A MATRIX APPROACH TO MULTILAYER OPTICS

by

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In this document the transfer-matrix method (TMM)is introduced. This method describes the electromagnetic plane wave that propagates between two media (medium i and j). At the interface of the two, there is a *interface matrix* M_{ij} which *transfers* the waves in medium j that propagates away from and to medium i ($\widetilde{E}_{j\rightarrow}$ and $\widetilde{E}_{j\leftarrow}$) to the ones in medium i ($\widetilde{E}_{i\rightarrow}$ and $\widetilde{E}_{i\leftarrow}$). Next to this interface matrix, a propagation matrix M_j is also obtained that describes the waves traveling through the (absorbent) layer j.

By performing matrix multiplications for every transition and propagation in a layer of a multilayer stack, the reflection, transmission and absorption can be obtained, and even the locally absorbed power can be derived. This works for both s and p polarized (oblique) incident waves. Next to the polarization and incidence angle, only the refractive indices and thicknesses of each layer in the stack are needed as input parameters.

1. INTRODUCTION

This document shows how to obtain a matrix approach to (thin) multilayer optics, with the aim of calculating reflection, transmission and absorption. It starts with summarizing some of the results that can (mostly) be easily found in optics textbooks, such as reflection and transmission coefficients for normal incidence, and Fresnel coefficients for purely dielectric (nonabsorbing) media. Next (in section 4) this is generalized (starting from the macroscopic Maxwell equations) to include both absorption and oblique incidence. The generalization concludes with a summary, focusing on how to implement this model, given a set of layers with given material properties.

2. NORMAL INCIDENCE

2.1. SOME DEFINITIONS

For starters, we mostly follow the notation of [1], in particular Sections 9.3 and 9.4 of that reference. We write the electric and magnetic field of an electromagnetic wave in a section of homogeneous (linear, isotropic) medium (with label j), propagating in the $+\hat{z}$ direction, polarized along $\hat{x}$ as:

$$\begin{aligned}\tilde{\vec{E}}_j(z,t) &= \hat{x}\tilde{E}_j e^{i(\tilde{k}z-\omega_0 t)},\\ \tilde{\vec{B}}_j(z,t) &= \hat{y}\frac{\tilde{k}}{\omega_0}\tilde{E}_j e^{i(\tilde{k}z-\omega_0 t)},\end{aligned} \tag{1}$$

i.e. use complex notation, while it is understood that the actual fields are the real part of each equation:

$$\begin{aligned}\vec{E}_j(z,t) &= \mathrm{Re}(\tilde{\vec{E}}_j(z,t)) = \frac{1}{2}\left(\tilde{\vec{E}}_j(z,t)+cc\right),\\ \vec{B}_j(z,t) &= \mathrm{Re}(\tilde{\vec{B}}_j(z,t)) = \frac{1}{2}\left(\tilde{\vec{B}}_j(z,t)+cc\right),\end{aligned} \tag{2}$$

with cc denoting the complex conjugate of the preceding expression. This allows for compact notation. For instance the complex wave vector $\tilde{k}$ can be written in terms of the complex refractive index $\tilde{n}$,

$$\tilde{k} = \tilde{n}k_0, \tag{3}$$

with

$$\tilde{n} = n + i\kappa, \tag{4}$$

with real part n (the usual refractive index) and imaginary part κ (the latter indicating losses in propagation). Values for n and κ can be found in the literature, and on websites, e.g. [2] [1].

$$k_0 = \frac{2\pi}{\lambda_0} = \frac{\omega_0}{c}, \tag{5}$$

is the vacuum wavevector (with λ_0 the wavelength in vacuum, and c the speed of light in vacuum). The vacuum wavevector k_0 is mainly used as a shorthand here for the

The computational method described in this chapter is implemented in the Python code Multilayers

[1] Note that [2] uses the notation $\tilde{n} = n + ik$. Here, we follow Ref. [1] and use κ for the imaginary part of the complex refractive index. This is mainly to distinguish it clearly from the various wavectors k_0, k_i, $\tilde{k}$, $\boldsymbol{k}$, etc.

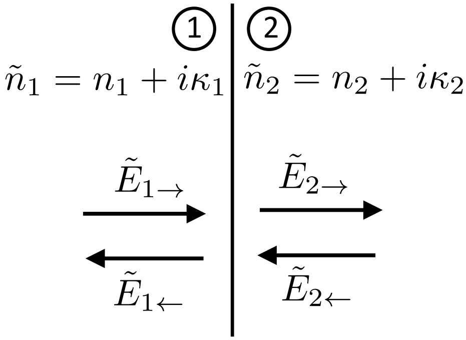

Figure 1: Interface between (linear) materials 1 and 2, with notation for complex-valued refractive index, and incident and outgoing fields indicated.

expression with angular frequency ω_0 (which does not change as the wave passes through various media). Note that the complex dielectric function is usually written as:

$$\tilde{\epsilon} = \epsilon_0 \tilde{n}^2 = \epsilon_0 (n^2 - \kappa^2 + 2in\kappa) = \epsilon_0(\epsilon_r + i\epsilon_i), \tag{6}$$

but later we will include the conductivity σ in n and κ, so we will refrain from expressing things in terms of ϵ.

2.2. THE USUAL IN-OUT MATRIX

At an interface between two linear media, as in figure 1, (and assuming for simplicity that the magnetic constants of the two media are identical, $\mu_1 = \mu_2$) the usual electromagnetic boundary conditions yield concerning the amplitude of the reflection coefficient r and transmission coefficient t at the interface between medium 1 and 2, that can be written in terms of

$$\beta = \frac{\tilde{k}_2}{\tilde{k}_1} = \frac{\tilde{n}_2}{\tilde{n}_1}, \tag{7}$$

as

$$t = \frac{2}{1+\beta} = \frac{2\tilde{n}_1}{\tilde{n}_1 + \tilde{n}_2}, \tag{8}$$

$$r = \frac{1-\beta}{1+\beta} = \frac{\tilde{n}_1 - \tilde{n}_2}{\tilde{n}_1 + \tilde{n}_2}. \tag{9}$$

The relation between the electric fields of the incoming and outcoming waves at the interface between media 1 and 2 can then be written in matrix form as:

$$\begin{pmatrix} \tilde{E}_{2\rightarrow} \\ \tilde{E}_{1\leftarrow} \end{pmatrix} = \begin{pmatrix} t & -r \\ r & \beta t \end{pmatrix} \begin{pmatrix} \tilde{E}_{1\rightarrow} \\ \tilde{E}_{2\leftarrow} \end{pmatrix}. \tag{10}$$

Here $\tilde{E}_{1\to}$ denotes the amplitude at the side of medium 1 traveling in the $+\hat{z}$ direction, while $\tilde{E}_{1\leftarrow}$ is the amplitude at the side of medium 1 travelling in the $-\hat{z}$ direction (obtained by replacing $\tilde{k}$ by $-\tilde{k}$ in equation (1)), etcetera. Also, to simplify the notation above we have written β instead of β_{12}, and similarly $r = r_{12}$, and $t = t_{12}$. When dealing with multiple interfaces, we will need to include the indices of the layers involved.

2.3. Interface matrix between media

For the purpose of multilayer systems, it is more convenient to rewrite equation (10) into a matrix transformation between the fields in medium 2 to those in medium 1. This is just a transformation of the above linear equations of equation (10), and yields

$$\begin{pmatrix} \tilde{E}_{1\to} \\ \tilde{E}_{1\leftarrow} \end{pmatrix} = \begin{pmatrix} \frac{1}{t} & \frac{r}{t} \\ \frac{r}{t} & \frac{r^2}{t} + \beta t \end{pmatrix} \begin{pmatrix} \tilde{E}_{2\to} \\ \tilde{E}_{2\leftarrow} \end{pmatrix}, \tag{11}$$

with $\tilde{E}_{1\to}$ (and similar) defined as before.

2.4. Matrix for homogeneous medium

For a linear, isotropic and homogeneous medium with thickness d, and wavevector $\tilde{k}$, the matrix relating the left-hand side (at low z) to the right-hand side (at higher z, $z_h = z_l + d$), is simply

$$\begin{pmatrix} \tilde{E}_{l\to} \\ \tilde{E}_{l\leftarrow} \end{pmatrix} = \begin{pmatrix} e^{-i\tilde{k}d} & 0 \\ 0 & e^{+i\tilde{k}d} \end{pmatrix} \begin{pmatrix} \tilde{E}_{h\to} \\ \tilde{E}_{h\leftarrow} \end{pmatrix}. \tag{12}$$

2.5. Multiple layers

For a stack of multiple layers, the total reflection and transmission can now be readily calculated as follows. First multiply the corresponding matrices of the various layers and interfaces, to obtain the (2 by 2) matrix of the total stack. Next, right-multiply this matrix with the vector $(1,0)$, to represent the situation that light is incident from the left (i.e.: no incident light from the right). This yields a vector with incident and reflected (complex) amplitude, scaled to unit transmitted amplitude. Finally, rescale to unit incident amplitude (and/or intensity) to obtain the reflection and transmission amplitudes (and/or intensities). For the intensities, do not forget to take into account the refractive index of the in- and outgoing media.

The mathematical expression for the transfer matrix, for a stack of layers labeled from 0 to m, is:

$$M_{\text{tot}} = M_{01} M_1 M_{12} M_2 \cdots M_{m-1\,m}, \tag{13}$$

with matrices for the interfaces

$$M_{ij} = \begin{pmatrix} 1/t_{ij} & r_{ij}/t_{ij} \\ r_{ij}/t_{ij} & r_{ij}^2/t_{ij} + \beta_{ij} t_{ij} \end{pmatrix}, \tag{14}$$

and for the propagation within each layer

$$M_j = \begin{pmatrix} e^{-i\tilde{k}_j d_j} & 0 \\ 0 & e^{+i\tilde{k}_j d_j} \end{pmatrix}, \tag{15}$$

To obtain transmission and reflection with light incident from layer 0 (i.e., no incident light from layer m), $E_{m\leftarrow} = 0$, we write:

$$\begin{pmatrix} \alpha_{0\rightarrow} \\ \alpha_{0\leftarrow} \end{pmatrix} = M_{\text{tot}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{16}$$

The amplitude transmission coefficient is then simply $1/\alpha_{0\rightarrow}$, while the amplitude reflection coefficient is $\alpha_{0\leftarrow}/\alpha_{0\rightarrow}$.

For intensities of transmission and reflection, we need to account for the local velocities, i.e. for layers 0 and m (and for each of the right- and left-travelling waves separately):

$$I_j = \frac{1}{2}\epsilon_0 n_j c E_j^2. \tag{17}$$

Note that we need to take the initial layer (0) and final layer (m) to have no absorption, otherwise total transmission and reflection are ill-defined (since in the presence of absorption, total transmission and reflection would depend on where in layer 0 and m you would you measure). Thus with the above, we obtain for the intensity transmission coefficient:

$$T = \left|\frac{1}{\alpha_{0\rightarrow}}\right|^2 \frac{n_T}{n_I}, \tag{18}$$

and the intensity reflection coefficient:

$$R = \left|\frac{\alpha_{0\leftarrow}}{\alpha_{0\rightarrow}}\right|^2, \tag{19}$$

and the total absorbed intensity fraction:

$$Abs = 1 - T - R. \tag{20}$$

2.6. LOCALLY ABSORBED POWER

Now, we would also like to have expressions for the locally absorbed power density. Taking isotropic, linear, homogeneous media, and, for simplicity, non-magnetic materials, $\mu = \mu_0$, the electromagnetic energy density is:

$$u = \frac{1}{2}\left(\epsilon E^2 + \frac{1}{\mu_0}B^2\right), \tag{21}$$

and the Poynting vector:

$$\vec{S} = \frac{1}{\mu_0}\vec{E} \times \vec{B}. \tag{22}$$

The cycle-averaged locally absorbed power density is then:

$$p = -\langle \vec{\nabla} \cdot \vec{S} \rangle. \tag{23}$$

Inserting a superposition of left- and right-travelling waves, and writing the local amplitudes in equation (1) as $\tilde{E}_{j\rightarrow} = \alpha_{\rightarrow} E_0$ and $\tilde{E}_{j\leftarrow} = \alpha_{\leftarrow} E_0$, leads to a relatively simple expression in terms of the (real-valued) value f:

$$f = \alpha_{\rightarrow}\alpha_{\rightarrow}^* + \alpha_{\leftarrow}\alpha_{\leftarrow}^* + \alpha_{\rightarrow}\alpha_{\leftarrow}^* + \alpha_{\leftarrow}\alpha_{\rightarrow}^*. \tag{24}$$

Namely,

$$
\begin{aligned}
p &= \frac{E_0^2}{\mu_0 \omega_0} n\kappa k_0^2 f \\
&= \epsilon_0 n c E_0^2 k_0 \kappa f.
\end{aligned}
\tag{25}
$$

This result may seem somewhat obvious, in hindsight. See below for a more general derivation, that for normal incidence also yields the above result.

The z-dependent $\alpha_{\rightarrow}$ and $\alpha_{\leftarrow}$ can be obtained using essentially the same procedure as in the previous section, namely by taking the product of the relevant matrices from the outgoing side (layer m) up to the position z, right-multiplying with $(1,0)$ to get the local amplitudes, and scaling to the incident amplitude $\alpha_{0\rightarrow}$ obtained from equation (16). In other words, first calculating

$$
\begin{pmatrix} \alpha_{\rightarrow}(z) \\ \alpha_{\leftarrow}(z) \end{pmatrix} = M(z) \begin{pmatrix} 1 \\ 0 \end{pmatrix},
\tag{26}
$$

the relative absorbed power density (scaled to the incident intensity obtained from equation (16) is:

$$
p_{\text{rel}}(z) = 2k_0 n_j \kappa_j f(z) \frac{1}{n_I |\alpha_{0\rightarrow}|^2}.
\tag{27}
$$

The numerically integrated relative local absorption should equal the total relative absorption, which can be used as a consistency check, i.e.

$$
\int p_{\text{rel}}(z)\, dz = A.
\tag{28}
$$

3. Oblique incidence

We now consider the situation where the incoming wave is not normal to the interface(s). We will still restrict ourselves to a planar situation, meaning that all interfaces are parallel.

When the incident light is at an angle, the situation becomes more complicated in several ways. For one, we now need to distinguish the two polarization directions, namely *in* the plane of incidence, and *perpendicular* to the plane of incidence. So instead of a 2×2 matrix, we will have at least two 2×2 matrices to deal with, and, if there is any coupling between in-plane and out-of-plane polarization, a 4×4 matrix per interface/propagation. Further, in the case of absorbing media, we need to distinguish propagation in the lateral direction (along the interfaces), from propagation normal to the interfaces. For incident plane waves (with a single wavevector $\vec{k}$), there is translational invariance of the waves along the lateral direction, so the amplitudes of the waves are independent of the lateral direction. Since for absorbing media the wave amplitudes *do* vary in the direction normal to the interfaces, this implies that the planes of constant amplitude will no longer be parallel to the planes of constant phase.

Anyway, let's get started by defining the relevant quantities, see figure 2. The polarization with its electric field along the plane of incidence is indicated by p, while light with its electric field perpendicular to the plane of incidence is traditionally denoted by s (for *senkrecht*).

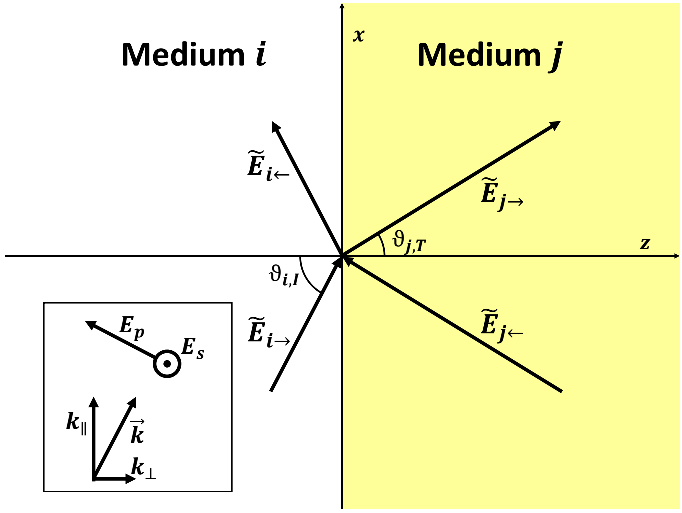

Figure 2: The plane of incidence (the xz plane), with (sketches of) wavevector and polarization definitions for oblique incidence.

3.1. NONABSORBING MEDIA

For nonabsorbing media, we can just use the standard Fresnel coefficient expressions. in particular, for p polarization we have [1]:

$$r_p = \frac{\alpha - \beta}{\alpha + \beta}, \tag{29}$$

$$t_p = \frac{2}{\alpha + \beta}, \tag{30}$$

with $\beta = k_2/k_1 = n_2/n_1$ as before, and

$$\alpha \equiv \frac{\cos\theta_T}{\cos\theta_I}, \tag{31}$$

with θ_I and θ_T the incident and transmitted angle, respectively. In terms of wavevectors, this is:

$$\alpha = \frac{k_{2\perp}}{k_2}\frac{k_1}{k_{1\perp}} = \frac{1}{\beta}\frac{k_{2\perp}}{k_{1\perp}}. \tag{32}$$

For s polarization (Prob. 9.17 of [1]) we have:

$$r_s = \frac{1 - \alpha\beta}{1 + \alpha\beta}, \tag{33}$$

$$t_s = \frac{2}{1 + \alpha\beta}. \tag{34}$$

4. Generalization

4.1. Macroscopic Maxwell equations

The macroscopic Maxwell equations [1] can be written as:

$$\begin{aligned} \vec{\nabla}\cdot\vec{D} &= \rho_f, &(35)\\ \vec{\nabla}\times\vec{E} &= -\frac{\partial\vec{B}}{\partial t}, &(36)\\ \vec{\nabla}\cdot\vec{B} &= 0, &(37)\\ \vec{\nabla}\times\vec{H} &= \vec{J}_f+\frac{\partial\vec{D}}{\partial t}. &(38)\end{aligned}$$

4.2. Complexified version of Poynting's theorem

For determining the locally absorbed power, it is useful to consider (the derivation of) Poynting's theorem for harmonic fields. We follow Sections 6.9 (and 6.7) of Jackson [3], adopting the following notation (a mix of the above and of [3]). We write the harmonically oscillating fields as:

$$\vec{E}(\boldsymbol{r},t)=\mathrm{Re}(\boldsymbol{E}(\boldsymbol{r})e^{-i\omega t})\equiv\frac{1}{2}\left[\boldsymbol{E}(\boldsymbol{r})e^{-i\omega t}+\boldsymbol{E}^*(\boldsymbol{r})e^{i\omega t}\right]. \tag{39}$$

Products such as $\vec{J}\cdot\vec{E}$ then can be rewritten as:

$$\vec{J}(\boldsymbol{r},t)\cdot\vec{E}(\boldsymbol{r},t)=\frac{1}{2}\mathrm{Re}\left[\boldsymbol{J}^*(\boldsymbol{r})\cdot\boldsymbol{E}(\boldsymbol{r})+\boldsymbol{J}(\boldsymbol{r})\cdot\boldsymbol{E}(\boldsymbol{r})e^{-2i\omega t}\right]. \tag{40}$$

When taking cycle-averages over time, the second term on the right-hand side then averages out. For the power dissipated, we are interested in the cycle-averaged value of $\vec{J}\cdot\vec{E}$, and hence in the first term on the right-hand side above. For harmonically oscillating fields, the macroscopic Maxwell equations then become:

$$\begin{aligned} \boldsymbol{\nabla}\cdot\boldsymbol{D} &= \rho_f, &(41)\\ \boldsymbol{\nabla}\times\boldsymbol{E} &= +i\omega\boldsymbol{B}, &(42)\\ \boldsymbol{\nabla}\cdot\boldsymbol{B} &= 0, &(43)\\ \boldsymbol{\nabla}\times\boldsymbol{H} &= \boldsymbol{J}_f-i\omega\boldsymbol{D}. &(44)\end{aligned}$$

Using the vector identity

$$\boldsymbol{\nabla}\cdot(\boldsymbol{a}\times\boldsymbol{b})=\boldsymbol{b}\cdot(\nabla\times\boldsymbol{a})-\boldsymbol{a}\cdot(\nabla\times\boldsymbol{b}), \tag{45}$$

and using the two Maxwell's equations for the curl (of $\boldsymbol{H}$ and $\boldsymbol{E}$ respectively), yields (a complex-valued version of) Poynting's theorem:

$$\frac{1}{2}\boldsymbol{J}_f^*\cdot\boldsymbol{E}=-2i\omega(u_e-u_m)-\boldsymbol{\nabla}\cdot\boldsymbol{S}, \tag{46}$$

with (potentially complex-valued) defined quantities

$$u_e=\frac{1}{4}\boldsymbol{E}\cdot\boldsymbol{D}^*, \tag{47}$$

$$u_m = \frac{1}{4}\boldsymbol{B}\cdot\boldsymbol{H}^*, \tag{48}$$

and

$$\boldsymbol{S} = \frac{1}{2}\boldsymbol{E}\times\boldsymbol{H}^*. \tag{49}$$

The real part of equation (46) expresses conservation of energy for the cycle-averaged quantities. In particular, $\mathrm{Re}(\boldsymbol{S})$ is the Poynting vector, and the imaginary part $\mathrm{Im}(u_e - u_m)$ accounts for dissipation in the material. The imaginary part of equation (46) relates to the reactive/stored energy and its alternating flow. In particular $\mathrm{Re}(u_e)$ is the instantaneous electric field energy density, and $\mathrm{Re}(u_m)$ the magnetic field energy density.

4.3. PLANE WAVES IN LINEAR MEDIA

We are interested in plane-wave solutions like before, as in equation (1), but need to keep the vectorial form, i.e. we write:

$$\boldsymbol{E}(\boldsymbol{r}) = \boldsymbol{E}_0 e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{50}$$

etcetera. Note that harmonic time-dependence is implied again here.

In a linear, isotropic and homogeneous medium, we may write constituent relations $\boldsymbol{D} = \tilde{\epsilon}(\omega)\boldsymbol{E}$, and $\boldsymbol{H} = \boldsymbol{B}/\tilde{\mu}(\omega)$. For simplicity we will limit ourselves to non-magnetic media ($\tilde{\mu} = \mu_0$). Furthermore, for a medium characterized by a conductivity $\sigma(\omega)$, we have $\boldsymbol{J}_f = \sigma(\omega)\boldsymbol{E}$. We will also take $\rho_f(\omega) = 0$ in the bulk of the medium. Note that below we will consider the boundary separately.

With this set of assumptions and simplifications, and inserting traveling-wave trial solutions of the form equation (50), the spatial and temporal derivatives lead to wave vector and angular frequency prefactors respectively:

$$\begin{aligned}
\boldsymbol{k}\cdot\boldsymbol{E} &= 0, && (51)\\
\boldsymbol{k}\times\boldsymbol{E} &= \omega\boldsymbol{B}, && (52)\\
\boldsymbol{k}\cdot\boldsymbol{B} &= 0, && (53)\\
i\boldsymbol{k}\times\boldsymbol{B} &= \mu_0\left[\sigma(\omega) - i\omega\tilde{\epsilon}(\omega)\right]\boldsymbol{E}. && (54)
\end{aligned}$$

Inserting section 4.3 into section 4.3 leads to:

$$\boldsymbol{k}\times(\boldsymbol{k}\times\boldsymbol{E}) = -\mu_0\left[\omega^2\tilde{\epsilon}(\omega) + i\omega\sigma(\omega)\right]\boldsymbol{E}. \tag{55}$$

Since $\boldsymbol{k}$ and $\boldsymbol{E}$ are orthogonal ($\boldsymbol{k}\cdot\boldsymbol{E} = 0$), the cross products on the left-hand side of the above simplify to $-(\boldsymbol{k}\cdot\boldsymbol{k})\boldsymbol{E}$, and section 4.3 simplifies to:

$$\boldsymbol{k}\cdot\boldsymbol{k} \equiv \tilde{k}^2 = \mu_0\left[\omega^2\tilde{\epsilon}(\omega) + i\omega\sigma(\omega)\right]. \tag{56}$$

Writing $\boldsymbol{k} = \vec{k}_0[n(\omega) + i\kappa(\omega)]$, with $|\vec{k}_0| \equiv k_0 \equiv \omega/c$ as before, and $\mu_0\epsilon_0 = 1/c^2$ results in:

$$\tilde{n}^2 = (n + i\kappa)^2 = \frac{1}{\epsilon_0}\left(\tilde{\epsilon} + \frac{i\sigma}{\omega}\right). \tag{57}$$

Thus, specifying n and κ of a (linear, isotropic, and homogeneous) material at a certain frequency, is sufficient to capture the behavior of electromagnetic waves in the material at that frequency. In particular, from the imaginary part of equation (57), we have:

$$2\epsilon_0 n\kappa = \mathrm{Im}\tilde{\epsilon} + \frac{\sigma}{\omega}. \tag{58}$$

4.4. Plane waves with a fixed incident angle

For a plane wave incident from a lossless medium, the incident field will have a constant amplitude at the interface, and the boundary conditions enforce that the transmitted wave will have the same spatial dependence along the interface. Thus, we can write:

$$\boldsymbol{k} = k_0(\vec{n} + i\vec{\kappa}), \tag{59}$$

with $\vec{\kappa}$ perpendicular to the interface, and the parallel part of $\vec{n}$ determined by the incoming wave. Note that $\boldsymbol{k}$, $\vec{n}$, and $\vec{\kappa}$ are all within the plane of incidence.

Starting from equation (59), we have

$$\tilde{k}^2 = \boldsymbol{k}\cdot\boldsymbol{k} = k_0^2(\vec{n}\cdot\vec{n} + 2i\vec{n}\cdot\vec{\kappa} - \vec{\kappa}\cdot\vec{\kappa}). \tag{60}$$

Thus, for a material with given n and κ, we need for the wavevector

$$\begin{aligned} \vec{n}\cdot\vec{n} - \vec{\kappa}\cdot\vec{\kappa} &= n^2 - \kappa^2, &(61)\\ \vec{n}\cdot\vec{\kappa} &= n\kappa. &(62)\end{aligned}$$

For a plane-wave boundary condition at a planar interface, the parallel part of $\vec{n}$ is fixed, $n_\parallel = k_\parallel/k_0$, and $\vec{\kappa}$ is strictly normal to the interface. Thus the above simplifies to:

$$\begin{aligned} n_\parallel^2 + n_\perp^2 - \kappa_\perp^2 &= n^2 - \kappa^2, &(63)\\ n_\perp\kappa_\perp &= n\kappa, &(64)\end{aligned}$$

and we have two equations with two unknowns ($n_\perp$ and $\kappa_\perp$), which can be solved directly. Namely with shorthand:

$$b = n^2 - \kappa^2 - n_\parallel^2, \tag{65}$$

$$\begin{aligned} n_\perp &= \sqrt{\frac{b + \sqrt{b^2 + 4n^2\kappa^2}}{2}}, &(66)\\ \kappa_\perp &= \frac{n\kappa}{n_\perp}. &(67)\end{aligned}$$

Note that for $n_\parallel = 0$ we recover $n_\perp = n$ and $\kappa_\perp = \kappa$, as should be. For what follows below, it is useful to define

$$\tilde{n}_\perp \equiv n_\perp + i\kappa_\perp. \tag{68}$$

In summary, then, with the coordinate system of figure 2, we have

$$\boldsymbol{k} = k_0\left[n_\parallel\hat{x} + (n_\perp + i\kappa_\perp)\hat{z}\right] = k_0\left(n_\parallel\hat{x} + \tilde{n}_\perp\hat{z}\right). \tag{69}$$

Out-of-plane polarization

For s polarization, the above can be worked out relatively easily, since $\boldsymbol{E}$ is perpendicular to the plane of incidence, while $\boldsymbol{k}$, $\vec{n}$, $\vec{\kappa}$, are within this plane.

As a consequence, the first Maxwell equation is satisfied, the second Maxwell equation ensures that $\boldsymbol{k}$ and $\boldsymbol{B}$ are orthogonal so that the third is automatically satisfied, and what remains is to satisfy equation (55). Thus we can write:

$$\begin{aligned} \boldsymbol{E}(\boldsymbol{r}) &= \tilde{E}_0\hat{y}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, &(70)\\ \boldsymbol{B}(\boldsymbol{r}) &= \frac{1}{c}\tilde{E}_0\left(n_\parallel\hat{z} - \tilde{n}_\perp\hat{x}\right)e^{i\boldsymbol{k}\cdot\boldsymbol{r}}. &(71)\end{aligned}$$

IN-PLANE POLARIZATION

For p polarization, the situation is similar, with the roles of $\vec{\tilde{B}}$ (which is now perpendicular to the plane of incidence) and $\vec{\tilde{E}}$ exchanged. For later convenience, we would like to keep the same phase definition of the $\hat{x}$ component of $\vec{\tilde{E}}$ leading to slightly more complicated expressions here. Namely,

$$\boldsymbol{E}(\boldsymbol{r}) = \frac{\tilde{E}_0}{N}\left(\hat{x} - \frac{n_\parallel}{\tilde{n}_\perp}\hat{z}\right)e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{72}$$

$$\boldsymbol{B}(\boldsymbol{r}) = \frac{\tilde{E}_0\hat{y}}{Nc}\left(\frac{n_\parallel^2}{\tilde{n}_\perp} + \tilde{n}_\perp\right)e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{73}$$

with normalization

$$N = \sqrt{1 + \frac{n_\parallel^2}{n_\perp^2 + \kappa_\perp^2}}. \tag{74}$$

4.5. REFLECTION AND TRANSMISSION FROM BOUNDARY CONDITIONS

To get to the boundary conditions, for the interface between two linear, isotropic and homogeneous media, we return to the macroscopic Maxwell equations. The medium with index j can then be characterized with dielectric function $\tilde{\epsilon}_j(\omega)$ and conductivity $\sigma_j(\omega)$. For media with nonzero conductivity, we can have (free) surface charge density σ_f built up at the interface. At charge conservation,

$$\boldsymbol{\nabla}\cdot\vec{J}_f = -\frac{\partial\rho_f}{\partial t}, \tag{75}$$

applied to the interface between media 1 and 2 then yields at frequency ω,

$$i\omega\sigma_f = -J_{f\perp 1} + J_{f\perp 2}, \tag{76}$$

and the boundary condition from the first Maxwell equation reads:

$$\left(\tilde{\epsilon}_1 + \frac{i\sigma_1}{\omega}\right)\tilde{E}_{\perp 1} = \left(\tilde{\epsilon}_2 + \frac{i\sigma_2}{\omega}\right)\tilde{E}_{\perp 2}. \tag{77}$$

Note that the same combination of $\tilde{\epsilon}$ and σ appears here as in the previous equations, so this can again be rephrased in terms of n_i and κ_i of the materials involved. Also, note that the above σ_1 and σ_2 are conductivities, not to be confused with the free surface charge density σ_f.

Again taking $\mu = \mu_0$ for all materials, for simplicity, and assuming there is no surface current density, the other boundary conditions are more common:

$$\vec{E}_{\parallel 1} = \vec{E}_{\parallel 2}, \tag{78}$$

$$B_{\perp 1} = B_{\perp 2}, \tag{79}$$

$$\vec{B}_{\parallel 1} = \vec{B}_{\parallel 2}. \tag{80}$$

For the discussion below, it is useful to state explicitly that for the wave vector in the direction of reflection, and the choice of coordinates of figure 2, we have

$$\boldsymbol{k}_R = k_0\left(n_\parallel \hat{x} - \tilde{n}_\perp \hat{z}\right), \tag{81}$$

while for the incident (and transmitted) direction we have

$$\boldsymbol{k}_I \equiv \boldsymbol{k} = k_0\left(n_\parallel \hat{x} + \tilde{n}_\perp \hat{z}\right), \tag{82}$$

as defined before.

Out-of-plane polarization

For s polarization, we write the electric and magnetic field of the reflected wave as:

$$\boldsymbol{E}_R(\vec{r}) = \tilde{E}_{R0}\hat{y}e^{i\boldsymbol{k}_R\cdot\boldsymbol{r}}, \tag{83}$$

$$\boldsymbol{B}_R(\vec{r}) = \frac{1}{c}\tilde{E}_{R0}\left(n_\parallel \hat{z} + \tilde{n}_\perp \hat{x}\right)e^{i\boldsymbol{k}_R\cdot\boldsymbol{r}}. \tag{84}$$

The first boundary condition is now automatically satisfied (since the perpendicular component of $\boldsymbol{E}$ is zero), while the rest yields the same expressions for the amplitude reflection and transmission coefficients:

$$r_s = \frac{1-\beta_s}{1+\beta_s}, \tag{85}$$

$$t_s = \frac{2}{1+\beta_s}, \tag{86}$$

with a modified β,

$$\beta_s = \frac{\tilde{n}_{\perp 2}}{\tilde{n}_{\perp 1}}. \tag{87}$$

These are readily shown to be consistent with the usual Fresnel expressions (without absorption) and the expressions for normal incidence (with absorption).

In-plane polarization

For p polarization, we write the electric and magnetic field of the reflected wave as:

$$\boldsymbol{E}_R(\boldsymbol{r}) = \frac{\tilde{E}_{R0}}{N}\left(\hat{x} + \frac{n_\parallel}{\tilde{n}_\perp}\hat{z}\right)e^{i\boldsymbol{k}_R\cdot\boldsymbol{r}}, \tag{88}$$

$$\boldsymbol{B}_R(\boldsymbol{r}) = -\frac{\tilde{E}_{R0}\hat{y}}{Nc}\left(\frac{n_\parallel^2}{\tilde{n}_\perp} + \tilde{n}_\perp\right)e^{i\boldsymbol{k}_R\cdot\boldsymbol{r}}, \tag{89}$$

and the boundary conditions lead to the same expressions for the reflection and transmission coefficients as before,

$$r_p = \frac{\alpha_p - \beta_p}{\alpha_p + \beta_p}, \tag{90}$$

$$t_p = \frac{2}{\alpha_p + \beta_p}, \tag{91}$$

with modified α and β,

$$\alpha_p = \frac{N_1}{N_2}, \tag{92}$$

$$\beta_p = \frac{\tilde{n}_2^2}{\tilde{n}_1^2}\frac{\tilde{n}_{\perp 1}}{\tilde{n}_{\perp 2}}\frac{N_1}{N_2}. \tag{93}$$

These are indeed consistent with the normal-incidence expressions (with absorption), and with the usual Fresnel (no absorption) expressions.

4.6. TRANSMITTED AND REFLECTED INTENSITY

To get to the transmitted and reflected intensity (per area of the interface), we need to take into account the angle between the interface and the wavefronts; this leads to an extra cosine term, i.e.

$$I = \frac{1}{2}\epsilon_0 n c E^2 \cos\theta, \tag{94}$$

for the incident, reflected and transmitted part of the waves. Thus, the intensity reflection and transmission coefficients are:

$$R = \frac{I_R}{I_I} = |r|^2, \tag{95}$$

and

$$T = \frac{I_T}{I_I} = |t|^2 \frac{n_T \cos\theta_T}{n_I \cos\theta_I}. \tag{96}$$

Note that $\theta_R = \theta_I$, and with θ_T given by Snell's law:

$$\frac{\sin\theta_T}{\sin\theta_I} = \frac{n_I}{n_T}. \tag{97}$$

4.7. LOCALLY ABSORBED POWER

Returning now to the issue of a useful expression for the locally absorbed (cycle-averaged) power, we now use the complex-valued version of Poynting's theorem, equation (46). For the linear, isotropic, homogeneous and non-magnetic ($\mu = \mu_0$) materials under consideration here, the real part of equation (46) yields

$$p \equiv -\mathrm{Re}\langle \boldsymbol{\nabla}\cdot\boldsymbol{S}\rangle = \frac{1}{2}\left[\sigma(\omega) + \omega\,\mathrm{Im}(\tilde{\epsilon}(\omega))\right]\langle \boldsymbol{E}^*\cdot\boldsymbol{E}\rangle. \tag{98}$$

Here, we encounter the same combination of σ and $\mathrm{Im}(\tilde{\epsilon})$ again, so that the result can be simplified in terms of $n\kappa$, as:

$$p = \epsilon_0 \omega n \kappa \langle \boldsymbol{E}^*\cdot\boldsymbol{E}\rangle. \tag{99}$$

Writing the field $\boldsymbol{E}(\boldsymbol{r})$ as a superposition of incoming and reflected wave amplitudes as $\tilde{E}_{I0}(\boldsymbol{r}) = \tilde{c}_I E_0$ and $\tilde{E}_{R0}(\boldsymbol{r}) = \tilde{c}_R E_0$, p can now be further worked out for both polarizations.

For s polarization the electric field points along $\hat{x}$ for both the transmitted and reflected direction, and the above simplifies to:

$$p = \epsilon_0 \omega n \kappa E_0^2 f_s, \tag{100}$$

with

$$f_s = (\tilde{c}_I + \tilde{c}_R)(\tilde{c}_I^* + \tilde{c}_R^*), \tag{101}$$

i.e. equivalent to f as defined before in equation (24).

For p polarization, the amplitudes of transmitted and reflected electric fields add along x, but subtract along z, and the result is

$$p = \epsilon_0 \omega n \kappa E_0^2 f_p, \tag{102}$$

with

$$f_p = \tilde{c}_I \tilde{c}_I^* + \tilde{c}_R \tilde{c}_R^* + \frac{1}{N^2}(\tilde{c}_I \tilde{c}_R^* + \tilde{c}_R \tilde{c}_I^*)\left(1 - \frac{n_\parallel^2}{n_\perp^2 + \kappa_\perp^2}\right), \tag{103}$$

or, equivalently,

$$f_p = (\tilde{c}_I + \tilde{c}_R)(\tilde{c}_I^* + \tilde{c}_R^*) - 2(\tilde{c}_I \tilde{c}_R^* + \tilde{c}_R \tilde{c}_I^*)\frac{n_\parallel^2}{n_\perp^2 + \kappa_\perp^2}. \tag{104}$$

So the absorbed power density relative to the incident intensity is

$$\frac{p}{I_I} = \frac{2k_0 n \kappa f}{n_I \cos\theta_I}, \tag{105}$$

with f set to f_s or to f_p depending on the polarization.

4.8. Implementation

In summary, to implement the above we can treat the combination of oblique incidence and multiple lossy layers as follows. First, from the incident angle and incident (lossless) medium with refractive index n_i calculate the parallel wavevector $k_\parallel = n_\parallel k_0$ and parallel index $n_\parallel$ from:

$$n_\parallel = n_i \sin(\theta_i), \tag{106}$$

and $k_0 = 2\pi/\lambda_0 = \omega_0/c$, with λ_0 the wavelength in vacuum. Next, for each layer, calculate $\tilde{n}_\perp$ from:

$$b = n^2 - \kappa^2 - n_\parallel^2, \tag{107}$$

$$n_\perp = \sqrt{\frac{b + \sqrt{b^2 + 4n^2\kappa^2}}{2}}, \tag{108}$$

$$\kappa_\perp = \frac{n\kappa}{n_\perp}, \tag{109}$$

and

$$\tilde{n}_\perp \equiv n_\perp + i\kappa_\perp. \tag{110}$$

Combine these to obtain

$$\boldsymbol{k} = k_0\left[n_\parallel \hat{x} + (n_\perp + i\kappa_\perp)\hat{z}\right] = k_0\left(n_\parallel \hat{x} + \tilde{n}_\perp \hat{z}\right), \tag{111}$$

and normalization factor

$$N = \sqrt{1 + \frac{n_\parallel^2}{n_\perp^2 + \kappa_\perp^2}}. \tag{112}$$

For each interface between (possibly lossy) media we then have complex-valued reflection and transmission coefficients:

$$r = \frac{\alpha - \beta}{\alpha + \beta}, \tag{113}$$

$$t = \frac{2}{\alpha + \beta}, \tag{114}$$

with $\alpha_s = 1$ and $\beta_s = \tilde{n}_{\perp 2}/\tilde{n}_{\perp 1}$ for out-of-plane polarization, and $\alpha_p = N_1/N_2$ and $\beta_p = \tilde{n}_2^2 \tilde{n}_{\perp 1} N_1 / \tilde{n}_1^2 \tilde{n}_{\perp 2} N_2$ for in-plane polarization. The matrix relating in- and outgoing waves then can be written as:

$$\begin{pmatrix} t & -r \\ r & \alpha\beta t \end{pmatrix}, \tag{115}$$

and the matrix relating the fields in the two media as:

$$\begin{pmatrix} \frac{1}{t} & \frac{r}{t} \\ \frac{r}{t} & \frac{r^2}{t} + \alpha\beta t \end{pmatrix}, \tag{116}$$

which actually simplifies to:

$$\frac{1}{2}\begin{pmatrix} \alpha + \beta & \alpha - \beta \\ \alpha - \beta & \alpha + \beta \end{pmatrix}, \tag{117}$$

inserting the proper α and β for either s or p polarization.

The propagation matrix within a layer (with thickness d) becomes

$$\begin{pmatrix} e^{-ik_0\tilde{n}_\perp d} & 0 \\ 0 & e^{+ik_0\tilde{n}_\perp d} \end{pmatrix}. \tag{118}$$

4.9. ACTUAL EXAMPLES

As a reference example, we will use light with a wavelength of $\lambda = 800\,\mathrm{nm}$, and model a thin film of Ru ($n = 5.89$ and $\kappa = 4.83$, corresponding tabulated properties of Ru at that wavelength [4]) on glass ($n_{\text{glass}} = 1.5$) in air ($n_{\text{air}} = 1.0$), with the light incident from the air side.

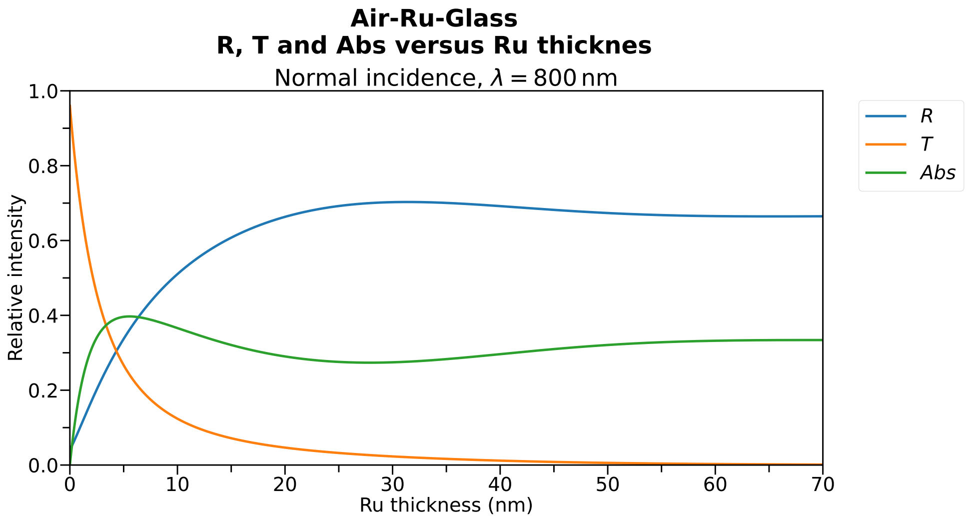

Figure 3: Reflection R, transmission T and total absorption Abs versus Ru thickness for a model air-Ru-glass structure illuminated with light with a wavelength $\lambda = 800\,\mathrm{nm}$ from the air side at normal incidence.

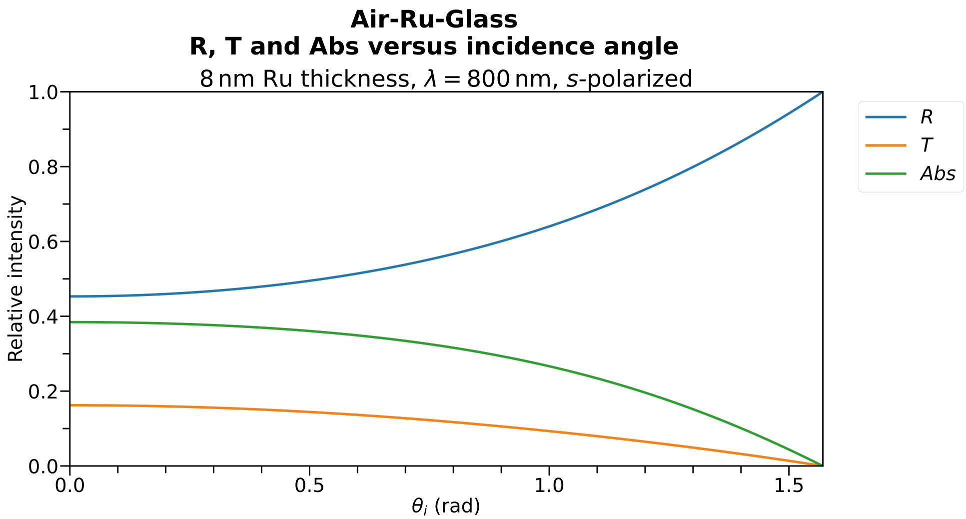

Figure 4: Reflection R, transmission T and total absorption Abs versus incident angle θ_i for a model air-Ru-glass structure, Ru thickness 8 nm, for s-polarized light with wavelength $\lambda = 800\,\mathrm{nm}$ incident from the air side.

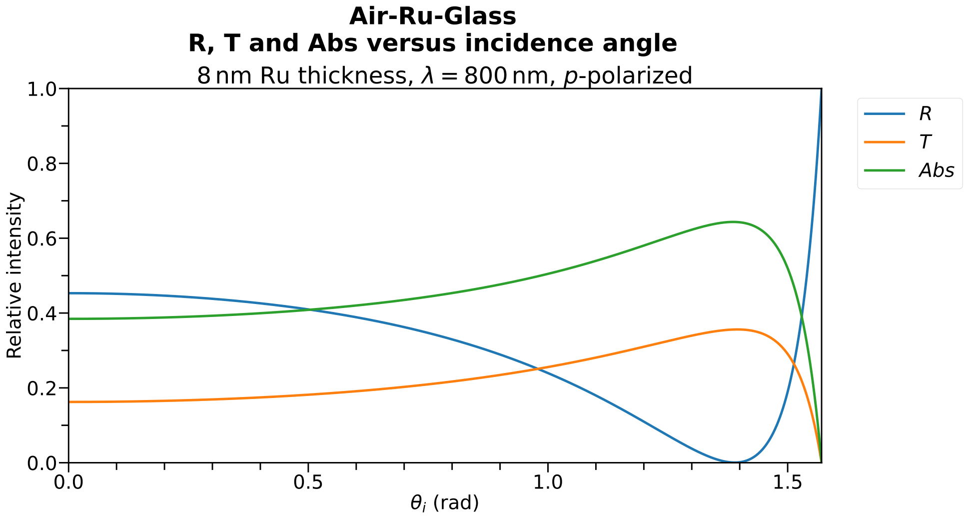

Figure 5: Reflection R, transmission T and total absorption *Abs* versus incident angle θ_i for a model air-Ru-glass structure, Ru thickness 8 nm, for p-polarized light with wavelength $\lambda = 800$ nm incident from the air side.

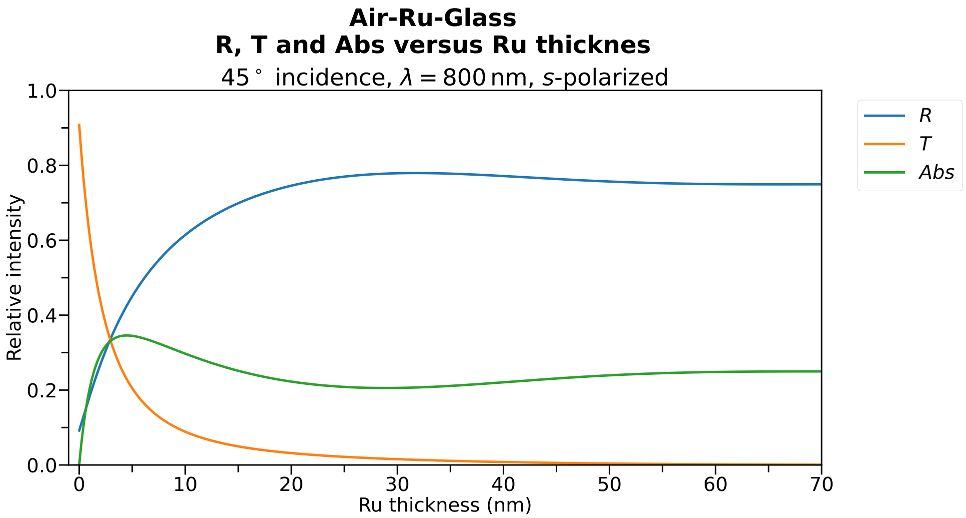

Figure 6: Reflection R, transmission T and total absorption *Abs* versus Ru thickness for a model air-Ru-glass structure illuminated with light with a wavelength $\lambda = 800$ nm from the air side for s polarization at 45° incident angle.

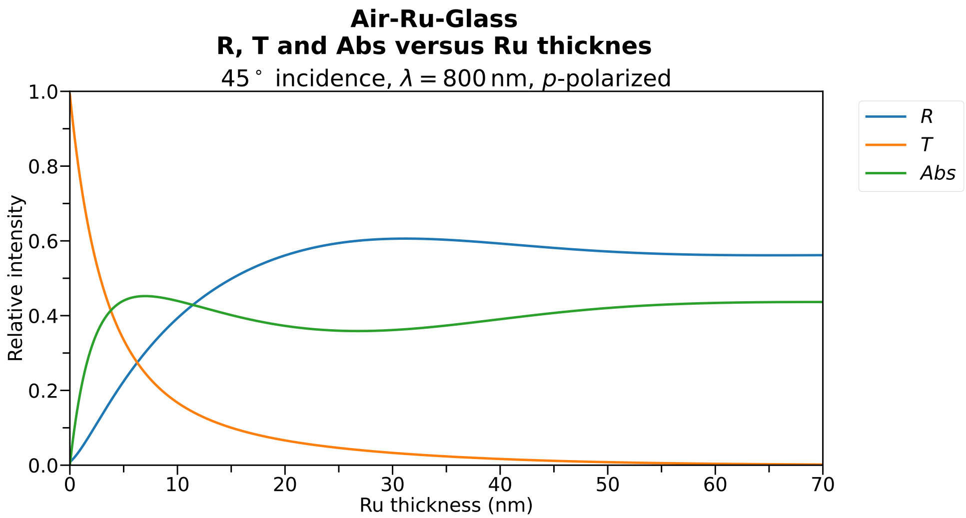

Figure 7: Reflection R, transmission T and total absorption Abs versus Ru thickness for a model air-Ru-glass structure illuminated with light with a wavelength $\lambda = 800\,\text{nm}$ from the air side for p polarization at 45° incident angle.

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