Supplemental Document

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# Monte Carlo simulation of a LSC based on stacked layers of fiber arrays with core-coating different absorbing properties: supplement

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# Monte-Carlo simulation of a LSC based on stacked layers of fiber arrays with core-coating different absorbing properties: supplemental document

## 1. Description of the Monte-Carlo model.

Fig. S1 shows the basic flow diagram for the Monte-Carlo simulation for studying the efficiency of the LSC:

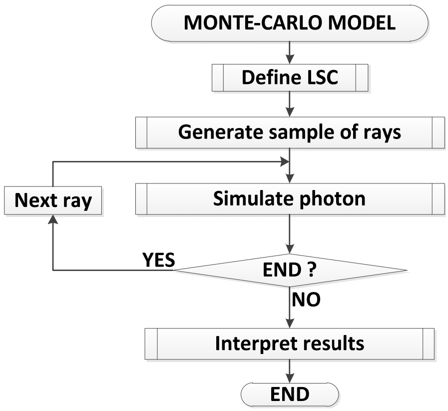


Fig. S1. Basic flow diagram of the Monte Carlo method for studying the LSC performance

In the first block, the optical and geometrical parameters of the LSC are defined. The LSC input geometrical parameters involve the fiber diameter $D_e$, the coating thickness $d$, the fiber length $L$ and the LSC thickness $w$, while the optical ones are the absorption coefficients of the host and the dopants, $\alpha_h$ and $\alpha_d$, respectively, the scattering coefficient $\alpha_{sc}$, the host refractive index $n$, the dopants emission quantum efficiency, $n_{PL}$, and their emission spectra $I_{em}$.

Then, a sample of rays, representative of the incident radiation, is generated. For this purpose, the spectral irradiance curve of the AM1.5G spectrum in terms of photon flux is sampled with a bandwidth of 1 nm. Every incident photon is defined by its wavelength and an incidence path, characterized by an initial position and a direction vector.

The next block incorporates the LSC model that simulates the physical processes that affect individual rays based on their incidence path and its wavelength. Absorption effects by the different absorbers are modelled by generating random path lengths $\Delta s$, according to the inverse cumulative density function, as (1), which the ray travels before absorption.

$$\Delta s = -\frac{log_{10}\xi}{\alpha(\lambda)} \qquad (1)$$

Where $\alpha(\lambda)$ is the decadic absorption coefficient and $\xi$ is a random variable uniformly distributed from 0 to 1. Three different absorption path lengths are generated for the inner host material, the outer host material and the QDs according to their respective absorption coefficients, $\alpha_{h,i}$, $\alpha_{h,e}$ and $\alpha_d$, by generating three random independent $\xi$ values.

In order to take into account the scattering effects, in the same manner as absorption, a scattering path length $\Delta s_{sc}$ is generated taking into account the scattering coefficient $\alpha_{sc}$ which the ray travels before a scattering event [2].

Ray propagation inside the fiber is tracked by its position vector in cartesian coordinates $\mathbf{r} = (r_x, r_y, r_z)$ while their successive positions $\mathbf{r}' = (r'_x, r'_y, r'_z)$ are obtained as $\mathbf{r}' = \mathbf{r} + \mathbf{u}\Delta s$, where $\mathbf{u}$ is the direction vector defined by its direction cosines $\mathbf{u} = (u_x, u_y, u_z)$ and a propagation distance $\Delta s$. Assuming fibers are positioned in the 3-D space with their axis parallel to $y$-axis and axis coordinates $(x_c, z_c)$ and $\Delta s$ is defined as the collision distance with the fiber surface of diameter $D_e$, its expression is:

$$\begin{aligned} \Delta s &= -b + \sqrt{b^2 - c} \\ b &= \frac{u_x(r_x - x_c) + u_z(r_z - z_c)}{u_x^2 + u_z^2} \\ c &= \frac{r_x^2 + r_z^2 - 2(r_x x_c + r_z z_c) + r_x^2 + r_z^2 - D_e^2/4}{u_x^2 + u_z^2} \end{aligned} \qquad (2)$$

The ray interaction with an interface is modelled following an stochastic approach where the ray is not divided when reaching the interface. Instead, it can be either a reflected or a transmitted to the refractive media with a probability given by the reflectance calculated from Fresnel's laws for planar waves incident in a flat surface. The reflectance expression $R_{\mathrm{sp}}$ is given by [1]:

$$R_{\mathrm{sp}} = \frac{1}{2}\left[\left|\frac{n_1 \cos\theta_i - n_2 \cos\theta_t}{n_2 \cos\theta_i - n_1 \cos\theta_t}\right|^2 + \left|\frac{n_2 \cos\theta_i - n_1 \cos\theta_t}{n_1 \cos\theta_i - n_2 \cos\theta_t}\right|^2\right] \qquad (3)$$

Where $n_1$ and $n_2$ are the refractive indexes of the incident and refractive media, respectively, assumed to be constant and independent of the light wavelength. $\theta_i$ s the incidence angle of the ray at the surface and $\theta_t$ is the refraction angle, given by Snell's law. In case of internal reflection ($n_1 > n_2$) and $\theta_i$ larger than the critical angle $\theta_c = arcsin\,(n_1/n_2)$, (3) yields a unity reflectance value and the ray is always reflected back, thus, modelling TIR phenomena.

The effect of absorption during propagation is taken into account by reducing the initial absorption path lengths, depending on the characteristics of the media traversed by the ray during its propagation. In our model, two types of media are considered: pure matrix and doped matrix. When the ray passes through pure matrix, only the absorption path length of the matrix is reduced, while the length corresponding to dopants, remains constant. As opposed, when it is propagated through a medium composed of doped matrix, both the path length of the matrix, as well as that of the dopants, is reduced. Finally, absorption takes place when the beam has traveled completely one the generated paths. In case the ray reaches a scattering center, it is deviated isotropically and a new scattering path length is generated in order to model successive scattering events.

Once a ray is absorbed by a QD, it can be re-emitted isotropically or undergo a non-radiant process, with a probability given by the quantum efficiency of the dopant. The emission direction is generated with a uniform probability in any direction in three-dimensional space. For this purpose, a sample $\boldsymbol{\xi}$ from the 3-D multivariant normal distribution $\boldsymbol{N}(\boldsymbol{\mu}, \boldsymbol{\sigma})$, with $\boldsymbol{\mu} = (0, 0, 0)$ and $\boldsymbol{\sigma}$ a 3×3 identity matrix, is generated and the new direction $\boldsymbol{\mu}$ is obtained by normalizing this value [3]. The emission wavelength of the dopant is generated by applying the rejection sampling method to the emission spectrum of the dopant. To ensure an energy photon down-shifting, it is imposed that the emission wavelength must be greater than the absorption wavelength. Finally, the loop is closed, generating a new set of optical path lengths for the re-emitted photons propagation.

After simulating each ray, prior to simulate the following one, the resulting event and the wavelengths at the start and at the time of the event are recorded. Each incident photon can result in any of the following events:

- Reflected: The photon does not penetrate inside of the LSC and, instead, it is reflected in its surface.
- Not absorbed: The photon passes through the LSC without being absorbed neither by the host matrix nor the dopants.
- Absorbed by the host matrix.
- Not re-emitted: The incident ray is dissipated into heat due to a non-radiant process in dopant in the first absorption event.
- Self-absorbed: The ray experiences at least two absorption events before being lost non-radiatively in a QD.
- Lost by waveguiding: The ray exits the LSC due to escape cone losses after an absorption-emission event, but without any previous scattering event.
- Lost by scattering: A emitted photon exits the LSC due to escape cone losses after an at least one previous scattering event.
- Captured: The ray manages to reach the surface limiting with the PV cell. Scattered photons can also be captured by the PV cell, or be lost by matrix absorption or self-absorption, but in these cases, they are classified as captured, absorbed, or self-absorbed, respectively.

Once all the photons in the sample have been simulated, the events that have taken place as a result of each of the simulated photons are recorded in a vector whose dimension is equivalent to the size of the sample. In another vector, the incident and final wavelengths of each simulated photon are collected. These data are interpreted by calculating the optical efficiencies of photon flux and radiant power. Furthermore, by using histograms, the regions of the incident spectrum exploited, the collected spectrum and the distribution of the losses, can be visualized.

## 2. Examples of ray tracing in LSC based of stacked layers of fiber arrays with core-coating different absorbing properties.

Fig. S2 presents the *xz* projections of a LSCs based on homogeneously doped PLMA fibers with a diameter of 240 μm, arranged in hexagonal and square packing and some random paths of different simulated photons resulting in different events. In Fig. S2(#4) a re-emitted photon is guided inside one of the fibers of the LSC in *y* direction towards the PV cells, following a propagation path similar to the ones shown in Fig 2 and Fig 3.

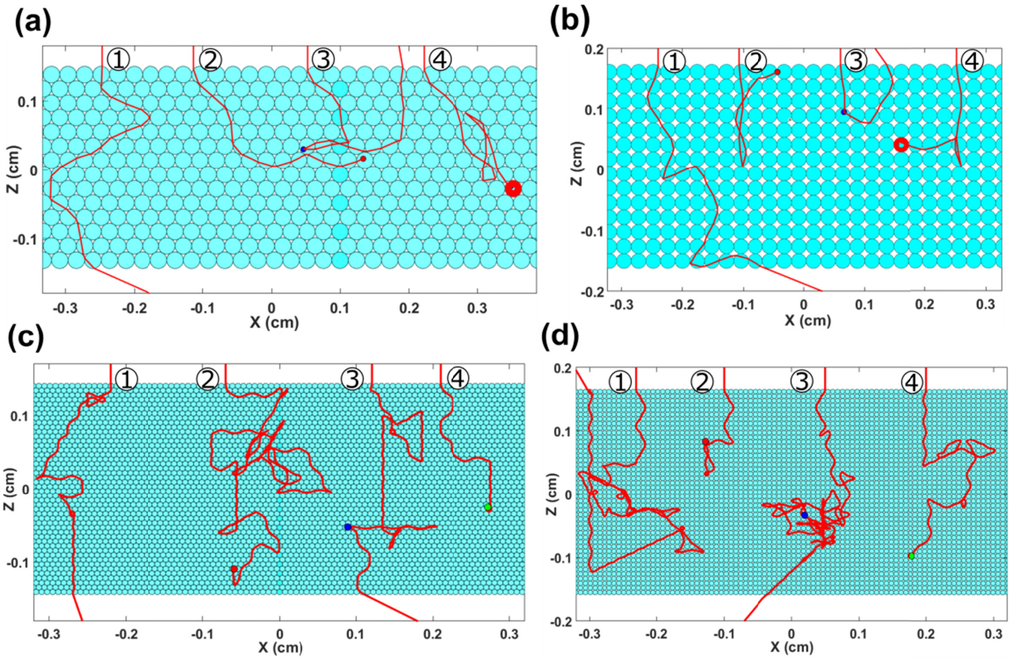


Fig. S2. *xz* projections of LSCs based on homogeneously doped PLMA fibers with diameters of 240 μm ((a),(b)), and 72 μm ((c),(d)), arranged in hexagonal (a) and square (b) packing and some random paths of different simulated photons resulting in different events: 1, photon not absorbed by the LSC; 2, photon lost as result of a non-radiative process (red dots) after being absorbed by a QD; 3, photon not trapped in the LSC after an absorption-emission event (blue dots); 4, photon guided inside a fiber after an absorption/re-emission event.

Despite having the same number of QDs as planar geometry, incident light absorption is not the same as in the plane LSC, while also decreases for shorter fiber diameters. To explain this effect an histogram of the resulting path lengths $\Delta s$ (Fig. S3(a)) travelled by $10^6$ photons simulated in a bulk-doped 30 μm fiber LSC with hexagonal packing and their corresponding absorption, according to $1-10^{-\alpha\Delta s}$ (Fig. S3(b)), are represented. Despite photons travel on average a longer absorption path length ($\overline{\Delta s}$ is higher than the planar LSC thickness $w$) the resulting average absorption is higher for the planar (fiber LSC mean absorption $\overline{A}$ is lower than the planar LSC absorption $A_p$) because of the high impact of photons travelling shorter distances on the absorption expression.

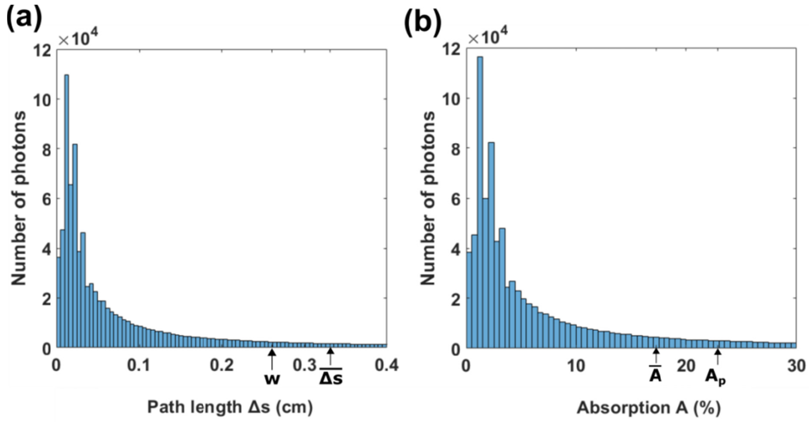


Fig. S3. Histograms of the resulting path lengths $\Delta s$ travelled by $10^6$ photons simulated in a bulk-doped 30 µm fiber LSC with hexagonal packing (a) and their corresponding absorption (b).

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