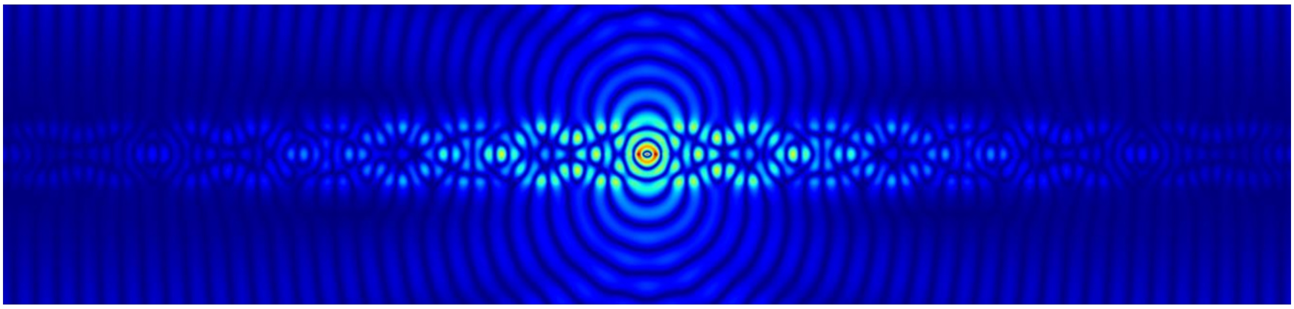
Pascal Institute

Clermont Auvergne University

University School of Physics and Engineering

Internship report presented by **Sakkali Amine**

The Simulation of Optical Properties of Multilayer Structures by the Admittance Method



Defend on June 12 ,2024

Internship supervised: MOREAU Antoine and LANGEVIN Denis

ACKNOWLEDGEMENT

I need to express my honest gratitude to all of the members of the ÉLÉNA Team at the Pascal Institute who warmly welcomed me from day number one and furnished me with all of the help I wished throughout my journey there.

I especially appreciate Mr. Langevin and Mr. Moreau and for their personal guidance, invaluable advice and unwavering support at each stage of this work.

It is also essential for me to explicit my gratitude to the other members individuals of the ÉLÉNA Team who warmly welcomed me, labored carefully with me on various occasions, and generously shared their information with me through their combined efforts.

My stay at the Institute with the ÉLÉNA Team has been an high-quality experience. It has allowed me to learn more about nanophotonics and the Python programming language while obtaining competencies in an effort to be beneficial for my career.

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General Introduction

The observe of multilayer structures based on reflection coefficients is a axial area of optics, having developed for greater than a century. The first attempts to calculate the reflectance of multilayers cycle back to the pioneering work of Lord Rayleigh. This study intensified withinside the mid-nineteenth century with the know-how and production of quarter-wave stacks, additionally known as Bragg mirrors or 1D photonic crystals.

Calculation of reflection and transmission coefficients in multilayer structures involves solving Maxwell`s equations with time dependence. These calculations require taking into consideration the continuity of the electrical and magnetic fields at the interfaces between the different layers of the material. Different formalisms, such as switch matrices, S matrices, admittance method, etc., had been evolved to solve those equations with increased stability and efficiency.

In this internship, we focus on making the admittance formalism work for transmission and reflection, using Python. This formalism helps us understand how light moves through different layers of materials. Its particularity is that it is very fast compared to other calculation methods. Using Python, we want to make this formalism even better, so that researchers can study complex layered structures quickly and accurately. It's easier and more accessible to everyone.

Chapter 1: Theoretical Background

Introduction

In this chapter we will see a presentation of the PyMoosh library in Python and also the concept of the admittance method based on Maxwell's equation.

I. Overview of PyMoosh library

PyMoosh (Python-based Multilayer Optics Optimization and Simulation Hub) is a simulation library developed in Python, designed to offer a complete set of numerical equipment for calculating the optical properties of multilayer structures. Designed for each study and education, PyMoosh locations precise emphasis on the usability and ease of its interface, even as presenting superior capabilities for professional users.

The number one intention of PyMoosh is to enable efficient and dependable computation of the optical properties of multilayer structures. This includes reflectance and transmittance below various conditions, absorption and Poynting flux in every layer, 2D Green`s functions, and the calculation of structural modes and their dispersion curves. Additionally, PyMoosh is designed to combine with optimization tools, making it particularly suitable for deep studying techniques and current optimization techniques.

II. Admittance Formalism for R and T coefficients

II. 1 The maxwell's equation

An electromagnetic wave obeys the maxwell's equations defined by

$$\vec{\nabla} \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t}, \qquad (1)$$

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \qquad (2)$$

$$\vec{\nabla} \cdot \vec{D} = \rho, \qquad (3)$$

$$\vec{\nabla} \cdot \vec{B} = 0, \qquad (4)$$

the vectors $\vec{E}$ et $\vec{H}$ represent the electric and magnetic fields, J is the current density, $\vec{D}$ and $\vec{B}$ are the electric and magnetic induction vectors, and ρ is the charge density.

With

$$\vec{E} = A^{+}\exp\,(iwt + i\vec{\beta}\,\vec{s}) \tag{5}$$

And :

$$\vec{\beta}.\vec{\beta} = k^2 = w^2\,\mu\epsilon\,,\ \vec{s} = \begin{matrix} x \\ y, \\ z \end{matrix} \tag{6}$$

According to Maxwell's equation, we obtain:

$$\begin{cases} \vec{H} = \frac{1}{w\mu}\vec{\beta}\times\vec{E} \\ \vec{E} = \frac{1}{w\epsilon}\vec{\beta}\times\vec{H} \end{cases} \tag{7}$$

we will base our calculation on these equations to determine the reflection and transmission coefficients. we consider a multilayer structure with p layer (see figure I.1).

The z-dependence of the elementary component of this incident wave is then described as

$$\overrightarrow{E_0} = \overrightarrow{A_0^{+}}\exp\,(i\alpha_0 z\,), \tag{8}$$

With : $\alpha_0 = \sqrt{k_0^2 - \sigma^2}$, $\sigma = k_{\,0}\sin\,(\theta_0)$ and $k_{\,0} = \frac{2\,\pi\,n_0}{\lambda}$ and $\overrightarrow{A_0^{+}}$ is the amplitude. We immediately observe that in the substrate there exists a unique progressive wave, whose z-dependence is written: $\overrightarrow{E_s} = \overrightarrow{A_s^{+}}\exp\,(i\alpha_s z\,)$, with: $\alpha_s = \sqrt{k_s^2 - \sigma^2}$, (9)

On the other hand, a stationary wave, resulting from the combination of a progressive and a retrograde wave, develops in the layer of rank **j (1 ≤ j ≤p) :**

$$\overrightarrow{E_j} = \overrightarrow{A_j^{+}}\exp\,(i\alpha_j z\,) + \overrightarrow{A_j^{-}}\exp\,(-i\alpha_j z\,),\text{ with } \alpha_j = \sqrt{k_j^2 - \sigma^2} \tag{10}$$

we have the shape of the standing wave changes according to the vertical position z inside the thin layer. Furthermore, the spatial variation σ remains the same in all layers, we can write

$$\sigma = k_j\sin\theta_j\ = cost >>>\ n_j\ \sin\theta_j\ =\ n_0\ \sin\theta_0 \tag{11}$$

Which is simply the Snell-Descartes invariant.

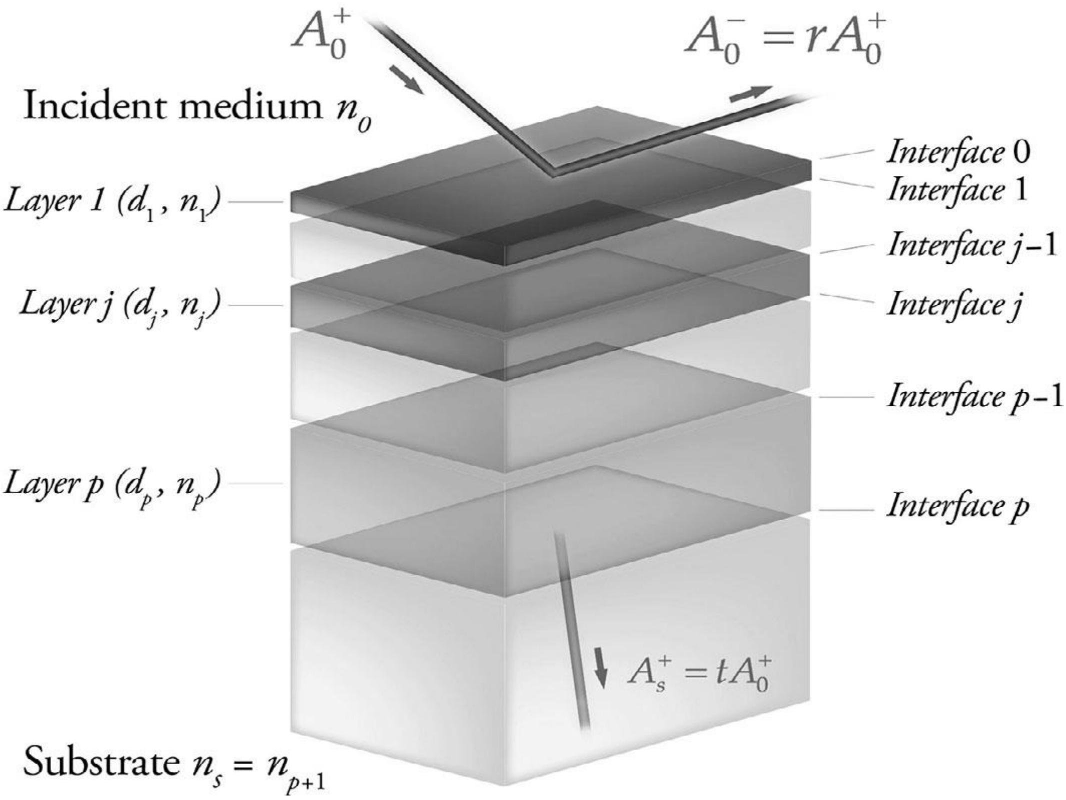

Figure I.1: general structure of a multilayer stack.

II. 2 the concept of effective reflective index

Consider a progressive wave propagating in the xOy plan a homogeneous medium. According to the equation (7) :

$$\begin{cases} \overrightarrow{B^+} = \frac{1}{w\mu}\overrightarrow{\beta^+} \times \overrightarrow{A^+} \\ \overrightarrow{A^+} = \frac{1}{w\epsilon}\overrightarrow{\beta^+} \times \overrightarrow{B^+} \end{cases} \quad \text{with } \overrightarrow{\beta^+} = \sigma\vec{x} + \alpha\,\vec{z} \tag{12}$$

At this point we need to introduce the polarization modes of light. We know that in transparent media the electric field lies in a plane perpendicular to the wave vector, so it can be described as the sum of two perpendicular fields in this plane, called the polarization modes.

II. 2-1 Transverse Electric Polarization TE

First of all, we consider a linearly polarized TE (Transverse Electric) plane wave, that is to say whose electric field vector is perpendicular to the plane of incidence xOz. Therefore, we can write in this case:

$$\overrightarrow{A^+} = A^+\,\vec{y} \tag{13}$$

Which leads to the following expression for $\overrightarrow{B^+}$

$$\overrightarrow{\mathrm{B}^+} = \frac{1}{\mathrm{w\mu}}\overrightarrow{\beta^+} \times \overrightarrow{\mathrm{A}^+} = \frac{1}{\mathrm{w\mu}}(\sigma\vec{\mathrm{x}} + \alpha\,\vec{\mathrm{z}}) \times \mathrm{A}^+\,\vec{\mathrm{y}} = \frac{\alpha}{\mathrm{w\mu}}\vec{\mathrm{z}} \times \overrightarrow{\mathrm{A}^+} + \frac{1}{\mathrm{w\mu}}\sigma\,\vec{\mathrm{z}} \tag{14}$$

and therefore to the following relationship between the tangential components (i.e. in the xOy plane) of the magnetic induction and the electric field:

$$\overrightarrow{\mathrm{B}_{tg}}^{+} = \frac{\alpha}{\mathrm{w\mu}}\vec{\mathrm{z}} \times \overrightarrow{A_{tg}}^{+} \tag{15}$$

The quantity $\tilde{n}$ is defined by:

$$\tilde{n} = \frac{\alpha}{\mathrm{w\mu}} \tag{16}$$

And is known as the effective refractive index, so the relationship between tangential components cans be written in the following compact from:

$$\overrightarrow{\mathrm{B}_{tg}}^{+} = \tilde{n}\,[\vec{\mathrm{z}} \times \overrightarrow{A_{tg}}^{+}], \tag{17}$$

We have w=k . c/n and n are refractive index

Therefore:

$$\tilde{n} = \frac{\alpha}{\mathrm{w\mu}} = \frac{\mathrm{n}\,\alpha}{\mathrm{k\,c\,\mu}} = \frac{1}{\eta_{\,v}\mu_r}\,\frac{n\,\alpha}{k} \text{ with } \eta_{\,v} = \sqrt{\frac{\mu_0}{\epsilon_0}} \tag{18}$$

II. 2-2 Transverse magnetic Polarization TM

Now, we consider a linearly polarized TM (Transverse magnetic) plane wave, that is to say whose magnetic field vector is perpendicular to the plane of incidence xOz. Therefore, we can write in this case:

$$\overrightarrow{B^+} = B^+\,\vec{y} \tag{19}$$

So ,

$$\vec{A} = -\frac{1}{\mathrm{w}\,\epsilon}\overrightarrow{\beta^+} \times \overrightarrow{\mathrm{B}^+} = -\frac{1}{\mathrm{w}\,\epsilon}(\sigma\vec{\mathrm{x}} + \alpha\,\vec{\mathrm{z}}) \times \mathrm{B}^+\,\vec{\mathrm{y}} = -\frac{\alpha}{\mathrm{w}\epsilon}\vec{\mathrm{z}} \times \overrightarrow{\mathrm{B}^+} - \frac{1}{\mathrm{w}\epsilon}\sigma\,\vec{\mathrm{z}} \tag{20}$$

we write relationship between the tangential components:

$$\overrightarrow{\mathrm{B}_{tg}}^{+} = \frac{\mathrm{w}\epsilon}{\alpha}\left[\vec{\mathrm{z}} \times \overrightarrow{A_{tg}}^{+}\right] = \tilde{n}\left[\vec{\mathrm{z}} \times \overrightarrow{A_{tg}}^{+}\right] \tag{21}$$

We can develop the expression of $\tilde{n}$ to:

$$\tilde{n} = \frac{w\epsilon}{\alpha} = \frac{1}{\eta_{v}\mu_{r}} \frac{nk}{\alpha} \tag{22}$$

II. 2-3 conclusion

The relationships established in the previous sections lead us to conclude that, in the case of the elementary component of a progressive wave, regardless of the polarization state, there exists a scalar $\tilde{n}$ such that:

$$\overrightarrow{B_{tg}}^{+} = \tilde{n}\,[\vec{z} \times \overrightarrow{A_{tg}}^{+}], \tag{23}$$

With

$$\tilde{n} = \begin{cases} \frac{w\epsilon}{\alpha} & in\ TM\ polarization \\ \frac{\alpha}{w\mu} & in\ TE\ polarization \end{cases} \tag{24}$$

Or

$$\tilde{n} = \frac{1}{\eta_{v}\mu_{r}} \begin{cases} \frac{nk}{\alpha} & in\ TM\ polarization \\ \frac{n\,\alpha}{k} & in\ TE\ polarization \end{cases} \tag{25}$$

The procedure is exactly the same in the case of a retrograde wave, except that now

the vector β is expressed as $\overrightarrow{\beta^{-}} = \sigma\vec{x} - \alpha\,\vec{z}$ which we obtain:

$$\overrightarrow{B_{tg}}^{-} = -\tilde{n}\,[\vec{z} \times \overrightarrow{A_{tg}}^{-}], \tag{26}$$

II. 3- the concept of the complex admittance

We must again establish the relationship between the tangential components of the electric and magnetic fields. To do this, recall that a standing wave is the sum of a progressive wave and a retrograde wave, and that the modulus of the wave varies with the height z.

The standing wave in layer j of the stack, illustrated in Figure I.1, is therefore described by the following equation:

$$\overrightarrow{E_{j,tg}} = \overrightarrow{A^{+}_{j,tg}}\exp\,(i\alpha_{j}z) + \overrightarrow{A^{-}_{j,tg}}\exp\,(-i\alpha_{j}z), \text{ with } \alpha_{j} = \sqrt{k_{j}^{2} - \sigma^{2}} \tag{27}$$

According to equation (7), it is easy to check that the tangential components of the to quantities $\overrightarrow{H_{J,\text{tg}}}$ et $\vec{z} \times \overrightarrow{E_{J,\text{tg}}}$ are parallel. Therefore, there exist a complex scalar Y such that we can write:

$$\overrightarrow{H_{J,\text{tg}}} = Y_j \, [\, \vec{z} \times \overrightarrow{E_{J,\text{tg}}}\,], \tag{28}$$

This quantity Y_j is simply a factor of proportionality between the tangential components of two files. Also is known as the complex admittance.
If we want to applicated at the upper 0 interface, we can write :

$$\overrightarrow{H_{0,\text{tg}}} = Y_0 \, [\, \vec{z} \times \overrightarrow{E_{0,\text{tg}}}\,], \tag{29}$$

Which leads to the following relation :

$$\overrightarrow{B^{+}_{0,\text{tg}}} + \overrightarrow{B^{-}_{0,\text{tg}}} = Y_0 \, [\, \vec{z} \times \overrightarrow{A^{+}_{0,\text{tg}}} + \ \vec{z} \times \overrightarrow{A^{-}_{0,\text{tg}}}], \tag{30}$$

The reflective coefficient r is defined by:

$$\overrightarrow{A^{-}_{0,\text{tg}}} = r \, \overrightarrow{A^{+}_{0,\text{tg}}} \tag{31}$$

Moreover, we have :

$$\overrightarrow{\mathrm{B}_{0,tg}{}^{-}} = -\tilde{n}_0 \, [\vec{\mathrm{z}} \times \overrightarrow{A_{0,tg}{}^{-}}\,] \quad \text{et} \quad \overrightarrow{\mathrm{B}_{0,tg}{}^{+}} = \tilde{n}_0 \, [\vec{\mathrm{z}} \times \overrightarrow{A_{0,tg}{}^{+}}\,], \tag{32}$$

By combining the tree equation ( ) , we obtain

$$\tilde{n}_0 \left[\vec{\mathrm{z}} \times \overrightarrow{A_{0,tg}{}^{+}}\right] - \tilde{n}_0 \, [\vec{\mathrm{z}} \times \overrightarrow{A_{0,tg}{}^{-}}\,] \ = Y_0 \, (1 + r) \, [\, \vec{z} \times \overrightarrow{A^{+}_{0,\text{tg}}}], \tag{33}$$

And hence

$$\mathrm{r} = \frac{\tilde{n}_0 - Y_0}{\tilde{n}_0 + Y_0} \tag{34}$$

The quantity Y_0, the complex admittance or reverse impedance of the component at the upper interface of the stack, depends not only on the angle of incidence and the polarization state, but also on all optical characteristics and geometrics of the multilayer. Equation (43) thus demonstrates that, for the calculation of the reflection, the multilayer component behaves like an artificial substrate with refractive index Y_0.

However, it is important to keep in mind that the equivalence between refractive index and admittance is only valid for reflection calculations; in fact, we will see that the transmission in the multilayer takes a different form from that of the single interface.

$$\mathrm{t} \neq \frac{2\,\tilde{n}_0}{\tilde{n}_0 + Y_0} \tag{35}$$

It now remains to define how to calculate this complex admittance in practice.

II. 4- Transfer Matrix

Consider inside the stack shown in figure I.2 the layer j of thickness d_j and refractive index n_j local between the (j-1) and the j-th interfaces. As noted previously, we are only interested in the tangential components of the field that are continuous throughout the stack. At an arbitrary point on the z abscissa within the thickness of the layer j, we can write

$$\begin{cases} \overrightarrow{E_{j,tg}} = \overrightarrow{A_{j,tg}^{+}} \exp(i\alpha_j z) + \overrightarrow{A_{j,tg}^{-}} \exp(-i\alpha_j z), \\ \overrightarrow{H_{j,tg}} = \overrightarrow{B_{j,tg}^{+}} \exp(i\alpha_j z) + \overrightarrow{B_{j,tg}^{-}} \exp(-i\alpha_j z), \end{cases} \tag{37}$$

The some for j-1:

$$\begin{cases} \overrightarrow{E_{j-1,tg}} = \overrightarrow{A_{j-1,tg}^{+}} \exp(i\alpha_{j-1} z) + \overrightarrow{A_{j-1,tg}^{-}} \exp(-i\alpha_{j-1} z), \\ \overrightarrow{H_{j-1,tg}} = \overrightarrow{B_{j-1,tg}^{+}} \exp(i\alpha_{j-1} z) + \overrightarrow{B_{j-1,tg}^{-}} \exp(-i\alpha_{j-1} z), \end{cases} \tag{38}$$

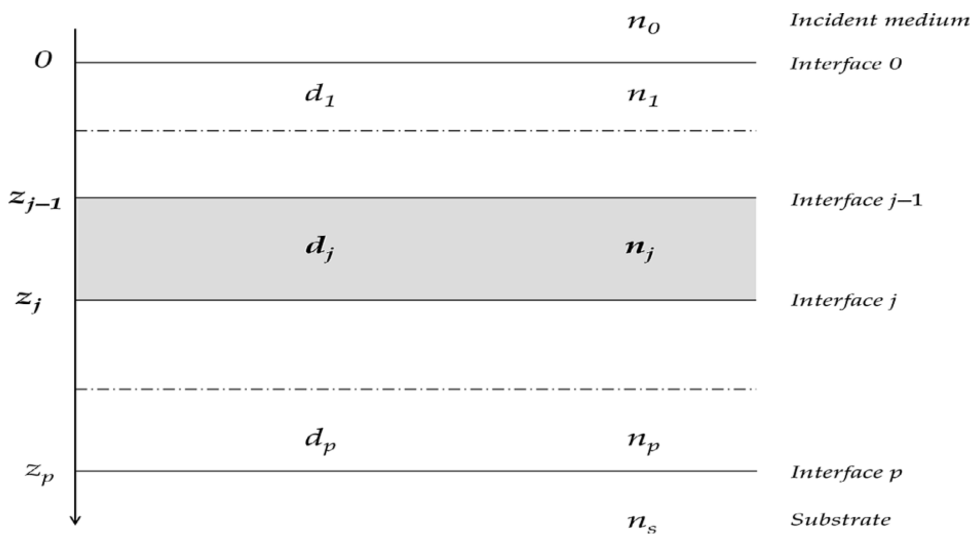

Figure I.2: layer j embedded in a stack of p layers

If we use equation (29) , and replacing in the equation (37) and (38) with :

$$\overrightarrow{B_{j,tg}}^{\pm} = \pm\tilde{n}_j \left[\vec{z} \times \overrightarrow{A_{j,tg}}^{\pm}\right], \tag{39}$$

We can obtain matrix:

$$\begin{bmatrix} \vec{z} \times \overrightarrow{E_{j,tg}} \\ \overrightarrow{H_{j,tg}} \end{bmatrix} = \begin{bmatrix} \cos\delta_j & i\sin\delta_j/\tilde{n}_j \\ i\tilde{n}_j \sin\delta_j & \cos\delta_j \end{bmatrix} \begin{bmatrix} \vec{z} \times \overrightarrow{E_{j-1,tg}} \\ \overrightarrow{H_{j-1,tg}} \end{bmatrix} \tag{40}$$

$$\begin{bmatrix} \vec{z} \times \overrightarrow{E_{j-1,tg}} \\ \overrightarrow{H_{j-1,tg}} \end{bmatrix} = Mj \begin{bmatrix} \vec{z} \times \overrightarrow{E_{j,tg}} \\ \overrightarrow{H_{j,tg}} \end{bmatrix} \tag{41}$$

With

$$\mathrm{Mj} = \begin{bmatrix} \cos\delta_j & -\, i \sin\delta_j/\tilde{n}_j \\ -i\tilde{n}_j \sin\delta_j & \cos\delta_j \end{bmatrix} \tag{42}$$

The matrix Mj is known as the transfer matrix associated with layer j, and makes it possible to calculate the quantities x at interface j-1, given the values of these same quantities at interface j.

By definition, the complex admittances of the interfaces j-1 et j are defined by

$$\overrightarrow{H_{\mathrm{j-1,tg}}} = Y_{j-1}\ [\, \vec{z} \times \overrightarrow{E_{\mathrm{j-1,tg}}}\ ], \tag{43}$$

$$\overrightarrow{H_{\mathrm{j,tg}}} = Y_j\ [\, \vec{z} \times \overrightarrow{E_{\mathrm{j,tg}}}\ ], \tag{44}$$

As a result, inserting these definitions into the matrix equation (40) and then constructing the ratio of the two equations thus obtained, we get:

$$Y_{j-1} = \frac{Y_j \cos\delta_j - i\,\tilde{n}_j \sin\delta_j}{\cos\delta_j \ - i\,Y_j \sin\delta_j/\tilde{n}_j} \tag{45}$$

or

$$Y_j = \frac{Y_{j-1} \cos\delta_j + i\,\tilde{n}_j \sin\delta_j}{\cos\delta_j + i\,Y_{j-1} \sin\delta_j/\tilde{n}_j} \tag{46}$$

Consequently, it remains to initialize these recurrence relations; a known admittance is required for this. For a progressive incident wave, this known admittance is given by the substrate.

The admittance of the substrate is therefore equal to its effective refractive index (Ys=ns), This makes it possible to initialize the recurrence relation (45) and, consequently, to progress to the value of the admittance at the first interface of the multilayer, i.e. $Y0$, then calculate the value of the reflection coefficient using equation (34).

II. 5-Transmission Coefficient of the Stack

we have that the reflection coefficient r is deduced from the admittance Y_0 by

$$\mathrm{r} = \frac{\tilde{n}_0 - Y_0}{\tilde{n}_0 + Y_0} \tag{47}$$

This coefficient t can be determined from equation (41) that relates the tangential components of the fields can be

$$\overrightarrow{E_{\mathrm{j-1,tg}}} = [\ \cos\delta_j - i\, Y_j \sin\frac{\delta_j}{\tilde{n}_j}\ ]\ \overrightarrow{E_{\mathrm{j,tg}}} \tag{48}$$

We immediately deduce a relationship between the variables $\overrightarrow{E_{0,\mathrm{tg}}}$ et $\overrightarrow{E_{\mathrm{p,tg}}}$, namely

$$\overrightarrow{E_{0,\mathrm{tg}}} = \prod_{j=1}^{p} [\ \cos\delta_j - i\ \sin\delta_j\ \ \frac{Y_j}{\tilde{n}_j}\ ]\ \overrightarrow{E_{\mathrm{p,tg}}}, \tag{49}$$

$$(1+r)\overrightarrow{A_{0,\mathrm{tg}}^{+}} = \prod_{j=1}^{p} [\ \cos\delta_j - i\sin\delta_j\ \frac{Y_j}{\tilde{n}_j}\ ]\ t\ \overrightarrow{A_{0,\mathrm{tg}}^{+}} \tag{50}$$

That is

$$\mathrm{t} = \frac{(1+r)}{\prod_{j=1}^{p} [\ \cos\delta_j - i\ \sin\delta_j\ \frac{Y_j}{\tilde{n}_j}\ ]} \tag{51}$$

Conclusion

In Chapter 1, we established the theoretical foundation for analyzing electromagnetic waves in layered structures using the PyMoosh library. We began by reviewing Maxwell's equations, which govern the behavior of electromagnetic fields. Then, we introduced crucial concepts for understanding light propagation in stratified media: effective refractive index, complex admittance, and transfer matrix. Finally, we explored the calculation of coefficient, a key parameter for analyzing light transmission and reflection through a multilayer stack.

Chapter 2: Practical Implementation of The Admittance method in PyMoosh

Introduction

In this internship, my work focused on finding practical solutions rather than simply developing the admittances formalism in PyMoosh. I was confronted with various challenges requiring innovative approaches and concrete solutions to improve the performance and efficiency of the formalism. This involved not only implementing the theoretical concepts of admittance and transfer matrices, but also optimizing algorithms and integrating new features to meet specific user needs.

I. Development and Integration in PyMoosh

As far as code development was concerned, I tried to apply exactly what we had demonstrated in the theoretical background chapter. I managed to obtain good results, but only for TE polarization, while the results for TM polarization were totally incorrect. After analyzing the code and results for each layer individually, I found a significant mismatch between the complex admittances. I explored all possibilities to solve this problem, but without premier success. Finally, I decided to use the same effective index of TE for delta calculation in both polarization modes, TE and TM. This approach enabled me to obtain good results for both polarization modes, showing that the unified effective index could correct the errors previously observed. This step was crucial in guaranteeing the accuracy and reliability of the PyMoosh simulations. For the complete code, l will leave the GitHub link at the end of the rapport.

```
n_s[0] = n[Type[0]] * np.cos(incidence)
n_s[1:] = np.sqrt(n[Type[1:]]**2 - n[Type[0]]**2 * np.sin(incidence)**2)
opp = np.imag(n_s) > 0
n_s = n_s - 2* n_s * (opp)
n_p = n[Type]**2 / n_s

delta = np.array(2*np.pi*thickness*n_s/wavelength)
temp = -1.j*np.tan(delta)
if polarization == 0:
    admittance = n_s
    Y = admittance[-1]
else:
    admittance = n_p
    Y = admittance[-1]
PR =1
for m in np.arange(g-2,-1,-1):
 Y = (Y + admittance[m+1]*temp[m+1])/(1 + Y*temp[m+1]/admittance[m+1])
 if (m != 0):
       PR *= (np.cos(delta[m]) - 1.j * Y * np.sin(delta[m])/admittance[m])
r = (admittance[0]-Y) / (admittance[0]+Y)
t = (r+1)/ (PR)
if (polarization == 1):
  r=-r
R = abs(r)**2
if polarization==0:
 admittance = n_s
 T = (admittance[-1].real/ admittance[0].real) * abs(t)**2
else:
  admittance = n_p
  T = (admittance[-1].real/ admittance[0].real) * abs(t)**2
return(r,t,R ,T)
```

Fugue II.1 : The code from the liberty PyMoosh of the admittance method

II. Testing and validation

After having developed the code, we run some preliminary tests in PyMoosh in order to use them as a standard benchmark then we calculate the error of all the methods as a function of the number of layers and distance. Speed tests of my coefficients for the admittance method were also done. To verify the accuracy and the efficiency of the code, we implemented some tests which are crucial and necessary for simulations of the optical properties of multilayer structures.

II.1 Numerical stability

Stability for multi-layered structures is essential in numerical simulations. The concept of numerical stability implies that the values that are arrived at through computation are dependable, and free of any catastrophic errors or instability in the presence of side-effects that might confuse the program. For all error calculations, we take the results of the S matrix as a reference.

- **Results for Absolute Error as a Function of Number of Layers for Normal, Intermediate, and large Incidence Angles**

The images below show the results of absolute error simulations as a function of the number of layers for normal, intermediate and large, comparing different methods: Abeles, D2N, T, and Impedance. The graphs are divided into two main categories: reflection (TER and TMR) and transmission (TET and TMT), each analyzed for TE and TM polarizations.

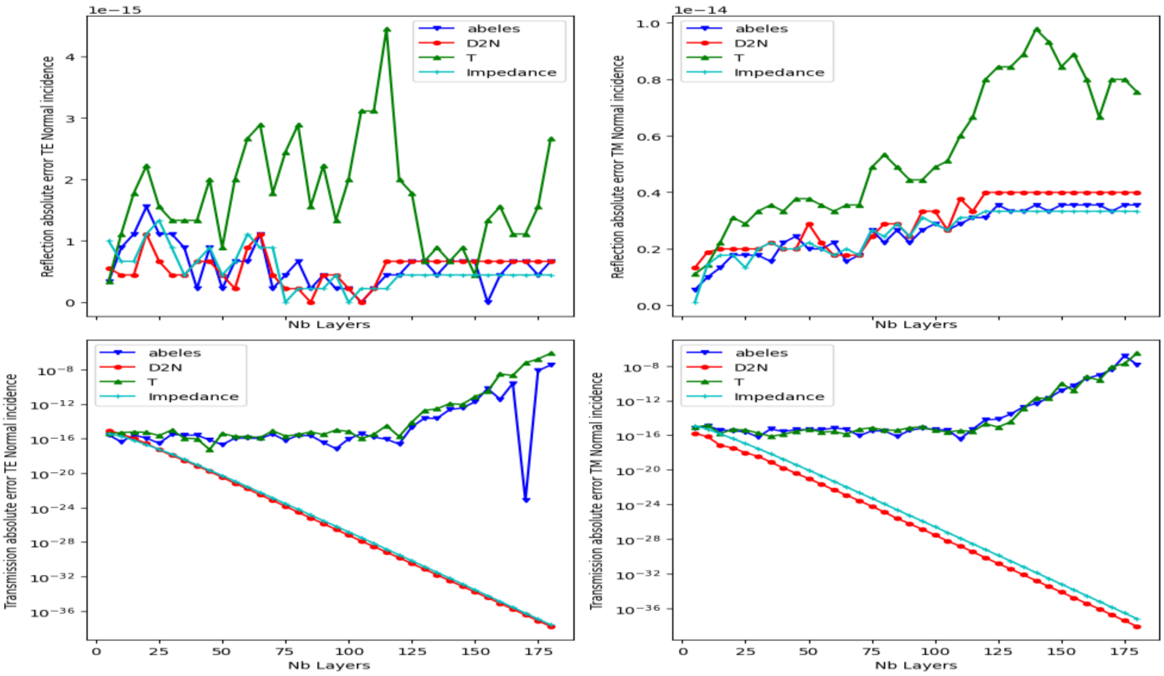

Figure II.2: Absolute Error as a Function of the Number of Layers for a normal Incidence

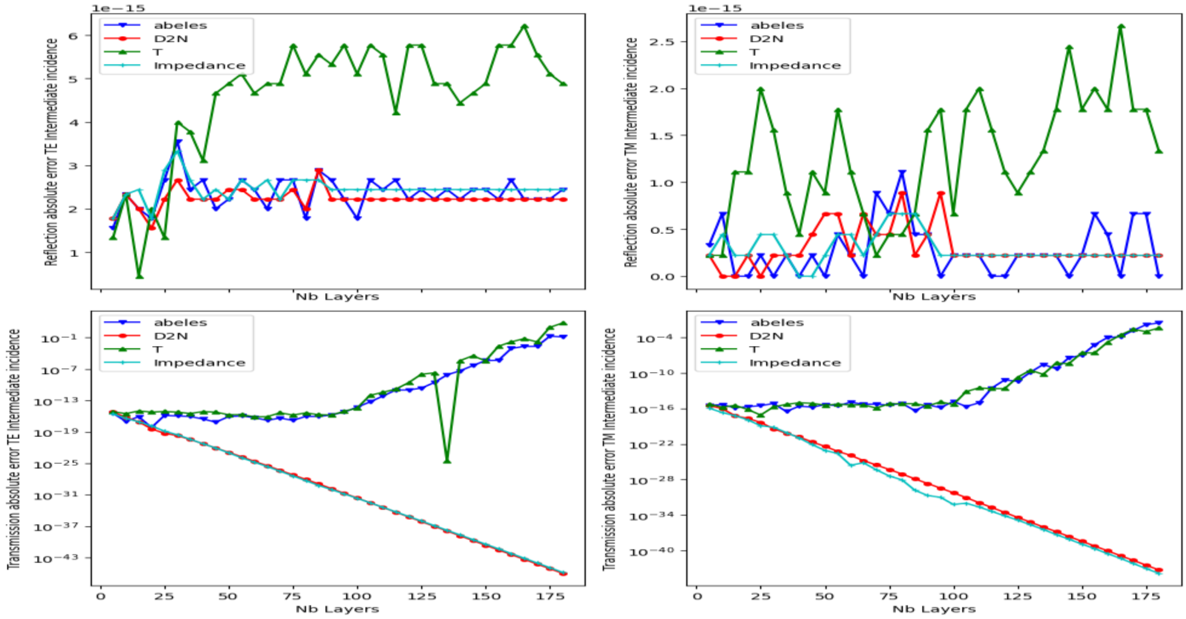

Figure II.3 : Absolute Error as a Function of the Number of Layers for an intermediate Incidence

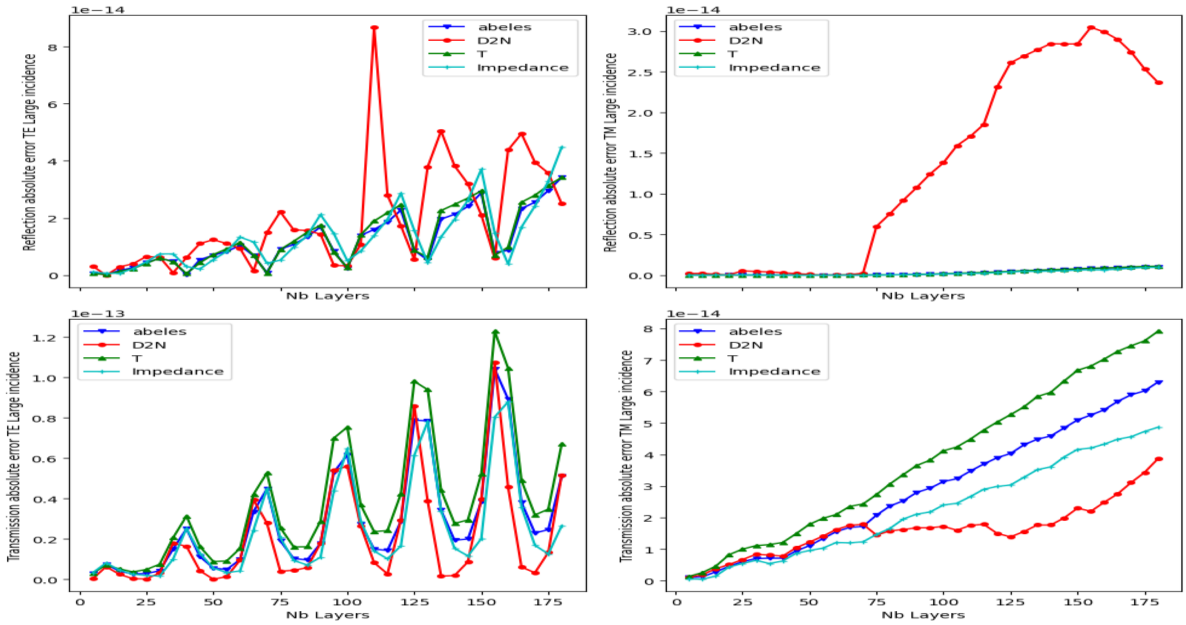

Figure II.4: Absolute Error as a Function of the Number of Layers for a large Incidence

These results indicate that, for multilayer configurations with different incidences, the admittance or impedance method offers relatively similar performances of matrix T and abeles for most configurations, with a slight superiority of the impedance method in terms of error stability in particular for transmission in TE and TM.

- **Results of total internal reflection Simulation**

The graphs show absolute reflection and transmission errors for TE (Transverse Electric) and TM (Transverse Magnetic) modes in the context of total internal reflection (TIR) as a function of distance (in nanometers). Methods compared include Abeles, D2N, T, and Impedance.

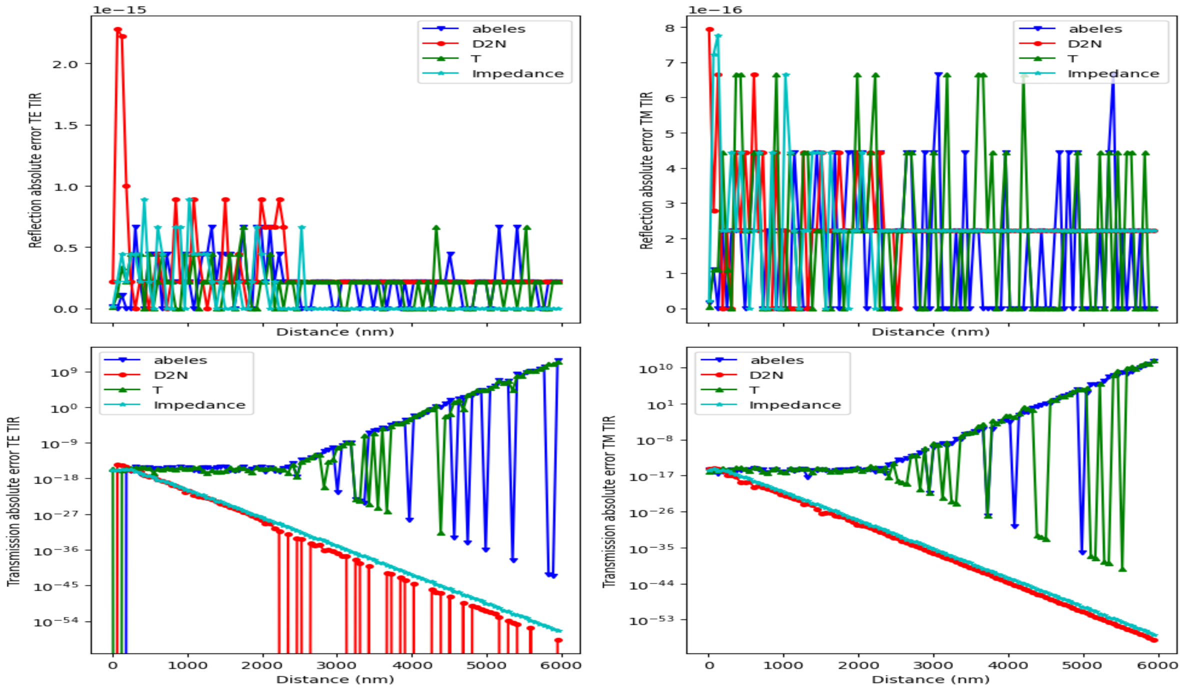

Figure II.5: Absolute Error as a Function of the distance of Layers for frustrated total internal reflection

In summary, the admittance or Impedance method is very stable and its TE and TM mode results have low errors. The D2N method ranked just behind Impedance, but it's not very stable; it performed similarly to Impedance and was only slightly less accurate.

From these results, it could be concluded that for extremely accurate TIR reflection and transmission calculations, the admittance or Impedance methods are more appropriate for such applications.

II.2 Analysis of the computational times of different methods

The graphs compare various methods to calculate calculation times depending on the number of layers on the x-axis, for Abeles, D2N, S, T, and Impedance. The calculation times are in seconds, and the number of layers goes from 0 to 175.

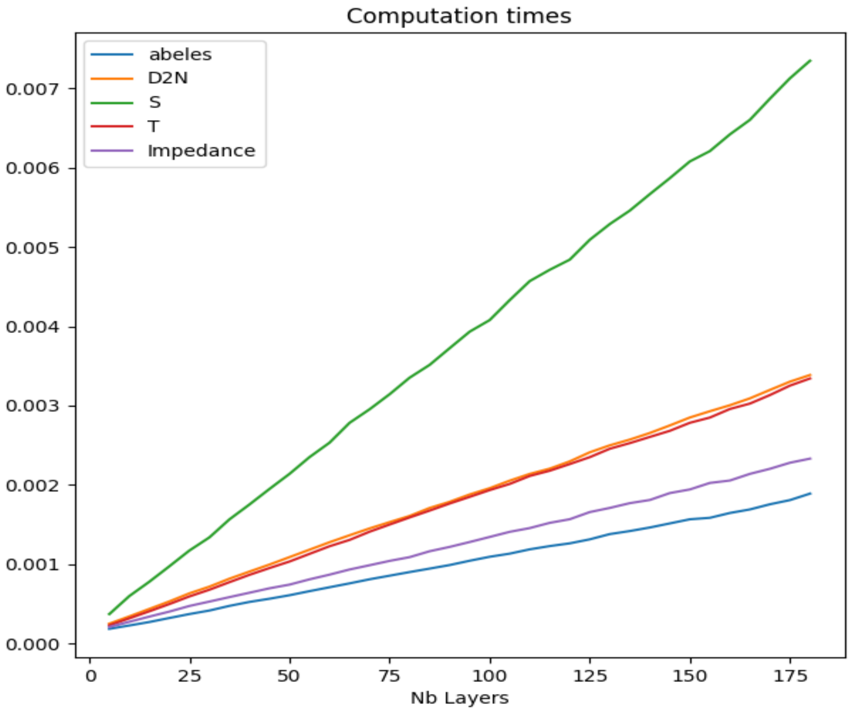

Figure II.6: The computational times of different methods

The results clearly show that for many layers, Abeles and Impedance are the fastest methods in terms of computation time, while S has the highest computation time. If you need to choose one of the available verification methods that are more moderate in terms of accuracy vs. speed, the Abeles and Impedance are recommended. Matrix T and D2N while they are marginally slower are still viable.

This data could help in choosing between the available methods by considering requirements, number of layers, and speed.

Conclusion

In Chapter 2 of this internship report, I focus on the practical implementation of the admittance method in PyMoosh. To do this, I not only had to understand and use the theoretical concepts of admittance and transfer matrices, but also optimize algorithms to improve the speed and efficiency of the formalism. Admittance matching problems for TM and TE polarizations of electromagnetic fields are discussed and the method was validated by means of stability and speed tests, demonstrating increased stability and accuracy in optical simulations of multilayer structures.

General Conclusion

The final conclusion part of this report emphasizes the objectives reached and the difficulties encountered during the run of this internship. The development and integration of the admittance method that we achieved into PyMoosh, has allowed us to drastically improve the simulation of the optical properties of multilayer structures. Particularly, this method presented comparable results in terms of accuracy compared to Abeles method even if it was not as fast as we had hoped at the beginning.

In particular the difficulties met, in particular the implementation complexity and performance comparison, were well dealt with. The results we obtained are promising and open up research paths for future optimizations to further decrease the computing time. This internship has therefore enriched PyMoosh, providing a new method that is both reliable for modeling multilayer structures and that opens the way to further improvements.

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***For the complete code, please visit the following GitHub repository**:*

https://github.com/A-sakkali/Simulation-with-admittance-method.git