Fundamentals of Multilayer Coating Design

Compiled by Dr. Nishikant Sonwalkar

1 Introduction

Multilayer coatings are essential in various optical applications, including anti-reflective coatings, mirrors, filters, and more. These coatings consist of multiple layers of materials with different refractive indices, designed to manipulate light through interference effects. This article covers the fundamentals of multilayer coating design, including the principles of coherence, the application of Fresnel equations, phase shift calculations, and the design of gradient index coatings.

2 Coherence and Incoherence in Multilayer Coatings

2.1 Coherent Light

Light is considered coherent if the phase relationship between the waves is maintained over the distance of interest. This typically occurs when the light source is monochromatic (single wavelength) and has a long coherence length (e.g., lasers).

In coherent layers, the phase of the light waves is preserved, and interference effects (constructive and destructive) are significant. The Fresnel equations and the transfer matrix method are used to calculate the reflectance and transmittance by considering the phase changes at each interface and within each layer.

2.2 Incoherent Light

Light is considered incoherent if the phase relationship between the waves is not maintained over the distance of interest. This typically occurs with broadband light sources (e.g., sunlight, LEDs) where the coherence length is short compared to the thickness of the layers.

In incoherent layers, the phase of the light waves is randomized, and interference effects average out. The reflectance and transmittance are calculated by considering the intensity of the light rather than the phase.

3 Application of Fresnel Equations

3.1 Fresnel Equations for a Single Interface

For an interface between two media with refractive indices n_1 and n_2:

3.1.1 Reflection Coefficients

For perpendicular (s-polarized) light:

$$r_s = \frac{n_1 \cos\theta_i - n_2 \cos\theta_t}{n_1 \cos\theta_i + n_2 \cos\theta_t}$$

For parallel (p-polarized) light:

$$r_p = \frac{n_2 \cos\theta_i - n_1 \cos\theta_t}{n_2 \cos\theta_i + n_1 \cos\theta_t}$$

3.1.2 Transmission Coefficients

For perpendicular (s-polarized) light:

$$t_s = \frac{2n_1 \cos\theta_i}{n_1 \cos\theta_i + n_2 \cos\theta_t}$$

For parallel (p-polarized) light:

$$t_p = \frac{2n_1 \cos\theta_i}{n_2 \cos\theta_i + n_1 \cos\theta_t}$$

Where:

- θ_i is the angle of incidence.
- θ_t is the angle of transmission, given by Snell's law: $n_1 \sin\theta_i = n_2 \sin\theta_t$.

4 Multilayer Coating Design

For a multilayer stack, the overall reflectance and transmittance are calculated by considering multiple reflections and transmissions at each interface. This is typically done using the transfer matrix method.

4.1 Transfer Matrix Method

4.1.1 Transfer Matrix for a Single Layer

For a layer with refractive index n_i, thickness d_i, and angle of incidence θ_i:

$$M_i = \begin{pmatrix} \cos\delta_i & i\eta_i \sin\delta_i \\ i\eta_i^{-1} \sin\delta_i & \cos\delta_i \end{pmatrix}$$

where:

$$\delta_i = \frac{2\pi n_i d_i \cos\theta_i}{\lambda}$$

is the phase thickness, and

$$\eta_i = \frac{n_i}{\cos\theta_i}$$

for s-polarized light, and

$$\eta_i = n_i \cos\theta_i$$

for p-polarized light.

4.1.2 Overall Transfer Matrix

For a stack of N layers, the overall transfer matrix M is the product of the individual layer matrices:

$$M = M_1 M_2 \cdots M_N$$

4.1.3 Reflectance and Transmittance

The overall reflectance R and transmittance T can be calculated from the elements of the overall transfer matrix M:

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}$$

Reflectance:

$$R = \left| \frac{M_{21}}{M_{11}} \right|^2$$

Transmittance:

$$T = \left| \frac{1}{M_{11}} \right|^2 \frac{\eta_N}{\eta_0}$$

where η_0 and η_N are the wave impedances of the incident and exit media, respectively.

5 Phase Angle and Phase Thickness

5.1 Actual Thickness

Actual Thickness (d): This is the physical thickness of the layer, measured in units such as micrometers (μm) or nanometers (nm).

5.2 Refractive Index

Refractive Index (n): This is a measure of how much the speed of light is reduced inside the material compared to the speed of light in a vacuum. It is a dimensionless quantity.

5.3 Optical Thickness

Optical Thickness: This is the product of the actual thickness and the refractive index of the layer. It represents the effective thickness of the layer in terms of the phase change experienced by light traveling through it.

$$\text{Optical Thickness} = n \cdot d$$

5.4 Phase Angle

Phase Angle (δ): This is the phase shift that a light wave undergoes as it travels through a layer of material. It is related to the optical thickness and the wavelength of the light.

5.5 Phase Thickness

Phase Thickness (δ): This is the phase shift expressed in radians. It is given by:

$$\delta = \frac{2\pi n d \cos\theta}{\lambda}$$

where:

- n is the refractive index of the layer.
- d is the actual thickness of the layer.
- θ is the angle of incidence inside the layer.
- λ is the wavelength of the light in a vacuum.

6 Relationships and Explanation

6.1 Actual Thickness vs. Optical Thickness

- The actual thickness d is the physical measurement of the layer.
- The optical thickness $n \cdot d$ takes into account the refractive index, indicating how the layer affects the phase of the light wave.

6.2 Phase Thickness

- The phase thickness δ represents the phase shift in radians that the light wave experiences as it travels through the layer.
- It depends on the optical thickness and the wavelength of the light.

6.3 Phase Angle

The phase angle is essentially the same as the phase thickness but is often referred to in the context of the phase shift experienced by the light wave.

7 Example Calculation

Let's consider a layer with:

- Refractive index $n = 1.5$
- Actual thickness $d = 100$ nm
- Wavelength of light $\lambda = 500$ nm
- Normal incidence ($\theta = 0$)

7.1 Optical Thickness

$$\text{Optical Thickness} = n \cdot d = 1.5 \cdot 100 \text{ nm} = 150 \text{ nm}$$

7.2 Phase Thickness

$$\delta = \frac{2\pi n d \cos\theta}{\lambda} = \frac{2\pi \cdot 1.5 \cdot 100 \text{ nm} \cdot \cos(0)}{500 \text{ nm}} = \frac{2\pi \cdot 150 \text{ nm}}{500 \text{ nm}} = \frac{2\pi \cdot 3}{10} = 6\pi/10 = 1.2\pi \text{ radians}$$

8 Gradient Index Coatings

8.1 Phase Shift in Gradient Index Coatings

In gradient index coatings, the refractive index varies continuously or in discrete steps through the thickness of the coating. This variation can be designed to achieve specific optical properties, such as minimizing reflection over a broad wavelength range or creating specific transmission characteristics.

8.2 Continuous Gradient Index

For a continuous gradient index profile, where the refractive index $n(z)$ varies smoothly with the position z within the layer, the phase shift δ is given by:

$$\delta = \frac{2\pi}{\lambda} \int_0^d n(z)\, dz$$

where:

- λ is the wavelength of the light in a vacuum.
- d is the total thickness of the gradient index layer.
- $n(z)$ is the refractive index as a function of position z within the layer.

8.3 Discrete Gradient Index

For a discrete gradient index profile, where the refractive index changes in steps, the phase shift δ is calculated by summing the contributions from each sub-layer:

$$\delta = \frac{2\pi}{\lambda} \sum_{i=1}^{N} n_i d_i$$

where:

- N is the number of sub-layers.
- n_i is the refractive index of the i-th sub-layer.
- d_i is the thickness of the i-th sub-layer.

9 Example Calculation

Let's consider a gradient index coating with a linear refractive index profile from n_0 to n_1 over a thickness d.

9.1 Continuous Gradient Index

For a linear gradient index profile:

$$n(z) = n_0 + \left(\frac{n_1 - n_0}{d}\right) z$$

The phase shift δ is:

$$\delta = \frac{2\pi}{\lambda} \int_0^d \left(n_0 + \left(\frac{n_1 - n_0}{d}\right) z\right) dz$$

Evaluating the integral:

$$\delta = \frac{2\pi}{\lambda} \left[n_0 z + \left(\frac{n_1 - n_0}{d}\right) \frac{z^2}{2}\right]_0^d$$

$$\delta = \frac{2\pi}{\lambda} \left(n_0 d + \frac{(n_1 - n_0)d}{2}\right)$$

$$\delta = \frac{2\pi}{\lambda} \left(n_0 d + \frac{n_1 d - n_0 d}{2}\right)$$

$$\delta = \frac{2\pi}{\lambda} \left(\frac{2n_0 d + n_1 d - n_0 d}{2}\right)$$

$$\delta = \frac{2\pi}{\lambda} \left(\frac{n_0 d + n_1 d}{2}\right)$$

$$\delta = \frac{2\pi d}{\lambda} \left(\frac{n_0 + n_1}{2}\right)$$

9.2 Discrete Gradient Index

For a discrete gradient index profile with N sub-layers, each with a constant refractive index n_i and thickness $d_i = \frac{d}{N}$:

$$\delta = \frac{2\pi}{\lambda} \sum_{i=1}^{N} n_i d_i$$

$$\delta = \frac{2\pi d}{\lambda N} \sum_{i=1}^{N} n_i$$

10 Gradient Index Design of the AR Coating Layer

10.1 Design Considerations

The design of a gradient index anti-reflective (AR) coating aims to minimize reflection over a broad wavelength range. This can be achieved by gradually changing the refractive index from the substrate to the outermost layer.

10.2 Example Design

Consider a substrate with a refractive index of $n_s = 1.5$ and air with a refractive index of $n_a = 1.0$. We want to design a gradient index AR coating with a total thickness of $d = 100$ nm.

10.2.1 Linear Gradient Index Profile

For a linear gradient index profile:

$$n(z) = n_s + \left(\frac{n_a - n_s}{d}\right) z$$

The phase shift δ is:

$$\delta = \frac{2\pi}{\lambda} \int_0^d \left(n_s + \left(\frac{n_a - n_s}{d}\right) z\right) dz$$

Evaluating the integral:

$$\delta = \frac{2\pi}{\lambda} \left[n_s z + \left(\frac{n_a - n_s}{d}\right) \frac{z^2}{2}\right]_0^d$$

$$\delta = \frac{2\pi}{\lambda} \left(n_s d + \frac{(n_a - n_s) d}{2}\right)$$

$$\delta = \frac{2\pi}{\lambda}\left(n_s d + \frac{n_a d - n_s d}{2}\right)$$

$$\delta = \frac{2\pi}{\lambda}\left(\frac{2n_s d + n_a d - n_s d}{2}\right)$$

$$\delta = \frac{2\pi}{\lambda}\left(\frac{n_s d + n_a d}{2}\right)$$

$$\delta = \frac{2\pi d}{\lambda}\left(\frac{n_s + n_a}{2}\right)$$

10.2.2 Discrete Gradient Index Profile

For a discrete gradient index profile with N sub-layers, each with a constant refractive index n_i and thickness $d_i = \frac{d}{N}$:

$$\delta = \frac{2\pi}{\lambda}\sum_{i=1}^{N} n_i d_i$$

$$\delta = \frac{2\pi d}{\lambda N}\sum_{i=1}^{N} n_i$$

11 Conclusion

Understanding the fundamentals of multilayer coating design, including coherence, the application of Fresnel equations, phase shift calculations, and gradient index coatings, is essential for designing and analyzing optical coatings with tailored properties. By carefully selecting the refractive indices, thicknesses, and profiles of the layers, you can achieve specific reflectance and transmittance characteristics for various applications.