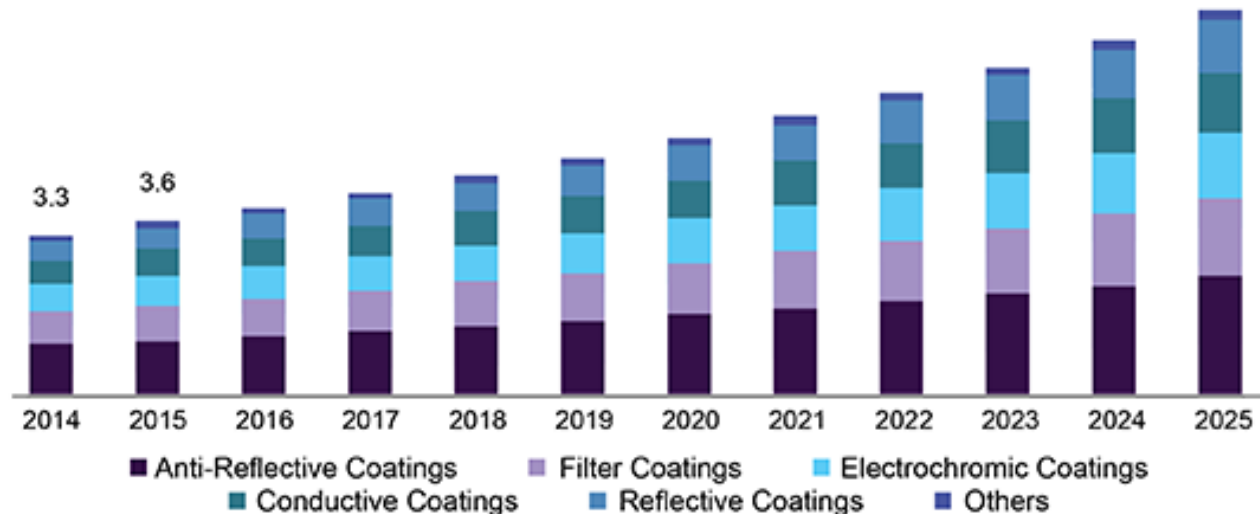


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Chapter 8A

Page 8A-19

U.S. optical coatings market size, by product, 2014 - 2025 (USD Billion)



Source: www.grandviewresearch.com

SMC030C *Future for Optical Coatings*, Business Communication Company, octobre 2006.

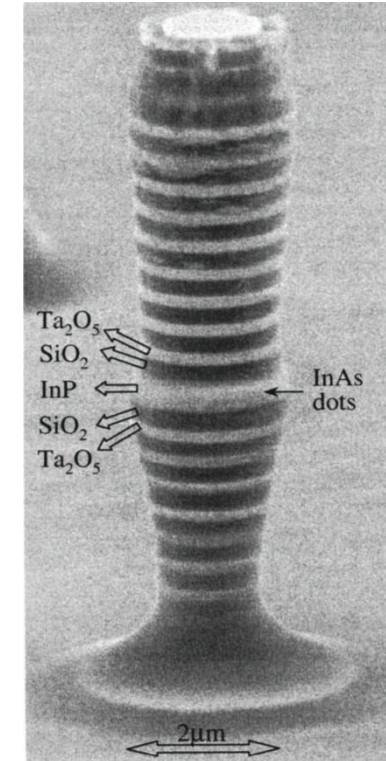
“The global market for optical coatings is expected to reach \$14.2 billion by 2021 from \$9.5 billion in 2016, rising at a compound annual growth rate (CAGR) of 8.3% from 2016 through 2021.”

Optical Coatings: Technologies and Global Markets, 2017, BCC Research Report.

8A – Present research interests



- Filters on polymers (AR, UV protection, mechanical protection).
- Integration with electronic devices.
- Adjustable/active optics.
- High-power applications.
- Micro-opto-electro-mechanical systems (MOEMS), screens.
- Biomedical imagery.
- Manufacturability studies, process control.
- Multifunctional coatings.
- Infrared optics.
- Metasurfaces.



Dan Dalacu *et al.*, «InAs/InP quantum-dot pillar microcavities using SiO₂/Ta₂O₅ Bragg reflectors with emission around 1.55 μm», *Appl. Phys. Lett.*, vol. 84, 2004, 3235–3237.



8A – Waves

- Light is a wave which can be described by its length: wavelength λ .
- In vacuum, light travels at

$$c = 299\,792\,458 \text{ m/s.}$$

- The period of a wave is given by:

$$\tau = \frac{\lambda}{c}$$

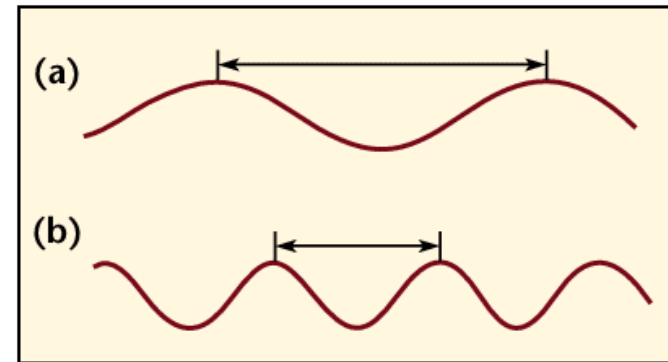
which corresponds to a frequency of:

$$f = \frac{1}{\tau} = \frac{c}{\lambda}.$$

- In all other media than vacuum, light travels at a speed $v < c$, this changes the wavelength to:

$$\lambda' = \frac{v}{c} \lambda = \frac{\lambda}{N}$$

where $N = c/v$, the refractive index of the medium. Neither f nor τ are affected.



Lawrence Berkeley National Laboratory

(www.lbl.gov)



8A – Waves: Exponential representation

- A wave propagating in the x direction can be expressed as:

$$\vec{A}(x,t) = |\vec{A}|\hat{i} \cos\left(2\pi\left(ft - \frac{1}{\lambda'}x\right)\right) = |\vec{A}|\hat{i} \cos\left(\omega t - \frac{2\pi}{\lambda'}x\right)$$

where $\omega = 2\pi f$ is the angular frequency of the wave.

- Light waves, which are electromagnetic, are typically expressed by their electric field:

$$\vec{E} = |\vec{E}|\hat{i} \cos\left(\overset{\text{Temporal}}{\omega t} - \overset{\text{Spatial}}{\frac{2\pi N}{\lambda}x}\right)$$

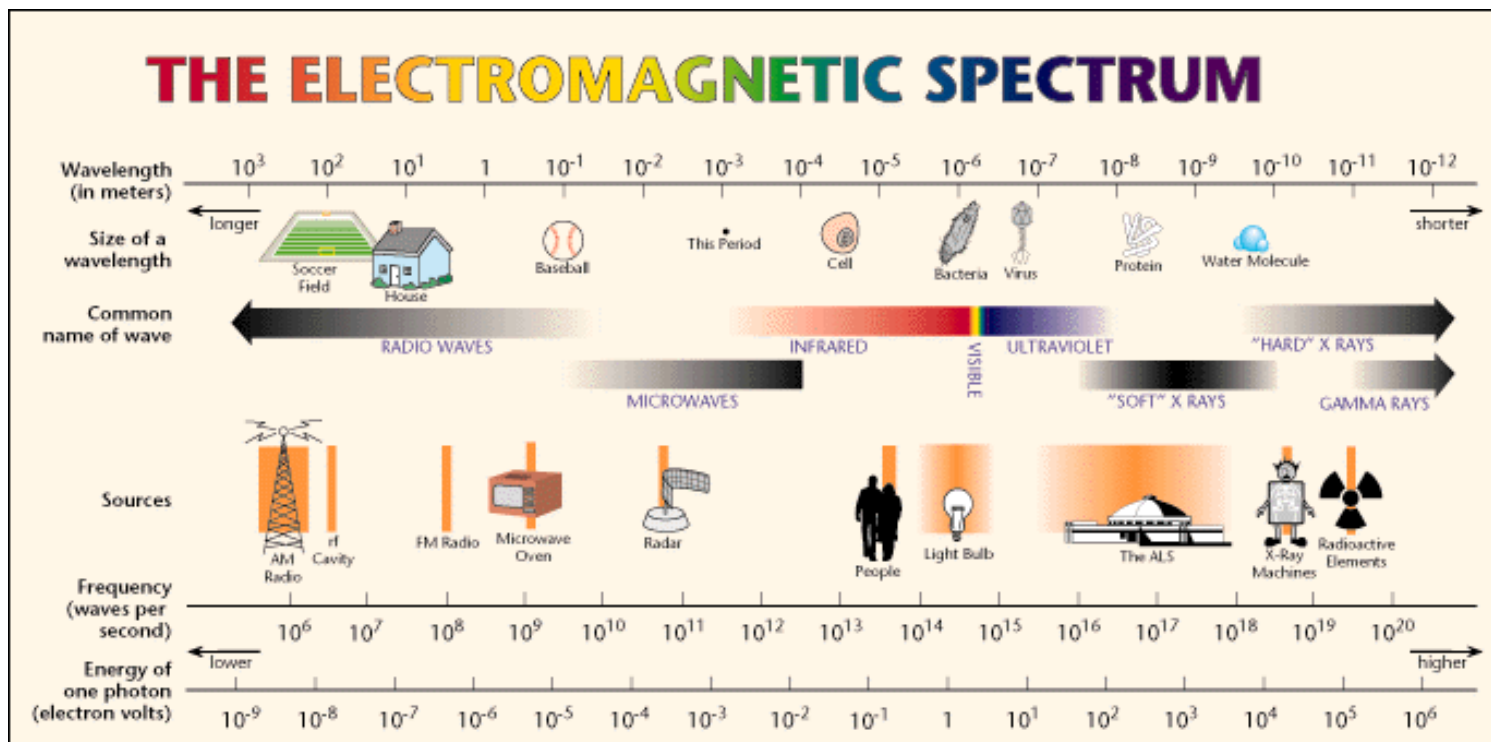
However, to simplify calculations, we will use an exponential notation:

$$\vec{E} = |\vec{E}|\hat{i} \exp\left[i\left(\omega t - \frac{2\pi N}{\lambda}x\right)\right] = |\vec{E}|\hat{i} \left[\cos\left(\omega t - \frac{2\pi N}{\lambda}x\right) + i \sin\left(\omega t - \frac{2\pi N}{\lambda}x\right)\right]$$

where the real part (or imaginary) represents the electric field.



8A – The electromagnetic spectrum



Lawrence Berkeley National Laboratory (www.lbl.gov)

E.g.: Gamma rays detected in 2019 of 450 trillion eV.

8A – Linear and non-linear optics

- A function is linear if:

$$f(A + B) = f(A) + f(B).$$

- All the following optics we will cover is linear:

- We can separate the light spectrum into its individual spectral components and analyze them separately.
- The light intensity does not influence the optical properties of the material.

- There exists many non-linear optical effects:

- Second-harmonic generation;
- Kerr effect;
- Raman scattering and Brillouin scattering;
- ...

- These phenomena occur almost exclusively for high light intensities.



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Nanoengineering of thin
films

Chapter 8A

Page 8A-24



8A – Maxwell's equations

- Light being an electromagnetic wave, it obeys Maxwell's equations:

$$\nabla \cdot \vec{D} = \rho,$$

Gauss's law for
electricity

$$\nabla \cdot \vec{B} = 0,$$

Gauss's law for
magnetism

$$\nabla \times \vec{H} = \vec{j} + \frac{\partial \vec{D}}{\partial t} \quad \text{and}$$

Ampere's law

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

Faraday's law of
induction

and the material equations:

$$\vec{D} = \epsilon \vec{E},$$

$$\vec{B} = \mu \vec{H} \quad \text{et}$$

$$\vec{j} = \sigma \vec{E},$$

where

\vec{E} is the electric field strength,

\vec{H} is the magnetic field strength,

\vec{D} is the electric displacement (electric flux density),

\vec{B} is the magnetic flux density,

\vec{j} is the electric current density,

ρ is the electric charge density,

σ is the electric conductivity of the material,

ϵ is the permittivity of the material

μ is the permeability of the material.

Divergence

$$\nabla \cdot$$

Measure of
the vector
flow out of a
surface
surrounding a
point

Curl

$$\nabla \times$$

measure of the
rotation of a
vector field



8A – The wave equation

- In the present case of optical materials, we will consider that there are no free charges ($\rho = 0$).
- One can solve the Maxwell equations to obtain an equation which only depends on the electric field (or magnetic field) :

$$\nabla^2 \vec{E} = \epsilon\mu \frac{\partial^2 \vec{E}}{\partial t^2} + \mu\sigma \frac{\partial \vec{E}}{\partial t}.$$

- This equation accepts a harmonic solution of the form:

$$\vec{E} = |\vec{E}| \hat{e} \exp\left(i\omega\left(t - \frac{x}{v}\right)\right)$$

where \hat{e} is a unit vector in the direction of the electric field.

$$\frac{\omega^2}{v^2} = \omega^2 \epsilon\mu - i\omega\mu\sigma$$

- In vacuum, $v = c$, $\epsilon = \epsilon_0 = 8,854187817... \times 10^{-12}$ F/m, $\mu = \mu_0 = 4\pi \times 10^{-7}$ H/m and $\sigma = 0$ and:

$$c^2 = \frac{1}{\epsilon_0 \mu_0}$$



8A – Refractive index

- For a material other than vacuum, we can divide

$$\frac{\omega^2}{v^2} = \omega^2 \epsilon \mu - i \omega \mu \sigma$$

by ω^2 , multiply by c^2 on the left and by $1/\epsilon_0 \mu_0 = c^2$ on the right to obtain:

$$\frac{c^2}{v^2} = \frac{\epsilon \mu}{\epsilon_0 \mu_0} - i \frac{\mu \sigma}{\omega \epsilon_0 \mu_0} = \epsilon_r \mu_r - i \frac{\mu_r \sigma}{\omega \epsilon_0}$$

where $\epsilon_r = \epsilon/\epsilon_0$ and $\mu_r = \mu/\mu_0$ are, the relative permittivity and permeability of the material, respectively.

- We recognize the presence of the refractive index in this equation $N = c/v$:

$$N^2 = \epsilon_r \mu_r - i \frac{\mu_r \sigma}{\omega \epsilon_0},$$

where the refractive index is shown to be a complex number:

$$N = n - ik.$$

8A – Refractive index continued

- By inserting the refractive index into the solution of the wave equation:

$$\vec{E} = |\vec{E}| \hat{e} \exp\left(i\omega\left(t - \frac{x}{v}\right)\right)$$

we obtain:

$$\begin{aligned}\vec{E} &= |\vec{E}| \hat{e} \exp\left(i\left[\omega t - \frac{2\pi N}{\lambda} x\right]\right) \\ &= |\vec{E}| \hat{e} \exp\left(i\left[\omega t - \frac{2\pi(n - ik)}{\lambda} x\right]\right) \\ &= |\vec{E}| \hat{e} \exp\left(-\frac{2\pi k}{\lambda} x\right) \exp\left(i\left[\omega t - \frac{2\pi n}{\lambda} x\right]\right).\end{aligned}$$

- The imaginary part of the refractive index results in a real exponential describing a decrease in intensity of the wave. Therefore, the real part of the index describes the wave's propagation and the imaginary part its absorption.



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Chapter 8A

Page 8A-28

8A - Orthogonality



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Chapter 8A

Page 8A-29

- Let us now suppose that the wave propagates in the direction described by the following unit vector:

$$\hat{s} = \alpha \hat{i} + \beta \hat{j} + \gamma \hat{k}.$$

- It can be demonstrated using Maxwell's equations, that :

$$\hat{s} \times \vec{H} = -\frac{N}{c\mu} \vec{E} \quad \text{et} \quad \frac{N}{c\mu} (\hat{s} \times \vec{E}) = \vec{H}.$$

- We can observe that the electric field, magnetic field and propagation vector all are mutually perpendicular and follow the right hand rule.



8A - Admittance

- Looking closely at the previous equations:

$$\hat{s} \times \vec{H} = -\frac{N}{c\mu} \vec{E} \quad \text{and} \quad \frac{N}{c\mu} (\hat{s} \times \vec{E}) = \vec{H},$$

we notice that:

$$\frac{|\vec{H}|}{|\vec{E}|} = \frac{N}{c\mu} = y$$

which we will call the optical admittance of the material. In vacuum, $N = 1$ and thus:

$$Y_0 = \frac{1}{c\mu_0} = \sqrt{\frac{\epsilon_0}{\mu_0}} = 2.6544187294 \times 10^{-3} \text{ S}$$

- In a material, $\mu_r = 1$ at optical frequencies,

$$y = \frac{N}{c\mu_r\mu_0} = \frac{N}{c\mu_0} = NY_0$$



8A – Poynting vector and irradiance

- The instantaneous rate of flow of energy across a unit area transported by an electromagnetic wave is given by the Poynting vector:

$$\vec{S} = \vec{E} \times \vec{H}.$$

- Since optical frequencies are much too high to observe the variations of the energy flux, we typically will be interested in the average flux; we call this value the irradiance. In the case of a harmonic wave, the irradiance can easily be calculated using the complex form of the wave:

$$\vec{I} = \frac{1}{2} \text{Re}\{\vec{E} \times \vec{H}^*\} = \frac{1}{2} \text{Re}\{\vec{E}\vec{H}^*\} \quad \text{since } \vec{E} \text{ and } \vec{H} \text{ are perpendicular.}$$

- Since we know that:

$$\vec{H} = y(\hat{s} \times \vec{E}),$$

we find that:

$$\vec{I} = \frac{1}{2} \text{Re}\{y\vec{E}\vec{E}^*\hat{s}\} = \frac{1}{2} y\vec{E}\vec{E}^*\hat{s} \quad \text{and}$$

$$|\vec{I}| = \frac{1}{2} y |\vec{E}|^2$$



8A – Simple boundary - continuity

- Let us now express two of the Maxwell equations in their integral form:

$$\oint \vec{E} \cdot d\vec{l} = -\frac{\partial}{\partial t} \iint \vec{B} \cdot d\vec{S} \quad (\text{Maxwell - Faraday law}) \quad \text{and}$$

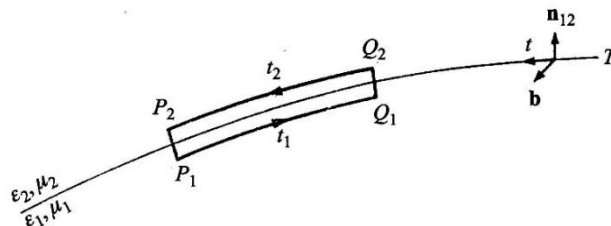
$$\oint \vec{H} \cdot d\vec{l} = \iint \left(\vec{j} + \frac{\partial \vec{D}}{\partial t} \right) \cdot d\vec{S} \quad (\text{Maxwell - Ampere law}),$$

where the first integral is taken on the contour of the surface of the second integral. In the absence of surface currents ($j = 0$) and for an infinitely thin contour, the surface integrals are null and the sides (P_1P_2 and Q_1Q_2) are negligible so that E et H are constant at P_1Q_1 et P_2Q_2 . The integrals can then be approximated by:

$$\left(\vec{E}_1 \cdot \vec{t}_1 + \vec{E}_2 \cdot \vec{t}_2 \right) \delta l = 0 \quad \text{and} \quad \left(\vec{H}_1 \cdot \vec{t}_1 + \vec{H}_2 \cdot \vec{t}_2 \right) \delta l = 0$$

and therefore, we can easily observe that the parallel (tangential) components of the electric and magnetic fields are continuous:

$$\vec{E}_{1,\text{par}} = \vec{E}_{2,\text{par}} \quad \text{et} \quad \vec{H}_{1,\text{par}} = \vec{H}_{2,\text{par}}.$$



Max Born and Emil Wolf, *Principles of Optics*, 7th (expanded edition), Cambridge University Press, 1999.

Fig. 1.2 Derivation of boundary conditions for the tangential components of \mathbf{E} and \mathbf{H} .



8A - Amplitude reflection and transmission at an interface

- Since the electric and magnetic field vectors are continuous at the interface,

$$\vec{E}_i + \vec{E}_r = \vec{E}_t \quad \text{and}$$

$$\vec{H}_i - \vec{H}_r = \vec{H}_t.$$

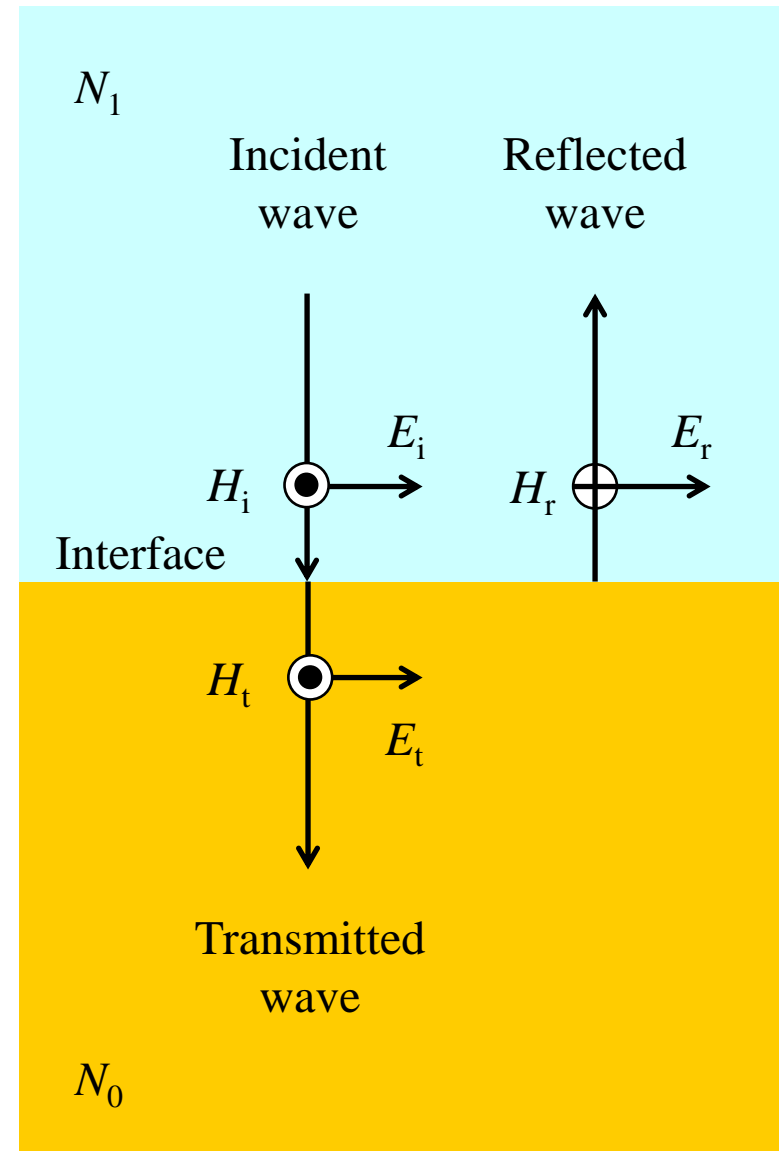
- Using the admittance of the materials we can express the magnetic fields as a function of the electric fields:

$$y_1 \vec{E}_i - y_1 \vec{E}_r = y_0 \vec{E}_t.$$

- We can then replace either the transmitted or reflected beams and obtain:

$$r = \frac{\vec{E}_r}{\vec{E}_i} = \frac{y_1 - y_0}{y_0 + y_1} = \frac{N_1 - N_0}{N_0 + N_1} \quad \text{and}$$

$$t = \frac{\vec{E}_t}{\vec{E}_i} = \frac{2y_1}{y_0 + y_1} = \frac{2N_1}{N_0 + N_1}.$$





8A – Reflectance and transmittance

- The amplitude of the reflected and transmitted beams are respectively,

$$\vec{E}_r = r\vec{E}_i \quad \text{and} \quad \vec{E}_t = t\vec{E}_i$$

- The irradiances of the incident, reflected and transmitted beams are therefore:

$$I_i = \frac{1}{2} y_1 |\vec{E}_i|^2,$$

$$I_r = \frac{1}{2} y_1 |\vec{E}_r|^2 = \frac{1}{2} y_1 |r\vec{E}_i|^2 = |r|^2 \frac{1}{2} y_1 |\vec{E}_i|^2 = |r|^2 I_i \quad \text{and}$$

$$I_t = \frac{1}{2} y_0 |\vec{E}_t|^2 = \frac{1}{2} y_0 |t\vec{E}_i|^2 = |t|^2 \frac{y_0}{y_1} \frac{1}{2} y_1 |\vec{E}_i|^2 = |t|^2 \frac{y_0}{y_1} I_i.$$

- The reflectance and transmittance (reflection and transmission in irradiance) are then given by:

$$R = \frac{I_r}{I_i} = |r|^2 \quad \text{and} \quad T = \frac{I_t}{I_i} = \frac{y_0}{y_1} |t|^2 = \frac{n_0}{n_1} |t|^2.$$

- It is simple to demonstrate that for a single interface, $R + T = 1$.
- R and T do not depend on the direction of the light (no absorption).



8A – Change in phase upon reflection

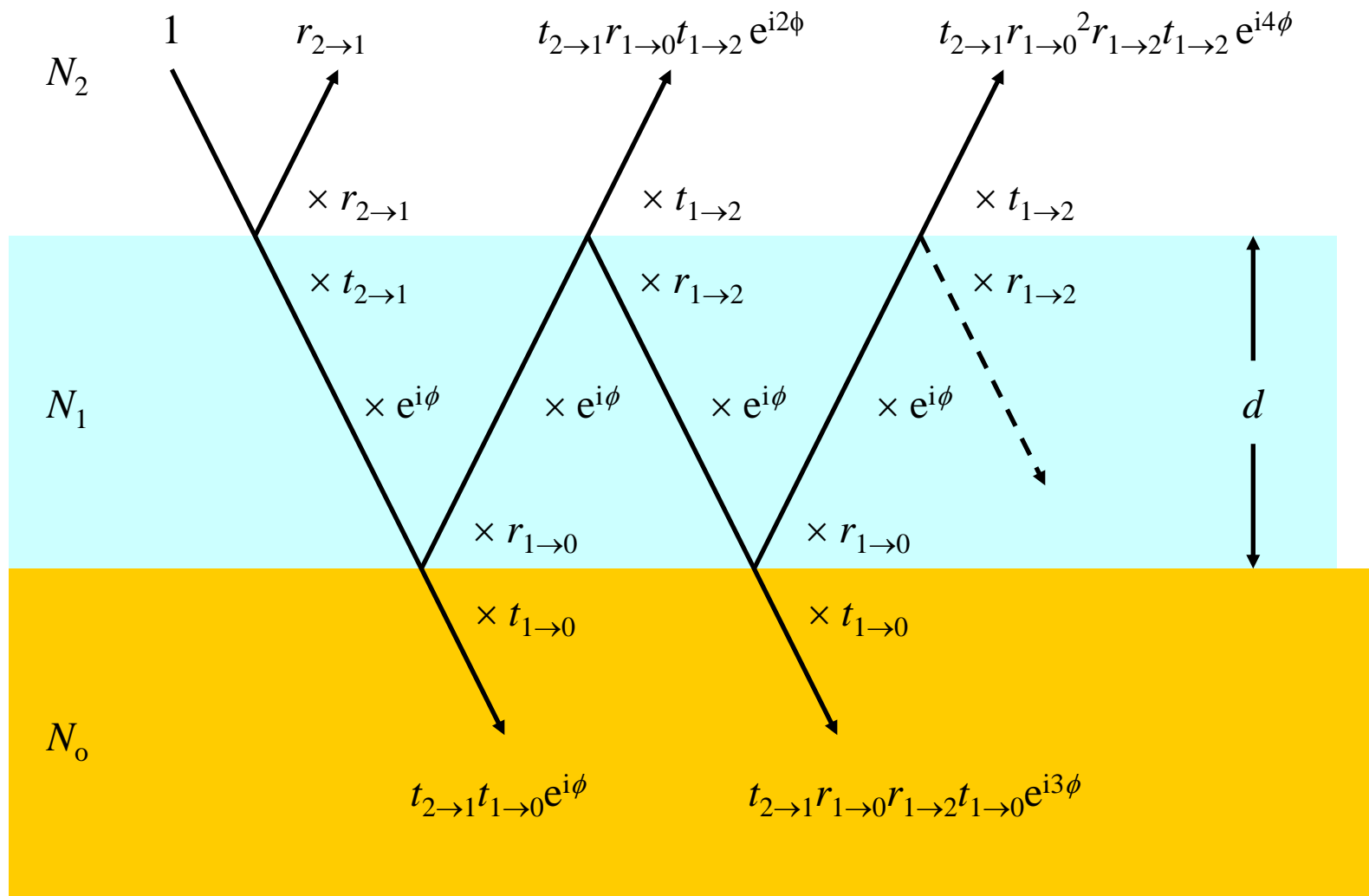
- The amplitude reflection and transmission are given by:

$$r = \frac{N_1 - N_0}{N_0 + N_1} \quad \text{and} \quad t = \frac{2N_1}{N_0 + N_1}.$$

- If the refractive indices are real, then the reflection and transmission coefficients are also real.
- The denominator is always positive.
- In the case of reflection,
 - the numerator is positive if $N_1 > N_0$, r is then positive; this corresponds to no change in phase upon reflection.
 - the numerator is negative if $N_1 < N_0$, r is then negative; this corresponds to a phase change of π upon reflection.
- The numerator is always positive in the case of transmission and there is therefore no phase change in transmission at an interface.
- Trick to remember:
 - *Low to high, phase shift π ,*
 - *High to low, phase shift 0.*



8A – Reflection and transmission of a thin film





8A – Reflection and transmission of a thin film continued

- The wavelength in a thin film of index N_1 is λ/N_1 . For a layer with thickness d , there are $d/(\lambda/N_1)$ waves which « fit » inside. A complete wave corresponds to a phase of 2π , and therefore, for a thin film, the phase is given by:

$$\phi = 2\pi \frac{N_1 d}{\lambda}.$$

- The amplitude reflection and transmission coefficients are then given by:

$$r_{2 \rightarrow 1} = \frac{N_2 - N_1}{N_2 + N_1},$$

$$t_{2 \rightarrow 1} = \frac{2N_2}{N_2 + N_1},$$

$$r_{1 \rightarrow 2} = \frac{N_1 - N_2}{N_1 + N_2} = -r_{2 \rightarrow 1},$$

$$t_{1 \rightarrow 2} = \frac{2N_1}{N_2 + N_1},$$

$$r_{1 \rightarrow 0} = \frac{N_1 - N_0}{N_1 + N_0} \quad \text{and}$$

$$t_{1 \rightarrow 0} = \frac{2N_1}{N_1 + N_0}.$$



8A – Reflection and transmission of a thin film continued

- To obtain the resulting reflection from a thin film, one must add all of the reflected components:

$$r = r_{2 \rightarrow 1} + t_{2 \rightarrow 1} r_{1 \rightarrow 0} t_{1 \rightarrow 2} e^{i2\phi} + t_{2 \rightarrow 1} r_{1 \rightarrow 0}^2 r_{1 \rightarrow 2} t_{1 \rightarrow 2} e^{i4\phi} + t_{2 \rightarrow 1} r_{1 \rightarrow 0}^3 r_{1 \rightarrow 2}^2 t_{1 \rightarrow 2} e^{i6\phi} + \dots$$

which are, with the exception of the first term, a geometric series:

$$r = r_{2 \rightarrow 1} + t_{2 \rightarrow 1} r_{1 \rightarrow 0} t_{1 \rightarrow 2} e^{i2\phi} \sum_{n=0}^{\infty} (r_{1 \rightarrow 0} r_{1 \rightarrow 2} e^{i2\phi})^n.$$

Incidentally, the sum of a geometric series is given by:

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$$

And therefore,

$$r = r_{2 \rightarrow 1} + \frac{t_{2 \rightarrow 1} r_{1 \rightarrow 0} t_{1 \rightarrow 2} e^{i2\phi}}{1 - r_{1 \rightarrow 0} r_{1 \rightarrow 2} e^{i2\phi}}.$$



8A – Reflection and transmission of a thin film continued

- We can simplify this equation by first posing that $r_{1 \rightarrow 2} = -r_{2 \rightarrow 1}$ and bringing all the elements under a common denominator:

$$\begin{aligned}
 r &= r_{2 \rightarrow 1} + \frac{t_{2 \rightarrow 1} r_{1 \rightarrow 0} t_{1 \rightarrow 2} e^{i2\phi}}{1 - r_{1 \rightarrow 0} r_{1 \rightarrow 2} e^{i2\phi}} = r_{2 \rightarrow 1} + \frac{t_{2 \rightarrow 1} r_{1 \rightarrow 0} t_{1 \rightarrow 2} e^{i2\phi}}{1 + r_{1 \rightarrow 0} r_{2 \rightarrow 1} e^{i2\phi}} = r_{2 \rightarrow 1} \frac{1 + r_{1 \rightarrow 0} r_{2 \rightarrow 1} e^{i2\phi}}{1 + r_{1 \rightarrow 0} r_{2 \rightarrow 1} e^{i2\phi}} + \frac{t_{2 \rightarrow 1} r_{1 \rightarrow 0} t_{1 \rightarrow 2} e^{i2\phi}}{1 + r_{1 \rightarrow 0} r_{2 \rightarrow 1} e^{i2\phi}} \\
 &= \frac{r_{2 \rightarrow 1} + r_{1 \rightarrow 0} r_{2 \rightarrow 1}^2 e^{i2\phi} + t_{2 \rightarrow 1} r_{1 \rightarrow 0} t_{1 \rightarrow 2} e^{i2\phi}}{1 + r_{1 \rightarrow 0} r_{2 \rightarrow 1} e^{i2\phi}} = \frac{r_{2 \rightarrow 1} + r_{1 \rightarrow 0} (r_{2 \rightarrow 1}^2 + t_{2 \rightarrow 1} t_{1 \rightarrow 2}) e^{i2\phi}}{1 + r_{1 \rightarrow 0} r_{2 \rightarrow 1} e^{i2\phi}}.
 \end{aligned}$$

and noting that

$$\begin{aligned}
 r_{2 \rightarrow 1}^2 + t_{2 \rightarrow 1} t_{1 \rightarrow 2} &= \left(\frac{N_2 - N_1}{N_2 + N_1} \right)^2 + \frac{2N_2}{N_2 + N_1} \frac{2N_1}{N_2 + N_1} = \frac{N_2^2 - 2N_2N_1 + N_1^2 + 4N_2N_1}{(N_2 + N_1)^2} \\
 &= \frac{N_2^2 + 2N_2N_1 + N_1^2}{(N_2 + N_1)^2} = \frac{(N_2 + N_1)^2}{(N_2 + N_1)^2} = 1.
 \end{aligned}$$

we obtain (a similar approach can be taken for the transmission),

$$r = \frac{r_{2 \rightarrow 1} + r_{1 \rightarrow 0} e^{i2\phi}}{1 + r_{2 \rightarrow 1} r_{1 \rightarrow 0} e^{i2\phi}} \quad \text{and} \quad t = \frac{t_{2 \rightarrow 1} t_{1 \rightarrow 0} e^{i\phi}}{1 + r_{2 \rightarrow 1} r_{1 \rightarrow 0} e^{i2\phi}}.$$



8A – Reflection and transmission of a thin film continued

- For the particular case where the exponential is equal to ± 1 . If $e^{i2\phi} = 1$,

$$r = \frac{r_{2 \rightarrow 1} + r_{1 \rightarrow 0}}{1 + r_{2 \rightarrow 1} r_{1 \rightarrow 0}} = \frac{N_2 - N_0}{N_2 + N_0} = r_{2 \rightarrow 0}$$

and the thin-film has no impact on the reflection. This situation arises when:

$$2\phi = 4\pi \frac{N_1 d}{\lambda} = m(2\pi) \Rightarrow N_1 d = \frac{m\lambda}{2}.$$

i.e. for a half-wave thin-film.

- If $e^{i2\phi} = -1$,
- $$r = \frac{r_{2 \rightarrow 1} - r_{1 \rightarrow 0}}{1 - r_{2 \rightarrow 1} r_{1 \rightarrow 0}}$$

the reflection will be lower if $N_2 < N_1 < N_0$ or higher (for $N_1 > N_0$). This is the case of a quarter-wave thin-film,

$$2\phi = 4\pi \frac{N_1 d}{\lambda} = (2m + 1)\pi \Rightarrow N_1 d = (2m + 1) \frac{\lambda}{4}.$$

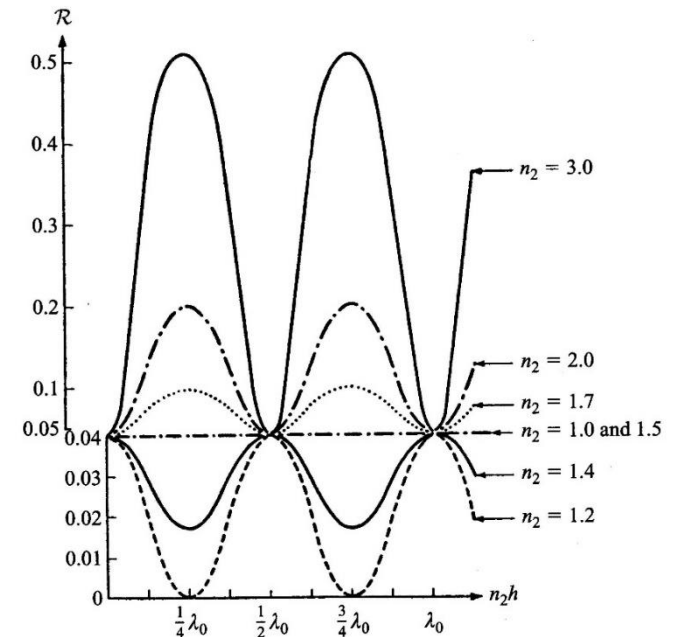


Fig. 1.18 The reflectivity of a dielectric film of refractive index n_2 as a function of its optical thickness. ($\theta_1 = 0$, $n_1 = 1$, $n_3 = 1.5$). [After R. Messner, *Zeiss Nachr.*, 4 (H9) (1943), 253.]

Max Born and Emil Wolf, *Principles of Optics*, 7th (expanded edition), Cambridge University Press, 1999. (Attention, la notation est différente.)

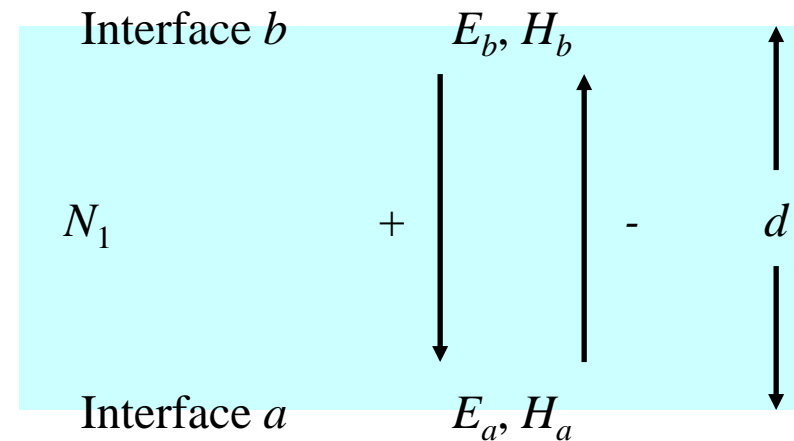


8A – The matrix approach

- The electric and magnetic fields being continuous at the interface, these values are of interest for optical filter calculations.
- At interface a ,

$$E_a = E_{1a}^+ + E_{1a}^-$$

$$H_a = H_{1a}^+ - H_{1a}^- = y_1 E_{1a}^+ - y_1 E_{1a}^-$$



where the + and – signs represent the waves propagating downwards and upwards in the thin film respectively. These fields at interface a are then given by:

$$E_{1a}^+ = \frac{1}{2}(H_a / y_1 + E_a)$$

$$E_{1a}^- = \frac{1}{2}(-H_a / y_1 + E_a)$$

$$H_{1a}^+ = y_1 E_{1a}^+ = \frac{1}{2}(H_a + y_1 E_a)$$

$$H_{1a}^- = -y_1 E_{1a}^- = \frac{1}{2}(H_a - y_1 E_a)$$



8A – The matrix approach continued

- The fields propagating in the positive direction undergo a phase shift of ϕ while those propagating in the negative direction undergo a phase shift of $-\phi$:

$$E_{1b}^+ = E_{1a}^+ e^{i\phi} = \frac{1}{2}(H_a/y_1 + E_a) e^{i\phi}$$

$$E_{1b}^- = E_{1a}^- e^{-i\phi} = \frac{1}{2}(-H_a/y_1 + E_a) e^{-i\phi}$$

$$H_{1b}^+ = H_{1a}^+ e^{i\phi} = \frac{1}{2}(H_a + y_1 E_a) e^{i\phi}$$

$$H_{1b}^- = H_{1a}^- e^{-i\phi} = \frac{1}{2}(H_a - y_1 E_a) e^{-i\phi}$$

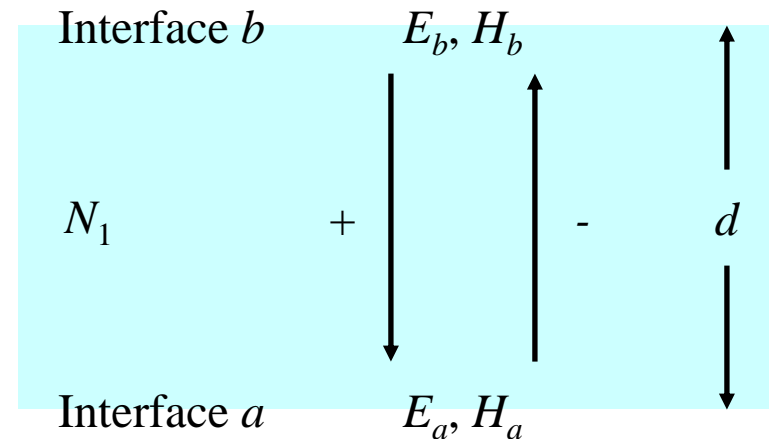
and as a result,

$$E_b = E_{1b}^+ + E_{1b}^- = E_a \frac{e^{i\phi} + e^{-i\phi}}{2} + \frac{H_a}{y_1} \frac{e^{i\phi} - e^{-i\phi}}{2}$$

$$= E_a \cos \phi + H_a / y_1 i \sin \phi$$

$$H_b = H_{1b}^+ + H_{1b}^- = E_a y_1 \frac{e^{i\phi} - e^{-i\phi}}{2} + H_a \frac{e^{i\phi} + e^{-i\phi}}{2}$$

$$= E_a y_1 i \sin \phi + H_a \cos \phi$$



8A – The matrix approach continued

- Finally, we can express

$$E_b = E_a \cos \phi + H_a / y_1 i \sin \phi$$

$$H_b = E_a y_1 i \sin \phi + H_a \cos \phi$$

or using a matrix form:

$$\begin{bmatrix} E_b \\ H_b \end{bmatrix} = \begin{bmatrix} \cos \phi & i / y_1 \sin \phi \\ i y_1 \sin \phi & \cos \phi \end{bmatrix} \begin{bmatrix} E_a \\ H_a \end{bmatrix}.$$





8A – The matrix approach (reflection and transmission)

- In medium 0, only a positive wave is propagating and thus,

$$H_0 = y_0 E_0 \Rightarrow H_a = y_0 E_a$$

and therefore, by dividing by E_a ,

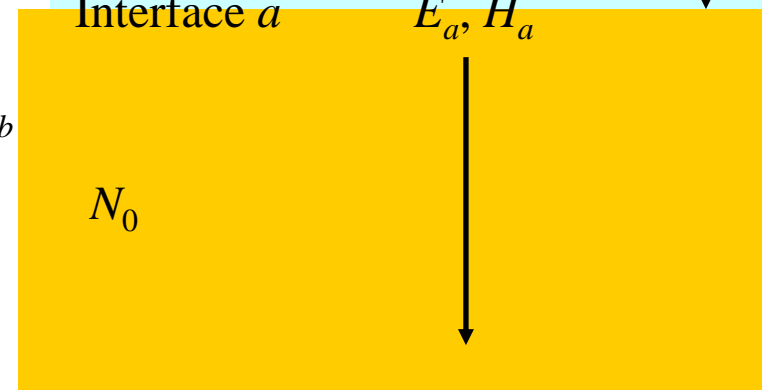
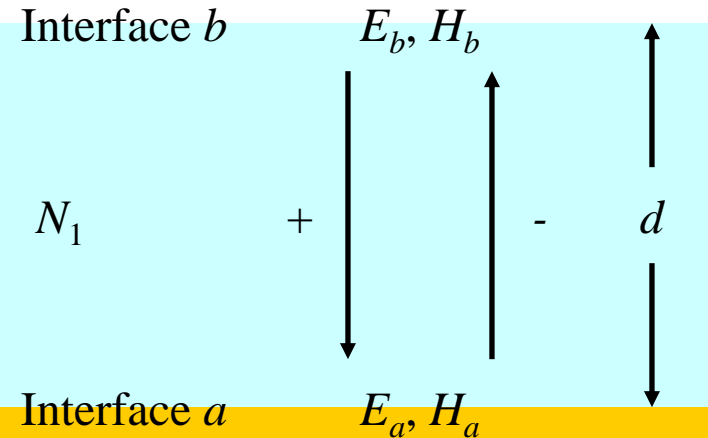
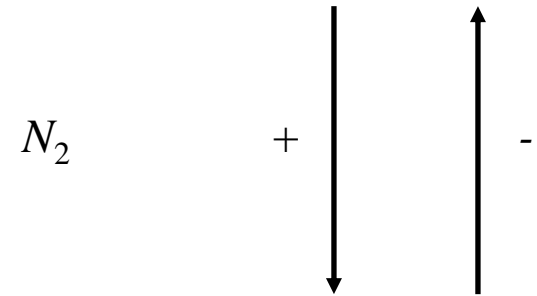
$$\begin{aligned} \begin{bmatrix} E_b/E_a \\ H_b/E_a \end{bmatrix} &= \begin{bmatrix} \cos \phi & i/y_1 \sin \phi \\ iy_1 \sin \phi & \cos \phi \end{bmatrix} \begin{bmatrix} E_a/E_a \\ H_a/E_a \end{bmatrix} \\ &= \begin{bmatrix} \cos \phi & i/y_1 \sin \phi \\ iy_1 \sin \phi & \cos \phi \end{bmatrix} \begin{bmatrix} 1 \\ y_0 \end{bmatrix} \end{aligned}$$

we can also define the admittance of the system:

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} E_b/E_a \\ H_b/E_a \end{bmatrix} \Rightarrow \frac{C}{B} = \frac{H_b/E_a}{E_b/E_a} = \frac{H_b}{E_b} = y_b$$

and finally,

$$r = \frac{y_2 - y_b}{y_b + y_2} \quad t = \frac{2y_2}{C + y_2 B}$$





8A – The matrix approach (multilayer system)

- For many interfaces, we can apply the matrix approach repetitively:

$$\begin{bmatrix} E_b \\ H_b \end{bmatrix} = \begin{bmatrix} \cos \phi & i/y_1 \sin \phi \\ iy_1 \sin \phi & \cos \phi \end{bmatrix} \begin{bmatrix} E_a \\ H_a \end{bmatrix}$$

$$\begin{bmatrix} E_c \\ H_c \end{bmatrix} = \begin{bmatrix} \cos \phi & i/y_1 \sin \phi \\ iy_1 \sin \phi & \cos \phi \end{bmatrix} \begin{bmatrix} E_b \\ H_b \end{bmatrix}$$

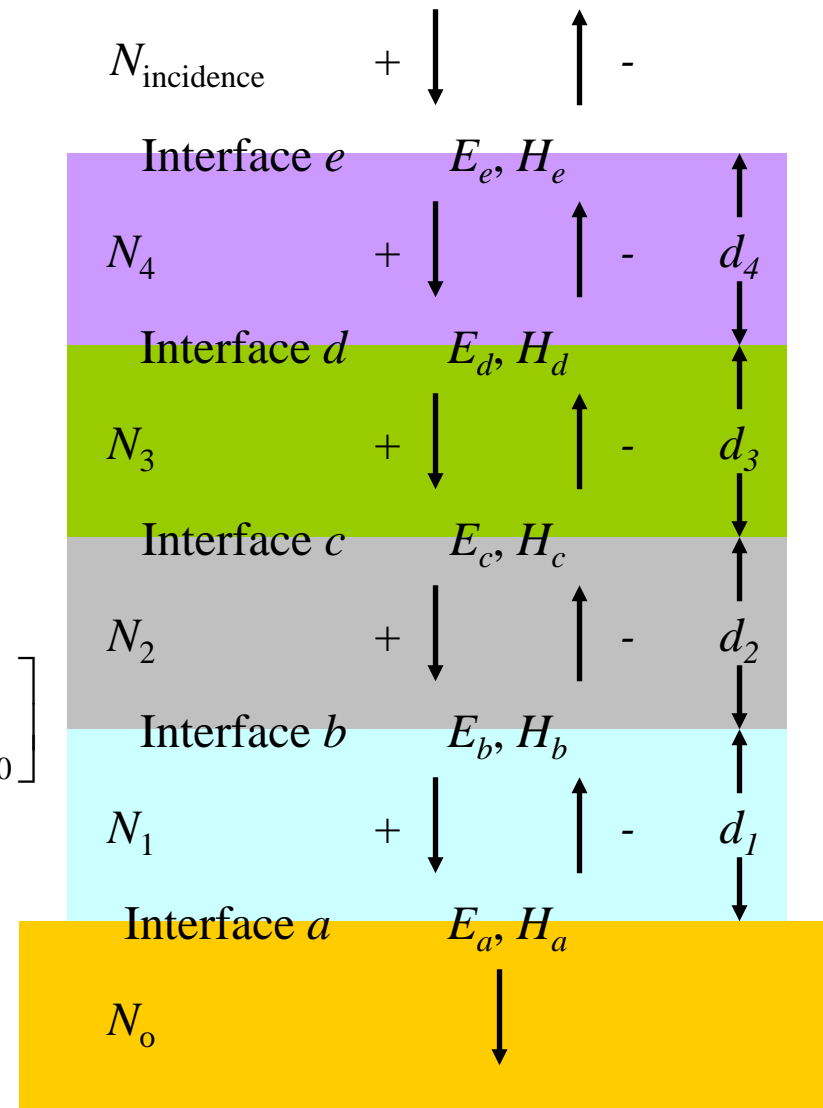
⋮

so that

$$\begin{bmatrix} B \\ C \end{bmatrix} = \left(\prod_n \begin{bmatrix} \cos \phi_n & i/y_n \sin \phi_n \\ iy_n \sin \phi_n & \cos \phi_n \end{bmatrix} \right) \begin{bmatrix} 1 \\ y_0 \end{bmatrix}$$

and since $y_{\text{system}} = C/B$ then

$$r = \frac{y_{\text{incidence}} - y_{\text{system}}}{y_{\text{system}} + y_{\text{incidence}}}$$





8A – The matrix approach (reflectance, transmittance and absorption)

- By dividing by the admittance of vacuum, Y_0 , and in the absence of a magnetic response, we can express the characteristic matrices as a function of the indices of the individual thin films:

$$\begin{bmatrix} B \\ C \end{bmatrix} = \left(\prod_n \begin{bmatrix} \cos \phi_n & i/N_n \sin \phi_n \\ iN_n \sin \phi_n & \cos \phi_n \end{bmatrix} \right) \begin{bmatrix} 1 \\ N_0 \end{bmatrix}$$

and $N_{\text{system}} = C/B$ so that:

$$r = \frac{N_{\text{incidence}} - N_{\text{system}}}{N_{\text{system}} + N_{\text{incidence}}} \quad t = \frac{2N_{\text{incidence}}}{C + N_{\text{incidence}} B}$$

- We now know how to calculate r et t for an assemble of thin films. We previously saw that

$$R = |r|^2 \quad \text{et} \quad T = \frac{n_0}{n_{\text{incidence}}} |t|^2.$$

However, contrary to a simple interface, $R + T$ can differ from 1 because of absorption in the layers:

$$R + T + A = 1.$$



8A – Quarter-wave layers

- When the optical thickness is equal to:

$$n_n d = (2m + 1) \frac{\lambda}{4}.$$

the characteristic matrix simplifies to:

$$\begin{bmatrix} \cos([2m + 1]\pi/2) & i/y_n \sin([2m + 1]\pi/2) \\ iy_n \sin([2m + 1]\pi/2) & \cos([2m + 1]\pi/2) \end{bmatrix} = \begin{bmatrix} 0 & \pm i/y_n \\ \pm iy_n & 0 \end{bmatrix}.$$

- In this case, we say that the layer is a quarter-wave.
- The admittance of a system composed of a quarter-wave is:

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} 0 & i/y_1 \\ iy_1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ y_0 \end{bmatrix} = \begin{bmatrix} iy_0/y_1 \\ iy_1 \end{bmatrix} \Rightarrow y = \frac{C}{B} = \frac{y_1^2}{y_0}.$$

- If there are two quarter-waves,

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} 0 & i/y_2 \\ iy_2 & 0 \end{bmatrix} \begin{bmatrix} 0 & i/y_1 \\ iy_1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ y_0 \end{bmatrix} \Rightarrow y = \frac{C}{B} = \frac{y_2^2 y_0}{y_1^2}.$$

8A – Quarter-wave layers continued

- For three quarter-waves,

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} 0 & i/y_3 \\ iy_3 & 0 \end{bmatrix} \begin{bmatrix} 0 & i/y_2 \\ iy_2 & 0 \end{bmatrix} \begin{bmatrix} 0 & i/y_1 \\ iy_1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ y_0 \end{bmatrix} \Rightarrow y = \frac{C}{B} = \frac{y_3^2 y_1^2}{y_2^2 y_0}.$$

- For four quarter-waves,

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} 0 & i/y_4 \\ iy_4 & 0 \end{bmatrix} \begin{bmatrix} 0 & i/y_3 \\ iy_3 & 0 \end{bmatrix} \begin{bmatrix} 0 & i/y_2 \\ iy_2 & 0 \end{bmatrix} \begin{bmatrix} 0 & i/y_1 \\ iy_1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ y_0 \end{bmatrix} \Rightarrow y = \frac{C}{B} = \frac{y_4^2 y_2^2 y_0}{y_3^2 y_1^2}.$$

- Therefore, for an odd number of quarter-waves:

$$y = \frac{\cdots y_5^2 y_3^2 y_1^2}{\cdots y_4^2 y_2^2 y_0}.$$

While for an even number:

$$y = \frac{\cdots y_6^2 y_4^2 y_2^2 y_0}{\cdots y_5^2 y_3^2 y_1^2}.$$





8A – One layer antireflective filter

- We've seen how the reflection is minimized when using a quarter-wave layer with a refractive index given by $N_2 < N_1 < N_0$. The index of such a system is given by:

$$N = \frac{N_1^2}{N_0}$$

and its reflection by

$$r = \frac{N_{\text{incidence}} - N}{N_{\text{incidence}} + N} = \frac{N_{\text{incidence}} - N_1^2/N_0}{N_{\text{incidence}} + N_1^2/N_0}$$

- The reflection is null if

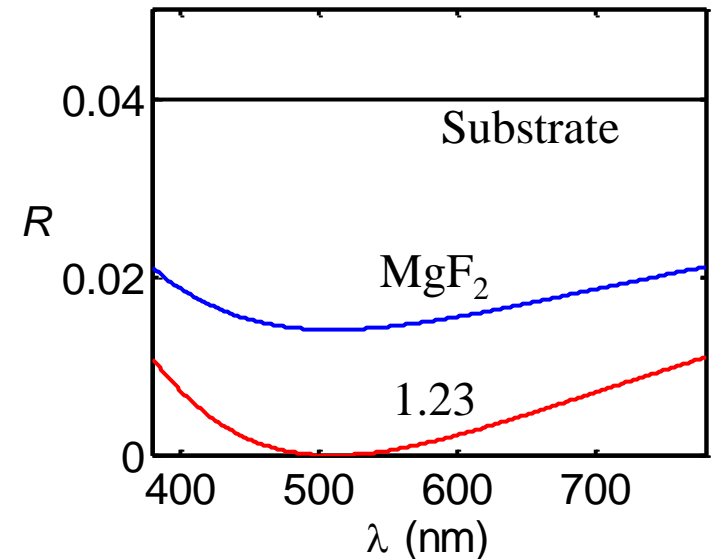
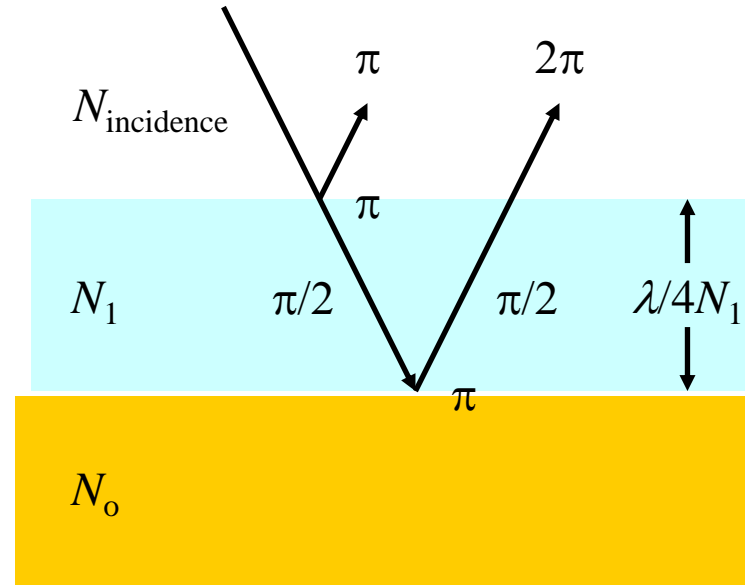
$$\frac{N_{\text{incidence}} - N_1^2/N_0}{N_{\text{incidence}} + N_1^2/N_0} = 0$$

$$\Rightarrow N_{\text{incidence}} - N_1^2/N_0 = 0$$

$$\Rightarrow N_1^2 = N_{\text{incidence}} N_0$$

- For glass ($N_0 = 1.52$) in air ($N_{\text{incidence}} = 1.00$) the layer's index must be:

$$N_1 = \sqrt{1.52 \cdot 1.00} = 1.23$$





8A – Two-layer antireflective filter

- The index of a two-layer filter composed of quarter-waves is

$$N = \frac{N_2^2 N_0}{N_1^2}$$

and its reflection is given by

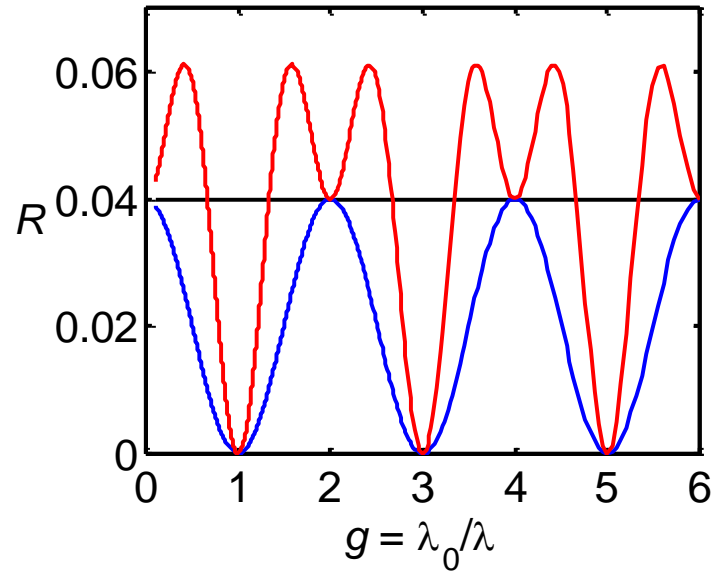
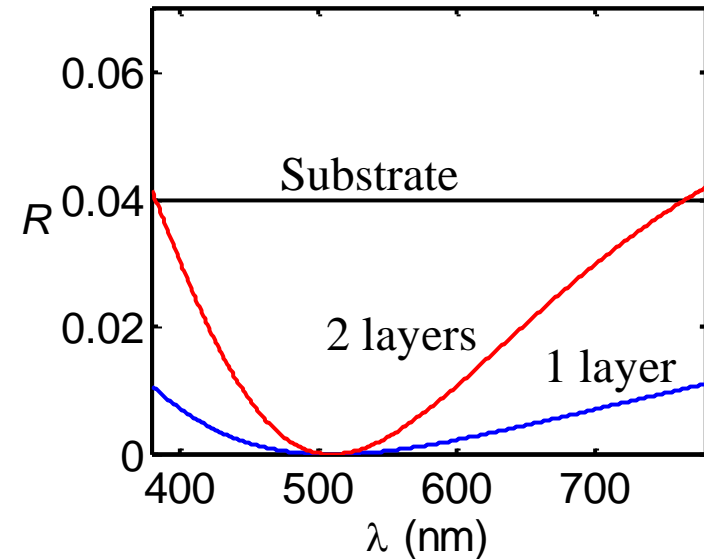
$$r = \frac{N_{\text{incidence}} - N_2^2 N_0 / N_1^2}{N_{\text{incidence}} + N_2^2 N_0 / N_1^2}$$

- Its reflection is null when

$$N_{\text{incidence}} - N_2^2 N_0 / N_1^2 = 0 \Rightarrow \frac{N_2^2}{N_1^2} = \frac{N_{\text{incidence}}}{N_0}$$

- Choosing $N_2 = 1.38$ (MgF_2), then

$$N_1 = N_2 \sqrt{\frac{N_0}{N_{\text{incidence}}}} = 1.38 \sqrt{\frac{1.52}{1.00}} = 1.70$$





8A – Quarter-wave reflector

- The effective index of a quarter-wave stack made of two materials with indices N_H et N_L is

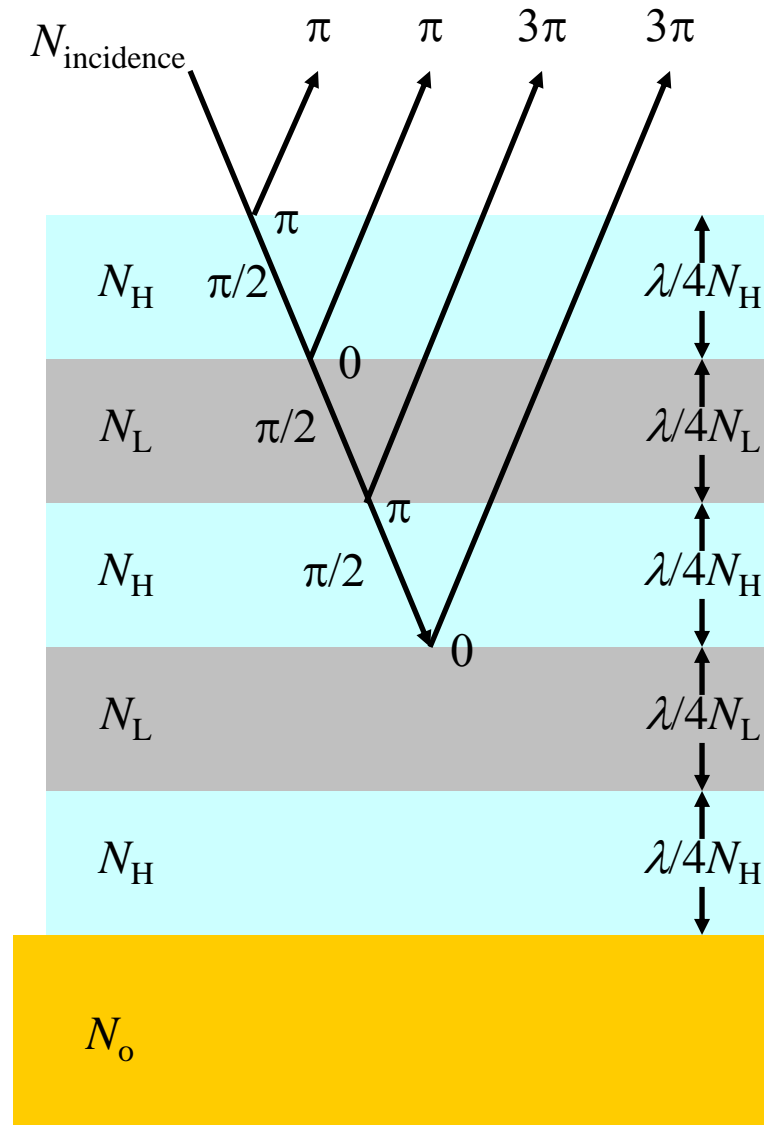
$$N = \frac{\dots N_H^2 N_H^2 N_H^2}{\dots N_L^2 N_L^2 N_0}$$

- The reflectance of such a system is

$$R = \left(\frac{N_{\text{incidence}} - N_H^{2m+2} / N_L^{2m} N_0}{N_{\text{incidence}} + N_H^{2m+2} / N_L^{2m} N_0} \right)^2$$

where $2m + 1$ is the total number of layers.

- To maximize the reflection, one needs to maximize the admittance y of the system; this can be done by maximizing the N_H/N_L ratio and/or by increasing the number of layers.



8A – Quarter-wave reflector continued

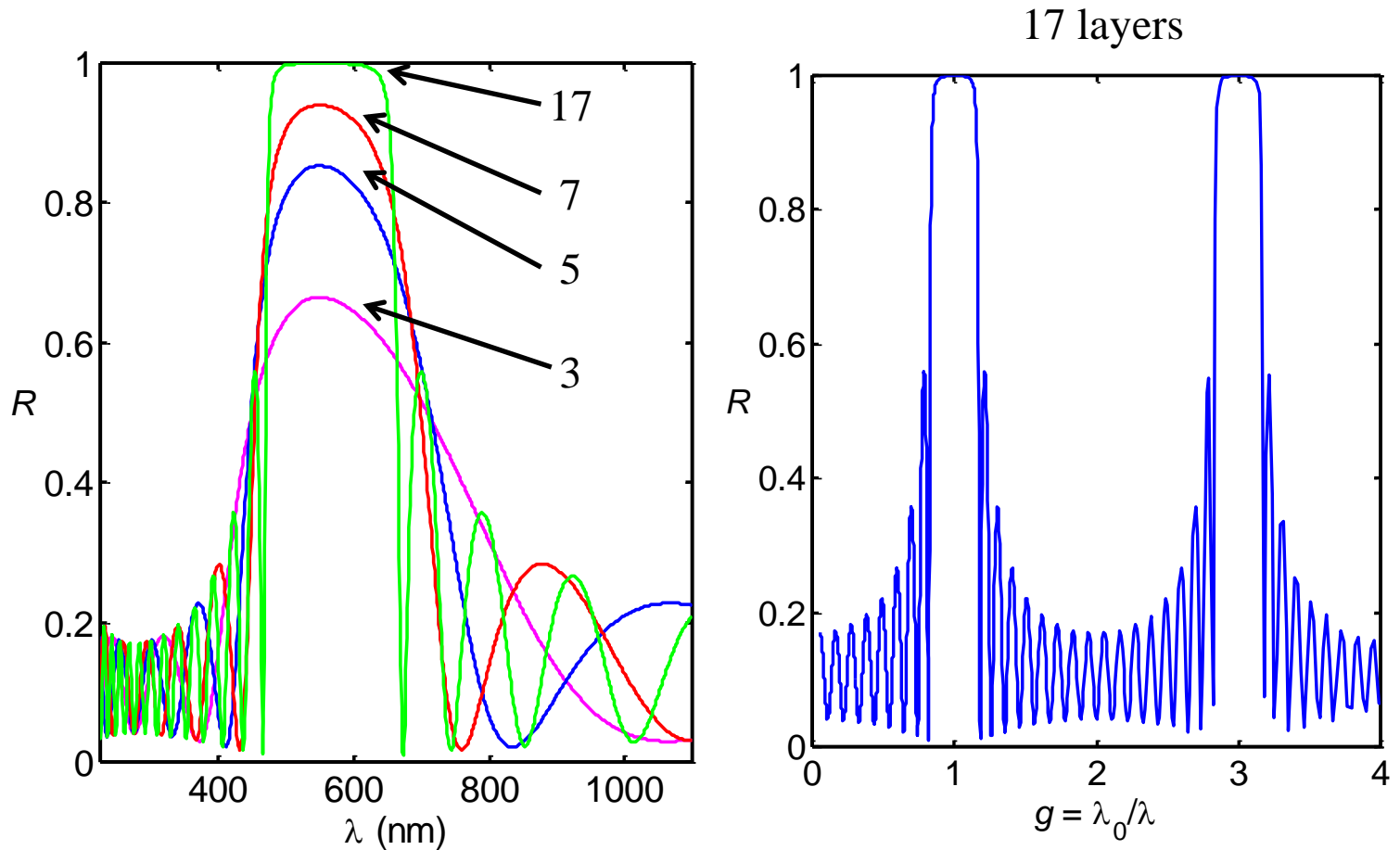


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Nanoengineering of thin
films

Chapter 8A

Page 8A-52





8A – Half-wave layer

- When the thickness of the layer is

$$n_n d = m \frac{\lambda}{2}.$$

the characteristic matrix simplifies to

$$\begin{bmatrix} \cos(2m\pi) & i/y_n \sin(2m\pi) \\ iy_n \sin(2m\pi) & \cos(2m\pi) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

which does not change the admittance of the system. These layers are simply « absent » and have no impact at the reference wavelength.

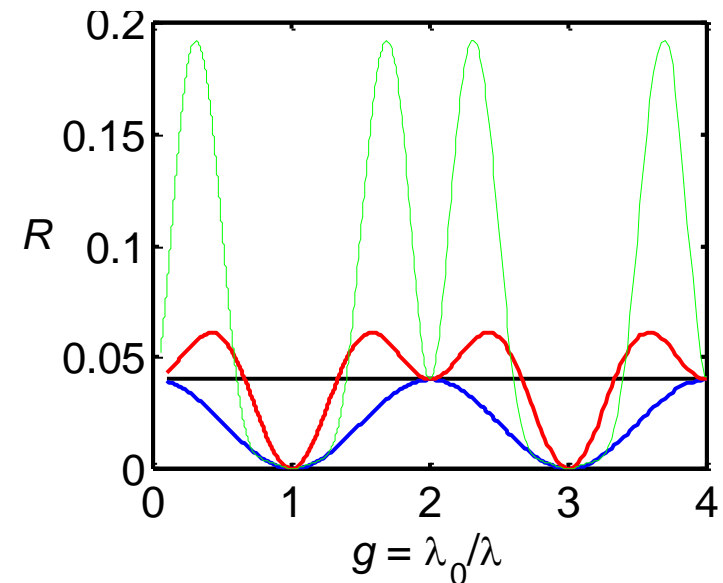
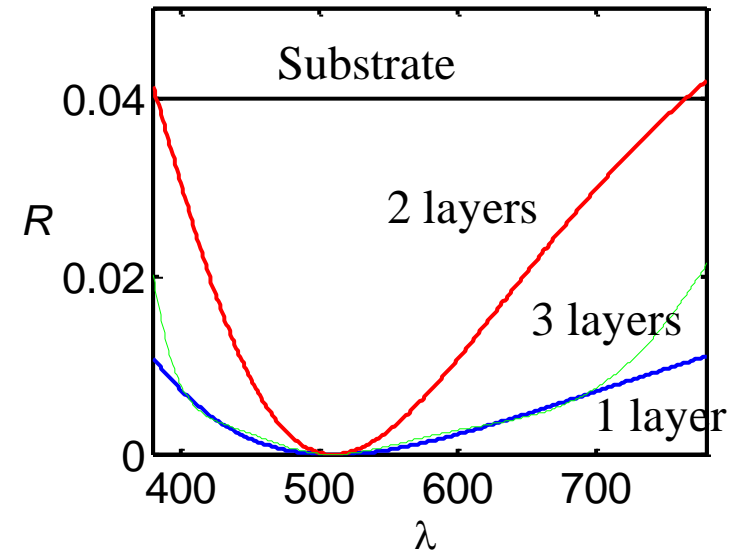
- When $nd = \lambda/2$, these layers are known as half-wave layers.



8A – Three-layer antireflective filter

- Since adding a half-wave layer does not impact the reflection at the reference wavelength, one can add one to modify the shape of the spectrum.
- Adding a high index layer (≈ 2.1) between the layers of a two-layer system, allows one to enlarge the minimum reflection region.

Substrate | $\frac{1}{4}$ 1.70 | $\frac{1}{2}$ 2.10 | $\frac{1}{4}$ 1.38 | Air





8A – Snell's law

- We've seen how the speed of light depends on the refractive index of the medium

$$N = \frac{c}{v}$$

this entails a change in the wavelength

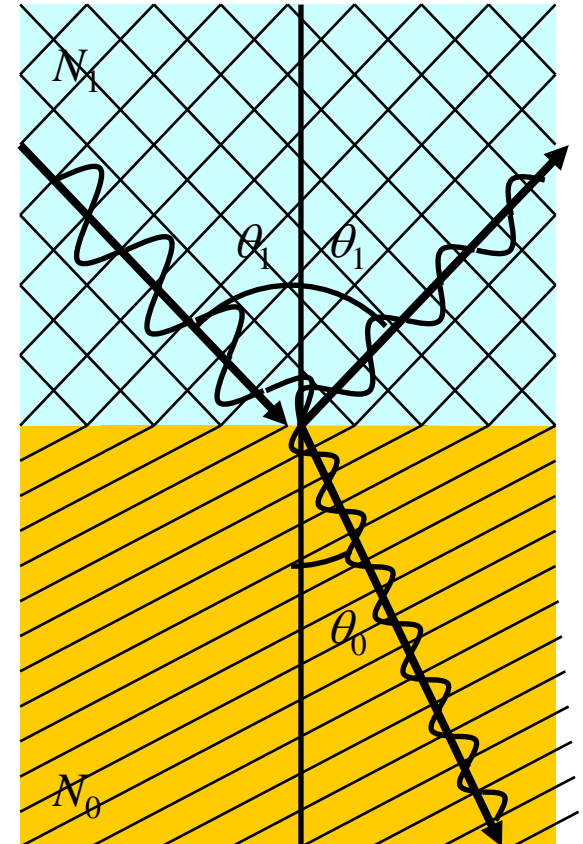
$$\lambda = \frac{\lambda_0}{N}$$

where λ_0 is the wavelength in vacuum.

- If light arrives at an interface at an oblique angle,

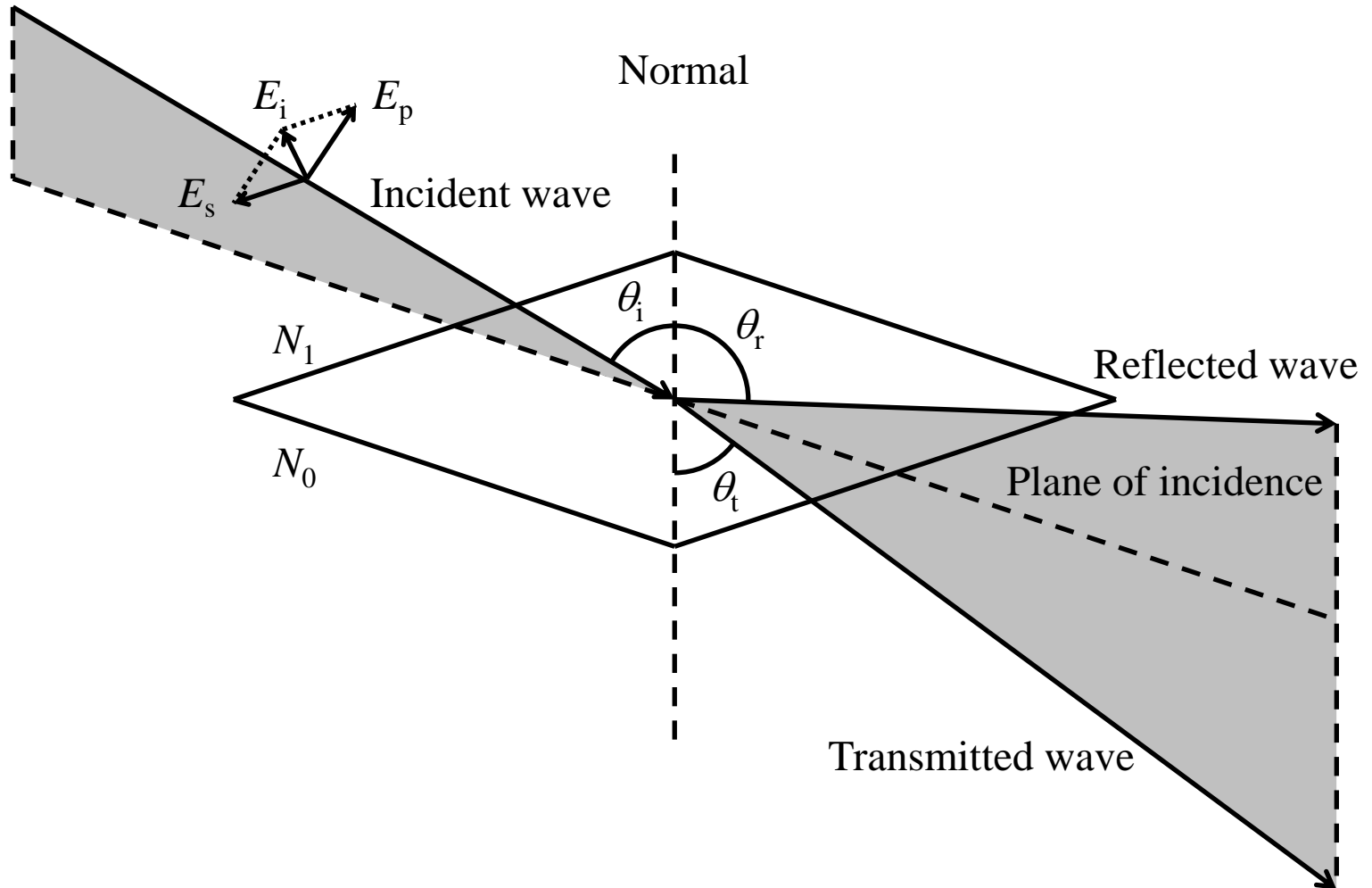
$$N_1 \sin \theta_1 = N_0 \sin \theta_0$$

to ensure the continuity of the electric and magnetic fields at the interface. In fact, $N_i \sin \theta_i$ is constant.





8A - Polarization



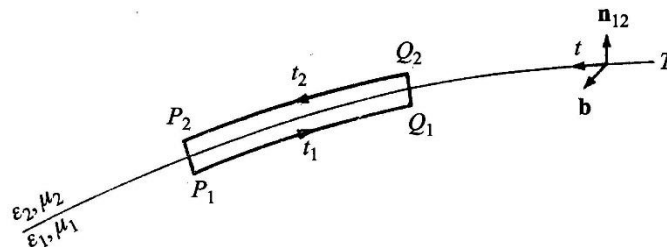


8A - Boundary conditions at oblique incidence

- Remember that the parallel (tangential) electric and magnetic fields are preserved at an interface:

$$\vec{E}_{1,\text{par}} = \vec{E}_{2,\text{par}} \quad \text{et} \quad \vec{H}_{1,\text{par}} = \vec{H}_{2,\text{par}}$$

- When considering oblique incidence, one must modify the reflection coefficients.



Max Born and Emil Wolf, *Principles of Optics*, 7th (expanded edition), Cambridge University Press, 1999.

Fig. 1.2 Derivation of boundary conditions for the tangential components of \mathbf{E} and \mathbf{H} .



8A - Boundary conditions at oblique incidence continued

s polarization

- The continuity conditions for s polarization are:

$$E_i + E_r = E_t \quad \text{and}$$

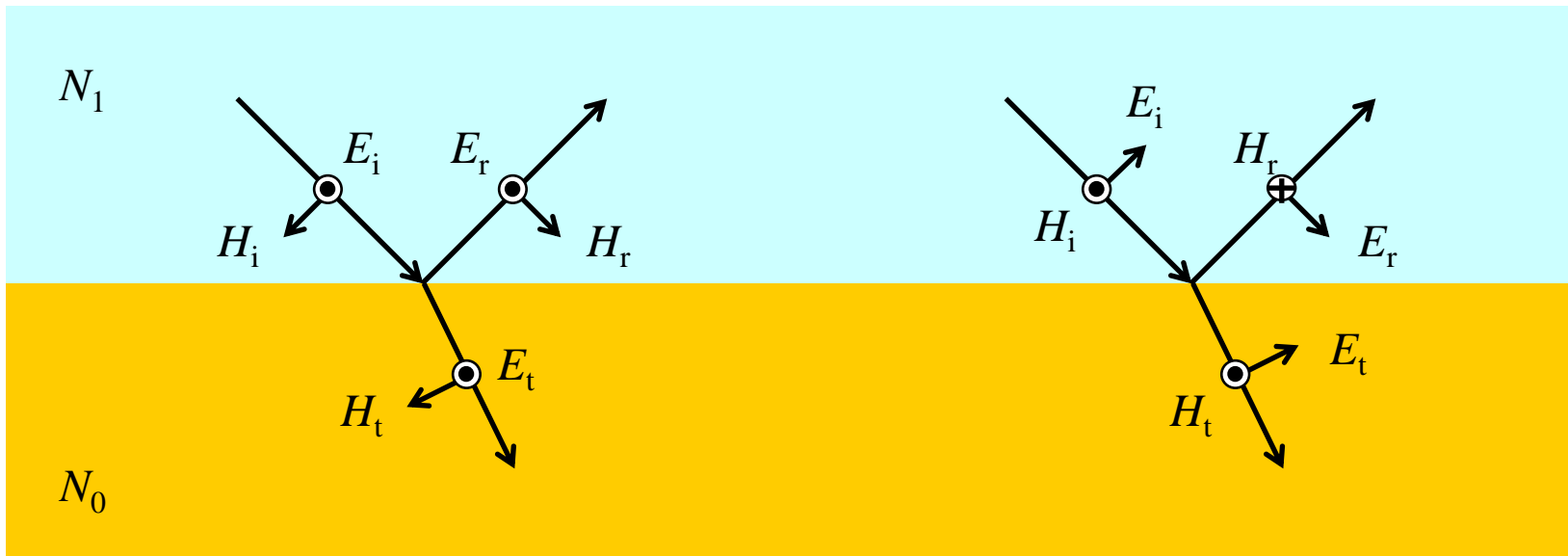
$$H_i \cos \theta_1 - H_r \cos \theta_1 = H_t \cos \theta_0$$

p polarization

- The continuity conditions for p polarization are:

$$E_i \cos \theta_1 + E_r \cos \theta_1 = E_t \cos \theta_0 \quad \text{and}$$

$$H_i - H_r = H_t$$





8A – Reflection and transmission at an interface at oblique incidence

s polarization

- The new continuity conditions result in a change of the reflection and transmission coefficients:

$$r = \frac{N_1 \cos \theta_1 - N_0 \cos \theta_0}{N_0 \cos \theta_0 + N_1 \cos \theta_1} \quad \text{and}$$

$$t = \frac{2N_1 \cos \theta_1}{N_0 \cos \theta_0 + N_1 \cos \theta_1}.$$

p polarization

$$r = \frac{N_1/\cos \theta_1 - N_0/\cos \theta_0}{N_0/\cos \theta_0 + N_1/\cos \theta_1} \quad \text{and}$$

$$t = \frac{2N_1/\cos \theta_1}{N_0/\cos \theta_0 + N_1/\cos \theta_1}.$$

Which brings us to define the pseudo indices

$$\eta_0 = N_0 \cos \theta_0$$

$$\eta_1 = N_1 \cos \theta_1$$

⋮

$$\eta_i = N_i \cos \theta_i$$

$$\eta_0 = N_0/\cos \theta_0$$

$$\eta_1 = N_1/\cos \theta_1$$

⋮

$$\eta_i = N_i/\cos \theta_i$$

And which allows one to write

$$r = \frac{\eta_1 - \eta_0}{\eta_0 + \eta_1} \quad \text{and} \quad t = \frac{2\eta_1}{\eta_0 + \eta_1}.$$

$$r = \frac{\eta_1 - \eta_0}{\eta_0 + \eta_1} \quad \text{and} \quad t = \frac{2\eta_1}{\eta_0 + \eta_1}.$$



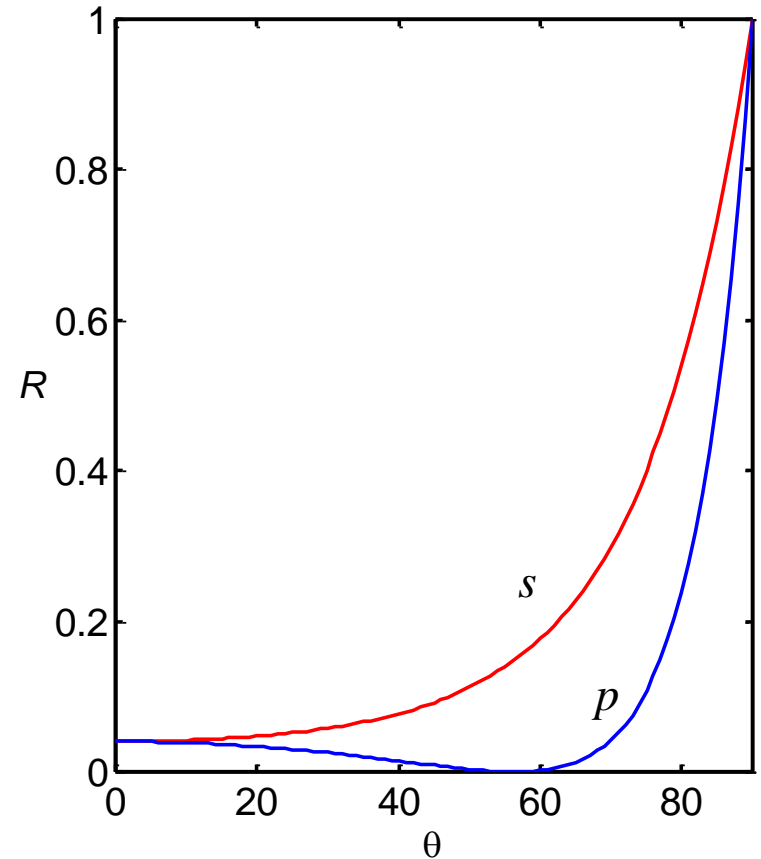
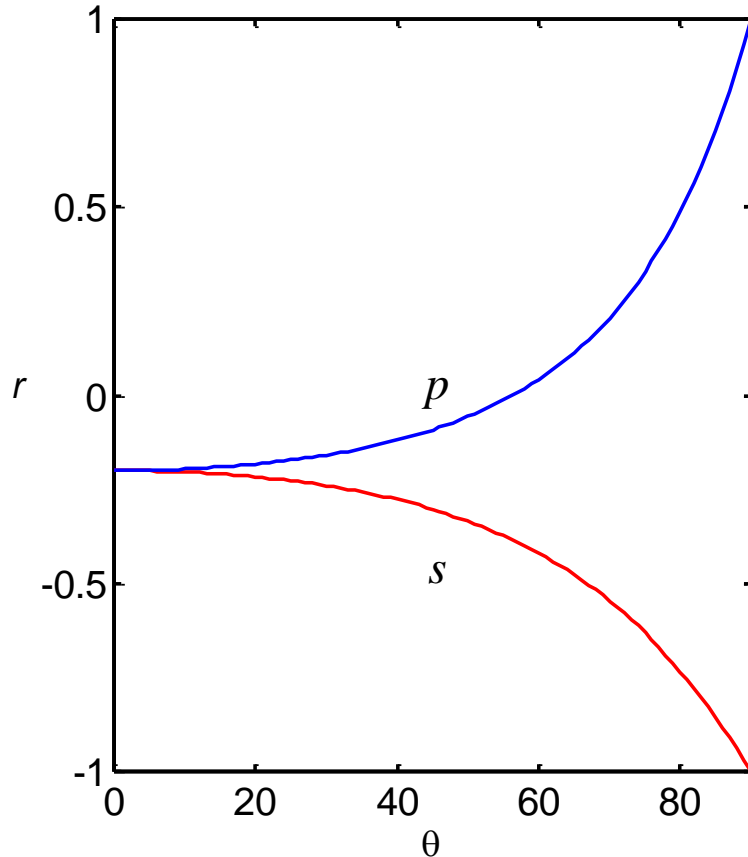
8A – Brewster angle



PHS6317 –
Nanoengineering of thin
films

Chapter 8A

Page 8A-60





8A – Matrix approach for oblique incidence

- The characteristic matrix can then be adapted for oblique incidence by using the pseudo indices:

$$\begin{bmatrix} B \\ C \end{bmatrix} = \left(\prod_n \begin{bmatrix} \cos \phi_n & i/\eta_n \sin \phi_n \\ i\eta_n \sin \phi_n & \cos \phi_n \end{bmatrix} \right) \begin{bmatrix} 1 \\ \eta_0 \end{bmatrix}$$

and by modifying the phase shift in the layers:

$$\phi_n = 2\pi \frac{N_n d}{\lambda} \cos \theta_n.$$