

Operation and physics of photovoltaic solar cells: an overview

Funcionamiento y física de celdas solares fotovoltaicas: una visión general

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ABSTRACT— Solar energy is considered the primary source of renewable energy on earth; and among them, solar irradiance has both, the energy potential and the duration sufficient to match mankind future energy needs. Nowadays, despite the significant potential of sunlight for supplying energy, solar power provides only a very small fraction (of about 0.5%) of the global energy demand. In order to increase the worldwide installed PV capacity, solar photovoltaic systems must become more efficient, reliable, cost-competitive and responsive to the current demands of the market. In this context, PV industry in view of the forthcoming adoption of more complex architectures requires the improvement of photovoltaic cells in terms of reducing the related loss mechanism, focusing on the optimization of the process design, as well as, reducing manufacturing complexity and cost. Hence a careful choice of materials, a suitable architecture and geometric distribution, passivation techniques and the adoption of a suitable numerical modeling simulation strategy are mandatory. This work is part of a research activity on some advanced technological solutions aimed at enhancing the conversion efficiency of silicon solar cells. In particular, a detailed study on the main concepts related to the physical mechanisms such as generation and recombination process, movement, the collection of charge carriers, and the simple analytical 1D p-n junction model required to properly understand the behavior of solar cell structures. Additionally, the theoretical efficiency limits and the main loss mechanisms that affect the performance of silicon solar cells are explained.

Keywords— *Electric field, electron-hole pair, energy bands, IBC solar cell, passivation technique, photovoltaic effect, p-n junction diode.*

RESUMEN— La energía solar es considerada la principal fuente de energía renovable en la tierra y tiene tanto el potencial energético como la duración suficiente para satisfacer las necesidades energéticas futuras de la humanidad. Hoy en día, a pesar del importante potencial de la luz solar para el suministro de energía, proporciona solo una fracción muy pequeña (de aproximadamente el 0,5 %) de la demanda mundial de energía. Para aumentar la capacidad fotovoltaica instalada en todo el mundo, los sistemas fotovoltaicos solares deben ser más eficientes, confiables, competitivos en costos y sensibles a las demandas actuales del mercado. En este contexto, la industria fotovoltaica requiere la mejora de las celdas fotovoltaicas centrándose en la optimización del diseño del proceso, así como en la reducción de la complejidad y el costo de fabricación. Por lo tanto, una elección cuidadosa de materiales, una arquitectura adecuada y una distribución geométrica, técnicas de pasivación y la adopción de una estrategia de simulación de modelado numérico adecuada son imprescindibles. Este trabajo es parte de una actividad de investigación detallada sobre los conceptos principales relacionados con los mecanismos físicos, como el proceso de generación y recombinación, el movimiento, la colección de portadores de carga y el modelo analítico simple de uniones p-n 1D requerido para comprender adecuadamente el comportamiento de las estructuras de las celdas solares. Además, se explican los límites de eficiencia teóricos y los principales mecanismos de pérdida que afectan el rendimiento de las celdas solares de silicio.

Palabras clave— *Campo eléctrico, par de orificios de electrones, bandas de energía, células solares IBC, técnica de pasivación, efecto fotovoltaico, diodo de unión p-n.*

1. Introduction

Nikola Tesla said that “the sun maintains all human life and supplies all human energy”. The sun furnishes with energy all forms of living, start from the photosynthesis process; plants absorb solar radiation and convert it into stored energy for growth and development, thus supporting life on Earth. For this reason, the sun is the

most important and plentiful sources of renewable energies. This star is about 4.6 billion years old with another 5 billion years of hydrogen fuel to burn in its lifetime. This characteristic gives to all living creatures a sustainable and clean energy source that will not run out anytime soon. In particular, solar power is the primary source of electrical and thermal energy, produced by

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directly exploiting the highest levels of the irradiated energy from the sun to our planet. Therefore, solar energy offers many benefits such as no-releasing greenhouse gases (GHG_s) or other harmful gases in the atmosphere.

It is economically feasible in urban and rural areas and evenly distributed across the planet. Moreover, as it was mentioned above, solar power is also essentially infinite, a reason why it is close to being the largest source of electricity in the world by 2050. Besides, most of the energy forms available on earth arise directly from the solar energy, including wind, hydro, biomass and fossil fuels, with some exceptions like nuclear and geothermal energies.

Solar cell also called photovoltaic (PV) cell is basically a technology that convert sunlight (photons) directly into electricity (voltage and electric current) at the atomic level. This can be obtained through the photovoltaic effect, process in which two dissimilar materials in close contact produce an electrical voltage when struck by light or other radiant energy. Essentially, solar cells are composed of two different types of semiconductors: an n- and a p-type that are joined together to create a p-n junction. By joining these two types of semiconductors, an electric field is formed in the region of the junction as electrons move to the positive p-side and holes move to the negative n-side. This field causes negatively charged particles to move in one direction and positively charged particles in the other direction, thus, producing an electrical voltage. On the other hand, PV energy is also a renewable, versatile technology that can be used for almost anything that requires electricity, from small and remote applications to large, central power stations. PV can be friendly and a great alternative to satisfy the steady growing energy-demand in the entire globe by producing clean electric power which also reduces the negative greenhouse effects (GHE). This work presents a concise review of the basic physical principles that characterize the method of function of solar cell devices.

Initially, a general report on a research activity on some advanced technological solutions aimed at increasing the conversion efficiency of silicon solar cells made in the photovoltaic industry since the middle of the 20th century is introduced. Furthermore, a description of the most used architectures of solar cells and an explanation of the main process-related to the PV effect is presented.

All these concepts support the comprehension of the working principle of silicon solar cells. Secondly, an analysis on the collection of charge carriers by using p-n junction and a review of the set of the basic equations that describe the ideal properties of semiconductor devices in

the drift-diffusion approximation is also included. Subsequently, the simple 1D diode model is first discussed in order to analytically derive the ideal solar cell illuminated I-V characteristics in order to complement the explanation of the physics mechanisms related to the solar cell operation.

2. Development of PV technology systems

Photovoltaic technology is one of the foremost ways to harness solar energy. A PV cell consists of an electrical device made out of certain semiconductor materials such as Silicon, that exhibit a particular property known as the *bulk photovoltaic effect*. The PV effect is a process that causes the absorption of photons of light and releases electrons, and when these free electrons are captured, an electric current is obtained. In other words, the PV system directly converts sunlight (photons) into electricity (voltage) without any intermediary. In 1954 the scientists Daryl M. Chapin, Calvin S. Fuller, and Gerald L. Pearson built the first modern silicon-based photovoltaic cell at Bell Laboratories in the United States, registering an efficiency of about 6% [3]. This paramount invention defines a new era for the current and future developments in the PV industry by offering advantages that include technical and environmental parameters, taking as a reference the positive and negative issues of conventional fossil-fuel power plants. By the early 1960s, laboratories started developing the first silicon solar cells to power space satellites. These applications were extremely expensive devices, unsuitable for terrestrial use. The first vast oil crisis, which occurred during the 1970s, gave a first important boost to the promotion of photovoltaics as an alternative energy-generation process for terrestrial use. Consequently, solar cells research and development experienced growing interest. As a result, solar cells began to quickly increase their energy-conversion efficiency (see figure 1) and the increase of the volume of cells produced for terrestrial use led to a significant reduction in solar cell manufacturing costs.

Therefore, in the late 1970s and 1980s, the developed PV systems were focused on terrestrial applications, and the first thin-film solar cell based on copper-sulphide/cadmium-sulphide junction amounted to an efficiency (η) above 10%.

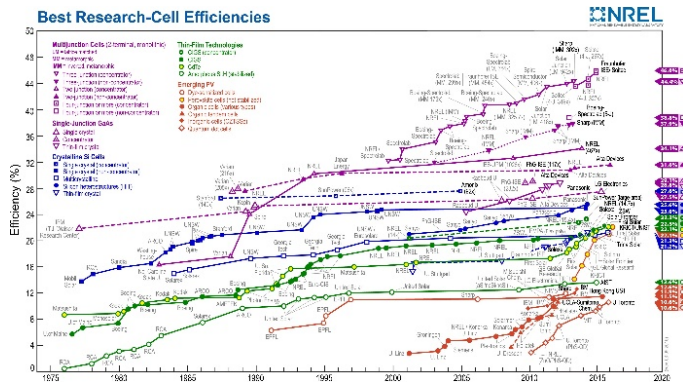


Figure 1. Evolution of conversion efficiency for different types of solar cells since 1975. Taken from www.nrel.gov/pv/

In contrast to this invention, in 1975 R. Schwartz initiated research of a new architecture known as back-contact solar cells, considered an alternative to photovoltaic cells, featuring both a front and rear contact [4]. In 1985, the University of New South Wales (UNSW) built crystalline silicon (*c*-Si) solar cells and reached efficiencies above 20%, and in 1999 they stated a new record of 25%, considered the world highest efficiency [16], [25]. The structure was also *c*-Si-based. In 1994, the National Renewable Energy Laboratory (NREL) from Colorado, U.S.A, built a solar cell based on indium-gallium-phosphide/gallium-arsenide tandem junction that exceeded 30% efficiency. Until the late 1990s, solar cell innovations continued to be introduced, pushing up the photovoltaic industry and the related manufacturing processes. Consequently, PV research and developments of solar cell systems were notably growing interest in North America, Europe, and Asia. To confirm this, the world total installed PV power systems in 1999 outstripped the 1 GW, defining a renewed beginning for the public discussion of solar energy, bearing in mind essential aspects such as the environment and the climate change, economy, health and the common welfare. In particular, at the end of 2011, the world-wide installed capacity of solar PV systems has reached more than 69,000 megawatts (MW), representing 0.5% of global electricity demand. Accordingly, photovoltaics is now, after hydro and wind power, the third most important renewable energy source in terms of global installed capacity [32]. Afterwards, many laboratories and companies continued developing silicon photovoltaic cells, achieving new conversion efficiency records of approximately 25% as in the case of SunPower & Panasonic in 2014 [35], [36]. Over the same year, the Australian National University designed an interdigitated back contact (IBC) solar cell featuring point contacts on the rear side achieving an efficiency of 24.4%, the

highest reported value to date for this promising back contact architecture [46]. Furthermore, at the end of 2016 Yoshikawa et. al from Kaneka Corporation built an interdigitated back contact (IBC) *c*-Si-based solar cell, obtaining the world's highest conversion efficiency of 26.33% [49]. Additionally, it is important to highlight that this kind of back contact-back junction (BC-BJ) solar cell structures are recognized by the many advantages over the conventional PV cells, but more complex configuration implies specific fabrication processes and higher costs. Anyhow, point contact cells have shown a pledging performance, thus representing a potential architecture to optimize by the extensive study carried out in this work [6]. It is worth mentioning, that each of these innovations have contributed significantly to the worldwide record growth of the photovoltaic market during the last years. Silicon is the second most abundant element in the Earth's crust (about 28%) after oxygen, and it is also a non-toxic material and represents a fundamental component in the microelectronic industry.

As silicon solar cells have shown satisfactory properties in creating an electric charge when exposed to sunlight, it has led the PV industry for more than the three decades and is still improving. Actually, this valuable semiconductor material offers a reliable technology that can easily achieve a large-scale deployment [43].

However, the key to accomplishing this objective is based on the understanding of the device operation and the reduction of the related loss mechanism, focusing on the optimization of the process design, increasing the conversion efficiency, as well as, reducing manufacturing complexity and cost.

3. Solar cell architecture

3.1 Conventional solar cells

A conventional solar cell structure is simply based on a semiconductor p-n junction diode that operates under solar illumination as sketched in figure 2. When sunlight strikes the surface of a semiconductor, a certain portion of photons is transmitted and, then, absorbed into the semiconductor material, thus giving rise to photogenerated electron-hole pairs, while the remainder is reflected from the surface. Some of these photogenerated charge carriers are separated by the internal built-in electric field of the p-n junction before they recombine and, then, they are collected at the cell terminals, thus contributing to the cell output current in the external circuit [28], [48]. On the other hand, one of the major disadvantages founded in this type of architecture is the shading losses effect caused by the presence of metal (front contacts) on the top surface of the solar cell which

prevents light from entering the solar cell. The shading losses are determined by the transparency of the top surface, which, for a planar top surface, is defined as the fraction of the top surface covered by metal. The transparency is determined by the width of the metal lines on the surface and on the spacing of the metal lines. An important practical limitation is the minimum line-width associated with a particular metallization technology [12], [21], [38].

In table 1 there is a summary of some of the latest published manufacturing data of *c*-Si solar cells and their certified efficiency records.

3.2 Advanced solar cells

During the last thirty years, the PV research community has been focusing their efforts on optimizing the solar cell design and performance, with the main scope of achieving highest efficiencies while reducing typical loss mechanisms and production costs. In this way, innovative cell designs have been studied and developed, stating that the best concepts so far are based on monocrystalline wafers [48]. Silicon-based structures, which feature the highest conversion efficiencies, are classified into three main groups:

- Passivated Emitter Rear Locally diffused (PERL) solar cell.
- Silicon Heterojunction solar cell (SHJ).
- Interdigitated Back Contact solar cell (IBC) (also called back contact-back junction solar cell (BC-BJ)).

In the following sections a short review of these kinds of solar cells is presented.

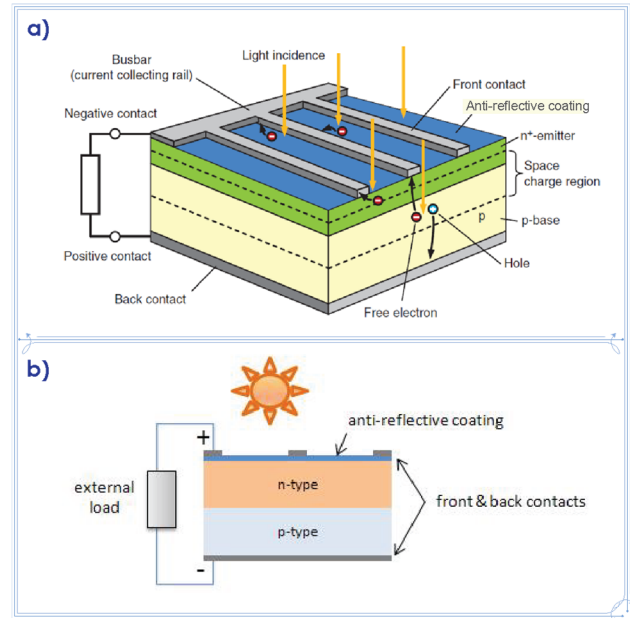


Figure 2. a) Three-dimensional (3D) view of a conventional solar cell featuring front and back contacts. b) Two-dimensional (2D) cross-section of a conventional solar cell. Taken from [26], [33].

3.2.1 Passivated Emitter Rear Locally diffused (PERL) solar cell

The *Passivated Emitter Rear Locally diffused* solar cell integrates two important concepts that minimise the recombination centers on the top and bottom of the solar cell. Substantially, the key features of PERL cells are listed as follows, the top surface of the solar cell is textured by using inverted-pyramid structures and covered by double-layer anti-reflecting coating (ARC) which significantly reduces the top surface reflection as well as the amount of carrier recombination. The front metal finger grids are defined by photolithography technology to be very thin therefore minimising metal shading loss. Both inverted-pyramid texturing and fine metal fingers decrease the optical losses which contribute to a higher current for the solar cell (see figure 3).

Conversely, at the rear side of the cell, a selective emitter technique is applied (heavily phosphorus diffused regions underneath the metal contacts) whilst the rest of the top surface is lightly diffused to keep excellent “blue response” (absorbing the short-wavelength photons). This can mitigate both contact resistance and recombination at the rear while keeping a good electrical contact. PERL solar cell uses micro-techniques to produce cells with efficiencies approaching 25% under the standard AM1.5 spectrum [16], [30], [47].

Table 1. Performance parameters of certified *c*-Si solar cells. (*da: designated area, *ta: total area, *ap: aperture area)

Device	Area [cm ²]	V _{oc} [mV]	J _{sc} [mA/cm ²]	FF[%]	η[%]	Reference
Kaneka IBC HIT	180.43 (da)	744	42.3	83.8	26.3	[49]
Panasonic IBC HIT	143.7 (da)	740	41.8	82.7	25.6	[35]
SunPower IBC	153.5 (ta)	737	41.3	82.7	25.2	[42]
Kaneka SHJ	151.9 (ap)	738	40.8	83.5	25.1	[39]
Fraunhofer ISE TOPCon	4.0 (da)	718	42.1	83.2	25.1	[34], [41]
UNSW PERL (<i>p</i> -type)	4.0 (da)	706	42.7	82.8	25.0	[16], [47]
Panasonic HIT	101.8 (ta)	750	39.5	83.2	24.7	[37]
EPFL MoOx SHJ	3.9 (ap)	725	38.6	80.4	22.5	[40]
IMEC PERT (<i>n</i> -type)	238.9 (ta)	695	40.2	80.5	22.5	[44], [45]
Trina solar mono-Si PERC (<i>p</i> -type)	243.7	680	40.5	80.3	22.1	[42]

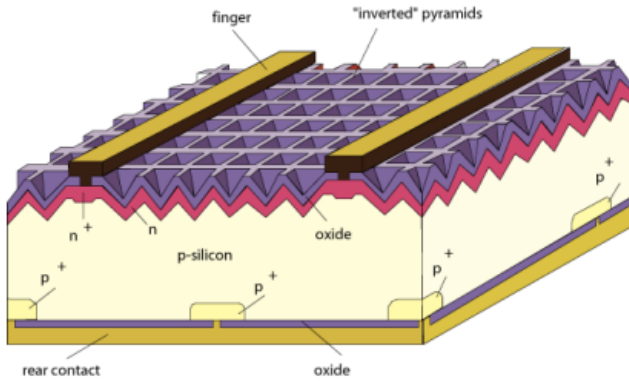


Figure 3. Structure of a high-efficiency PERL Solar cell. Reprinted from [13].

3.2.2 Silicon Heterojunction (SHJ) solar cell

The *Silicon Heterojunction* solar cell is a structure made out of two different silicon-based semiconductor materials. One of these materials is applied as a thin layer between silicon and metal. This technique commonly considers the deposition of a thin amorphous silicon (*a*-Si) layer, demonstrating an evident increment of the open circuit voltage V_{oc} with no need of an expensive patterning process. Since *a*-Si has a wide band-gap layer, V_{oc} is enhanced and the high surface recombination in active metal contacts is lessened. A schematic of a two-dimensional cross view and a band diagram of a typical silicon heterojunction (SHJ) solar cell are illustrated in figure 4. The latest performance record for the heterojunction silicon-based (*c*-Si) concept has reported an open circuit voltage value of $V_{oc} = 0.74V$ and a conversion efficiency equal to $\eta = 25.6\%$ [42].

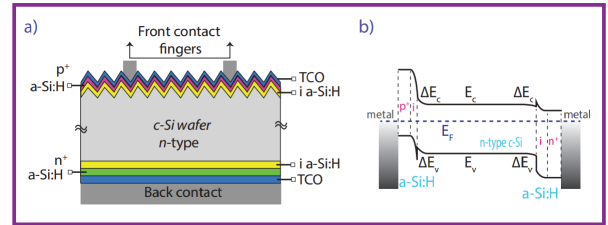


Figure 4. a) Two-dimensional (2D) cross section of a silicon heterojunction (SHJ) solar cell. b) Corresponding band diagram in dark at equilibrium. Reprinted from [33], [48].

3.2.3 Interdigitated Back Contact solar cell (IBC)

This architecture is also known as *back contact-back junction solar cell* (BC-BJ) and consists of a design where both metal contacts are located on the bottom of the *c*-Si wafer, simplifying the cell interconnection at module level. These characteristics of IBC cells also allow boosting the solar cell conversion efficiency η due to the absence of front contact shadowing losses. In fact, this is the opposite case of traditional PV cells, where metal grids at the front surface are the main cause of electrical shading losses and an attenuated short circuit current J_{sc} . Since back contact-back junction cells are an evolution of conventional solar cells, they offer many other advantages as the possibility of coplanar interconnection and low series resistance, due to the facility of making much larger metallization coverage on the rear side. Nonetheless, some critical parameters must be kept in mind. Usually, carriers are generated near the top surface because most energetic photons are absorbed almost immediately within the first microns of the wafer. Subsequently, since BC-BJ has the junction on the rear side of the cell, charge carriers have to travel through the whole substrate to reach their respective collection centers, avoiding recombination. With regards to this,

$$E = h \cdot \nu \quad (1)$$

back contact-back junction solar cells are very sensitive to recombination mechanisms such as SRH in the bulk and at the interfaces [23]. These process can occur due to an inadequate passivation (i.e. a way to suppress the defects present in the crystal lattice) on the front and back surfaces, and also because of a low effective bulk lifetime τ_{Bulk} , as well as, a high surface recombination velocity at front surface. Basically, the cell structure has both *n*-type and *p*-type sides alternating on the bottom of the substrate, and they are represented by the BSF and emitter regions, respectively. These regions are responsible for collecting the charge carriers selectively, by directing electrons into the BSF and holes into the emitter. Consequently, collected carriers must flow through their corresponding metal-point contacts located just below the *n*-type and *p*-type regions in order to extract power from the PV cell, as illustrated in figure 5.

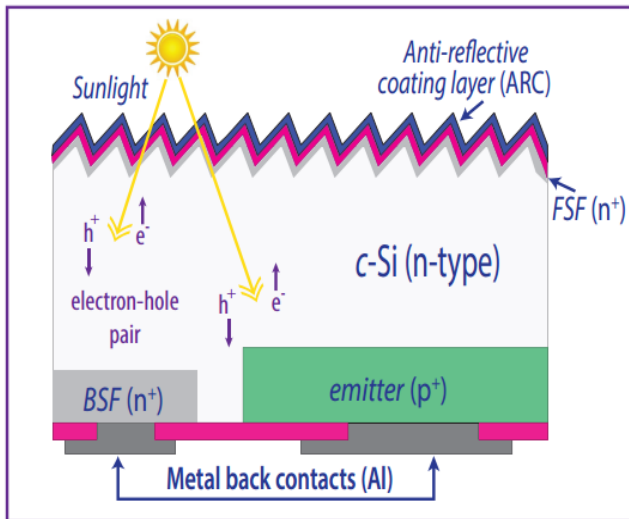


Figure 5. Schematic of a simple single-junction back contact solar cell structure, where the photogeneration of electron-hole pairs is exhibited. Re-designed from [29].

4. Solar cell operating principle

The working principle of a silicon solar cell is based on the well-known photovoltaic effect discovered by the French physicist Alexander Becquerel in 1839 [1]. As described in section 2 this effect generates an electric field at the junction of two materials in response to electromagnetic radiation (photons). It is worth noting that the PV effect is closely related to the photoelectric effect which was explained by Albert Einstein in 1905.

Basically, he assumed that photons are quantum energy which are present in light, and this energy is given by the following expression,

Where, h is Planck's constant and ν is the frequency of the light. This scientific explanation granted Einstein the Nobel Prize in Physics in 1921 [2]. Accordingly, the photovoltaic effect takes places in a solar cell, a structure based on two types of semiconductor materials that are joined together to create a p-n junction diode that operates under solar illumination (see figure 5). Essentially, the PV effect is described by three basic process:

1. **Generation of charge carriers (electron-hole pair) due to the absorption of light.** When sunlight hits the semiconductor surface, a portion of photons is transmitted and, then, absorbed into the material producing photo-generated electron-hole pair; while the rest is reflected.

2. **Separation of the photo-generated charge carriers in the junction.** The electron-hole pair is separated by the internal built-in electric field of the p-n junction before they recombine.

3. **Collection of the photo-generated charge carriers at the terminals of the junction.** The charge carriers are extracted from the solar cell with electrical contacts, thus contributing to the output current in the external circuit. Finally, the chemical energy of the charge carriers is converted to electric energy. At this point, as electrons have passed through the circuit, they will recombine with holes at a metal absorber interface, as sketched in figure. 6 [48].

5. Device physics of solar cells

5.1 Semiconductor model equations

Once the electron-hole pairs are generated due to the light absorption process, they move around inside the crystal lattice and before recombining they should be collected in order to extract power from the PV cell. The way these electrical currents are generated is due to the transport of the electron-hole charges. Therefore, the well known Drift-Diffusion (D-D) model transport is the appropriated mechanism to describe the operation of charge carriers in the substrate under the influence of light and/or electric field, thus leading to a variation from the thermal equilibrium conditions. Basically, the D-D approximation consists in the solution of a set of five basic equations which derive the ideal properties of semiconductor devices including *Si* solar cells.

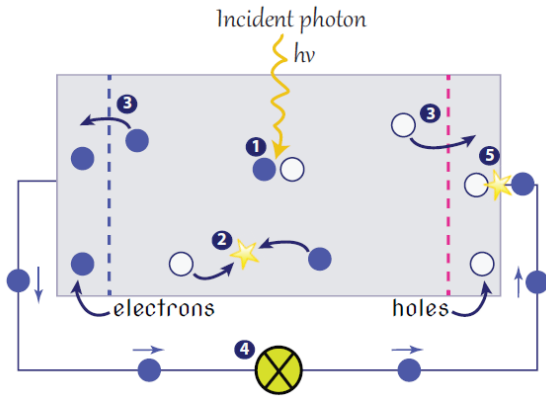


Figure 6. Schematic of a very simple solar cell model.

① Absorption of a photon leads to the generation of an electron-hole pair. ② Normally, the electrons and holes will recombine. ③ Electrons and holes can be separated by the n-type and p-type materials. ④ The separated electrons can be used to drive an electric circuit. ⑤ After the electrons have passed through the circuit, they will recombine with holes. Taken from [48].

5.1.1 Poisson equation

Poisson equation describes the electrostatics by relating the divergence of the static electric field ξ to the charge density ρ :

$$\nabla \cdot \xi = \nabla^2 \varphi = \frac{\rho}{\varepsilon} \quad (2)$$

where ρ is the electrostatic potential and ε is the material permittivity. The charge density in a semiconductor device is given by,

$$\rho = q(p - n + N_D^+ - N_A^-) \quad (3)$$

where n and p are the electron and hole densities, and N_D^+ and N_A^- are the densities of ionized donors and acceptors, respectively.

5.1.2 Drift-Diffusion transport model equations

It is widely known that the electrical current flow in a semiconductor device is generated by the transport of electrons and holes. This is possible through the two basic drift-diffusion (D-D) transport processes. First of all, drift mechanism takes place when applying an electric field ξ across the semiconductor, whereas diffusion transport process is driven by a concentration gradient.

Accordingly, the total current densities of electrons and holes denoted by, J_n and J_p are defined as,

$$J_n = q\mu_n n \xi + qD_n \nabla_n \quad (4)$$

$$J_p = q\mu_p p \xi + qD_p \nabla_p \quad (5)$$

where μ_n and μ_p are the electron and hole mobilities, and D_n and D_p are the electron and hole diffusion coefficients, respectively. The first terms on the right side of equation (4) and equation (5) represent the drift currents, whereas the second terms denote diffusion currents approximation. The mobility and diffusion coefficients are related through the Einstein relationship, as follows,

$$D_n = \mu_n \frac{kT}{q} \quad \text{and} \quad D_p = \mu_p \frac{kT}{q} \quad (6)$$

For the case of solar cell devices, the simulator estimates charge distribution and transport mechanisms according to the well known Drift Diffusion (D-D) Model.

5.1.3 Continuity equations

In order to define the complete set of semiconductor equations, two more expressions are required. These last equations associate the divergence of the current densities to the generation and recombination rates of the related charge carriers. Besides, they take into account the law of conservation of charges. Under steady-state conditions, the electron and hole continuity equations can be defined as,

$$\frac{1}{q} \nabla \cdot J_n = R_n - G_n \quad (7)$$

$$\frac{1}{q} \nabla \cdot J_p = R_p - G_p \quad (8)$$

where G represents the optical generation rate of electron-hole pairs and, R_n and R_p are the recombination rates for electrons and holes respectively. For a uniformly doped semiconductor; band-gap, electric permittivity, mobility and diffusion coefficients are independent of position. Therefore, the equations (2), (4), (5), (7) and (8) represent the base for obtaining the reduced version of semiconductor equations.

6. 1D p-n junction diode model

An ideal PV cell illuminated I - V characteristics and output dark can be easily solved, from the set of equations already presented in the previous section 5.1. To achieve this, it is mandatory to adopt a simple 1D p - n junction diode model for a silicon solar cell featuring a constant doping in the n - and p -type regions, and a blunt doping

step transition, as well as additional simplified assumptions [31].

6.1 Electrostatics of the p – n junction

As already explained a conventional solar cell is simply formed by the well-known $p-n$ junction. It consists of a simple union of two oppositely doped silicon blocks that allows the operation of the device, aggregating all carrier transport (e.g., drift and diffusion effects) as illustrated in figure 7. The n -type block has a large number of free electrons negatively charged. Meanwhile, p -type block has also a big amount of free holes positively charged. Both charged carriers can move freely through the semiconductor material. When two pieces of n -type and p -type doped semiconductors are brought into contact, electrons diffuse from the region of high concentration (n -type side) to the region of low concentration (p -type side), due to the concentration gradient between the two types of material. Similarly, holes diffuse from p -type side to n -type side. As a consequence, the electrons diffusion current from the n -doped to the p -doped region creates a charge imbalance in the n -type side, leading to a positively charged region in that side (see figure 8). Likewise, the holes diffusion causes a negative charge in the p -type side. This leads to the creation of an electric field that opposes the diffusion transport, thus resulting in an equilibrium situation.

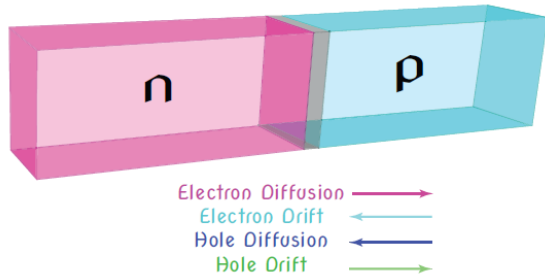


Figure 7. Sketch of a 3D $p-n$ junction semiconductor diode. Re-designed from [20].

The transition region between the n -type and p -type of the semiconductor material, where the electric field E is present, is known as the *depletion region* (denoted by W), since it is depleted of free carriers (i.e. electrons and holes swept by the E electric field) [18], [22]. With regards to the energy band diagrams, the main concepts are illustrated in figure 9 a) where a structure of an n -type interdigitated back contact (IBC) crystalline silicon solar cell is sketched and features two phosphorus diffusions ($n+$) to create the top region known as *front surface field*

(FSF) and the bottom region called *back surface field* (BSF). The junction is at the back by the injection of Boron in the emitter region. On the other hand, figure 9 b) the $p-n$ junction is in equilibrium. It shows a constant Fermi level E_F , thus causing the band bending of the conduction energy band E_C and the valence band E_V .

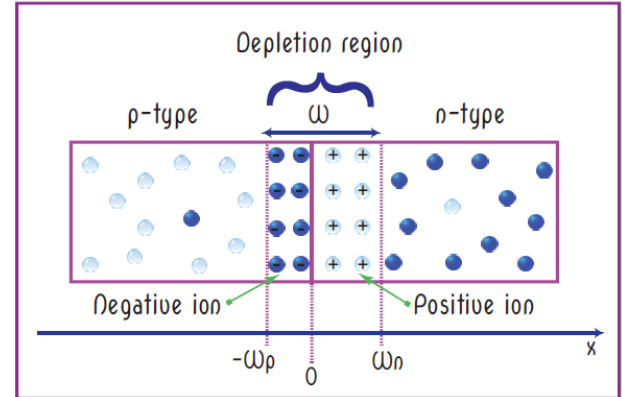


Figure 8. Simple solar cell schematic showing a 1D $p-n$ junction. The junction is in $x = 0$, W is the width of the depletion region, whereas W_p and W_n represent the edges of the depletion region [27].

In figure 9 c) the Fermi energy level splits into two quasi-Fermi energy levels when the solar cell is working in a maximum power point. This is a consequence of the excess concentration of carriers generated by the one-sun illumination. A small gradient of the quasi-Fermi energy levels drives electrons to fall (as balls) to the left, whereas holes rise up (as bubbles) to the right side. This directional flow of electron-hole carriers is due to the fact that, electron density is several orders of magnitude higher than hole density on the left ($n+$ region), and the opposite happens on the right side ($p+$ region), as shown in figure 9 d). In terms of energy bands, the Fermi levels E_f of two separated p - and n -doped regions are different.

Instead, the $p-n$ junction in equilibrium shows a constant Fermi level, thus causing the band bending of the conduction energy band E_C and the valence energy band E_V (see figure 9 b)). From figure 9 b), the electrostatic potential difference across the junction, known as the built-in potential j_0 , can be expressed as:

$$q\phi_0 = E_g - E_1 - E_2 \quad (9)$$

where $E_g = E_1 - E_2$ is the energy band-gap between the conduction and valence band edges. E_1 and E_2 can be derived from the Boltzmann expressions of the free

carrier concentrations for non-degenerate doped semiconductors at thermal equilibrium, assuming that the dopants are fully ionized [5]:

$$n_0 = N_D = N_C \exp\left(-\frac{E_C - E_F}{kT}\right) \quad (10)$$

$$p_0 = N_A = N_V \exp\left(-\frac{E_F - E_V}{kT}\right) \quad (11)$$

where N_C and N_V are the effective densities of states of the conduction and valence bands, respectively. The electrostatics of the p-n junction is defined by Poisson equation see equation (2).

7. Carrier Recombination Mechanisms

As discussed in section 4, generation and recombination of charge carriers are fundamental to the operation of several optoelectronic semiconductor devices such as solar PV cells. Moreover, it is crucial to know that both processes take place continuously in the crystal structure *c*-Si, where electrons and holes are created and then annihilated. On top of this, under equilibrium conditions, they are equal, and carrier density is constant. The recombination rate U per unit time and volume can be defined as the difference between the recombination rate R and the generation rate G ,

$$U = R - G \quad (12)$$

The generation of the electron-hole pair is originated when a piece of semiconductor is illuminated by a light pulse with photon energy bigger than the band gap energy; enhancing the transition of electrons from the valence band to the conduction band, leaving holes behind in the valence band. In order to reach the thermal equilibrium in the system, the reverse process must also occur, the excess electrons in the conduction band will recombine with holes and the energy is released in the may recombine before they contribute to the collected current. These losses are frequently classified according to the region of the cell where they take place [33], [48].

Thus, the most common recombination mechanisms which contribute to the electrical losses are located in both, the bulk and the surface of the wafer. The first one is an intrinsic recombination process, i.e. they are inherent to the existence of separated energy bands of the material.

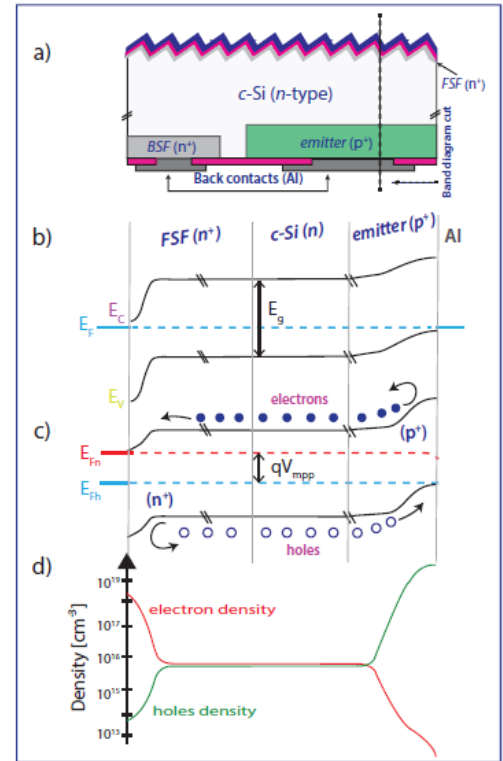


Figure 9. Energy band diagrams of a) simulated interdigitated back contact (IBC) *n*-type (5) *c*-Si solar cell featuring main regions such as bulk, FSF, BSF, and emitter. b) p-n junction in equilibrium. c) maximum power point operation. d) electron-hole density or concentration in the FSF, bulk and emitter regions, respectively.

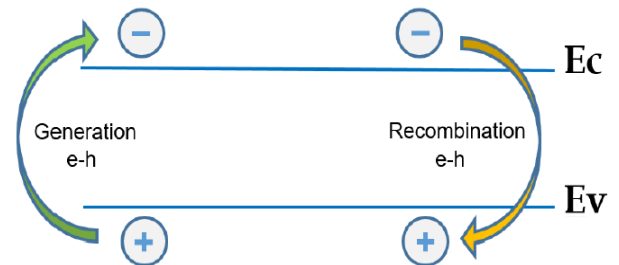


Figure 10. Sketch of a semiconductor in thermal equilibrium. E_v represents the valence band energy and E_c the conduction band energy, respectively. The electron-hole pair is denoted by **e-h**. [18].

In the substrate of a single-crystal structure, the basic recombination mechanism is composed by the Radiative, Shockley-Read-Hall (SRH) and Auger (see figure 11).

The effects of the different recombinations add together to form a total rate of recombination in the bulk, as described in equation (13),

$$R_{Bulk} = (R_{RAD} + R_{AUGER} + R_{SRH}) \quad (13)$$

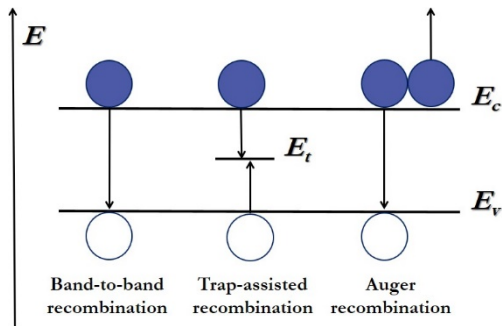


Figure 11. Schematic of the bulk recombination mechanisms in semiconductors. Taken from [20].

However, there is another important type of recombination which significantly impacts the performance of a semiconductor device, and we refer to it as *surface recombination*. This type is promoted by the presence of impurities and crystallographic imperfections at the surface, interface or within the material causing a high local recombination rate. These defects are denominated *dangling bonds* and generally are originated by interruptions to the periodicity of the silicon crystal lattice. Essentially, the dangling bond occurs when valence electrons on the silicon surface cannot find a partner to create a covalent bond with, leaving an abrupt discontinuity of the crystal lattice, as exhibited in figure 12 a). As a consequence, dangling bonds enhance the creation of surface energy states in the forbidden band-gap, acting as trapping (recombination) centers for the minority carriers, inducing to *SRH* recombination (see figure 12 b)) [22]. In very pure semiconductors, recombination might be dominated by surface recombination.

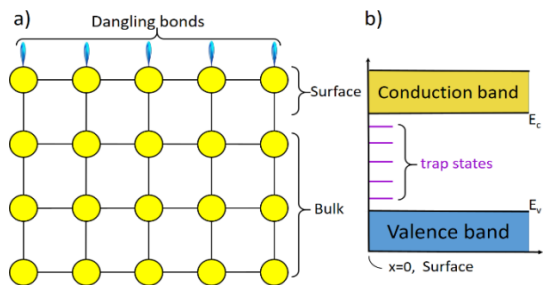


Figure 12. a) Diagram of dangling bonds (surface defects or crystallographic imperfections) on a semiconductor surface; b) Sketch of the trapping state centers within the band-gap created by the dangling bonds. Taken from [48].

It is worth noting that, the presence of dangling bonds

or defect (recombination) centers minimizes the *effective lifetime* of the excess minority carriers within the semiconductor, limiting the conversion efficiency η of the solar cells. For this reason, in order to boost the performance and quality of the solar cells, it is crucial to have a low *surface recombination velocity* S_r and hence reduce the number of dangling bonds in the silicon crystal lattice. This can be accomplished in two different ways:

1. First, S_r can be made low by reducing the trap density N_{sT} . In semiconductor technology, by depositing a thin layer of a suitable material onto the semiconductor surface can reduce the defect density. Because of this layer, the valence electrons on the surface can form covalent bonds, such that N_{sT} is reduced. This technique is known as *surface passivation* and it will be discussed in section 8.
2. Secondly, the excess minority carrier concentration (of electrons and holes) at the surface can be reduced by high doping of the region just underneath the surface in order to create a barrier. Because of this barrier, the minority carrier concentration is reduced and hence the recombination rate.

8. Surface passivation techniques

As it was mentioned above, silicon solar cells efficiency continues being degraded and limited by the recombination losses of photogenerated carriers (i.e. electron-hole pairs) that take places at the interfaces and surfaces of the device. However, currently there is a large research activity focus on the implementation of effective processes to minimize the contamination control during fabrication and harmful surface defects. In order to enhance the quality and performance of solar cells, it is essential to limit the presence of crystallographic defects and external undesirable impurities (i.e. dangling bonds), while also keeping the surface recombination as low as possible. This is accomplished by the growth of an appropriate passivating film on the semiconductor surface (chemical passivation), or by immersing the sample into polar liquids [9], [17], [19]. *Surface passivation* is achieved by the chemical process of depositing a thin layer of a different material on top of a semiconductor surface, which partially restores the bonding periodicity of the atoms in the silicon crystal lattice [7], [8], [10], [11], [15], [24]. This leads to a lessened interface defect density of traps N_{sT} and a reduced surface recombination velocity S_r at the *Si* surface [14].

9. Conclusion

Solar PV cells are quite simple devices that convert sunlight into voltage or electric current by exploiting the

capabilities of semi-conducting materials (e.g., *c*-Si) to absorb light and to deliver a portion of energy to carriers of electrical current. Reasoning from this fact, solar cell specialists have been contributing to the development of advanced PV systems from a costly space technology to affordable terrestrial energy applications.

Actually, since the early 1980s, PV research activities have been obtaining significant improvements in the performance of diverse photovoltaic applications. A new generation of low-cost products based on thin films of photoactive materials (e.g., amorphous silicon, copper indium diselenide (CIS), cadmium telluride (CdTe), and film crystalline silicon) deposited on inexpensive substrates, increase the prospects of rapid commercialization. It is worth mentioning that the photovoltaic market is dominated by the crystalline silicon *c*-Si solar cell devices because of the specific and beneficial characteristics of this semiconductor material in the electronics industry. Particularly, *Si* is abundant in nature and can be processed at relatively low costs, thus leading to a lowering on the energy payback time. In particular, the research on *c*-Si has a fundamental importance especially due to the low-costs achieved and the promising wide enhancements on the future electronic applications. Consequently, the photovoltaic industry has focused on the development of feasible and high-efficiency solar cell devices by using accessible semiconductor materials that reduce production costs.

Nonetheless, photovoltaic applications must improve their performance and market competitiveness in order to increase their global install capacity. In this context, the design of innovative solar cell structures along with the development of advanced manufacturing process are key elements for the optimization of a PV system. Therefore, the understanding of the basic physical principles, loss mechanism and the adoption of a proper solar cell design, passivation techniques, materials, and doping profiles are fundamental to the operation of several optoelectronic semiconductor devices such as solar PV cells.

Accordingly, photovoltaic energy generates electricity in a distributed, clean and inexhaustible manner, being able, theoretically, to fully cover the worldwide energy demand, or at least an important portion.

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