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Single-Layered Thin Film Coatings for Anti-Reflective Purposes: An Optical Study

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Abstract:

This paper delves into the application of thin films in an essential area: anti-reflective coatings (ARCs) for lenses. Through a comprehensive review of existing literature, the paper establishes critical formulas and criteria for evaluating material performance in these applications. It primarily delves into the properties of refraction, dispersion, reflectance and interference. To explore ARCs on lenses, the paper employs a combination of theoretical analysis and simulations based on interference and impedance principles, to provide values for the optimal refractive index and optimal film thickness of the lens. The theoretical values are obtained from common rules or equations utilised, whereas the simulation utilises a gradient-descent algorithm on Python to identify the optimal parameters for lenses. This simulation serves to identify the optimal refractive index and thickness for single-layer ARCs, providing valuable insights into enhancing lens performance. Furthermore, this research posits insights into potential further areas of study, describing the use of ARCs in current and future applications including flexible display screens and AR headsets.

Keywords **—**Lens, Anti-reflective Coatings, Thin films, Optics

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I. INTRODUCTION

Among the many areas of study, anti-reflective coatings (ARCs) for lenses stand out as a crucial and essential field. The reduction of unwanted reflections from lens surfaces is paramount in enhancing optical efficiency and visual clarity. This research paper embarks on a comprehensive exploration of the utilization of thin films in ARCs, aiming to establish critical formulas and evaluation criteria for material performance in these applications. By employing theoretical analysis and advanced simulations based on interference and impedance principles, we delve into the optimal refractive index and thickness for single-layer ARCs. Our findings shed light on valuable insights that can significantly improve lens performance, contributing to the advancement of optical devices and elevating our visual experiences. This study holds the promise of propelling future innovations in thin film technology and revolutionizing lens design for diverse applications in various fields.

II. LITERATURE REVIEW

Prior to delving into the two discussed coatings and their respective applications, it is essential to define and review basic optical properties through a thorough secondary literature review. Optical (from opticus "of sight or seeing," in mediaeval Latin) refers to the manner in which matter interacts with light. Optical properties consist of a large range of features, including but not limited to: refractive index, dispersion, scattering, dichroism, photosensitivity, reflectivity, transmittance and absorption. This section will discuss a few of the relevant properties for the study of electrochromic coatings and ARCs in detail.

A. Refraction and Refractive Indices

In simple terms, the refractive index is a property of a material that indicates the amount of bending light undergoes as it passes from one medium to the material (second medium).[1] The refractive index of a material is a dimensionless quantity, and can also be expressed as the ratio of the speed of light travelling through a vacuum with respect to the speed of light in the second medium. This is delineated by the formula[2]:

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

Where 'n' is the refractive index of the material, 'c' is the speed of light in a vacuum, and 'v' is the speed of light in the material.

TABLE 1: COMMON REFRACTIVE INDICES THAT WILL BE USED THROUGH THE REPORT

Material	Refractive Index (correct to 2 decimal places)
Air	1.00[3]
Tungsten Trioxide (WO_3)	1.99[4] (with a wavelength of 550 nm)
Magnesium Fluoride (MgF_2)	1.38[5] (with a wavelength of 550 nm)
Silicon Dioxide (SiO_2)	1.46[6] (with a wavelength of 550 nm)
Titanium Dioxide (TiO_2)	2.65[7] (with a wavelength of 550 nm)
Glass Lens	1.52[8]

Additionally, another aspect of refraction can be understood from Snell's law. This law is based on an interpretation of Fermat's principle, which explains the tendency of light to travel in the path which yields the shortest time. Snell's law[9] can be visually depicted as follows:

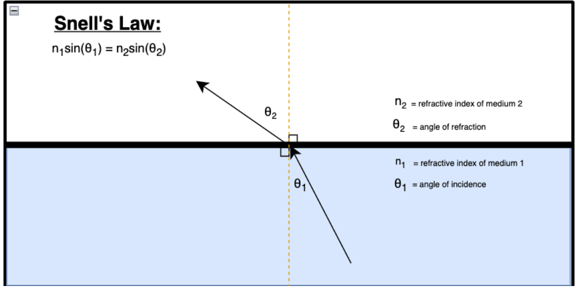

Fig 1.1: A diagram illustrating Snell's Law through exploring the path taken by an electromagnetic wave.

Here, n_1 and n_2 are the refractive indices of the media, and θ_1 and θ_2 refer to the angle of incidence and the angle of refraction respectively.

The phenomenon of refraction is especially pertinent to the study of ARCs, since light refracts a minimum twice as it passes through a lens, whether it is convex or concave - as the light passes from air to the glass medium, and back to the air medium. Furthermore, the refractive index plays an important role in the amount of light transmitted, and thereby is of paramount significance for ARCs.

B. Dispersion

'Dispersion' refers to the variation in the refractive index of a material based on the wavelength of the incoming electromagnetic radiation. The mathematical explanation of this phenomenon involves two fundamental formulae[10]:

$n = \frac{c}{v}$, as discussed before, and

$$v = \lambda \times f$$

Where:
'n' is the refractive index of the medium
'c' is the speed of light in a vacuum (in metres per second)
'v' is the velocity of the wave (in metres per second)
'λ' is the wavelength of the wave (in metres)
'f' is the frequency of the wave (in hertz)

Since the refractive index is related to the velocity of the wave, and the velocity of the wave is directly proportional to the wavelength, it follows that the refractive index would be based on the wavelength of the light that enters it. Thus, if a beam with light of many different wavelengths enters the material, each wavelength will be bent to a different amount, and thus split up or disperse.

The amount of dispersion of light caused by a material is measured through a parameter referred to as 'Abbe's number.' [11] This number can be obtained through calculation[12] as follows:

$$V_D = \frac{n_d - 1}{n_F - n_C}$$

Here,
V_D refers to the abbe's number
n_d refers to the refractive index of the blue F line of the emission spectra of hydrogen
n_F refers to the refractive index of the yellow D lines of the emission spectra of sodium
n_C refers to the refractive index of the red C line of the emission spectra of hydrogen

A higher Abbe's number corresponds to lower dispersion over the visual spectrum.[13]

Dispersion is an important phenomenon for this study since it is the underlying phenomenon responsible for chromatic aberration in optical devices which use lenses such as eyeglasses or cameras. The primary function of lenses is to focus all the light that is refracted at one particular point, referred to as the focal point. However, since the visible spectrum electromagnetic radiation contains a range of wavelengths, the light is refracted differently, thereby causing chromatic aberration - a defect where in coloured fringes are formed, distorting the image quality.

C. Reflectance and Reflection Coefficient

Reflectance is a dimensionless quantity that expresses the amount of light that is reflected off a surface as a ratio between the reflected radiant energy and the incident radiant energy. It depends on the optical frequency of light, angle of incidence and the polarisation of light. The underlying phenomenon that leads to reflectance is the 'response of the electronic structure of the material' to the incident light. In order to calculate reflectance, specifically hemispherical reflectance, the following formula can be used:

$$R = \frac{\phi_e^r}{\phi_e^i}$$

Where:
ϕ_e^r refers to the radiant flux reflected by the material,
ϕ_e^i refers to the radiant flux received by the material,
The study of reflectance is relevant in that it can be used to ensure the constant nature of coating for either electrochromism or anti-reflection, and to make sure that the coating has no defects or surface damage. Furthermore, reflectance can be used as a parameter to test the efficacy of the ARC used.

The reflection coefficient of a material is another extremely significant property, and is related to the refractive index discussed in section 1.1. When a wave encounters a sudden change in the medium it is propagating through (a change in the refractive index), it undergoes both transmission and reflection. The reflection coefficient quantifies the relationship between the amplitude of the reflected wave and the amplitude of the incident wave.

This can be understood mathematically through the Fresnel equations. While they have diverse complex

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forms (for s-polarised and p-polarised light) which will be explored through the coding simulation in section 3.3, the basic equation for the reflection coefficient for light that is normally incident on the interface between two media with different refractive indices is as follows[14]:

$$R = \left|\frac{n_1 - n_2}{n_1 + n_2}\right|^2$$

Where:
R is the reflection coefficient
n_1 is the refractive index of the first medium
n_2 is the refractive index of the first medium

This equation is applicable since when the angle of incidence and refraction are both equal to 0, there is no distinction between s-polarisation and p-polarisation.[15]

This concept, as well as the Fresnel equations[16] are an extremely important concept in optics, and will be referred to and utilised throughout the paper. With reference to electrochromism we can gain an understanding of the manner in which the refractive index of the electrochromic material affects the transmittance through it. Within ARCs, the Fresnel equations help minimise the reflectance through indicating the ideal refractive index of the ARCs.

D. Interference

With reference to anti-reflective coating on glasses, the optical concept of 'interference' plays an important role. For ARCs, multiple layers of coating are often used, with varying refractive indices.

The properties of these coatings, such as the thickness and material are decided based upon a phenomenon referred to as thin film interference. Examples of this phenomenon in daily lives include the colours seen in soap bubbles or an oil layer. Here, upon reflection off a medium of higher refractive index than the medium of propagation, a ray of light will undergo a phase change of π radians or 180º.[17] This can be explained through an example as displayed below:

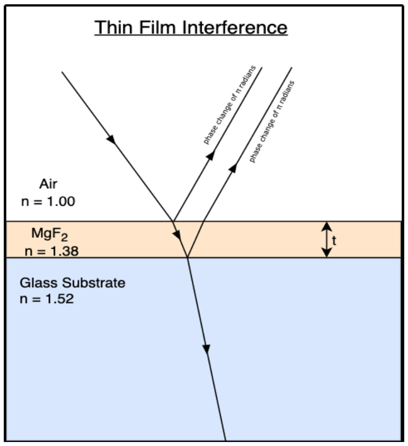

Fig 1.4 - Thin film interference caused by a single layer of MgF_2 on a glass substrate.

The path difference between the two waves would be approximately 2t (2 multiplied by the film thickness). In order to calculate parameters for the film width for constructive and destructive interference, the following formulae can be used.[18] These are displayed in a tabular form for easier calculation:

TABLE 2
FORMULAE[19] ASSOCIATED WITH INTERFERENCE

	1 phase change	0 or 2 phase changes
Constructive Interference	$2\,t\,n = (m + \frac{1}{2})\,\lambda$	$2\,t\,n = m\,\lambda$
Destructive Interference	$2\,t\,n = m\,\lambda$	$2\,t\,n = (m + \frac{1}{2})\,\lambda$

Here,
't' is the width or thickness of the film
'n' is the refractive index of the film with respect to air
m is the order number and takes the form of any constant: 0, 1, 2…

These are extremely important equations since they provide information about the wavelengths of light that will undergo constructive and destructive interference with a particular film thickness, therefore contributing to the anti-reflective nature of the coating. (The reflected wavelength that suffers destructive interference will be absent in the

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[14] Fresnel's equations for reflection and transmission - Brown University. Accessed June 19, 2023. [illegible]

reflected light). A single layer of anti-reflective coating could function to eliminate one wavelength, whereas multiple coatings are used for eliminating a larger range of wavelengths.

III. ANTI-REFLECTIVE COATINGS (ARCS)

A. Background Information

All ARCs are applied on various apparati, notably eyeglasses, camera lenses, photovoltaic cells for solar panels and display screens in order to provide optimised visual features for the respective application. When light rays are incident on an uncoated lens, the change in refractive index (optical property described in section 1.1) causes some light to be reflected. This reflected light thus reduces the transmission of light through the lens, and can cause glare, reduce contrast, and diminish overall optical performance. In order to reduce the amount of light reflected and increase the intensity of transmitted light, an ARC is applied. The principle behind thisfunctions on 2 main phenomena:

1) Interference: A coated lens surface will cause light to reflect from two different layers, leading to a phase difference and thus destructive interference (as discussed in section 1.6). This would mean the reflected waves can be cancelled out and thereby reduced in intensity, subsequently increasing the optical performance of the device.[20]

2) Impedance matching: The primary cause of the reflection of light at the boundary of the two media is the mismatch of impedance (the resistance that a wave encounters when propagating through a medium). The ARCs aid in decreasing this impedance, assisting in a smoother transmission of light.[21]

Essentially, ARCs work to decrease reflection and increase the transmission of light through the lens. This is done through providing destructive interference and assisting in impedance matching. In most ARCs multiple layers of varying thickness and varying refractive index are utilised, in order to minimise reflections over a broader range of wavelengths.

B. Types of ARCs

There are various types of structures used for ARCs, including a single-layer coating, gradient index coating and multilayer stacks.[22]

Single layer coating - This refers to one layer of thin film between the two surfaces that has an intermediary refractive index. This would lead to a reduction in the reflection coefficient (as obtained from the Fresnel equations), as well as a destructive interference effect where the reflectance is cancelled out.

Gradient Index Coating [23] - This refers to a coating with layers gradually decreasing in refractive index. The amount by which the decrease takes place and the number of coatings both impact the anti-reflective properties. These coatings primarily tend to be used for scanners, microscopes and photovoltaic applications. Although single- and double-layer ARCs only reduce the reflectance for particular wavelengths, a graded index coating helps eliminate this constraint and allows sustained, reduced reflectance over a large range of wavelengths.

Multilayer Stacks - this refers to alternating layers of high and low refractive indices. A common multilayer stack used consists of alternating layers of TiO2 and SiO2 thin films, in order to sufficiently decrease the reflected light and increase transmission. Referring to data from table 1, TiO_2 has a high refractive index, of about 2.65, while SiO_2 nanoparticles have a much lower refractive index of only 1.46. Carefully controlling the thickness of these layers, the type of interference can be controlled. For destructive interference applications, such as ARCs, the coatings are deliberately adjusted in a way that reflected waves from adjacent layers have a phase difference of a half-integer multiple of the wavelength. In this case, the waves cancel each

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other out, leading to reduced reflection at certain wavelengths.

C. Python Simulation-based Approach for a Single-Layer ARC

In order to identify the optimal thickness and material for a single-layered ARC, a secondary review was performed to identify established formulae and norms, and subsequently a simulation-based method was employed to corroborate the findings. [24][25]

For single layer coating in the case of an air (refractive index of 1) and glass (refractive index of (1.46) interface, the material used is conventionally magnesium fluoride (MgF_2) with a refractive index of 1.38. The optimal refractive index of the film, would be the geometric mean of the refractive indices of the two surfaces:

$$\sqrt{n_0 \times n_s} \approx 1.23$$

(where n_0 is the refractive index of air and n_s is the refractive index of the glass substrate)

Magnesium fluoride can easily be coated through physical vapour deposition and has a close refractive index of 1.38.

To calculate the reflection coefficient for a glass substrate with a refractive index of 1.52 and air with a refractive index of 1.00, without any ARC, we can use the formula discussed in section 1.4:

$$R = \left|\frac{n_1 - n_2}{n_1 + n_2}\right|^2$$

$$R = \left|\frac{1 - 1.52}{1 + 1.52}\right|^2$$

$$R = 0.0425799\ldots$$

$$R \approx 4.26\%$$

This is the percentage of light reflected without an ARC, only accounting for the first surface of a lens. Now, implementing an ARC with refractive index of 1.38, for normal incidence, the reflection coefficient can be calculated as follows:

$$R = \left|\frac{1 - 1.38}{1 + 1.38}\right|^2 + \left|\frac{1.38 - 1.52}{1.38 + 1.52}\right|^2$$

$$R = 0.02722866\ldots$$

$$R \approx 2.72\%$$

Thus, as can be seen, the reflected light at 550 nm is almost halved with an ARC of refractive index 1.38.

Furthermore, MgF_2 has a high Abbe's number (as explained in section 1.3) of approximately 95. This is beneficial because it reduces chromatic aberrations and colour separation, leading to improved colour uniformity and optical performance.

Subsequently, a simulation was run with the code below to identify the optimal refractive index of the coating material.

Code 1.0 - To identify refractive index which provides the least reflectance.

```
import numpy as np
import matplotlib.pyplot as plt

defcalculate_reflectance(refractive_ind
ex_arc, refractive_index_lens):
n_air = 1.0# refractive index of air
reflectance = ((n_air -
refractive_index_arc) / (n_air +
refractive_index_arc))**2 +
((refractive_index_lens -
refractive_index_arc) /
(refractive_index_lens +
refractive_index_arc))**2
return reflectance

# Constant Values
refractive_index_lens = 1.52#
refractive index of the lens material
(glass)

# Range of refractive indices for ARC
refractive_indices_arc =
np.linspace(1.1,1.5,100)

# Calculate reflectance for different
ARCs
reflectances = []
```

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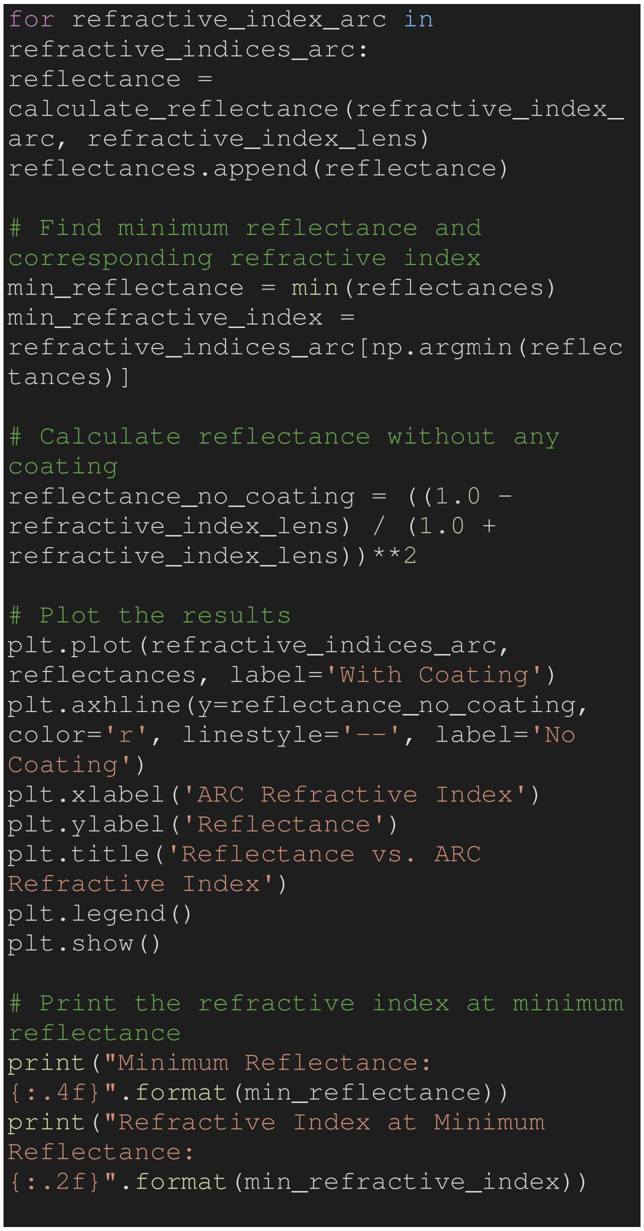
[24] Fontanot, Tommaso, Ujjayanta Bhaumik, Ravi Kishore, and Youri Meuret. “POCAL: A Python-Based Library to Perform Optical Coating Analysis and Design.” *Optics Continuum* 2, no. 4 (2023): 810. https://doi.org/10.1364/optcon.484972.



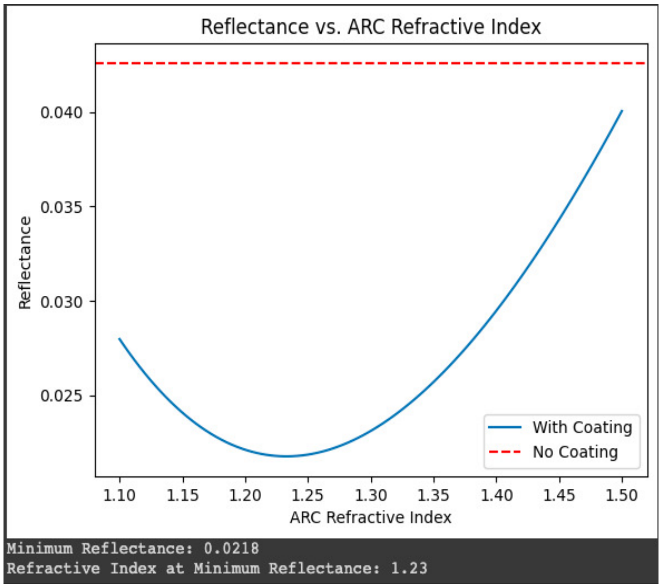
```
for refractive_index_arc in
refractive_indices_arc:
reflectance =
calculate_reflectance(refractive_index_
arc, refractive_index_lens)
reflectances.append(reflectance)

# Find minimum reflectance and
corresponding refractive index
min_reflectance = min(reflectances)
min_refractive_index =
refractive_indices_arc[np.argmin(reflec
tances)]

# Calculate reflectance without any
coating
reflectance_no_coating = ((1.0 -
refractive_index_lens) / (1.0 +
refractive_index_lens))**2

# Plot the results
plt.plot(refractive_indices_arc,
reflectances, label='With Coating')
plt.axhline(y=reflectance_no_coating,
color='r', linestyle='--', label='No
Coating')
plt.xlabel('ARC Refractive Index')
plt.ylabel('Reflectance')
plt.title('Reflectance vs. ARC
Refractive Index')
plt.legend()
plt.show()

# Print the refractive index at minimum
reflectance
print("Minimum Reflectance:
{:.4f}".format(min_reflectance))
print("Refractive Index at Minimum
Reflectance:
{:.2f}".format(min_refractive_index))
```



```
Minimum Reflectance: 0.0218
Refractive Index at Minimum Reflectance: 1.23
```

Fig 3.1 - Results of the simulation, Reflectance vs ARC refractive index.

As can be seen, the code results corroborate with the theoretical understanding, yielding an optimal refractive index of 1.23, where the reflectance is 2.18% for light with a wavelength of 550nm. A coating particularly tending to the centre of the visible spectrum displays good anti-reflective properties across the spectrum. The lack of solid materials with a low refractive index causes the utilisation of MgF_2 (with a close refractive index). Several fluoropolymers have lower refractive indices, but are difficult to synthesise and coat.[26]

Using the concepts of destructive interference, it is theoretically devised that the optimum thickness for a single-layer ARC should be 1/4th of the wavelength intended to be blocked. In order to ensure good performance across the visual spectrum, 550 nm is often taken to be the intended wavelength. To test this derivation, I employed a sophisticated simulation as displayed below, which uses the gradient descent update rule to adjust the film thickness in the direction that reduces the reflectance.

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[26] "Coating Materials." ISR Corporation > Products > Optical Materials > OPSTAR. Accessed July 2, 2023. [illegible]

Code 2 - to identify optimal thickness

```
import numpy as np
import matplotlib.pyplot as plt

defcalculate_reflectance(n1, n2,
theta_i, wavelength):
theta_t = np.arcsin((n1 / n2) *
np.sin(theta_i))
r_parallel = (n1 * np.cos(theta_i) - n2
* np.cos(theta_t)) / (n1 *
np.cos(theta_i) + n2 * np.cos(theta_t))
r_perpendicular = (n2 * np.cos(theta_i)
- n1 * np.cos(theta_t)) / (n2 *
np.cos(theta_i) + n1 * np.cos(theta_t))
reflectance = (np.abs(r_parallel)**2 +
np.abs(r_perpendicular)**2) / 2
return reflectance

defoptimize_film_thickness(n1, n2,
wavelength):
theta_i = np.deg2rad(0)# Incident angle
(assumed normal incidence)
t = (wavelength / (4 * n2))# Initial
film thickness guess (quarter-
wavelength)

# Gradient descent optimization
learning_rate = 0.001
precision = 1e-6
max_iterations = 10000
iteration = 0

while iteration < max_iterations:
reflectance = calculate_reflectance(n1,
n2, theta_i, wavelength)
if reflectance < precision:
break
dR_dt = -(wavelength / (8 * np.pi * n2))
* (np.sin(2 * n2 * t * np.pi /
wavelength) - np.sin(2 * n2 * (t -
wavelength / (4 * n2)) * np.pi /
wavelength))
t = t - learning_rate * dR_dt
iteration += 1

return t

defplot_optimal_thickness(n1, n2,
wavelengths):
optimal_thicknesses = []

for wavelength in wavelengths:
t = optimize_film_thickness(n1, n2,
wavelength)
optimal_thicknesses.append(t)

# Plotting the results
plt.plot(wavelengths,
optimal_thicknesses, marker='o')
plt.xlabel('Wavelength (nm)')
plt.ylabel('Optimal Film Thickness
(nm)')
plt.title('Optimal Film Thickness for
Anti-Reflective Coating')
plt.grid(True)

# Adding data labels
for x, y inzip(wavelengths,
optimal_thicknesses):
label = f'{y:.2f} nm'
plt.text(x, y, label, ha='center',
va='bottom')

# Adding additional text
plt.text(400,0.9 *
max(optimal_thicknesses),f'Refractive
Index (Film): {film_refractive_index}',
fontsize=10)

plt.show()

# Main program
air_refractive_index = 1.00
lens_refractive_index = 1.52
film_refractive_index = 1.23
wavelengths = np.linspace(400,700,7)#
Wavelengths in nanometers

plot_optimal_thickness(air_refractive_i
ndex, lens_refractive_index,
wavelengths)
```

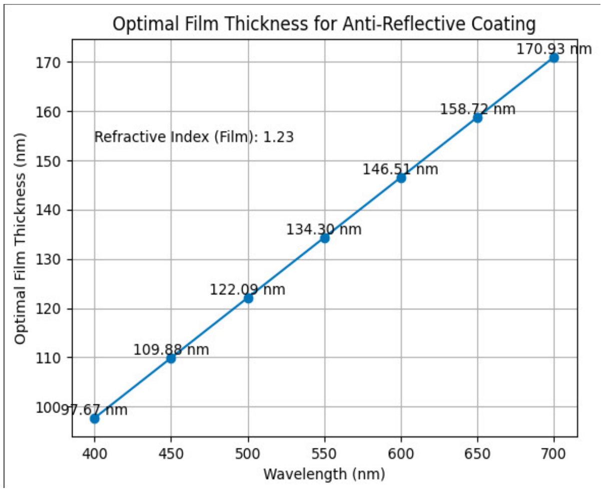

Fig 3.2 - Results of the simulation, optimal film thickness at different wavelengths.

The optimal film thickness at 550 nm should be 137.5 nm if the quarter-wavelength rule is used, however the simulation yields a value of 134.3 nm. This discrepancy can be attributed to the various assumptions made while deriving the solution theoretically, including that the quarter-wavelength rule assumes a specific interference condition, primarily for minimising reflectance due to destructive interference. It does not account for other factors like multiple reflections, complex refractive index profiles, polarisation effects, and other potential considerations specific to the application.

IV. CONCLUSIONS

This paper reviews the optical properties relevant to Anti-Reflective Coatings (ARCs). In the context of ARCs, a combination of theoretical and simulation-based approaches is employed to optimise properties for a single-layer ARC. The study identifies an optimal refractive index of 2.3 and a thickness of 134.3 nm for a wavelength of 550 nm. In addition to lenses for glasses, ARCs have a myriad of potential applications in the future. This includes their use in photovoltaic cells to maximise the energy and efficiency for renewable energy generation.[27] They can also be employed in emerging display technologies, such as flexible display screens and AR headsets. Additionally, their ability to remove glare indicates their importance in the automotive industry for windscreens and rear-view mirrors.[28] After a thorough study, several parallels between the applications of electrochromic materials and ARCs emerge, including the eyeglass industry, automotive industry, and for display screens. The gradient descent algorithm provides us with an accurate estimation of the optimal results for the lens.

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