International Journal of ChemTech Research
CODEN (USA): IJCRGG ISSN: 0974-4290
Vol.7, No.2, pp 594-599, 2014-2015

ICONN 2015 [4th -6th Feb 2015]
International Conference on Nanoscience and Nanotechnology-2015
SRM University, Chennai, India

Monte Carlo Simulation to Analyze the Performance of the Crystalline Silicon Solar Cell

Manikandan A V M[1]*, Prasobh C[2], Nachammal C[3], Shanthi Prince[4]

[1,2,3,4]**Department of ECE, SRM University, Kattankulathur-603203, Tamilnadu, India**

Abstract : A physical model describing photon absorption mechanism is presented in the context of photovoltaic applications. We present a dynamical Monte Carlo Method (MCM) for the calculation of quantum efficiency for crystalline silicon solar cells. The quantum efficiency is given as a function of wavelength. The MCM is widely used in various fields including photovoltaics, to simulate the processes which are repeated several times. In MCM, each particle is traced until it loses all its energy, and thus the various processes that occur can be interpreted on a probability basis.

The Monte Carlo model simulates the processes underlying the absorption of photons in the bulk of the solar cell. The aim is to gain some insight into absorption, reflection, refraction, transmission and scattering of light in various layers of solar cell.

The solar cell model takes into account the reflection at the front surface computed using Fresnel's equation, transmission angle computed using Snell's Law, scattering theory and path length calculation, and absorption condition stated using Beer-Lambert Law. An Anti-Reflective Coating (ARC) of Silicon Dioxide (SiO_2) is applied at the surface of the solar cell to reduce reflection. The reflectance is reduced by choosing proper ARC thickness. It has been shown that the external quantum efficiency of the solar cell has enhanced from 65% without ARC to about 81% with a double-layer ARC (SiO_2 and SiN_4).

1. Introduction

The generation of photocurrent in crystalline silicon solar cells starts with a photon being absorbed in the active layer and creating an excited electron/hole pair (exciton). The exciton is mobile and dissociates into electron and hole at an interface between donor and acceptor material, unless it decays before it reaches the interface. If they do not recombine, the charge carriers migrate toward the appropriate electrode and contribute to the photocurrent. Thus, the efficiency of crystalline silicon solar cells depends strongly on the geometry and electronic properties of the donor/acceptor materials[1].

Simulating in detail the processes described above is of interest since it enables the modeling of devices with different architectures and materials properties. Since processes such as exciton absorption, electron hopping, and recombination take place on vastly different time scales, we employ an event-driven Monte Carlo algorithm to simulate the performance of the solar cell.

2. Monte Carlo

Monte Carlo algorithms are stochastic and are used to solve complex physical or mathematical problems. When the number of variables is great and the solution is complex, exploring the solution space or events space randomly can give an accurate estimate of the solution. In a typical Monte Carlo algorithm, random draws following given distributions define a chain of local events characterizing the global even and leading to a final state. By repeating this numerous times an approximation of the solution is obtained. The accuracy of this solution depends on how well the problem is modeled and how many draws are made[2].

3. Methodology

Ray tracing is a technique from geometrical optics to model the path taken by light in an environment by following rays of light. This ray tracing approach gives the photons a particle's behaviour rather than that of a wave. The photons are given a position and a direction and the future position is defined by the current position, the direction and the travelled distance[3].

A light beam is partially reflected and partially refracted at interfaces; similarly, it may be partially absorbed and partially reemitted in a medium. A light beam could be simulated by tracing it until the next interface, compute the reflected part and the refracted part and then trace the two resulting beams, reduced in intensity. This process would have to be repeated at each intersection for each resulting beams creating an exponentially growing number of beams to track. This is complicated and often involves a lower threshold for intensity of tracked beams and some beams are discarded. When absorption and reemission are considered, the complexity of the problem grows further. At each reemission, the beam is reemitted in several directions. This makes the above described "beam split" approach unsuitable and for this reason photons will be "shot" one by one rather than in beams. In this approach a single photon arriving at an interface may be refracted or reflected with a particular probability and similarly, the photon may be absorbed at a random point in the medium and then reemitted in a random direction. As it will be explained shortly, numerous of those events are quantum effects and depend on the wavelength of the light, this suggests the use of a Monte Carlo algorithm where the wavelength of each incoming photon and the occurrence of numerous quantum events in the materials are drawn randomly.

4. The Solar Cell Model

In our work, a crystalline silicon solar cell is chosen because of structural simplicity. The program developed to analyse the performance of the solar cell is simple and quite general, and can be easily applied to other kinds of solar cells, such as heterojunction solar cells, tandem cells, with little modifications.

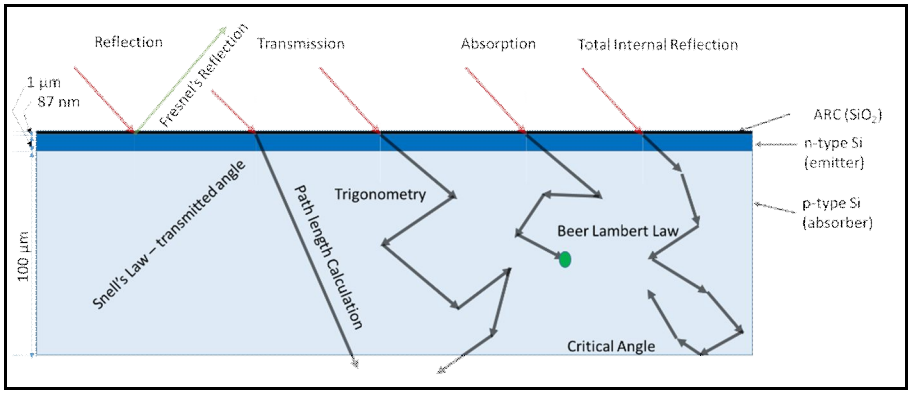

Figure-1: Solar cell model for calculation of quantum efficiency

If some materials are luminescent it can be explained by the behavior of light inside them. Figure-2 explains the different events that happens inside the solar absorber, and demonstrates reflection, refraction, internal reflection, absorption, reemission and multiple reemission as printed from left to right and top to bottom. Due to classical optic proprieties of the materials, light may be reflected at the interface with air and not enter the collector. If it is not reflected, light will be refracted inside the collector with a specific angle determined by Snell's law. Once inside the collector more specific luminescent proprieties come into play and light may be absorbed. If it is not, it traverses the material, arrives at the bottom interface where it may again be

reflected or refracted. The absorbed light can be reemitted, once or several times. The following figure illustrates those events [3].

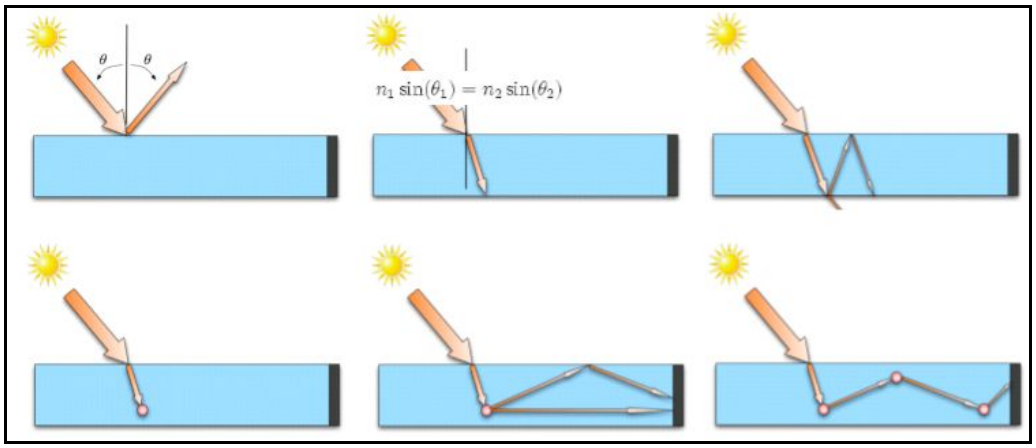

Figure-2: Different events inside a solar absorber

The non-absorbed light is reflected back through the stack to increase the absorbed proportion of light and therefore the reemitted, collected light. This makes it possible to use less solar cell surface with more efficiency.

5. Modelling light and its interactions with the medium

The following graph resumes the possible chains of events in a photons "life", the initial state is "Birth", rectangles represent states and rhombuses symbolize decisions [3].

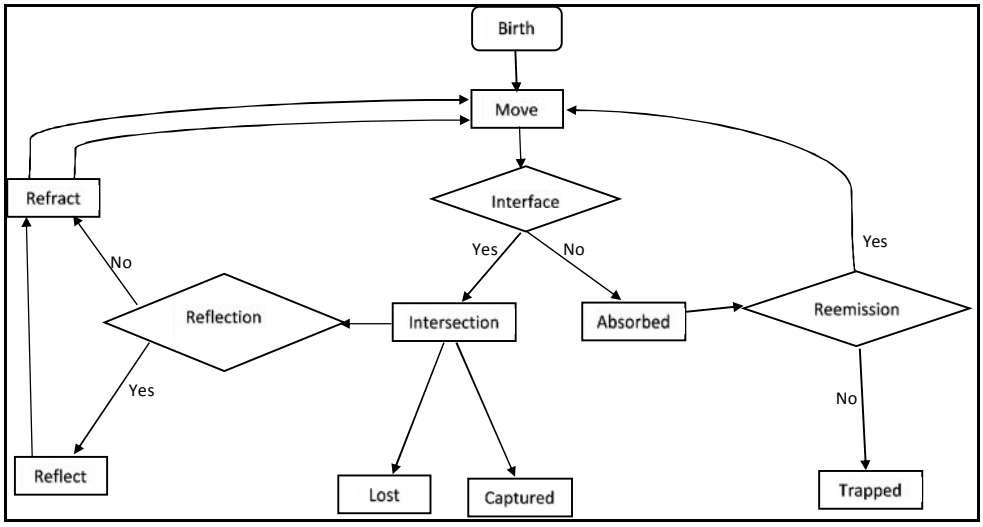

Figure-3: State machine of a photon's life

After its birth, a photon has a determined direction and travels a certain distance. If it does not strikes an interface along its path it will be absorbed, once absorbed it can be trapped and the next photon is shot. If reemitted, it will travel further and may hit an interface. At an interface the photon may either be reflected or refracted and set into motion in the corresponding direction. An interface can also mean the photon quits the system or is detected.

Birth of photon, the source

The AM1.5 spectrum for direct light from the National Renewable Energy Laboratory (NREL) is used with a defined angle cone in which the rays are distributed uniformly.

Reflection and Refraction

Refraction is a well-known phenomenon making light "bend" at the interface between two different mediums. It can be observed as a straw is half immersed in water and appears bended. The angle of refraction of light is defined by Snell's law:

$$n_1 \sin(\theta_i) = n_2 \sin(\theta_t)$$

where θ_i and θ_t are the angle of incidence and refraction, respectively, and n_1 & n_2 are the refractive indices of the two media with $n_2 > n_1$.

However, the values for the refraction indices are not constant and depend on the wavelength. Therefore, each material should define values for the refraction index at different wavelengths. This defines the refracted angle, but as it is stated by Fresnel's equations, refraction does not occur for the totality of the incident beam. A part of this beam is reflected and the other part is refracted. These proportions depend on the incident angle and the refractive index of the materials at each side of the interface. The proportions also depend on the polarization of light, but as the simulation does not take polarization into account yet, the mean value between orthogonally and parallel polarized light will be used. The values of Fresnel's equations yield the proportions of reflected and refracted light in a beam depending on the incoming angle. Because we consider only a single photon at a time, a random number between 0 and 1 is drawn at every intersection with an interface and if it is greater than the reflected percentage of light R, the photon is refracted, else it is reflected.

$$R_\perp = r_\perp^{\,2} = \left(\frac{\sin(\theta_i - \theta_t}{\sin(\theta_i + \theta_t} \right)^2 \qquad T_\perp = 1 - R_\perp$$

$$R_\parallel = r_\parallel^{\,2} = \left(\frac{\tan(\theta_i - \theta_t}{\tan(\theta_i + \theta_t} \right)^2 \qquad T_\parallel = 1 - R_\parallel$$

where $R_\perp$ and $R_\parallel$ are the reflectance or reflectivity for s-polarized and p-polarized light, respectively. $T_\perp$ and $T_\parallel$ are its transmittances.

If the incident light is unpolarised (containing an equal mix of s- and p-polarisations), the reflectance and transmittance is

$$\overline{R} = \left(\frac{R_\parallel + T_\perp}{2} \right) \qquad \overline{T} = 1 - \overline{R}$$

A remarkable angle is the critical angle above which there is total internal reflection. This angle exists only if the refraction index of the incident material is greater than the one of the material beyond the interface:

$$\theta_{crit} = \arcsin\left(\frac{n_2}{n_1} \right)$$

Above this critical angle, the reflectance value is equal to one and the transmittance inexistent.

Absorption

A central phenomenon that has to be modeled is the absorption of light by the material. This phenomenon is essential to simulate luminescent collectors but is not exclusive to them and happens in many materials. The intensity of a light beam diminishes exponentially with the distance x in the material.

$$I(x) = I_O e^{-\alpha x}$$

where I(x) is the photon intensity at a distance x, I_O is the initial photon intensity, α is the coefficient of absorption which depends on the material and the wavelength of incoming light, and x is the distance at which the photon is situated. This law defines the intensity at a given distance inside the material and it can also be considered as the probability distribution function for the penetration depth inside the material.

In our MCM simulation of solar cell, each particle is followed until it has lost all its energy and the various processes that occur are interpreted on a probability basis. Since the sum of the probabilities of the various processes at each step is of course equal to unity, a random number between zero and unity is consequently chosen in order to decide the kind of process which should occur. In our case, for instance, in

order to select a photon from the solar spectrum, the integral of its energy distribution is normalized to unity and the random number chosen by the program is compared with the normalized partial integrals of the energy distribution [4]. For the subsequent process, light absorption in the cell, the problem can be solved analytically since the probability of absorption between x and x + dx is given by

$$\frac{dI}{I_O} = \alpha \exp(-\alpha x)dx$$

which is obviously normalized to unity, and thus the random number R is given by the following expression:

$$\alpha \int_0^d \exp(-\alpha x)dx = 1 - \exp(-\alpha d) = 1 - R$$

Therefore, the penetration depth of the involved photon can be obtained from the equation

$$d = -\frac{\ln R}{\alpha(\lambda)}$$

where α (λ) being the absorption coefficient at the selected photon wavelength.

If a random penetration depth is drawn for every photon, it will result in beam intensity according to the expected law at any depth in the material.

Table-1: Typical device Parameters used as input for Monte Carlo Simulation

Thickness of absorber layer (p-type Si)	100 μm
Thickness of emitter layer (n-type Si)	1 μm
Choice of material for ARC	SiO_2 (single-layer) SiO_2 & SiN_4 (double-layer)
Thickness of ARC	87 nm
Incident angle	54^o
Photon trail	10,000
Light Source	One-SUN (AM1.5G, 100 mW/cm^2)

Reemission

It depends on the internal quantum yield (QY), which is the number of reemitted photon divided by the number of absorbed photon for a single quantum dot. The quantum yield value depends on the wavelength of the absorbed photon. The probability for an absorbed photon to be reemitted is equal to this QY. For each photon, a random number is draw and if it is greater than the QY, the photon is lost, trapped inside the material else it is reemitted. When a photon is reemitted, its direction of reemission follows a uniform spherical distribution.

Results and Discussions

Our work may be considered as an example of the possibility of using the MCM in the simulation of solar cells. We modelled the photon transportation inside crystalline silicon solar cell with ARC. The Monte Carlo model suggested that the external quantum efficiency of a bulk homojunction silicon solar cell has increased considerably from 65% without any ARC to about 74% with single layer ARC, to 81% with double layer ARC (Figure-4) in the wavelength of range 380 - 780 nm (visible light spectrum). In the calculation of the QE, we have assumed that each absorbed photon generate an exciton, and each generated exciton get collected. That is quantum efficiencies are calculated without taking into consideration the recombination of electrons in the silicon solar cell. Absorption of photons in the ARC layer has also been neglected for the simulation study. The Monte Carlo model presented here will provide a useful tool in suggesting optimum thickness of the solar cell layers and the choice of material for ARC.

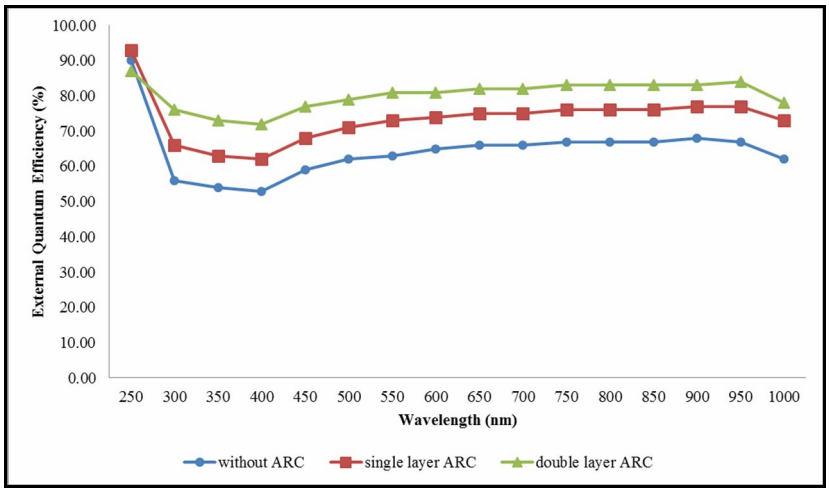

Figure-4: Comparison of AR performance of crystalline silicon solar cell

A proper combination of thicknesses and refractive indices of the SiO_2 and SiN_4 [5] as a double-layer anti-reflective coatings are applied to the silicon solar cell to analyse its performance for quantum efficiency calculation. The ARC films showed efficiency as high as 81% in the visible light spectrum.

Conclusions

The work presented here is a Monte Carlo simulation that can model the processes that govern the conversion of light to electrical power. The Monte Carlo simulation describes how the interacting particles in the solar cell move and behave. This simulation can provide insight to how the structure of the cell can influence both charge creation and charge collection. It has been shown that the external quantum efficiency of the solar cell has enhanced from 65% without ARC to about 81% with a double-layer ARC (SiO_2 and SiN_4). The double-layer ARC reported in this paper can be used as a significant tool for efficiency improvement for large area crystalline silicon solar cells by minimizing the optical loss.

Our work can be extended to simulate the short-circuit current by determining the drift and diffusion current, the open-circuit voltage, the current-voltage characteristics, the fill factor and conversion efficiency.

References

1. Takakura, H., Hamakawa, Y., "Device simulation and modeling of microcrystalline silicon solar cells", Journal of Solar Energy Materials and Solar Cells, Volume 74, Issues 1-4, Pages 479-487, September 2002.
2. Akira Usami., "Theoretical simulations of optical confinement in dye-sensitized nanocrystalline solar cells", Journal of Solar Energy Materials and Solar Cells, Volume 64, Issue 1, Pages 73-83, September 2000.
3. André Kostro., "Photonsim: Development of a Monte Carlo Ray Tracing Software for the Simulation of Solar Concentrators", Masters Thesis in Computer Science, LESO-PB, EPFL 2006.
4. Manfredotti, C., Meliga, M., "Monte Carlo simulation of solar cells", Journal of Solar Cells, Volume 10, Issue 3, Pages 211–222, December 1983.
5. Suresh Kumar Dhungel., "Double-Layer Antireflection Coating of MgF_2/SiN_x for Crystalline Silicon Solar Cells", Journal of the Korean Physical Society, Vol. 49, No. 3, September 2006, pp. 885-889.

*****