OTSunWebApp: Manual of materials

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Introduction

This manual shows how to generate optical materials for simulation with OTSunWebApp.

The set of optical materials available in OTSunWebApp is very diverse, since there is a wide variety of materials used in solar harvesting technologies. There are two main different types of optical materials, *volume materials* and *surface materials*, corresponding to objects that can be considered three-dimensional or two-dimensional, respectively. These materials can be generated using a submodule inside OTSunWebApp named "Creator of Materials", available at `http://otsun.uib.es/otsunwebapp/material`, and which we describe in this section.

In all cases the first parameter to be introduced is the material name, which will be used as identifier of the material when it is used in an optical system (referenced as `material` in the FreeCAD project). The other parameters to be entered are specific to each type of material, as specified in this section and summarized in Tables 1, 2, 3 and 4. At the end of the process of description of a material, the user gets a file with extension `otmaterial` which is, in fact, a json file representing the properties of the material. To proceed with the simulations, the webapp requires a zip file containing the json optical materials.

1 Volume materials

Volume materials provide optical properties to 3D objects in which light can travel through them. When the user chooses to generate a volume material, a drop-down menu appears in order to choose which kind of materials has to be created. In the description below (and also in the description of two-dimensional materials in Section Surface materials) we identify each of them with the label that is shown in the drop-down menu of the webapp.

- *Constant refractive index*: Material with constant optical properties, given by its index of refraction, n, and attenuation coefficient, α (in mm^{-1}). For instance, this material can be used to simulate the so called *water white* glass, taking $n = 1.52$ and $\alpha =$

0.004mm^{-1} [1]. When a ray hits on a material of this kind, it can either be reflected or refracted, according to the probabilities calculated using the Fresnel equations. In case of reflection, the reflected ray is computed using the law of reflection; if the ray is refracted, it takes a new direction according to the Snell's law, and its energy is attenuated according to the Beer-Lambert model, that is $E = E_0 e^{-\alpha(\lambda)\ell}$. Here ℓ is the length of ray path inside the 3D object and E_0 is the initial ray energy when it hits the volume material.

- *Variable refractive index*: Material with non-constant optical properties, where the complex refraction refraction index $\tilde{n} = n - i\kappa$ depends on the wavelength. We note that this is the most accurate way to emulate isotropic materials considering the geometrical optics approach [2, Ch. 2]. In order to define such a material, the user must provide a text file where each row gives the data $(\lambda, n(\lambda), \kappa(\lambda))$, where λ is the wavelength (in nanometers), n is the index of refraction and κ is the extinction coefficient. As in the *constant refractive index* case, the Fresnel's equations are used to determine if the ray is reflected or refracted. If the ray is refracted the attenuation coefficient is calculated as $\alpha = 4\pi\kappa/\lambda$ and the Beer-Lambert model is applied. We show below (part of) an example of such a data file, corresponding to a BK7 glass. Note that lines starting with the symbol # are ignored and hence can be used to include comments.

```
# https://refractiveindex.info/?shelf=glass&book=BK7&page=SCHOTT
# lambda        n                 k
300.00        1.552770264        2.86E-06
300.50        1.552613438        2.79E-06
301.00        1.552456612        2.71E-06
301.50        1.552299786        2.64E-06
-        -                 -
-        -                 -
2498.00        1.486055635        8.09E-06
2498.50        1.486046154        8.10E-06
2499.00        1.486036672        8.11E-06
2499.50        1.486027191        8.12E-06
```

- *PV material*: Material used to simulate active materials in PV cells such as Silicon, Germanium, perovskite, ... As in the *variable refractive index* material, a data file with the wavelength-dependent complex refractive index $\tilde{n} = n - i\kappa$ must be provided. In this kind of materials, the absorbed ray energy (determined by the Beer-Lambert law) converts the absorbed photons into electrons, which give rise to the current generated by the solar cell. The number of electron-hole pairs (per second, surface and wavelength) that are generated is given by the equation

$$N = \frac{I\lambda}{hc} E_0 (1 - e^{-\alpha(\lambda)\ell}), \tag{1}$$

where I is the light irradiation per wavelength (in $W/m^2\lambda$) emitted by the source, h is the Planck constant, c is the speed of light, ℓ is the length of the path of the ray inside the material, $\alpha(\lambda) = 4\pi\kappa(\lambda)/\lambda$ is the attenuation coefficient, and E_0 is the initial ray energy when it hits the PV material.

- *Thin film material*: Material that represents a multilayer medium, composed of several flat thin layers where light interference takes place. See Fig. 1, where a sketch illustrates a thin film material composed by N layers between two adjacent optical media (front and back). This kind of materials can be used to model, for instance, anti-reflective coatings, spectral filters, first surface reflectors ... In order to generate such a material, the user must upload a text file where each row gives the data $(\lambda, \theta, R_s(\lambda,\theta), R_p(\lambda,\theta), T_s(\lambda,\theta), T_p(\lambda,\theta))$, where λ is the wavelength (in nanometers), θ is the incidence angle (in degrees), R and T denote respectively the coefficients of power reflection and transmission, and subindexes s and p denote respectively the perpendicular and parallel ray polarization. In case of transmission through the thin material, the ray energy is attenuated by a factor of $1 - T_p$ (or $1 - T_s$, depending on the polarization). If the ray is not transmitted, then it is specularly reflected. We show below an excerpt of the data file corresponding to the anti-reflective material used in [3].

```
# https://doi.org/10.1115/1.4039329
# lambda           theta          Rs           Rp          Ts           Tp
285.0 0.0 0.0467927901 0.0467927901 0.9480563372 0.9480563372
285.0 2.0 0.0468673894 0.0467203856 0.9479805130 0.9481267446
285.0 4.0 0.0470916560 0.0465028053 0.9477525740 0.9483383314
-        -        -        -        -        -
-        -        -        -        -        -
285.0 86.0 0.7624711413 0.5713919240 0.2356909338 0.4254094793
285.0 88.0 0.8729302473 0.7564589080 0.1260847307 0.2417205862
285.0 90.0 1.0000000000 1.0000000000 0.0000000000 0.0000000000
290.0 0.0 0.0467825157 0.0467825157 0.9482420140 0.9482420140
290.0 2.0 0.0468544781 0.0467075081 0.9481688459 0.9483150856
290.0 4.0 0.0470708085 0.0464821744 0.9479489003 0.9485346096
-        -        -        -        -        -
-        -        -        -        -        -
290.0 86.0 0.7598469773 0.5718014740 0.2383584719 0.4251141057
290.0 88.0 0.8714236938 0.7567179981 0.1276137719 0.2415266632
290.0 90.0 1.0000000000 1.0000000000 0.0000000000 0.0000000000
-        -        -        -        -        -
-        -        -        -        -        -
4000.0 0.0 0.0374686553 0.0374686553 0.9624826412 0.9624826412
4000.0 2.0 0.0375308148 0.0374074471 0.9624204715 0.9625438275
4000.0 4.0 0.0377179367 0.0372237388 0.9622333187 0.9627274698
-        -        -        -        -        -
-        -        -        -        -        -
4000.0 86.0 0.7751516450 0.5695102186 0.2248330053 0.4304576618
4000.0 88.0 0.8803031859 0.7552537090 0.1196886304 0.2447279968
4000.0 90.0 1.0000000000 1.0000000000 0.0000000000 0.0000000000
```

  The standard way to compute this data is by using the Transformation Matrix Method (TMM), to account for interference in coherent/incoherent mediums [4]. The python package [5] can be used to generate it.

  In order to fully characterize the optical properties of the thin film, the user must also define the materials that are adjacent to its front and back sides. For each of these two sides, the user must upload a file with the table of refraction index values (as in

the case of *variable refractive index* material) characterizing the adjacent material; in case that no file is uploaded, then the adjacent material is assumed to be air.

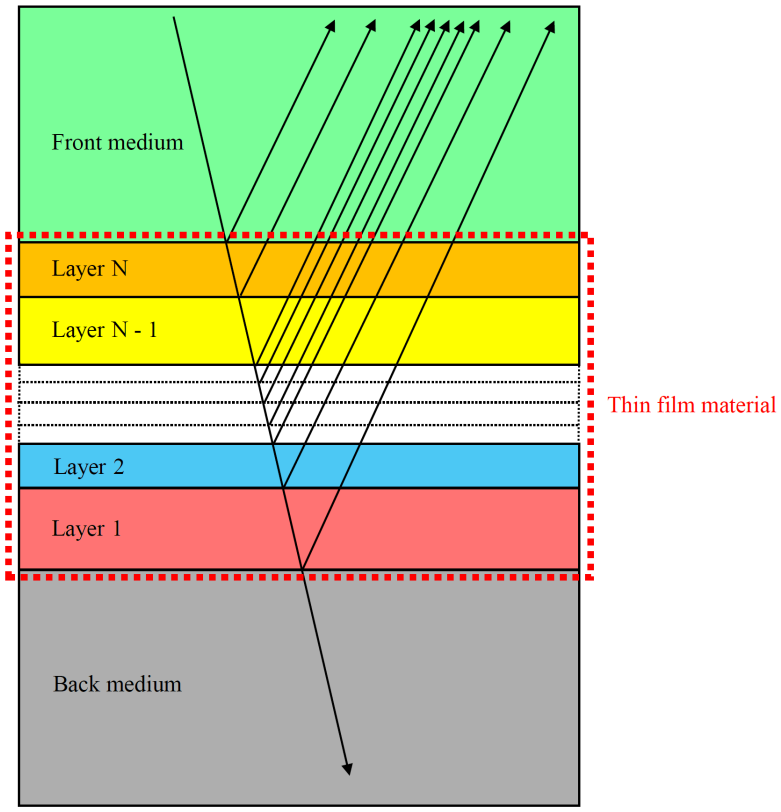

Figure 1: Stack with N thin layers composing a thin film material between the front and back mediums. One ray hits the stack of layers and multiple reflections occurs in each interface.

We summarize in Table 1 the data inputs that are required to create each kind of volume materials.

Notice that the materials that we have introduced in this section are volume materials, and hence their properties are associated to the volume itself, not to its faces. However, it is also feasible to assign additional specific optical properties to (some or all of) its faces, by assigning to them a surface material (as described in the next section). In order to obtain the limiting faces of a volumetric object, and hence being able to assign materials to them, we provide a helper FreeCAD macro, available at `https://otsun-uib.github.io/macros/faces_of_a_solid.FCMacro`. This procedure is very useful to ensure perfect contact between surfaces and 3D objects, as would be the case for second surface silvered-glass reflectors.

2 Surface materials

Surface materials are used to give optical properties to two-dimensional objects in a FreeCAD project. This model physical components whose thickness can be considered negligible in

Kind of volume material	
Input name as it appears in OTSunWebApp	*Data to input or upload*
Constant refractive index	
Index of refraction	Real number
Attenuation coefficient [mm-1]	Real number
Variable refractive index	
Refractive index data	Text file with rows $(\lambda, n(\lambda), \kappa(\lambda))$
PV material	
PV data	Text file with rows $(\lambda, n(\lambda), \kappa(\lambda))$
Thin film material	
Thin film data	Text file with rows $(\lambda, \theta, R_s(\lambda, \theta), R_p(\lambda, \theta), T_s(\lambda, \theta), T_p(\lambda, \theta))$
Refractive index data for front material (leave it empty if it is Vacuum)	Text file with rows $(\lambda, n(\lambda), \kappa(\lambda))$
Refractive index data for back material (leave it empty if it is Vacuum)	Text file with rows $(\lambda, n(\lambda), \kappa(\lambda))$

Table 1: Summary of data needed to define each of the different kinds of volume materials. We give the input names under which they are specified in the webapp OTSunWebApp and the data to be input or uploaded.

the simulation.

In terms of their functionality, they are classified as: absorber, reflective and transparent. Also, depending on how they reflect light rays, they can present lambertian or gaussian scattering properties.

2.1 Opaque/absorber materials

This kind of materials are characterized by the property that when a light ray hits them, then it (mainly) gets absorbed, either giving rise or not to usable energy. We provide different classes of such materials.

- *Opaque simple layer*: Material that absorbs any ray that hits it, without generating any kind of usable energy. It is used to model materials that block rays.
- *Absorber simple layer*: Material characterized by the property that when a ray hits this surface, it is either absorbed (with a constant *probability of absorption* that the user must input) or reflected. If the ray is absorbed the ray energy is accounted as useful thermal energy; otherwise, the ray is reflected specularly keeping its energy.
- *Absorber lambertian layer*: Material with the same behaviour as in the *absorber simple layer* case, but in case of reflection of the ray, a lambertian scattering is also applied (with a given probability). See paragraph Lambertian scattering model for details and which parameters define this behaviour.
- *Absorber TW model layer*: Absorber material where the absorption probability, a, depends on the incidence angle, θ, according to the Tesfamichael-Wäckelgård model [6], $a = a_0 \left\{1 - b\left(\frac{1}{\cos\theta} - 1\right)^c\right\}$, where a_0 is the absorption probability at normal incidence and b, c are parameters that are often obtained experimentally and that the user must input. If the ray is not absorbed, then it is specularly reflected.
- *Absorber polarized coating layer*: Material used to simulate wavelength-dependent selective absorbers. The user must upload a data file analogous to the described in the case of *thin film material*, but without the T_s and T_p columns, since no transmittance is possible. The ray energy will be absorbed according to the absorption probability, computed as $1 - R_{s/p}$. If the ray is not absorbed, then it is specularly reflected.

2.2 Reflective materials

This kind of materials is used to simulate surfaces whose main purpose is to reflect light.

- *Reflector specular layer*: Material characterized by the property that when a ray hits it, then the ray is reflected with a given *probability of reflection* (that the user must provide) or otherwise, it is blocked, without producing usable energy. In case of reflection, a gaussian scattering may take place; see paragraph Gaussian scattering model for details and the parameters that are needed.

- *Reflector lambertian layer*: Material with the same behaviour as in the case of *reflector specular layer* case but now with lambertian instead of gaussian scattering. See paragraph Lambertian scattering model for details on how to define this scattering.
- *Reflector specular metallic layer*: Material whose reflectance is determined by the Fresnel's Equations. Hence, the complex refractive index must be given as in the case of materials of the kind *variable refractive index*. This material is used to simulate highly reflective materials such as silver, gold and aluminium. Note also that since the Fresnel's equations are used, the reflectance depends on the incidence angle, wavelength and light polarization. In the case of a reflected ray, the specular or scattering model is applied according to its input parameters, as described in paragraph Gaussian scattering model.
- *Reflector lambertian metallic layer*: Material with same properties as in the case of *reflector specular metallic layer*, but now now with lambertian instead of gaussian scattering. See paragraph Lambertian scattering model for details.
- *Reflector polarized coating layer*: Material similar to the case of *absorber polarized coating layer*, with the difference that if the ray is absorbed, then no energy is collected. This material is useful for simulating first surface coating mirrors [3]. In case of reflection, a gaussian scattering effect can be applied, as explained in paragraph Gaussian scattering model.

2.3 Transparent materials

Materials whose main purpose is to let light pass through them.

- *Transparent simple layer*: Material characterized by the property that when a ray hits it, then with a constant *probability of transmission* (that the user has to provide), the ray passes through the layer (keeping its direction). Otherwise, it is reflected.
- *Transparent polarized coating layer*: Material used to simulate thin transparent coatings, such as anti-reflective coatings [3], where the thickness can be neglected in the simulation. The data values are given as in the case *thin film material*. If the ray is transmitted, its energy is absorbed according to the absorption probability calculated as $1 - T_{s/p}$. If the ray is not transmitted, then it is specularly reflected.

2.4 Composed materials

In addition, it is possible to create a surface material by combining two surface materials:

- *Two layers material*: Material whose optical properties depend on which side of the layer is hit by the ray, and where each of those two behaviours is modeled by one of the materials introduced so far. In order to define such a material, the user has to enter the identifiers of the two layers (front and back, respectively) that form the material. Note that the `otmaterial` files describing these two layers must also be included in the zipfile with all the materials that the user has to upload when launching a computation.

In Table 2 we summarize the data inputs required to create each of the surface materials.

Kind of surface material	
Input name as it appears in OTSunWebApp	*Data to input or upload*
Opaque simple layer	
No input is needed	
Absorber simple layer	
Probability of absorption	Real number $\in [0, 1]$
Absorber lambertian layer	
Probability of absorption	Real number $\in [0, 1]$
Data defining the lambertian scattering model (see Table 3)	
Absorber TW model layer	
Probability of absorption	Real number $\in [0, 1]$
b constant	Real number > 0
c constant	Real number > 0
Absorber polarized coating layer	
Coating absorber file	Text file with rows $(\lambda, \theta, R_s(\lambda, \theta), R_p(\lambda, \theta))$
Reflector specular layer	
Probability of reflection	Real number $\in [0, 1]$
Data defining the gaussian scattering model (see Table 4)	
Reflector lambertian layer	
Probability of reflection	Real number $\in [0, 1]$
Data defining the lambertian scattering model (see Table 3)	
Reflector specular metallic layer	
Refractive index data	Text file with rows $(\lambda, n(\lambda), \kappa(\lambda))$
Data defining the gaussian scattering model (see Table 4)	
Reflector lambertian metallic layer	
Refractive index data	Text file with rows $(\lambda, n(\lambda), \kappa(\lambda))$
Data defining the lambertian scattering model (see Table 3)	
Reflector polarized coating layer	
Coating reflector file	Text file with rows $(\lambda, \theta, R_s(\lambda, \theta), R_p(\lambda, \theta))$
Data defining the gaussian scattering model (see Table 4)	
Transparent simple layer	
Probability of transmission	Real number $\in [0, 1]$
Transparent polarized coating layer	
Coating transparent file	Text file with rows $(\lambda, \theta, R_s(\lambda, \theta), R_p(\lambda, \theta), T_s(\lambda, \theta), T_p(\lambda, \theta))$

Table 2: Summary of data needed to define each of the different kinds of surface materials. We give the input names under which they are specified in the webapp OTSunWebApp and the data to be input or uploaded.

Reflection scattering parameters	
Input name as it appears in OTSunWebApp	*Data to input*
Lambertian weight	Real number $\in [0, 1]$
Lambertian kind	Choose either Total or Cosine

Table 3: Data needed to define the lambertian scattering model. We give the input names under which they are specified in the webapp OTSunWebApp and the data to input.

2.5 Lambertian scattering model

As shown before, some surface materials can be modeled so that, in case of reflection, the direction of the ray is affected by a phenomenon of lambertian scattering. Namely, with a given probability that the user must define, called the *weight parameter*, the direction of the ray is modified as explained below; otherwise an specular reflection is applied.

The lambertian scattering can be of two different kinds. In case of *total* dispersion, the probability distribution of the outgoing ray is uniform in all possible directions. In case of *cosine* dispersion, the distribution follows Lambert's cosine law, where the probability density function (pdf) is equal to the cosine of the angle θ between the reflected ray and the normal, that is $f(\theta) = \cos(\theta)$.

2.6 Gaussian scattering model

As mentioned when describing the different surface materials, some materials include the possibility of adding gaussian scattering phenomenon when a reflection takes place.

The basic model of gaussian scattering reflectance is that described by Johnston [7], which was applied to describe the surface error distribution of mirrors on concentrated solar collectors. This model gives a probability density function for the deviation angle θ_s between a measured surface normal vector and the ideal surface normal (see Fig. 2 for a depiction of this situation),

$$f(\theta_s) = \frac{\theta_s}{\sigma_s^2} e^{-\frac{\theta_s^2}{(2\sigma_s^2)}}, \tag{2}$$

called the *Generalised Rayleigh* pdf, where σ_s is the standard deviation.

However, experimental results show that the reflectance profile of some solar mirrors cannot be modeled by a single gaussian. Indeed, as found by Pettit [8], the reflectance profile of certain mirrors appeares to be composed of a sharp central beam together with a broad background reflectance curve. This leads to the assumption that the pdf for θ_s is given by a linear combination of two different Raleigh distributions,

$$f(\theta_s) = k\frac{\theta_s}{\sigma_{s_1}^2} e^{-\frac{\theta_s^2}{(2\sigma_{s_1}^2)}} + (1-k)\frac{\theta_s}{\sigma_{s_2}^2} e^{-\frac{\theta_s^2}{(2\sigma_{s_2}^2)}}, \tag{3}$$

where two gaussian distributions with standard deviation σ_{s_1} and σ_{s_2} are ponderated according to a weight parameter $k \in [0, 1]$.

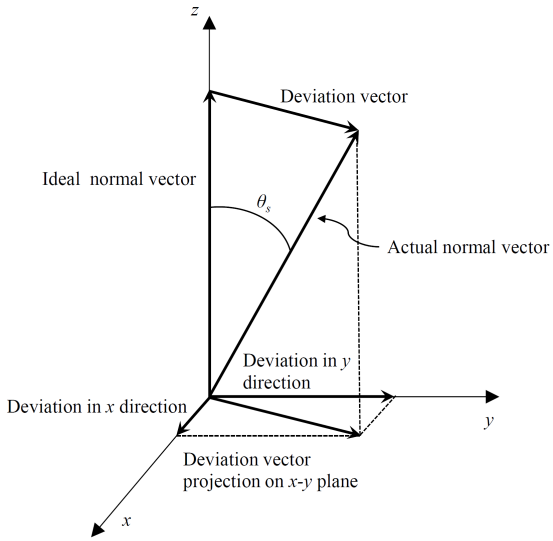

Figure 2: Angular deviation θ_s between the measured surface normal vector and the ideal surface normal vector.

Thus, the cumulative distribution function for the random deviation angle φ_s is given integrating Eq. 3, giving

$$F(\varphi_s) = [1 - ke^{-\frac{\varphi_s^2}{(2\sigma_{s_1}^2)}} - (1-k)e^{-\frac{\varphi_s^2}{(2\sigma_{s_2}^2)}}]. \tag{4}$$

In order to define a gaussian scattering on surface materials, the user must give the parameters σ_{s_1}, σ_{s_2} (both in mrad) and k. See Table 4. Notice, however, that if only one of two standard deviations is given, then a single Raleigh distribution will be used.

We now compare the parameters used in the model we are using with those in Sutter et al. [9], used for the characterization of first and second surface mirrors. In their model, the specular reflectance is given by

$$\rho(\lambda, \theta_i, \varphi) = \rho(\lambda, \theta_i, h)[1 - ke^{-\frac{\varphi^2}{(2\sigma_1^2)}} - (1-k)e^{-\frac{\varphi^2}{(2\sigma_2^2)}}], \tag{5}$$

where $\rho(\lambda, \theta, h)$ is the hemisferical reflectance at wavelength λ and at an incidence angle θ_i, σ_1 and σ_2 are the statistical standard deviations, and φ is the acceptance angle (half-space). It is worth to mention that the aforementioned work [9] is part of ongoing developments in the SolarPaces Task III reflectance work group, aiming to satisfy the demand for standarization in the qualification procedures of solar mirrors. In order to compare both models, notice that in Eq. 4, the angle φ_s is the deviation of the normal surface vector, while in Eq. 5, the angle φ is the deviation of the dispersed reflected ray. From the reflection law, it follows that $\varphi_s = \frac{\varphi}{2}$ (see Fig. 3). With this remark, and comparing the two equations, it follows that the standard deviations that define both models are related by the equalities $\sigma_{s_1} = \frac{\sigma_1}{2}$ and $\sigma_{s_2} = \frac{\sigma_2}{2}$. This should be taken into account when the user has to input the parameters in the webapp.

Finally, we show in Fig. 4 the distribution of the reflected ray deviation determined by simulation with OTSunWebApp using the *reflector specular layer* material for two scattering cases: $\sigma_s = 3$ mrad (Fig. 4(a)) and $\sigma_{s_1} = 1.2$ mrad, $\sigma_{s_1} = 8$ mrad, $k = 0.92$

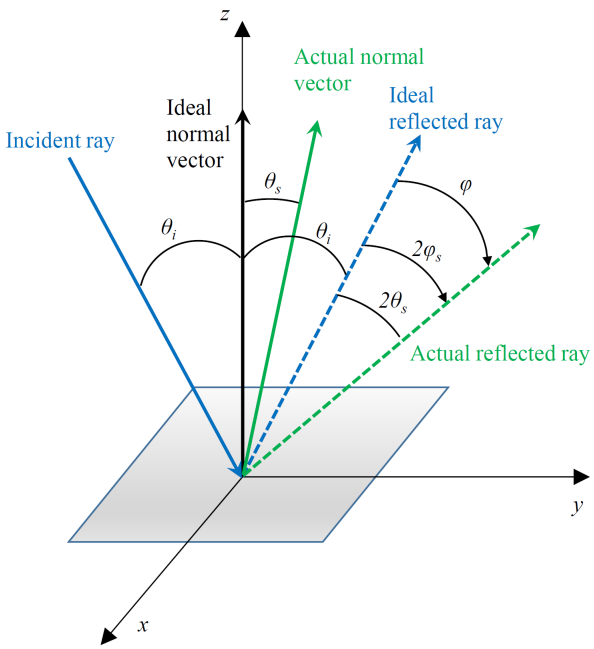

Figure 3: Specular deviation by scattering: in blue ideal vector directions and in green actual vector direction due surface normal vector deviation.

Reflection scattering parameters	
Input name as it appears in OTSunWebApp	*Data to input*
σ_{s_1} [mrad]	Real number > 0 (or empty if no σ_{s_1} distribution)
σ_{s_2} [mrad]	Real number > 0 (or empty if no σ_{s_2} distribution)
weight for σ_{s_1} distribution	Real number $\in [0, 1]$ (or empty if no σ_{s_2} distribution)

Table 4: Data needed to define the gaussian scattering model. We give the input names under which they are specified in the webapp OTSunWebApp and the data to input.

(Fig. 4(b)). The former is also determined by simulation with Tonatiuh (version 2.2.4) (Fig 4(c)). The scripts and other auxiliary files can be found at the repository `https://github.com/otsun-uib/OTSunWebAppSuppMat`. We can observe in Figs. 4(a) and 4(b) that the ray deviation histograms calculated using OTSunWebApp approximate well the theoretical Rayleigh distribution (with the correction on standard deviations commented before), which serves as validation of the model we have implemented. In Fig. 4(c) we compare this theoretical distribution with the results obtained using Tonatiuh. The discordance between them could be due to the procedure that Tonatiuh uses to determine the scattering angle.[1]

[1]See lines 186–188 of the source file for Tonatiuh in `https://github.com/iat-cener/tonatiuh/blob/master/TonatiuhProject/plugins/MaterialOneSideSpecular/src/MaterialOneSideSpecular.cpp`

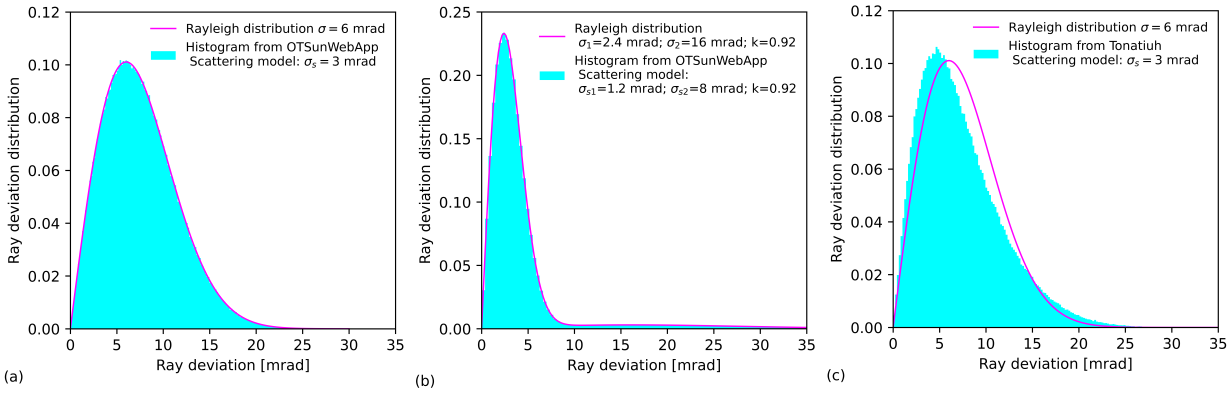

Figure 4: Distribution of the deviated ray angle for several cases using OTSunWebApp (a) and (b) and Tonatiuh (c).

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