Introduction

Introduction

The worldwide energy demand is forecast to rise dramatically due to the combined effect of the global growing population and the rise in the per capita energy consumption of developing economies [1, 2]. In addition, the pressing climate change crisis creates the need for the source of this energy to be as low in carbon emissions as possible to stop the increase of the greenhouse effect [3–5]. Given this, photovoltaics, among other renewable [6, 7] energy technologies have experimented a great development since the first cells based on single crystalline or polycrystalline silicon wafers that were developed in the 1950s [8–10] that are the currently worldwide dominant commercialized solar technology, due to the high power conversion efficiency (PCE) reached by them (24.4 % and 19.9%).

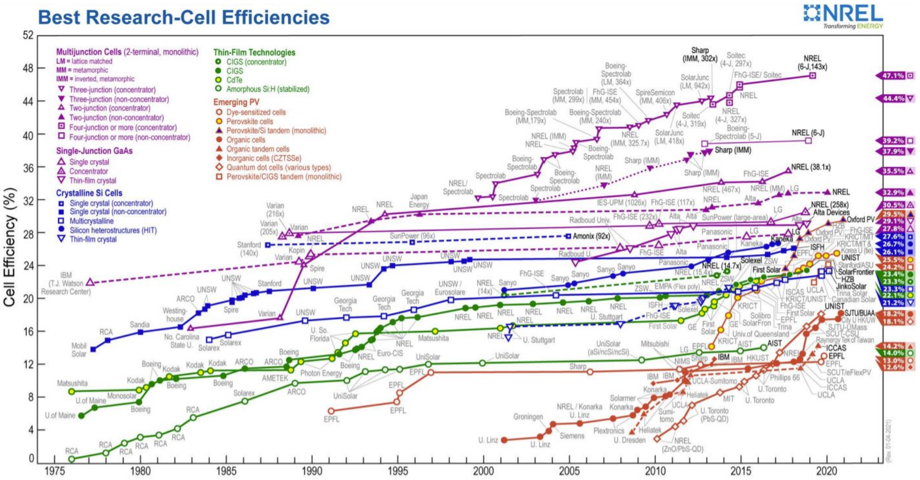

FIGURE 1: Best research-cell efficiency chart with the highest confirmed conversion efficiencies for a range of photovoltaic technologies from 1976 to the present by National Renewable Energy Laboratory (NREL) (Consulted the 1^{st} july 2021).

The high manufacturing costs caused by the extensive amount of high purity materials led to the rising in the 1970s of a second generation of thin-film solar cells including cadmium telluride (CdTe) [11], copper indium gallium selenide (CIGS) [12] or amorphous silicon [13]. The low availability of the raw materials used and the high energy requirements during the manufacturing process settled the basis for the recent development of the third generation of PV devices, based on abundant and cheap materials with limited toxicity and environmental impact such as organic photovoltaic (OPV) [14], dye-sensitized solar cells (DSSCs) [15] and more recently Perovskite-based solar cells [16].

How do photovoltaics work?

This kind of material rely on the photoelectric effect described by the Nobel Prize winners and internationally renowned scientists Max Planck [17] and Albert Einstein [18] at the beginning of the XX Century to generate electricity using light as an energy source. Although there are several works [19–21] developing and characterizing materials that can convert in an efficient manner the artificial indoors light into electricity, the most common application of these materials is the photoconversion of the solar radiation as in Figure 2.

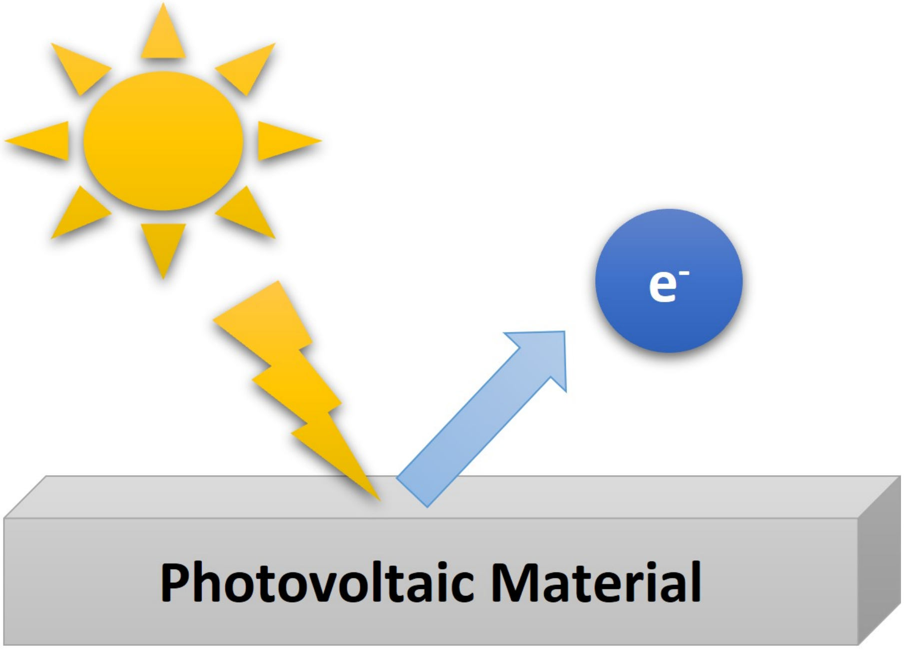

FIGURE 2: Simple schema of the photovoltaic effect.

The materials that are used for this kind of application are generally semiconductors that are capable of absorbing the energy of the photons by exciting the valence electrons to higher energy levels where they can move.

The empty state that is produced by this excitation of the electron is known as a hole, which has the same electrical charge that an electron but is opposite. These electrons and holes show a potential difference, which creates the need for an electric field that ensures the separation of the charge carriers [22].

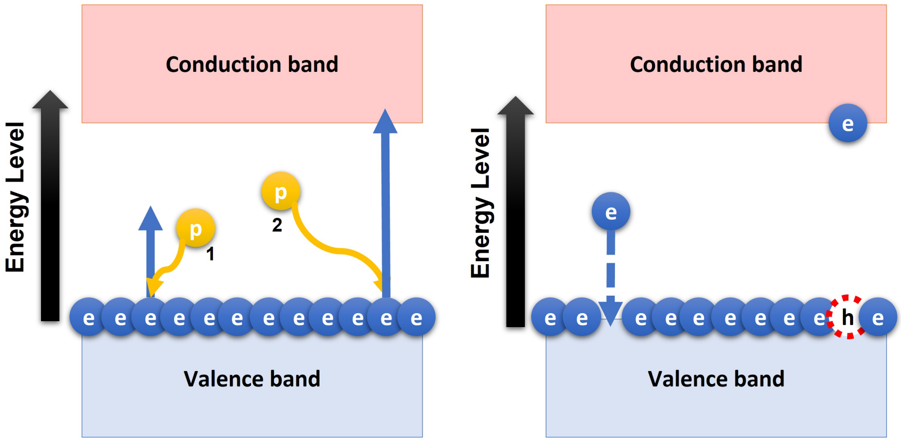

FIGURE 3: Basic schema of the different causalities that can happen when photons of different energies reach the photovoltaic material.

Due to the Pauli Exclusion Principle applied to crystals, the energy levels where electrons may exist as free electrons are limited. The intermediate energy levels between the valence band where the non-excited electrons remain and the conduction band where the excited electrons can exist are known as forbidden bands, and the difference in the energy levels between the valence and conduction band is called bandgap, which is one of the main parameters used to assess the photovoltaic performance of a certain material [23]. As can be observed in Figure 4, photon number 1 energy is not enough for the excited electron to reach the conduction band so since it can not cross the forbidden gap, goes back to the valence band. Photon 2 energy, on the other hand, allows the excited electron to reach the conduction band.

As it has been explained before, the bandgap indicates the minimum energy that a photon needs to have in order to permit the excited electron to "jump" from the valence band to the conduction band. The Planck-Einstein Relation combines the findings of both scientists regarding the photoelectric effect to determine the energy of a single photon via the equation:

$$E = h\nu = \frac{hc}{\lambda} \tag{1}$$

Where E is the energy of the photon, h is the Planck constant, ν is the frequency of the photon, c the speed of the light in the vacuum, and λ the wavelength of the photon. This indicates that a material of a certain bandgap will only be able to absorb photons of a certain wavelength range of the radiation spectrum.

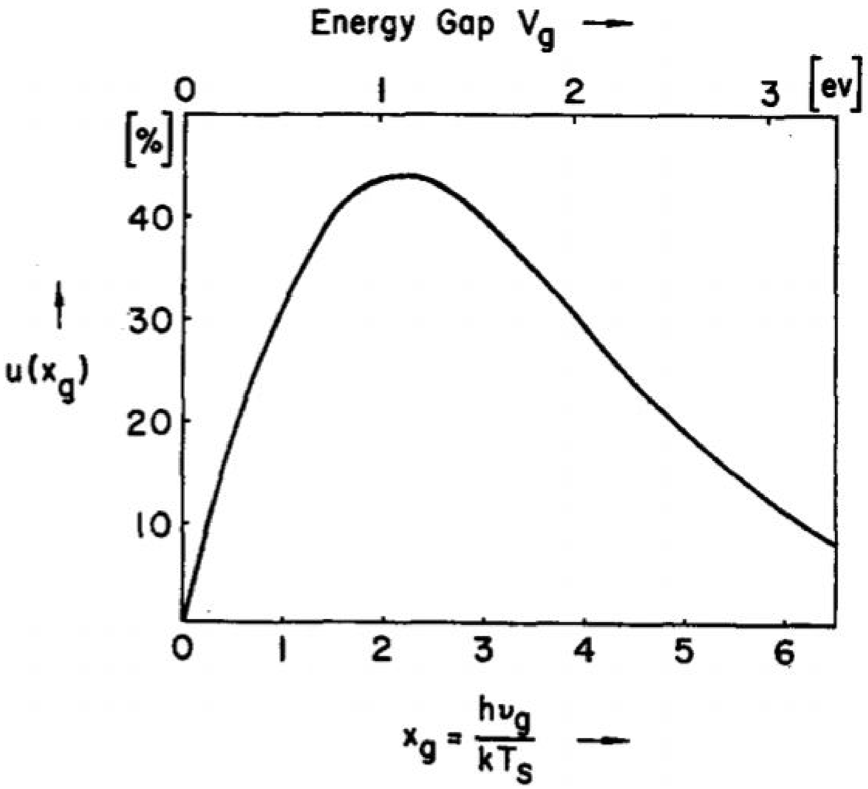

FIGURE 4: Dependence of the maximum theoretical efficiency upon the energy bandgap of the semiconductor (Figure 3 of the work by William Shockley and Hans J. Queisser). [24]

In 1961, William Shockley and Hans J. Queisser [24] calculated the theoretical maximum efficiency (30% at 1.1 eV bandgap) for a single p-n junction solar cell where the only source of loss of collected power is radiative recombination. As can be appreciated in Figure 1, there is still room for improvement to reach this theoretical limit of efficiency. These calculations were made considering a 6000K black body spectrum. However, in 2016 S. Rühle repeated the calculations considering the AM 1.5G measured global spectra, correcting this theoretical maximum efficiency to 33.7% with a bandgap of 1.34 eV. [25]

As a summary, to show a good photovoltaic performance these materials need to meet some fundamental requirements [26]:

- The bandgap of the material should be equal or lower than the energy of the majority of incident photons in the material.
- There has to be an electric field that ensures the separation of the free electron and hole carriers so they can be successfully collected by the electrodes of the device.
- It needs to include a p-n junction that allows the separation of electron and hole carriers so an usable electric potential is produced.

The current-voltage curve

The main characterization technique used to assess the performance of a certain material or device is the current-voltage curve or jV curve. This technique is a voltammetric measurement that records the photocurrent generated by the photovoltaic material under a fixed illumination during a linear increase of an external potential applied to the device.

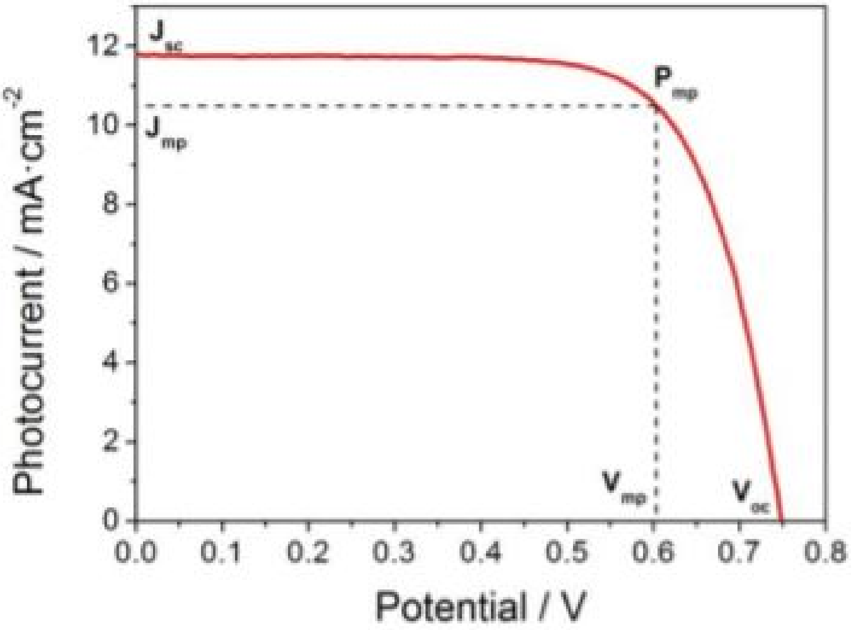

FIGURE 5: Example of a jV curve with the main photovoltaic parameters that characterize a solar cell and that can be extracted from this curve.

An example of a typical jV curve is shown in Figure 5. Its behavior can be described by the diode equation. The most meaningful photovoltaic parameters that can be extracted from this curve are:

- *Jsc*. The short circuit photocurrent density is the maximum generated photocurrent by the device under the illumination applied. It is obtained when the applied voltage is zero.
- *Voc*. The open-circuit voltage is the applied voltage where the generated photocurrent is balanced to zero by the dark current.
- P_{mp}. The maximum power point is the maximum output power of the device per unit area. It is defined by the square under the IV curve with the largest area associated with a voltage and a photocurrent.
- *FF*. The Fill Factor is a parameter that estimates the squareness of the IV curve and it is an approximation of how close the maximum output power of the cell

is to the theoretical limit defined by the Jsc and the Voc of the device. It can be calculated as:

$$FF = \frac{P_{mp}}{V_{oc} \cdot J_{sc}} \tag{2}$$

- *PCE*. The power conversion efficiency of the device is the overall conversion of the solar cell and can be calculated as

$$PCE = \frac{J_{sc} \cdot V_{oc} \cdot FF}{P_{in}} \tag{3}$$

Where P_{in} is the the incident light power density, which in the case of 1 sun conditions is 1000 W $\cdot\, m^{-2}$

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Quantum Efficiency

Quantum Efficiency

Solar Irradiation

The Sun releases a huge amount of power in all directions due to the hydrogen fusion to helium that occurs in its inside. This energy source is what makes planet Earth habitable, sustains the biosphere by ensuring the photosynthesis of plants that will feed other living beings like animals, whose biomass will ultimately form the hydrocarbons we burn nowadays for energy. The power of the Sun is also the driving force of the wind in our planet and of the water cycle that feeds hydroelectric power. In other words, almost all the electricity generated on our planet comes directly or indirectly from the Sun.

The power that is released by the Sun is in the form of photons, which can be directly harvested by photovoltaic devices. Each photon has the potential of generating an electron-hole pair, so we can compare the incident photon flux in a device to the photogenerated electric current and assess how efficient this conversion is. This is by definition the quantum efficiency.

After traveling through space, the average photon flux reaching the Earth's atmosphere is 1366 W/cm^2, which is known as the Solar constant and shows a similar spectrum to a blackbody at 5670K [1]. However, before reaching the surface of the Earth, the solar radiation is affected by the atmospheric conditions, changing its intensity and distribution [2]. The irradiation reaching the surface depends on the angle at which it crosses the atmosphere because the longer the path length, the higher the attenuation that will suffer. This attenuation is determined by the Air Mass (AM) parameter that is defined as

$$AM = \frac{1}{\cos(\Phi)} \tag{4}$$

where Φ is the angle of elevation of the Sun. The standard spectral distribution considered for photovoltaics applications is AM 1.5G, corresponding to a Φ of 48.2° [2, 3]. This atmosphere thickness implies an attenuation of the solar radiation that makes the mean irradiance in the surface be 900 W/cm^2. However, for consensus, this standard spectrum is normalized in a way that the integrated irradiance of this spectrum is 1000 W/cm^2, which is known as 1 sun illumination [1].

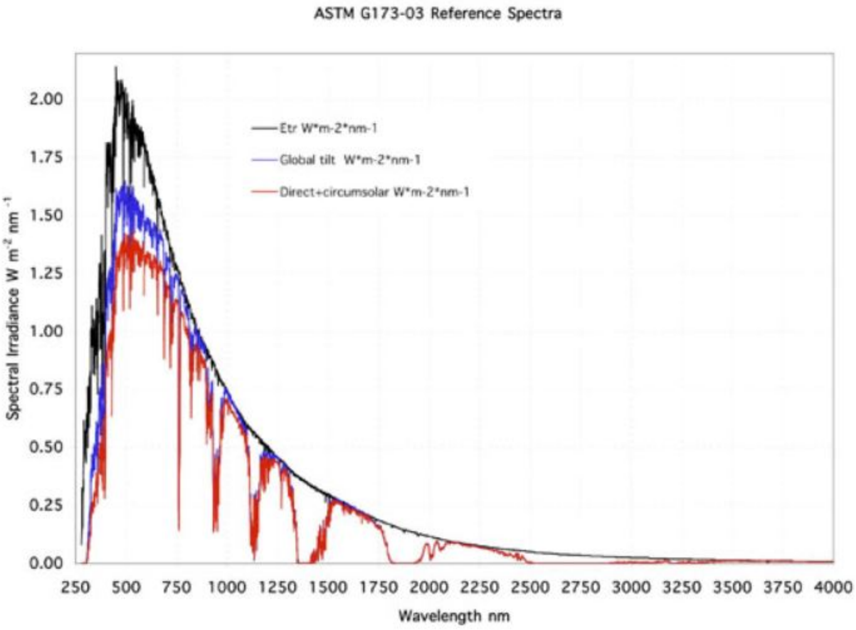

FIGURE 6: Spectra of a blackbody at 5670K, extraterrestrial and terrestrial (AM 1.5) solar spectrum

IPCE

The External Quantum Efficiency (EQE) or Incident Photon to Current Efficiency (IPCE), is defined as the number of electrons delivered extracted to the external circuit from the photovoltaic device compared to the number of incident photons, for a given wavelength [1, 4, 5].

$$EQE(\lambda) = \frac{h \cdot c \cdot J_{sc}(\lambda)}{q \cdot \lambda \cdot P_{light}(\lambda)} \tag{5}$$

where c is the light velocity, λ is the wavelength, q is the elementary charge, J_{sc} is the short-circuit photocurrent at a given wavelength, and P_{light} is the power density of the incident light.

This technique is a useful tool to assess the performance of the device converting the incident photons with different wavelengths into available electrical energy. In particular, the EQE is determined by the combination of three different processes [1]:

- The absorption coefficient of the active material.
- The efficiency of charge separation, driven by the interfacial charge transfer processes.
- The efficiency of charge collection at the contact, that depends on the charge recombination.

Integrated short-circuit photocurrent

As it was stated in the introduction, the short-circuit current (J_{sc}) is the maximum photocurrent that can be extracted from a photovoltaic device, in absence of resistances. This parameter can be calculated overlapping the IPCE results with the spectral photon flux of the incident irradiation [6]

$$J_{sc} = q \int_{\lambda_{min}}^{\lambda_{max}} I_0(\lambda) \cdot IPCE(\lambda) \cdot d\lambda \tag{6}$$

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Diode Equation

Diode Equation Derivation

As it has been stated previously, a solar cell is a particular diode favoring the current flow in one direction, preventing it in the opposite. The general shape of the jV curve observed in the Introduction is a consequence of the relation of two antagonistic mechanisms.

- Current generation produced by light-induced charge separation.
- Charge loss processes caused by recombination mechanisms.

When an external voltage larger than V_{oc} is applied under dark conditions, a charge injection generates a current into the cell due to the potential difference between both selective contacts. This depends on the applied external voltage and it is known as dark current that flows as opposed to the photocurrent. For an ideal diode this dark current can be expressed as [1, 2]

$$J_{dark}(V) = J_0(e^{\frac{qV}{k_B T}} - 1) \tag{7}$$

where J_0 is the saturation current in the dark, q is the elementary charge, k_B is the Boltzmann constant and T is the absolute temperature.

On the other hand, under illumination, charge carriers are photogenerated. These carriers are collected by the selective contacts due to the potential difference at the interfaces, which depends on the externally applied potential and the Fermi level of the material under illumination. This process acts as a driving force that counters the dark current, so the maximum generated photocurrent [3], known as short-circuit photocurrent, is obtained when J_{dark} is 0. This is when the recombination processes are minimized. Therefore, if the superposition principle applies, the photocurrent of the device at each applied potential can be described as

$$J(V) = J_{sc} - J_{dark} \tag{8}$$

This means that for an ideal diode the photocurrent is written as

$$J = J_{sc} - J_0(e^{\frac{qV}{k_B T}} - 1) \tag{9}$$

However, a real solar cell shows a behavior that is usually expressed by a non-ideal diode equation

$$J = J_{sc} - J_0(e^{\frac{qV}{mk_BT}} - 1) \tag{10}$$

Where m is a parameter called ideality factor that indicates how close to an ideal diode the device behaves. Its value is ranged between 1 and 2, being 1 for an ideal diode.

Parameters

When using the diode equation section of SolarPVsoft, several parameters need to be included as inputs. A brief description of the meaning of these values is included below.

Shunt and Series Resistances

The performance of the device is affected not only by the internal processes happening in the cell but also by parasitic resistances that can harm the performance of the device, especially diminishing the Fill Factor of the current-voltage curve. The two main sources of these additional losses are:

- Series resistance (R_s). It is the resistance of the cell material to the current flow.
- Shunt resistance (R_{sh}). It is the resistance caused by the leakage of currents through the device, around the edge of the device, and between the contacts [1].

Dark Saturation and Light Generated Currents

The current flow in the device is determined by the balance between the dark saturation current and the photogenerated current. In order to obtain good performances the first needs to be as small as possible while the second has to be maximized.

- Dark saturation current (J_0). It is an intrinsic parameter of the material, which changes from one diode to another. It can be considered as a measure of the recombination in the device or the leakage of current under dark conditions [4].
- Short circuit photocurrent (J_{sc}. The photogeneration of carriers is crucial for the good performance of the device. It is known as the process of conversion of the energy of a photon into an electron-hole pair that will eventually produce electrical energy. This parameter will depend on the incident photon flux, the absorption of the material and its thickness, and can be expressed as

$$J_{sc} = \alpha F_{ph} e^{-\alpha x} \tag{11}$$

Where α is the absorption coefficient, which is a particular property of the material, which varies depending on the wavelength excitation, F_{ph} is the photon flux at the surface of the device and x is the thickness of the active layer.

Ideality Factor

As it has been stated in the diode equation, the ideality factor represents a numerical parameter that determines how close is the behavior of the cell to an ideal diode. It can be used as a source of information of the main recombination process responsible for the current losses in the device. Typical ideality factor values are 1, 2, and 2/3, which accounts for radiative, Shockey-Read-Hall, and Auger recombination, respectively for an intrinsic semiconductor [5].

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Drift Diffusion

Drift-Diffusion Model

The two major mechanisms driving the transport in a semiconductor like the ones used to make solar cells are drift and diffusion. Drift is the process that occurs when an electric field is applied to the device, forcing the flow of the carriers following the electric field (holes in the same direction as the field and electrons in the opposite direction). Diffusion, on the other hand, is a driving force caused by the gradient of photogenerated carriers which accumulates at the surface under illumination, leading to a slow flow from high to low carrier concentration regions seeking the uniformity of the carrier concentration across the entire device [1].

The drift-diffusion model used in this software is an application of the numerical model developed by Zhou and Gray-Weale [2] based on the continuity equations and Poisson's equation. This particular implementation consists on a time-dependent drift-diffusion model [3]

In one spatial dimension, the contribution of the drift and diffusion processes can be described as [1, 2, 4, 5]

$$\frac{\delta c}{\delta t} = D\frac{\delta}{\delta x}\left(\frac{qc}{k_B T}\frac{\delta \Phi}{\delta x} - \frac{\delta c}{\delta x}\right) + G - R \tag{12}$$

where c is the particle density, D the carrier diffusion coefficient, q the elementary charge, k_B the Boltzmann constant, T the temperature, Φ the electric potential, G all the generation, and R the combination of the recombination processes.

The electric potential Φ is determined by Poisson equation

$$\frac{\delta^2 \Phi}{\delta x^2} = -\frac{\rho}{\epsilon} \tag{13}$$

being ρ the charge density of the device and ϵ the permittivity of the material. As for the generation term, it can be calculated with a Beer-Lambert profile as it was described in the Diode equation section

$$J_{sc} = F_{ph}\alpha e^{-\alpha x} \tag{14}$$

with F_{ph} as the incident photon flux, α the absorptivity of the photovoltaic material, and x the thickness of the active layer of the device.

The last recombination element would include the sum of all possible recombination processes is the combination of bimolecular (direct relaxation across the bandgap) and Shockley-Read-Hall recombination

$$R_{bulk} = \beta(np - n_i^2) + \frac{(np - n_i^2)}{\tau_n p + \tau_p n} \tag{15}$$

where β is the bimolecular recombination constant, n and p account for the electron and hole densities, τ_n and τ_p accounts for the lifetimes of electrons and holes, respectively and n_i is the intrinsic carrier density given by

$$n_i = np = N_C N_V e^{\left(-\frac{E_g-(qV)}{2k_BT}\right)} \tag{16}$$

being N_C and N_V the density of states at the conduction and valence bands and E_g the bandgap of the material.

This time-dependent drift-diffusion model [3] solves these equations for electrons and holes and for the electrical field using a discretized scheme and the Forward Time Central Space method [4] considering as boundary conditions [2] that the electron and hole densities are fixed by the applied voltage, whereas transfer of electrons is blocked at the hole selective contact while the transfer of holes is blocked at the electron selective contact. As for the electric field, it is considered that the screening effect of the ions cancels the field within the active layer [6, 7]. SolarPVsoft allows for working considering or neglecting the influence of the ions by activating or deactivating this electric field as an input option.

As for the values of the electron and hole densities at the boundaries, they are calculated using

$$n_0(x=0,V) = N_c e^{\left(-\frac{E_c-E_{f(n)}}{k_BT}\right)} (17)$$

$$p_0(x=d,V) = N_v e^{\left(-\frac{E_v-E_{f(p)}}{k_BT}\right)} (18)$$

where $E_{f(n)}$ and $E_{f(p)}$ are the quasi-Fermi levels of electrons and holes, respectively, and N_c/N_v and E_c/E_v are the density of states and the conduction/valence band and the conduction/valence band edge.

After solving the equation, the photocurrent density for each given value of the potential V is obtained from the stationary density profile at the contacts, allowing to obtain the full current-voltage curve

$$J = \left(\frac{dn(x,t)}{dx}\right)_{x=0} = \left(\frac{dp(x,t)}{dx}\right)_{x=d} \tag{19}$$

Parameters

Thickness

This parameter account for the width of the active layer of the device that is being simulated. It affects the optical properties of the device, taking part in the Beer-Lambert profile that determines the absorbed photon flux. In addition, this thickness will determine the the amount of photogenerated carriers that reach the contacts before being recombined to be extracted in the selective constants.

Bandgap

The bandgap is determined by the energy difference between the conduction and the valence bands and represents the minimum energy required for an electron to be excited from the valence to the conduction band and, therefore, to be involved in the photogeneration process.

Illumination

This will determine the incident photon flux per area unit that will arrive at the surface of the device. Each photon will have the potential of generating one sole electron-hole pair, but the rate of success doing this will be determined by the absorption of the material. SolarPVsoft uses AM 1.5 standard solar flux (see section 2) or monochromatic light with a given absorption coefficient.

Absorbance

Each semiconductor material holds its specific optical properties, determining the ratio of photons of certain photon energy will be absorbed and therefore, will have the potential of generating an electron-hole pair. The absorption profile is closely related to the bandgap of the semiconductor, since no photon with energy below this bandgap will be absorbed, and the higher the excitation energy is, the larger number of excitations of electrons will happen. SolarPVsoft reads the wavelength dependent absorption coefficient in m^{-1} (for white AM 1.5G light) or a single value of the absorption coefficient in m^{-1} (for monochromatic light).

Dielectric constant

The dielectric constant, or relative permittivity, is a material property that is defined as the ratio of the electric permeability of the material to the electric permeability of free space [8], determining the ease of electric fields to cross the material.

Density of states

The density of states of the material is a property that accounts for the ratio of occupied states at the valence and conduction energy levels. [9] This parameter will determine the intrinsic electron and hole carriers that are available for the conduction of photogenerated charges.

Electronic diffusion coefficient

The diffusion coefficient determines the average rate of flow of the electronic carriers across the semiconductor material following the gradient created by the excess of photogenerated carriers in the surface of the material [10]. The higher this value is, the more likely the carriers will be able to cross the entire active layer reaching the selective contacts before being lost by recombination.

Bimolecular recombination constant

This recombination term accounts for the bulk radiative recombination that is caused by direct relaxation across the bandgap, also known as "band to band" recombination. When this recombination happens, the combination of an electron and a hole produces a photon with equivalent excitation energy to the bandgap, so it can be absorbed again. Although it is dominant for direct bandgap semiconductors, its importance in most solar cells based on indirect bandgap semiconductors is very low. [1]

Lifetimes

The lifetime is a way to consider the average time that electron and hole carriers take before being lost by recombination, so it is the opposite of the recombination rate of the device. If the lifetime of the carriers is long enough to allow the carriers to reach the selective constants the performance of the device is higher. Note that this parameter is closely linked to the electronic diffusion coefficient since the faster the carrier moves, the longer the distance will be able to travel during its lifetime. For this reason, both parameters are usually treated together as *diffusion length* [1]. The lifetimes enter the SolarPVsoft calculation via Eq. 15.

Discretization points

This is a numerical parameter that is not related to the physics involving the calculations but has a crucial role in mathematical calculations. It determines the number of sections the full thickness of the device is split in. [11]

Time steps

As the model is a time-dependent drift-diffusion, in addition to the split of the spatial dimension determined by the discretization points, the time range where the simulation is happening can also be discretized by different time steps. [11] The longer you want your calculation to span, the larger this parameter must be.

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