

Local absorption via transfer matrices

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In order to calculate the local absorbed energy density $a(z)$ with a transfer matrix formalism, we are going to follow this 5- step process:

1. Calculate r_s/t_s or r_p/t_p for every layer under consideration using Fresnel's formula
2. Calculate all the transfer matrices for each layer M_n
3. Calculate $\tilde{M} = M_0 \cdot M_1 \cdot M_2 \cdots \Rightarrow$ total reflectivity at layer 0 r ; total transmission at last layer t
4. Use t and M_n to obtain v_n, w_n , i.e. amplitude of forward- backward traveling wave for each layer.
5. Use all v_n, w_n to obtain the local absorption $a(z)$ at each point z

Each section will correspond to functions in the code. That is, step 1) will be executed in the "**fresnel()**" function; step steps 2) and 3) will be evaluated by the "**TM()**" function; step 4) will be executed by the "**layerAmpl()**" - and step 5) will finally be computed in the "**absorbtion()**"- function.

1 Fresnel formula

In order to represent the electric field, we want to use a superposition of an incoming and outgoing wave.

$$E(r) = E_f \cdot e^{ik_z r} + E_b \cdot e^{-ik_z r} \quad (1)$$

where,

$$k_z = \frac{2\pi n \cos(\theta)}{\lambda_{vac}} \quad (2)$$

If we are considering multiple layers, at each transition there will be a certain part that is going to be reflected and a part that is going to be transmitted $\rightarrow r_{n,n+1}, t_{n,n+1}$. To obtain the parameters $r_{n,n+1}$ and $t_{n,n+1}$ one can use the Fresnel formulas. Those vary slightly from s to p - polarized light. For s - polarized light one can find [1],

$$\begin{aligned} r_s &= \frac{n_1 \cos(\theta_1) - n_2 \cos(\theta_2)}{n_1 \cos(\theta_1) + n_2 \cos(\theta_2)} \\ t_s &= \frac{2n_1 \cos(\theta_1)}{n_1 \cos(\theta_1) + n_2 \cos(\theta_2)} \end{aligned} \quad (3)$$

and for p -polarized light

$$\begin{aligned} r_p &= \frac{n_2 \cos(\theta_1) - n_1 \cos(\theta_2)}{n_2 \cos(\theta_1) + n_1 \cos(\theta_2)} \\ t_s &= \frac{2n_1 \cos(\theta_1)}{n_2 \cos(\theta_1) + n_1 \cos(\theta_2)} \end{aligned} \quad (4)$$

2 Transfer Matrices

We can use this formulation to express a system of equations, where we formulate the intensity of the forward- and backward traveling wave at each layer n .

$$\begin{bmatrix} v_n \\ w_n \end{bmatrix} = M_n \cdot \begin{bmatrix} v_{n+1} \\ w_{n+1} \end{bmatrix} \quad (5)$$

where,

$$M_{n \geq 1} = Tr \cdot Pr = \begin{bmatrix} e^{-i\phi_n} & 0 \\ 0 & e^{i\phi_n} \end{bmatrix} \cdot \begin{bmatrix} 1 & r_{n,n+1} \\ r_{n,n+1} & 1 \end{bmatrix} \frac{1}{t_{n,n+1}} \quad (6)$$

with,

$$\phi_n = \frac{\delta_n 2\pi n \cos(\theta_n)}{\lambda_{vac}} \quad (7)$$

where δ_n = thickness of layer n and θ_n is the incident angle of the beam at each layer according to Snell's law.

2.1 Total reflectively/ transitivity

Following the expression of eq. (5) we can now multiply the matrices M_n for all layers under consideration, and formulate an expression which relates the amount of intensity reflected at the first layer r and the amount of intensity transmitted through the last layer t .

$$\begin{bmatrix} 1 \\ r \end{bmatrix} = \tilde{M} \cdot \begin{bmatrix} t \\ 0 \end{bmatrix} = \begin{bmatrix} \tilde{M}_{00} & \tilde{M}_{01} \\ \tilde{M}_{10} & \tilde{M}_{11} \end{bmatrix} \begin{bmatrix} t \\ 0 \end{bmatrix} \quad (8)$$

where $\tilde{M} = M_0 M_1 M_2 M_3 \dots$ and $M_0 = \begin{bmatrix} 1 & r_{0,1} \\ r_{0,1} & 1 \end{bmatrix}$

Equation (8), shows that, if we are multiplying the matrices M for every layer under consideration, we can obtain information about the total reflected and the total transmitted intensity. I.e. $t = \frac{1}{\tilde{M}_{00}}$ and $r = \frac{\tilde{M}_{10}}{\tilde{M}_{00}}$.

3 Forward- backward amplitudes for each layer

In order to calculate the amplitude of the forward- and backward traveling wave, one can execute matrix- vector multiplications for each layer. If we look at eq. (5), we see that if the forward- backward amplitude, v_{n+1}, w_{n+1} , for layer $n + 1$ is known we can obtain those parameters for the layer before it, i.e. layer n . Since the amplitudes of the last layer have just been obtained, see eq. (8), we can go from the last wave amplitudes to the first.

$$\begin{bmatrix} v_{n-1} \\ w_{n-1} \end{bmatrix} = M_{n-1} \begin{bmatrix} t \\ 0 \end{bmatrix} \Rightarrow \begin{bmatrix} v_{n-2} \\ w_{n-2} \end{bmatrix} = M_{n-2} \begin{bmatrix} v_{n-1} \\ w_{n-1} \end{bmatrix} \dots \quad (9)$$

This is, once t , the amplitude of the transmitted wave after the last layer is obtained, we can go from there and solve a system of equations for every layer, in order to obtain the amplitude of the forward- backward traveling wave of the layer before.

Absorbed density

Once the amplitudes v_n, w_n are obtained for every layer, the absorbed energy density $a(z)$ can be calculated as a function of space. In order to do so, the steps in the algorithm 1 are executed for every layer $j \in 1, 2, 3 \dots N - 1$ [1].

Algorithm 1 Absorbtion

```
1: for j=0 to N-1 (for every layer) do
2:   Calculate  $k_z = \frac{2\pi n_j \cos(\theta_j)}{\lambda_{vac}}$ 
3:    $z = [0, \delta_j]$ 
4:    $E_f = v_j e^{i \cdot k_z \cdot z}$ 
5:    $E_b = w_j e^{-i \cdot k_z \cdot z}$ 
6:   if polarization == p then
7:      $abs_j = \frac{Im[n_j \cos(\theta_j^*) k_z |E_f - E_b|^2 - k_z^* |E_f + E_b|^2]}{Re[N_0 \cos(\theta_0^*)]}$ 
8:   end if
9:   if polarization == s then
10:     $abs_j = \frac{|E_f + E_b|^2 Im[n_j] \cos(\theta_j) k_z}{Re[n_0 \cos(\theta_0)]}$ 
11:   end if
12:    $abs_{tot} = \text{append}(abs_{tot} \text{ with } abs_j)$ 
12: end for
```

In the algorithm 1, δ_j is the respective thickness for each layer, n_j is the complex refractive index of each layer and θ_j is the incident angle of the beam. In line 3, $z = [0, \delta_i]$ means that we are resetting the grid each time. Next the forward E_f and backward E_b traveling wave can be calculated with the respective amplitudes v_j and w_j which were obtained in the steps before. Then, the local absorption abs_j for each layer is calculated, dependent on whether the wave is s or p polarized. At the end all the local absorption grids are appended together, to form the entire absorption profile abs_{tot} .

Summarizing the process in brief we see that in order to construct the transfer matrices M_n we need to compute their elements using Fresnel's formula.

Once all the matrices are obtained, we can multiply them together and get the transmitted and reflected wave amplitude r and t , see (8).

Using t and M_n we can obtain the amplitudes for the forward and backward traveling wave in each layer, see (9).

Calculating those amplitudes for every layer is then the key to obtain the local energy absorption evaluated at every point under consideration, see algorithm 1.

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References

- [1] Steven J. Byrnes. Multilayer optical calculations. *arXiv:1603.02720v3*, 2018.