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Behavior of free electrons and excitons, due to their mobility under the effects of optoelectric parameters in a silicon heterojunction cell (HIT): Interdependence of physical phenomena acting on free and bound load carriers

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Abstract For to better understand the interdependence of the physical phenomena that convert photon energy $h.\nu$

into electrical energy of photovoltaic origin: The theory of creation of free or linked electron-hole pairs and the study of the phenomena of relaxations (multiphonon and intraband) of charge carriers are developed to introduce basic physical knowledge.

Solving the system of continuity equations by a numerical method minimizes simplifying assumptions unfavorable to parameter dependence (kinematic and intrinsic) and facilitates interactions between physical phenomena in the cell (HIT).

Since most of the conversion of photovoltaic energy takes place with the mobility of the load carriers, then the mobilities are first evaluated as a function of temperature. Diffusion lengths, carrier densities, carrier photocurrent densities and internal quantum efficiency are then studied as a function of carrier mobility to conclude on the interdependence of free electrons and excitons.

Keywords Mobility, Diffusion lengths, Interdependence, Excitons, Optoelectric, Heterojunction cell (HIT)

1. Introduction

In this paper, we study the physical phenomena explaining not only the movement of charge carriers through their mobilities, but also the interdependence of optoelectric parameters through free or bound charge carriers (excitons). Since some authors have already studied these physical phenomena, in other fields or in other circumstances, it is then necessary to refer to them to better understand the subject, in order to contextualize it in our field of study.

Matthew C. Beard, Kelly P. Knutsen, Pingrong Yu, Joseph M. Luther, Qing Song, Wyatt K. Metzger, Randy J. Ellingson, and Arthur J. Nozik used a process of multiple exciton generation in colloidal silicon nanocrystals to increase the solar conversion efficiency of homojunction photovoltaic cells [1].

Richard Corkish, Daniel S. P. Chan, and Martin A. Green have shown that excitons, although neutral, can participate in the current of photovoltaic devices by diffusing towards the junction where they can be dissociated by the electric field, using the generalized theory of three-particle transport (electron, hole and exciton) in semiconductors [2].

P.N. Rao, E.A. Schi, L. Tsybeskov and P. Fauchet, using electron drift mobilities and very low hole drift mobilities $(\mu_{e,t} \prec 10^4 cm^2 N^{-1} s^{-1})$ compared to homogeneous crystalline silicon, concluded that drift mobilities are limited

by nanoporous geometry and not by localized disordered states acting as traps [3].

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H. Hillmer, A. Forchel, S. Hansmann, M. Morohashi and E. Lopez studied the mobility of two-dimensional excitons in $GaAs/Ga_{1-x}Al_xAs$ -type quantum wells. Comparison of the experimental results with the calculated mobility limits shows that diffusion disorder at the alloy barrier only significantly affects exciton mobilities in narrow $GaAs/Ga_{1-x}Al_xAs$ quantum wells [4].

Richard D. Schaller, Milan Sykora, Jeffrey M. Pietryga and Victor I. Klimov have demonstrated experimentally that by using semiconductor nanocrystals, they can reduce energy losses at the gap to an almost absolute minimum allowed by energy conservation by producing multiple single photon excitons. Specifically, by generating seven excitons from a single photon with an energy of 7.8 energy differences, which corresponds to only 10.0 % energy losses, whereas under normal conditions (one photon produces one exciton) 90.0 % of the energy of the photon would be dissipated as heat [5].

M. Faye, M. Niane, S. Ndiaye, O. Ngom, C. Mbow and B. Ba have developed a numerical model applicable to inorganic semiconductors in the presence of excitons. They have shown that the generation of minority carriers (electrons and excitons) depends on the absorption and temperature mean associated with the volume coupling coefficient ($b = 10^{-2} T_{moy}^{-2} + 2.5.10^{-6} T_{moy}^{-0.5} + 1.5.10^{-7}$). They also showed that absorption can be dominated by electrons (f = 1) or by excitons (f = 1) [6]

electrons $(f_e = 1)$ or by excitons $(f_x = 1)$ [6].

All these authors, in one way or another, have used mobility phenomena [3,4] or the contribution of excitons [1,2,5,6] to improve the power production efficiency of the studied photovoltaic devices or heterostructures.

The accomplishment of this work is possible thanks to a theoretical study on the notion of free or bound electronhole pair, an interdependence of charge carriers by a multiphonon or intraband relaxation method and a mathematical modelling solved by a numerical method well elaborated in the reference [7].

2. Theory

2.1. The formation of free or bound electron-hole pairs (excitons):

In semiconductors, the absorption of a photon of energy greater than or equal to the width of the band gap causes the transition of an electron from the valence band to the conduction band. The transit electron creates a hole, which behaves as a charge carrier as opposed to the electron.

The electron and the hole can bind by Coulomb interaction [8] to form a hydrogen complex: the exciton [9,10]. It is an uncharged quasiparticle, formed by an electron-hole pair linked by an attractive or coulombic force. The electron of the exciton has an energy slightly lower than that of the electron of a free electron-hole pair given by the sum of the energies of the two isolated charges.

To create an electron-free-hole pair [11,12,13], it is necessary to bring an energy greater than or equal to the value of the absorption Gap in the material. These two charge carriers are free to propagate in the crystal from one step to another without the influence of the band gap.

The energy level dispersion equation is defined by:

$$E_n(z) = \frac{\hbar^2 k_n(z)^2}{2m} \tag{1}$$

With $m = m_e$ (mass of the electron) at the conduction band and $m = m_t$ (mass of the hole) at the valence band allows us to represent the energy levels by parabolas because the energy (E_n) is a function of the wave vector (k_n) which in turn is a function of the thickness z of the cell. The energy levels are quantified [14,15] with the main quantum number (n).

Since the absorption of the energy photon $h.\nu$ is near the value of the wave vector $k_n = 0$, then the parabolic curves can be assimilated to their tangents at this point, all the more so since the phenomenon under study takes place at very small dimensions around the nanometers (nm); hence the often single-band representation of the energy levels in semiconductors.





Figure 1: Process of creating free or linked electron-hole pairs (excitons)

Excitonic energy levels are localized in the band gap, hence their instability with respect to the charge carriers housed there. Before the material comes into contact with light or temperature, the electrons at the last filled band (valence band) are in the ground state. In the presence of a thermal or light source, some electrons, if they do not have sufficient energy to reach the conduction band, will occupy excitonic energy levels and others sufficiently charged will occupy the conduction band. These charge carriers can undergo relaxation phenomena by passing from one energy level to another lower level before being recombined.

2.2. Relaxation of charge carriers

The energy of an excited electron can dissipate in the crystal matrix through phonons. This increases the vibration amplitude of the atoms in the matrix and shortens the observed lifetime of free charge carriers and excitons.



Figure 2: Relaxation process of free or linked electron-hole pairs (excitons).

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This relaxation can be achieved by means of one or more phonons, and is referred to as multiphonon relaxation [16] if the recombination energy is greater than the quantized value of the crystal vibrations. In the case of an indirect process (non-resonant excitation), relaxations by phonons (vibrations) take place which lower the energy level of the pair thus formed.

The discretization of energy levels requires the use of several phonons for intraband relaxation [17], which theoretically should slow down the carrier recombination process. Moreover, combinations between intraband and multiphonon relaxations ensuring the principle of energy conservation are rare. Nevertheless, the existence of excited energy levels allows electron-hole pairs, after going through multiphonon relaxation, to relax directly from one energy level to the other (intraband relaxation) before recombining.

These relaxation phenomena are described in figure 2.

3. Modeling

We consider a silicon heterojunction cell (a-Si:H/c-Si) of np type, length L, illuminated (n^+p) monochromatic light in the presence of excitons.



Figure 3: Structure of an $(n^+ p)$ *-type silicon heterojunction photopile* (a - Si: H/c - Si)

3.1. Mathematical model:

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The mechanisms of generation, recombination and diffusion govern the continuity equations. In the (p)-type doped base, the minority carriers are charge electrons (-q). These electrons come from free electron-hole pairs and excitons. The electron density obeys the charge conservation law described by the system of continuity equations.

$$\begin{cases} D_{e} \frac{\partial^{2} n_{e}}{\partial z^{2}} + \mu_{e} \frac{\partial [n_{e} E_{P}(z)]}{\partial z} = \frac{n_{e} - n_{e0}}{\tau_{e}} + b N_{A} (n_{e} - n_{e0}) - \frac{n_{x} - n_{x0}}{\tau_{d}} - G_{e} \\ D_{x} \frac{\partial^{2} n_{x}}{\partial z^{2}} + \mu_{x} \frac{\partial [n_{x} E_{P}(z)]}{\partial z} = \frac{n_{x} - n_{x0}}{\tau_{a}} - b N_{A} (n_{e} - n_{e0}) + \frac{n_{x} - n_{x0}}{\tau_{d}} - G_{x} \end{cases}$$
(2)

The two equations of system (2) are closed by the following initial and for boundary conditions:

a) For electrons from free electron-hole pairs:

$$\begin{bmatrix}
D_e \frac{dn_e}{dz} \\
\sum_{z=0} = S_e \left[n_e(0) - n_{e0} \right] \\
\begin{bmatrix}
D_e \frac{dn_e}{dz} \\
\sum_{z=L_p} = -S_e \left[n_e(L_p) - n_{e0} \right]
\end{cases}$$
(3)

b) For electrons from excitons:

$$\begin{cases} \left[D_x \frac{dn_x}{dz} \right]_{z=0} = S_x \left[n_x(z) - n_{x0} \right] \\ \left[D_x \frac{dn_x}{dz} \right]_{z=L_p} = -S_x \left[n_x(L_p) - n_{x0} \right] \end{cases}$$
(4)

After adimensionalization and discretization of the systems of equations (2), (3) and (4) we find ourselves with the following algebraic system of equations.

3.2. Numerical (algebraic) model of continuity equations in the base:

$$\begin{cases}
b_{1,k} \cdot n_{k,I_0} - c_{1,k} \cdot n_{k,I_0+1} = d_{1,k} & i = I_0 \\
-a_{w,k} \cdot n_{k,i-1} + a_{M,k} \cdot n_{k,i} - a_{r,k} \cdot n_{k,i+1} = S_{m,k} & I_0 + 1 \le i \le I_m - 1 \\
-n_{k,I_m-1} + b_{m,k} \cdot n_{k,I_m} = d_{m,k} & i = I_m
\end{cases}$$
(5)

With here:

$$\begin{aligned} b_{1,k} &= a_{M1,k} - 2.C_{dk}.a_{w1,k} & ; & c_{1,k} = a_{r1,k} - a_{w1,k} & ; & d_{1,k} = S_{1,k} - 2.C_{dk}.a_{w1,k}.n_{k0} \\ a_{m,k} &= 1 & ; & b_{m,k} = 1 + C_{Lk} & ; & d_{m,k} = C_{Lk}.n_{k0} \end{aligned}$$

The coefficients $a_{w,k}$, $a_{M,k}$ and $a_{r,k}$ are evaluated at the control volume interfaces using the power law diagram.

They represent the combined conduction and diffusion flows. The expressions of these coefficients are given in references [7,18].

The algebraic system is solved by a line-by-line relaxation method of the Gauss Seidel type see [7].

3.2. Photocurrent densities:

The photocurrent densities of electrons and excitons are the sums of two contributions: diffusion and conduction currents.

c) For electrons:

$$J_e = q.n_e.\mu_e.E(\lambda) + q.D_e.\frac{dn_e}{dz}$$
(6)

d) For excitons:

$$J_x = q.n_x.\mu_x.E(\lambda) + q.D_x.\frac{dn_x}{dz}$$
⁽⁷⁾

3.3. Internal quantum efficiency:

The internal quantum efficiency (IQE) takes into account the photon flux absorbed by the active layer of the cell. It can also be defined as the ratio between the external quantum efficiency [7] and the absorption coefficient of the z-thick layer.

$$IQE = \frac{EQE(\lambda)}{A(\lambda)}$$
(8)

With here: $A(\lambda) = [1 - R(\lambda)][1 - e^{\alpha(\lambda)z}]$ being the absorption coefficient of the layer of thickness z.

4. Results and Discussion

In this paper, we set ourselves the objective of studying the behavior of free electrons and excitons due to charge carrier mobility on the optoelectric parameters of a HIT cell.

The base of the cell is c-Si(p) with a thickness $L = 0.025 \ cm$ and a doping rate $N_A = 1.14 \cdot 10^{17} \ cm^{-3}$. The emitter is constituted by the a-Si:H(n) very heavily doped in donor atoms: $N_D = 1.5 \cdot 10^{19} \ cm^{-3}$, the recombination rates of the electrons and excitons: $S_e = S_x = 6.0 \cdot 10^6 \ cm.s^{-1}$. Taking into account the effective electron mass $m_e = 2.85689 \cdot 10^{-31} \ Kg$, we were able to evaluate the intrinsic parameters on which the mass depends. Indeed,

the excitons in inorganic semiconductors being pseudo particles whose electron and hole pairs are weakly linked, we can therefore choose a very low volume coupling coefficient ($b = 10^{-16} cm.s^{-1}$) in c-Si(p).

In addition to the physical parameters related to the study and the intrinsic parameters, we can give the values of the physical constants involved in this work:

 $k_{b} = 1.380662.10^{-23} J.K^{-1}, \ c = 2.997924562.10^{8} m.s^{-1}, \ h = 6.626176.10^{-34} J.s^{-1}, \ \varepsilon_{0} = 8.842.10^{-12} A^{2}.s^{4}.k_{g}^{-1}.m^{-3}.$

4.1. Mobility of charge carriers (electrons and excitons) as a function of temperature:

Given the physical conditions that allowed us to define the studied phenomena. We found ourselves with mobility coefficients between $1.3.10^2 cm^2 V^{-1} s^{-1}$ and $3.3.10^3 cm^2 V^{-1} s^{-1}$. In addition, we used a monochromatic illumination with a wavelength $\lambda = 1.1 \mu m$ which corresponds to an energy close to the gap energy of crystalline silicon.

Figure 4 shows the mobility coefficients of electrons and excitons as a function of temperature. As the temperature increases, we observe an increase in electron mobility and a decrease in exciton mobility. Specifically, when the temperature is increased, the exciton mobility is significantly reduced from $3.5.10^3 cm^2 V^{-1} s^{-1}$ to $2.5.10^2 cm^2 V^{-1} s^{-1}$ and the electron mobility is increased from $2.0.10^2 cm^2 V^{-1} s^{-1}$ to $3.0.10^3 cm^2 V^{-1} s^{-1}$.



Figure 4: Mobility of charge carriers (electrons and excitons) as a function of temperature

At temperatures below 254 *K*, corresponding to a mobility of $8.7.10^2 cm^2 V^{-1} s^{-1}$, we find that the mobility of the excitons is more intense than that of the electrons, and at temperatures above 254 *K*, the electrons are more mobile than the excitons.

The mobility of the charge carriers depends on the photon energy absorbed by the material, the electric field at the space charge zone (SCZ) level and the temperature. Temperature plays an exciting role by taking electrons out of their orbits and allowing them to find themselves in excited positions (excitons). In addition to the fact that the electrons are in an interstitial position, thermal agitation is another factor that causes the atoms to vibrate, leading to instability in the molecular organization of the semiconductor (silicon). These vibrations are often unfavorable to the cell, as they tend to recombine or relax the excitons because of their instability. Hence, the mobility of the excitons decreases with increasing temperature, i.e. when the vibrations within the semiconductor become more and more intense.

The instability of the semiconductor under consideration will not only put the electrons in an excited state, thus creating recombinant sites and a congestion of the excited states, but will also cause them to vibrate, which is synonymous with mobility. In addition, the thermal source brings a surplus of energy to the sufficiently charged electrons. This clearly explains the physical phenomena observed in figure 4.

The notion of excitons more stable than electrons at low temperatures and electrons more stable than excitons at high temperatures is verified in reference [7].

Since the physical phenomena observed in a photovoltaic cell under illumination are often created by parameters external to the semiconductor (photon energy, electric field and temperature), knowing the behavior of temperature with respect to charge carrier mobility, we can already be interested in a study of charge carrier mobility in a silicon heterojunction cell. We can therefore be interested in the diffusion length of electrons and excitons.

4.2. The diffusion lengths of electrons and excitons as a function of electron mobility:

Figures 5 and 6 show the diffusion lengths of electrons and excitons as a function of electron mobility on the one hand and exciton mobility on the other.

In Figure 5, we can see with certainty an increase in the electron diffusion length, ranging from about $2.6.10^{-3} cm$ for an electron mobility of $1.9.10^{2} cm^{2} . V^{-1} . s^{-1}$ to $2.3.10^{-2} cm$ for an electron mobility of $3.4.10^{3} cm^{2} . V^{-1} . s^{-1}$. While figure 6 shows the electron and exciton diffusion coefficients with very adequate scales, allowing to observe a simultaneous increase of the electron and exciton diffusion lengths. Here, the diffusion length of the excitons is well represented and increases from a value of $2.6.10^{-3} cm$ for an electron mobility of $1.9.10^{2} cm^{2} . V^{-1} . s^{-1}$ to a value of $3.4.10^{-3} cm$ for an electron mobility of $1.9.10^{2} cm^{2} . V^{-1} . s^{-1}$ to a







Figure 6: Diffusion lengths of electrons and excitons at different scales as a function of electron mobility Generally, the terms mobility and diffusion seem to have the same meaning, but their physical meanings are different, as a particle may be mobile and not diffusive. When a particle vibrates, it is mobile, but it does not diffuse, for the simple reason that diffusion is a displacement in a well-defined direction. Hence the study of the length at which carriers diffuse as a function of mobility.

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The mobility of electrons depends on the energy of the photons stored by the charge carriers, the thermal potential of the SCZ which influences the electric field at the SCZ. Since this electric field is at the origin of the mobility of the charge carriers, the charge carriers (electrons and excitons), by conserving the stored energy and being more mobile, can only diffuse as far as possible.

Knowing that the mobility of electrons favors a diffusion of electrons and excitons, we are now going to discover what it is about the mobility of excitons over the diffusion lengths of electrons and excitons.

4.3. The diffusion lengths of electrons and excitons as a function of the mobility of the excitons:

In contrast to electron mobility, an increase in exciton mobility leads to a decrease in the diffusion lengths of electrons and excitons (Figure 8). A mobility value of $2.7.10^3 cm^2 V^{-1} s^{-1}$ corresponds to a charge carrier (electron and exciton) diffusion length of $2.6.10^{-3} cm$. Using this value as a reference, we can see two physical phenomena described in Figure 7:

For lower mobility values $3.4.10^3 cm^2 V^{-1} s^{-1}$, electrons are more diffusible than excitons;

While for higher mobility values $3.4.10^3 cm^2 V^{-1} s^{-1}$, the excitons are more diffusible than the electrons.



Figure 7: Electrons and excitations diffusion lengths as a function of exciton mobility



Figure 8: Diffusion lengths of electrons and excitons at different scales as a function of the mobility of the excitons

Exciton mobility better describes the exciting effect of temperature on semiconductors making atoms vibrate. These vibrations, when they become intense, make the molecular structure of the material unstable. Thus, free electrons and excitons diffuse less and less as the mobility of the excitons increases. In addition, the instability of

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the molecular structure of silicon leads not only to the creation of other excited states, but also to the creation of recombinant sites that reduce the diffusion of free electrons by simple recombination or relaxation phenomena. This explains why, at a mobility greater than $3.4.10^3 cm^2 V^{-1} s^{-1}$, the excitons are more diffusible than the electrons.

Knowing the effect of carrier mobility on diffusion lengths, we are going to deepen the study of mobility on charge carrier densities.

4.4. Charge carrier densities (electrons and excitons) as a function of electron mobility:

In this section, the objective is not to study charge carrier densities as a function of depth of crystalline silicon [7]. Therefore, it is essential to take into account the mobility of electrons and excitons on the charge carrier densities, and then the dependence of the two types of charge carriers for comparison.



Figure 9: Electron density as a function of depth of crystalline silicon with different values of electron mobility



Figure 10: Electron density as a function of depth of crystalline silicon with different values of exciton mobility



Figure 11: Exciton density as a function of depth of crystalline silicon with different values of electron mobility





In Figures 9 and 10, we see that an increase in electron and exciton mobility respectively leads to a decrease in electron density and an increase in exciton density respectively.

On the other hand, the density of the excitons increases with the mobility of the electrons and decreases with the mobility of the excitons: see figures 11 and 12.

The more the free electrons are mobile, the more they relax from the permitted levels to the excited levels, which decreases the electron density and increases the density of the excitons. A very high mobility leads to the creation of new excited states.

Since free electrons and excitons interact, increasing the mobility of the excitons tends to lead to lower temperatures. That is, the molecular structure of crystalline silicon becomes more and more stable allowing the excitons in the semiconductor to remain stable. This does not prevent the recombination of the free electrons, some of which will undergo relaxation phenomena in order to pass into excited states, thus forming other excitons. Hence the fact that the electron density decreases to the detriment of the density of the excitons.

The physical phenomena analyzed and interpreted have allowed us to see that with or without the excitons, the same phenomena are observed, but with photocurrent densities higher in number than those of the excitons. Their numbers being described by the density of the charge carriers since we need to collect them to produce electricity, so it is necessary that they are well ordered to be able to move towards the receiving electrodes. This orderly



movement of charge carriers in a photovoltaic cell is nothing more than the photocurrent density of the charge carriers.

4.5. Photocurrent densities of charge carriers as a function of electron and excitation mobilities:

Figure 13 shows the electron, excitation and total photocurrent densities as a function of electron mobility coefficients, respectively. Here, we notice an increase in the electron photocurrent density and a decrease in the excitation density. For a mobility value of $1.8.10^2 cm^2 V^{-1} s^{-1}$, we obtain a photocurrent density of electrons and excitons equal to $3.0 \ mA.cm^{-2}$, then an increase in the photocurrent density of electrons up to $14.0 \ mA.cm^{-2}$ and at the same time a decrease in the photocurrent density of excitons up to $1.4 \ mA.cm^{-2}$. By combining the two types of charge carriers, we find ourselves first with the same variations as that of electrons, then with photocurrent densities of $15.4 \ mA.cm^{-2}$ for a mobility of $3.4.10^3 cm^2 V^{-1} s^{-1}$.

However, when the photocurrent densities are evaluated as a function of the mobility of the excitons (Figure 14), the opposite effect is observed, i.e. a decrease in the electron photocurrent density from 14.0 $mA.cm^{-2}$ to 2.4 $mA.cm^{-2}$ and an increase in the excitation photocurrent density from 1.4 $mA.cm^{-2}$ to 3.2 $mA.cm^{-2}$. With mobility coefficients below 2.8.10³ cm².V⁻¹.s⁻¹ the electron photocurrent is predominant and with higher mobility coefficients 2.8.10³ cm².V⁻¹.s⁻¹ the photogenerated carriers from the excitons become more numerous.



Figure 13: Photocurrent density of electrons, excitons and total as a function of electron mobility



Figure 14: The photocurrent density of electrons, excitons and total as a function of the mobility of the excitons. The mobility of the charged electrons depends on the electric field created at the SCZ which orients the charge carriers in a well-defined direction, thus favoring the orderly movement of the free charge carriers which makes

them free from the phenomena of relaxations and recombinations. This gives us the result obtained in figure 13 on the photocurrent of the free carriers. Contrary to the photocurrent of free electrons, the excitons, not having received enough supplement from sufficiently charged electrons and the fact that they are unstable are physical phenomena that cause the excitons to decrease as the mobility of the electrons becomes intense.

This is not the case when the mobility of the excitons is made to act on the photocurrent densities of the charge carriers. The mobility of linked electron-hole pairs (excitons) is synonymous with disorder. This disorder disadvantages the free electrons by direct recombination or relaxation (exciton creation), the disorder created by the mobility of the excitons does not favor an orderly movement of the free charge carriers. Nevertheless, the mobility of the excitons allows them not only to be stable for some time, given their lifetimes, but also to benefit from a surplus of free electrons that relax to occupy other excited energy levels. For a mobility of excitons higher than $2.8.10^3 cm^2 N^{-1} s^{-1}$, the structure of silicon will start to disorganize by creating recombinant sites leading to excited states (excitons). This explains why the photocurrent density of excitons is higher than that of free electrons.

Whether with the mobility of electrons or with that of excitons, we have a minimum contribution of $1.4 \ mA.cm^{-2}$ and a maximum of $3.2 \ mA.cm^{-2}$ of the exciton photocurrent density on the total photocurrent generated by the silicon heterojunction cell. These contributions can be expressed as a percentage in terms of internal quantum efficiency.

4.6. Internal quantum efficiency of charge carriers:

Since the study here is based on monochromatic light and the quantum efficiency focuses on the quantity of photons absorbed and that photogenerated, given the high gap of the ITO window layer, synonymous with its transparency, it could not be otherwise, because the very character of monochromatic light: a single wavelength, could only give profiles similar to those of photocurrent density, but with different meanings in physics. In this part, we obtain internal quantum efficiencies of the order of 65.4 % for electrons and an internal quantum efficiency of excitons of 6.5 % for a mobility of $3.4.10^3 \ cm^2 N^{-1} s^{-1}$. Hence a total yield of 71.9 % due to the participation of the excitons. We also observed an internal quantum efficiency of 14.0 % for an electron mobility coefficient of $1.8.10^2 \ cm^2 N^{-1} s^{-1}$ and for an exciton mobility coefficient of $2.8.10^3 \ cm^2 N^{-1} s^{-1}$ before the efficiency of excitons takes over that of electrons (Figure 16).



Figure 15: Internal quantum efficiency of electrons, excitons and total as a function of electron mobility



Figure 16: Internal quantum efficiency of electrons, excitons and total as a function of exciton mobility After all these physical phenomena that have allowed us to better understand the photocurrent densities of charge carriers, we can explain the cell's profitability in terms of photoelectric energy production.

And after analyzing the results obtained, we realized that the mobility of free electrons is favorable to the internal quantum efficiency of the carriers. This can be explained by the fact that the electrons are generated in greater numbers than the excitons: verified by the fact that the total internal quantum efficiency varies in the same way as that of the free electrons despite the presence of the excitons.

On the other hand, the mobility of the excitons considerably reduces the internal quantum efficiency, due to its destructive nature, which leads to a disorganization of the atomic structure of silicon.

As we have pointed out from the beginning, the physical parameters interact with each other, and one cannot act on a physical phenomenon without it in turn having an effect on the other physical phenomena. Therefore, to decrease the mobility of the excitons, it is enough to increase the mobility of the electrons in order to have the best possible efficiency.

To sum up, there are excitonic phenomena that reduce the diffusion length and photocurrent density of the free electrons in a photovoltaic cell, but this in no way has a negative effect on the participation of the excitons in the photocurrent. On the other hand, the excited levels have allowed us to photogenerate carriers (excitons) that would never have been photogenerated if they had not been taken into account. So, we can clearly state that the excitons are not harmful to the cell's energy production.

Taking into account all the physical phenomena studied in this paper, we have been able to verify the antagonistic behavior of electron and excitation mobilities in the following table:

| | | Diffusion lengths | | Densities | | Photocurrent | | Variation |
|-------------|-----------|---|----------|-----------|----------|--------------|----------|----------------|
| | | Electrons | Excitons | Electrons | Excitons | Electrons | Excitons | (] |
| Mobility | Electrons | + | 1 | + | + | + | + | |
| | Excitons | Ļ | Ļ | + | + | Ļ | + | |
| Observation | | The mobility writes the antagonistic property of electrons and excitons | | | | | | Ō |

Table:Summary of the interactions between the physical parameters studied.

At the atomic or molecular scale, free electrons and excitons coexisting in the molecular structure of silicon interact through phenomena of mobility, diffusion, generation, relaxation and recombination. The relaxed and generated electrons participate, through the excitons, in the photocurrent density to increase the internal quantum efficiency of the photovoltaic cell.

5. Conclusion

Once again, we can see the interdependence of kinematic and intrinsic parameters. We can also, given the results obtained, conclude with certainty on the dependence of free electrons and excitons by a multiphonon relaxation process. In this study, the phenomena of particle vibrations in materials are highlighted. These vibration

phenomena caused by a thermal excitation of the material lead to a multiphonon relaxation allowing the free charge carriers to be in excited positions (excitons) before their recombination. Relaxation also allows some free charge carriers to participate in the charge carrier density and photocurrent. In terms of efficiency, charged electrons that would not even have the possibility to diffuse into the photovoltaic cell without recombining, participate up 6.5 % to 14.0 % via the excitons. Hence the usefulness of taking the latter into account in practical experiments or in the design of photovoltaic cells in order to be able to approach the theoretical yields of photovoltaic cells.

The result is a solar cell model that has internal quantum efficiencies of up to 71.9 % in our field of study.

References

- Matthew C. Beard, Kelly P. Knutsen, Pingrong Yu, Joseph M. Luther, Qing Song, Wyatt K. Metzger, Randy J. Ellingson, et Arthur J. Nozik; Multiple Exciton Generation in Colloidal Silicon Nanocrystals; Nano Letters, Vol. 7, No. 8, (2007) 2506–2512.
- [2]. Richard Corkish, Daniel S.-P. Chan, and Martin A. Green; Excitons in silicon diodes and solar cells: A three-particle theory; J. Appl. Phys., Vol. 79, No. 1, (1996) 195–203.
- [3]. P.N. Rao, E.A. Schiff, L. Tsybeskov et P. Fauchet; Photocarrier drift-mobility measurements and electron localization in nanoporous silicon; Photocarrier drift-mobility measurements and electron localization in nanoporous silicon; Chemical Physics, Vol. 284, Issues 1–2, (2002) 129–138.
- [4]. H. Hillmer, A. Forchel, S. Hansmann, M. Morohashi, et E. Lopez; Optical investigations on the mobility of two-dimensional excitons in *GaAs/Ga_{1-x}Al_xAs* quantum wells; The American Physical Society, Vol. 39, No. 15, (1989) 10901–10912.
- [5]. Richard D. Schaller, Milan Sykora, Jeffrey M. Pietryga, and Victor I. Klimov; Seven Excitons at a Cost of One: Redefining the Limits for Conversion Efficiency of Photons into Charge Carriers; Nano Letters, Vol. 6, No. 3, (2006) 424–429.
- [6]. M. Faye, M. Niane, S. Ndiaye, O. Ngom, C. Mbow, B. Ba; Numerical Modeling of Effects of Excitons on Photoelectric Properties of Cells; Journal of Scientific and Engineering Research, Vol. 6, No. 6, (2019) 138–146.
- [7]. Ousmane Ngom, Modou Faye, Mamadou Mbaye, Cheikh Mbow, Bassirou Ba. Numerical Study of the Effect of Temperature on the Performance of a Silicon Heterojunction Solar Cell (HIT) in the Presence of Excitons. International Journal of Materials Science and Applications. Special Issue: Advanced Materials for Energy Storage and Conversion Applications. Vol. 8, No. 4, (2019) 56-67.
- [8]. Bairen Zhu, Xi Chen and Xiaodong Cui; Exciton Binding Energy of Monolayer WS₂; Science Rapports 5, No. 9218, (2015) 1-5.
- [9]. B. Goller, S. Polisski, H. Wiggers and D. Kovalev; Freestanding spherical silicon nanocrystals: a model system for studying confined excitons; Appl. Phys. Lett. Vol. 97, Issue 4, (2010) 1-3.
- [10]. S. W. Koch, M. Kira, G. Khitrova and H. M. Gibbs; Semiconductor excitons in new light; nature materials, Vol. 5, (2006) 523-531.
- [11]. Stanislav NeJpGrek, VéraCimrova, JitiPfleger and Ivan Kminek; Free Charge Carrier Formation in Polymers under Illumination; Polymers for Advanced Technologies, Volume 7, Issue 5-6, (1996) 459– 470.
- [12]. GytisSliauzys, KestutisArlauskas, and VidmantasGulbinas; Photogeneration and recombination of charge carrier pairs and free charge carriers in polymer/fullerene bulk heterojunction films; Phys. Status Solidi A, Vol. 209, No. 7, (2012) 1302–1306.
- [13]. Tomasz Janik and Bogdan Majkusiak, Influence of carrier energy quantization on threshold voltage of metal-oxide-semiconductor transistor, Phys. Status Solidi a, Vol. 209, No. 7, (2012) 1302–1306.
- [14]. T. Hiroshima and R. Lang, Effect of conduction-band nonparabolicity on quantized energy levels of a quantum well, Appl. Phys. Lett. Vol. 49, Issue 8, (1986) 456–457.
- [15]. Svetlana V. Kilina, Dmitri S. Kilin, Victor V. Prezhdo, and Oleg V. Prezhdo; Theoretical Study of Electron-Phonon Relaxation in PbSe and CdSe Quantum Dots: Evidence for Phonon Memory; J. Phys. Chem., Vol. 44, No. 115, (2011) 21641–21651

- [16]. Bryan T. Spann and Xianfan Xu, Ultrafast Spectroscopy of CdSe Nanocrystals: Morphological and Environmental Effects on Nonradiative and Nonadiabatic Relaxation, J. Phys. Chem., Vol. 5, No. 118, (2014) 2844–2850.
- [17]. Hangleiter, R. Hacker; Enhancement of band-to-band Auger recombination by electron-hole correlations; Phys. Rev. Lett., Vol. 2, No. 65, (1990) 215–218.
- [18]. Daniel Herrmann, Sabrina Niesar, Christina Scharsich, Anna K€ohler, Martin Stutzmann, and Eberhard Riedle; Role of Structural Order and Excess Energy on Ultrafast Free Charge Generation in Hybrid Polythiophene/Si Photovoltaics Probed in Real Time by Near-Infrared Broadband Transient Absorption; J. Am. Chem. Soc, Vol. 45, No. 133, (2011) 18220–18233.