Deep-level traps and recombination centers effects on photovoltaic conversion efficiency of GaAs based crystalline solar cell

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Abstract. In this work, we proceed to analytical and numerical resolutions, using finite difference method, of semiconductor four equations system governing the variations of electrostatic potential, electrons and holes densities, density profile of occupied levels associated to deep-level traps as well as concentration profile of occupied levels related to recombination centers, in one-dimensional thin-film crystalline solar cell based on Gallium Arsenide (GaAs). In addition to physical quantities mentioned above, the problem resolution, achieved using Maple computer algebra software, enables us to retrieve electrostatic field, electrons and holes current densities as well as energy band diagram throughout the device. Ultimately, particular attention is devoted to specific phenomena related to semiconductors such as the presence of deep-level traps or recombination centers whose levels are in the middle of the gap. In this way, we show that the presence of deep-level traps or recombination centers leads, via Shockley-Read-Hall mechanisms, to a decrease of solar cell photovoltaic conversion efficiency. We also show that these effects are dependent on energy levels of traps and defects, on traps and defects concentrations as well as their electron and hole capture cross sections.

1. Introduction
Nowadays, global energy needs are growing exponentially. This is essentially due to increased energy demand of newly industrialized Asian countries such as India and China, and also of emerging countries all around the world such as Indonesia, Brazil, Turkey and South Africa. Now, all climate specialists agree on the fact that excessive consumption of fossil fuels such as oil, coal or natural gas leads to an increase of carbon dioxide, methane and nitrous oxide rates in the atmosphere. Unfortunately for us and for our planet Earth, these gas emissions have two major negative environmental effects, they lead to an increase of greenhouse gases rates in the atmosphere and make air pollution more pronounced which brings about climatic changes that result in acute droughts or catastrophic floods. Nowadays, there is only one alternative that satisfy growing energy needs while contributing to the protection of the environment: renewable energies. The main source of renewable energy is the Sun. With its two components solar thermal and solar photovoltaic, the Sun represents an inexhaustible source of energy which is able to fulfill all energy needs of humanity. Here, we are interested in converting incoming solar radiation into energy via crystalline photovoltaic solar cells. Now, the main component in solar photovoltaics is silicon solar cell technology but thin film technology is gaining importance since it offers high efficiency and in some cases low cost solar cells. In the present work, we perform the simulation of a thin-film crystalline semiconductor solar cell based on Gallium Arsenide (GaAs). We are particularly interested in the effects of deep-level traps and recombination centers, whose energy levels are in the middle of the gap, on solar cell photovoltaic conversion efficiency. The present paper is divided into six sections. After the present general introduction, we present, in the second section, the four semiconductor fundamental equations driving electrostatic potential, densities of charge carriers, density of occupied levels associated with deep-level traps as well as density of occupied levels associated with recombination centers, in the case of a one-dimensional crystalline solar cell. In the third section, we present the photonic part of our work. We particularize to the case of Gallium Arsenide
based solar cell and give refractive index and extinction coefficient of GaAs. Then, we calculate the reflectance and the transmittance of air/GaAs interface as well as the absorption coefficient of the material. Next, we calculate the generation rate of electron-hole pairs in GaAs under real solar illumination corresponding to an air mass equal to 1.5 (AM1.5). In the fourth section, we perform the normalization of semiconductor fundamental equations. Then, we proceed to numerical and analytical resolutions of three coupled differential equations system obtained in the stationary case. In the fifth section, we present the results of numerical and analytic calculations. We show that the presence of deep-level traps or recombination centers leads to a decrease of open-circuit voltage, maximum power point coordinates and photovoltaic conversion efficiency of thin-film crystalline semiconductor solar cell. Finally, we end our article with a general conclusion.

2. Theoretical framework - Electronics background

2.1. Semiconductor fundamental equations formulated as functions of natural variables $V(x), n(x), p(x)$

The semiconductor fundamental equations as they have been established by W. Van Roosbroeck for a one-dimensional electronic device are [1]:

$$
\frac{d^2 V(x)}{dx^2} + \frac{q}{\varepsilon_0 \varepsilon_r} \left( p(x) - n(x) + N_D^+(x) - N_A^-(x) \right) = 0 \tag{2.1}
$$

$$
\frac{dn(x)}{dt} = \frac{1}{q} \frac{dJ_n(x)}{dx} - R_n(x) + G_n(x) \tag{2.2}
$$

$$
\frac{dp(x)}{dt} = -\frac{1}{q} \frac{dJ_p(x)}{dx} - R_p(x) + G_p(x) \tag{2.3}
$$

$$
\frac{dN_{np, def}(x)}{dt} = R_n(x) - R_p(x) \tag{2.4}
$$

$q$ is the elementary charge, $\varepsilon_0$ is the vacuum dielectric permittivity and $\varepsilon_r$ is the semiconductor relative permittivity. The first equation is Poisson equation. It expresses the variations of electrostatic potential $V(x)$ and electrostatic field $E(x)$ as functions of total charge volume density $\rho(x)$. $N_D^+(x)$ and $N_A^-(x)$ are respectively donor-type and acceptor-type impurity density profiles. The second and the third equations are respectively electrons and holes continuity equations. They describe the conservation of electrons charge $-qn(x)$ and holes charge $qp(x)$ through the device. $R_n(x)$ and $R_p(x)$ are respectively the terms describing electrons and holes recombination. $G_n(x)$ and $G_p(x)$ are respectively electrons and holes generation rates. The fourth equation represents the continuity equation of deep-level traps or defects. $N_{np}(x)$ ($N_{def}(x)$) is deep-level traps (defects) density profile. $J_n(x)$ and $J_p(x)$ are current densities due to electrons and holes flows:

$$
J_n(x) = -q\mu_n n(x) \frac{dV(x)}{dx} + qD_n \frac{dn(x)}{dx} \tag{2.5}
$$

$$
J_p(x) = -q\mu_p p(x) \frac{dV(x)}{dx} - qD_p \frac{dp(x)}{dx} \tag{2.6}
$$

$D_n$ and $D_p$ are electrons and holes diffusion coefficients. They are related to mobilities of electrons $\mu_n$ and holes $\mu_p$ by Einstein’s relations:

$$
\frac{D_{n,p}}{\mu_{n,p}} = \frac{K_B T}{q} \tag{2.7}
$$

In the stationary case and for normal operating conditions, all impurities are ionized. So, semiconductor fundamental equations as functions of natural variables become:
\[
\frac{d^2V(x)}{dx^2} + \frac{q}{\varepsilon_0\varepsilon_r}(p(x) - n(x) + N_D(x) - N_A(x)) = 0
\] (2.8)

\[
D_n \frac{d^2n(x)}{dx^2} + \mu_n E(x) \frac{dn(x)}{dx} + \mu_n n(x) \frac{dE(x)}{dx} - R_n(x) + G_n(x) = 0
\] (2.9)

\[
D_p \frac{d^2p(x)}{dx^2} - \mu_p E(x) \frac{dp(x)}{dx} - \mu_p p(x) \frac{dE(x)}{dx} - R_p(x) + G_p(x) = 0
\] (2.10)

\[
R_n(x) - R_p(x) = 0
\] (2.11)

2.2. Recombination-generation mechanisms in semiconductors

In the present study, we take into account the following recombination-generation mechanisms:

2.2.1. Direct band-to-band or bimolecular recombination

Direct band-to-band recombination is a radiative recombination involving one electron from conduction band and one hole from valence band. Its rate is given by [2]:

\[
R_{rad} = B_i \left( n.p - n_i^2 \right)
\] (2.12)

Where \( B_i \) is band-to-band recombination coefficient [3, 4] and \( n_i \) is the intrinsic concentration of charge carriers.

2.2.2. Indirect Shockley-Read-Hall (SRH) recombination of shallow impurities

Indirect Shockley-Read-Hall recombination of shallow impurities is a non-radiative recombination involving one electron and a donor-type hydrogenic impurity or one hole and an acceptor-type hydrogenic impurity. Its rate is given by [2]:

\[
R_{SRH}^{Shallow} = \frac{n.p - n_i^2}{\tau_e(n + n_i) + \tau_h(p + p_i)}
\] (2.13)

\( \tau_e (\tau_h) \) is the electron (hole) lifetime. \( n_i = n_i \exp\left( (E_D - E_F) / k_B T \right) \) and \( p_i = n_i \exp\left( -(E_A - E_F) / k_B T \right) \). \( E_D \) and \( E_A \) are, respectively, energy levels of donors and acceptors. \( E_F \) is the intrinsic Fermi level.

2.2.3. Indirect Shockley-Read-Hall (SRH) recombination of deep-level traps or recombination centers

Indirect Shockley-Read-Hall recombination of deep-level traps or recombination centers is a non-radiative recombination involving one charge carrier and a deep-level trap or a recombination center in the middle of the gap. Its rate is given by [2]:

\[
R_{SRH}^{Deep} = \sigma_n \sigma_p \nu_e^{\theta} \nu_h^{\theta} N_i \left( n.p - n_i^2 \right)
\]

\[
\sigma_n \nu_e^{\theta} \left( n + n_i \right) + \sigma_p \nu_h^{\theta} \left( p + p_i \right)
\]

\( N_i \) is deep-level traps (recombination centers) concentration. \( \sigma_n (\sigma_p) \) is electron (hole) capture cross-section by deep-level traps or recombination centers. \( n_i = n_i \exp\left( (E_D - E_F) / k_B T \right) \) and \( p_i = n_i \exp\left( -(E_A - E_F) / k_B T \right) \). \( E_D \) (\( E_A \)) is the energy of deep-level traps (recombination centers).

\( \nu_e^{\theta} = \sqrt{3k_B T / m_e} \) \( \left( \nu_h^{\theta} = \sqrt{3k_B T / m_h} \right) \) is the electron (hole) velocity due to thermal agitation.
3. Theoretical framework - Photonics background

3.1. Electron-hole pairs generation rate

The generation rate $G(x)$ of electron-hole pairs in an illuminated semiconductor at a distance $x$ from air/semiconductor interface receiving incoming light is written as [2]:

$$G(x) = \int_0^\lambda (1 - R(\lambda)) \alpha(\lambda) \frac{\lambda}{hc_0} I(\lambda) e^{-\alpha(\lambda)x} d\lambda$$  \hspace{1cm} (3.1)

$I(\lambda)$ is the real spectral solar irradiance. $R(\lambda)$ is the reflectance of illuminated air/semiconductor interface. $\alpha(\lambda)$ is the semiconductor absorption coefficient. $\lambda_c$ which is the critical value of wavelength beyond which semiconductor material is transparent, is linked to semiconductor energy band-gap by the expression $\lambda_c = hc/E_g$.

3.2. Real solar spectrum

In the present study, we carry out the simulation of a GaAs based thin-film crystalline solar cell exposed to a real illumination corresponding to an air mass AM1.5, which means an incident solar radiation making an angle $\theta = 48.2^\circ$ with the zenith [5] and whose incident power $P_{in}$ is equal to 1000.37 W/m$^2$ (see figure 1).

![Figure 1. Spectral irradiance $I(\lambda)$ for an extra-terrestrial collector (AM0) and a tilted terrestrial collector making an angle $\theta = 48.2^\circ$ with the zenith (AM1.5) [5].](image)

3.3. Optical and dielectric properties of the semiconductor

The reflectance and the transmittance of air/semiconductor interface are expressed as [6]:

$$R(\lambda) = \frac{1 - n'(\lambda)^2}{1 + n'(\lambda)^2} \hspace{1cm} (3.2)$$

$$T(\lambda) = 1 - R(\lambda) \hspace{1cm} (3.3)$$

$n'(\lambda)$ is the semiconductor complex refractive index. It may be expressed as:

$$n'(\lambda) = n(\lambda) - ik(\lambda) \hspace{1cm} (3.4)$$

Where $n(\lambda)$ and $k(\lambda)$ are respectively refractive index and extinction coefficient of semiconductor. The absorption coefficient $\alpha(\lambda)$ of semiconductor is related to the extinction coefficient $k(\lambda)$ by the following equation:

$$\alpha(\lambda) = 4\pi \frac{k(\lambda)}{\lambda} \hspace{1cm} (3.5)$$
In figure 2, we present the variations of refractive index \( n(\lambda) \) and extinction coefficient \( k(\lambda) \) of Gallium Arsenide as functions of incoming photon wavelength [7, 8].

![Figure 2](image2.png)

**Figure 2.** Real \( n(\lambda) \) and imaginary \( k(\lambda) \) parts of Gallium Arsenide complex refractive index \( n'(\lambda) \) as functions of incident photon wavelength [7, 8].

In figure 3, we plot the variations of air/Gallium Arsenide interface reflectance \( R(\lambda) \) and transmittance \( T(\lambda) \) as functions of incoming photon wavelength.

![Figure 3](image3.png)

**Figure 3.** Reflectance \( R(\lambda) \) and transmittance \( T(\lambda) \) profiles of air/Gallium Arsenide interface as functions of incident photon wavelength.

Figure 4 presents the variations of Gallium Arsenide absorption coefficient \( \alpha(\lambda) \) versus incoming photon wavelength [7, 8]. The reader can easily remark that for photons of wavelength \( \lambda > \lambda_c (GaAs) = \frac{hc}{E_g (GaAs)} = 873.128 \text{ nm} \), the absorption coefficient \( \alpha(\lambda) \) vanishes.

![Figure 4](image4.png)

**Figure 4.** Variation of Gallium Arsenide absorption coefficient \( \alpha(\lambda) \) as a function of photon wavelength [7, 8].
In figure 5, the variations of electron-hole pairs generation rate $G(x)$ (cf. eq 3.1) are plotted against the depth $x$ in GaAs material. After a careful analysis of generation rate profile, we show that the process of photons absorption and electron-hole generation occurring in Gallium Arsenide at a distance $x$ from illuminated air/semiconductor interface may be described by the following equation

$$G(x) = Ae^{-ax} + Be^{-bx}$$

where $A = 0.9574 \times 10^{28} \text{ m}^3$, $B = 0.2345 \times 10^{28} \text{ m}^3$, $a = 24.0456 \times 10^6 \text{ m}^{-1}$ and $b = 2.6758 \times 10^6 \text{ m}^{-1}$.

![Figure 5. Electron-hole pairs generation rate $G(x)$ profile drawn versus the distance $x$ to air/GaAs illuminated interface.](image)

4. Theoretical framework - Normalization and scaling of semiconductor equations

4.1. Normalization and scaling of semiconductor equations

Equations (2.8) to (2.10) are coupled non-linear non-homogeneous second order differential equations. In order to make easier numerical handling and computational treatment of the system composed by these equations via Maple computer algebra software [9], and also in order to avoid precision loss due to the large difference between orders of magnitude of $x$, $V(x)$, $n(x)$ and $p(x)$, we proceed to a normalization of all physical quantities involved by using the parameters given in table 1.

| Symbol with dimension | Symbol dimensionless | Meaning | Normalization parameters |
|-----------------------|----------------------|---------|--------------------------|
| $x$ | $X$ | Length | $L = w_{p0} + w_{n0}$ |
| $V, \varphi, \varphi_p$ | $U, F_n, F_p$ | Electrostatic potential, Electrons and holes quasi-Fermi levels | $k_BT/q$ |
| $n(x), p(x)$ | $n'(X), p'(X)$ | Electrons and holes densities | $n_i$ |
| $J_n(x), J_p(x)$ | $J'_n(X), J'_p(X)$ | Electrons and holes current densities | $qn_i D_{n,p}/L$ |

In the table above, $w_{p0}$ and $w_{n0}$ denote penetration depths of the quasi-depletion layer, i.e. the space charge zone respectively into P-type and N-type regions at thermodynamic equilibrium, in the dark and without polarization.

4.2. Normalized semiconductor equations system

After normalization, the basic equations of one-dimensional semiconductor device are expressed via dimensionless potential $U(X)=qV(X)/k_BT$, electrons density $n'(X)=n(X)/n_i$ and holes density $p'(X)=p(X)/n_i$, where dimensionless variable $X=x/L$:
\[
\frac{d^2U(X)}{dx^2} - \frac{L_d^2}{L_{dx}^2} \left( n'(X) - p'(X) - \frac{N_p(X) - N_A(X)}{2n_i} \right) = 0
\]
(4.1)

\[
\frac{d^2n(X)}{dx^2} - \frac{dU(X)}{dx} \frac{dn(X)}{dx} - n'(X) \frac{d^2U(X)}{dx^2} + \frac{R_p(X)}{D_p n_i} L_d^2 + \frac{G_p(X)}{D_p n_i} L_d^2 = 0
\]
(4.2)

\[
\frac{d^2p'(X)}{dx^2} + \frac{dU(X)}{dx} \frac{dp'(X)}{dx} + p'(X) \frac{d^2U(X)}{dx^2} - \frac{R_n(X)}{D_n n_i} L_d^2 + \frac{G_n(X)}{D_n n_i} L_d^2 = 0
\]
(4.3)

Where \( L_{dx} \) is the Debye length of charge carriers in intrinsic semiconductor:

\[
L_{dx} = \sqrt{\frac{e^2 \kappa \kappa T}{2n_i q^2}}
\]
(4.4)

### 4.3. Analytical and numerical resolutions

The system of three coupled differential equations (4.1) to (4.3) is solved in the case of the thin-film Gallium Arsenide crystalline solar cell presented in figure 6. The resolution of this system is carried out both analytically and numerically in P-type quasi-neutral region \((-X_n < X < -W_p)\) and N-type quasi-neutral region \((W_n < X < X_n)\). The resolution is performed numerically via finite difference approach in the space charge zone \((-W_p < X < W_p)\). In all regions, analytical and numerical calculations are achieved using Maple computer algebra software [12].

### 5. Results and discussions

In the present section, we investigate the variations of total current density \(J=J_n+J_p\) as well as power density \(P = J(V)\cdot V\) delivered by the solar cell as functions of applied voltage \(V\). We also calculate the form factor \(FF=J_{max}V_{max}/J_{SC}V_{oc}\) and solar cell photovoltaic conversion efficiency \(\eta = P_{max}/P_{in}\).

In figure 7, we present the variations of Gallium Arsenide based crystalline thin-film solar cell characteristics \(J=f(V)\), in the dark and under an illumination corresponding to AM1.5 air mass. The solar cell emitter length \(x_p\) and base length \(x_n\) are both equal to 50.50\(\mu\)m. Acceptors doping profile \(N_p(x)\) in P-type region and donors doping profile \(N_n(x)\) in N-type region are uniform and respectively equal to 5.10\(^5\) cm\(^{-3}\) and 10\(^6\) cm\(^{-3}\). When the solar cell is illuminated with real solar spectrum, we get a short circuit current density \(J_{SC} = -20.445\) mAcm\(^{-2}\), an open-circuit voltage \(V_{oc} = 0.92\) V, a maximum power point whose current density \(J_{max} = -19.96\) mAcm\(^{-2}\) and voltage \(V_{max} = 0.833\) V (see figure 8). One can easily deduce that the form factor \(FF = 88.39\%\) and solar cell photovoltaic conversion efficiency \(\eta = 16.62\%\). The results obtained above show that, for similar acceptors and donors doping profiles and concentrations, efficiency of GaAs based solar cells is clearly higher than efficiency of Si based solar cells. We also remark that these results are in very good agreement with those given by solar cells.
modelling and simulation software used in photovoltaic field such as AMPS1D [2], PC1D [13, 14] and SCAPS3300 [15].

Figure 7. GaAs based thin-film crystalline solar cell characteristics \( J=f(V) \) in the dark and under real solar spectrum illumination corresponding to AM1.5 air mass.

In figure 9, GaAs based solar cell characteristics under illumination \( J=f(V) \) are drawn versus applied voltage for different values of uniform deep-level traps concentration: \( N_t = 0, 5.10^{12}, 10^{13}, 10^{14} \) and \( 5.10^{15} \text{cm}^{-3} \). The energy of deep-level traps \( E_t = 0.46 \text{eV} \) [16]. Electrons capture cross-section \( \sigma_e = 10^{-12} \text{cm}^2 \) [16]. Holes capture cross-section \( \sigma_h = 10^{-14} \text{cm}^2 \) [16]. One can notice that deep-level traps concentration has a small influence on short-circuit current density \( J_{sc} \). On the other hand, increasing deep-level traps concentration leads to an appreciable decrease of open-circuit voltage and also implies a significant decrease of maximum power point coordinates (see figure 10).

Figure 9. GaAs based thin-film crystalline solar cell characteristics \( J=f(V) \) under real solar spectrum illumination corresponding to AM1.5 air mass for different concentrations of deep-level traps.

Figure 10. GaAs based thin-film crystalline solar cell power density characteristics \( P=f(V) \) under real solar spectrum illumination corresponding to AM1.5 air mass for different concentrations of deep-level traps.
Figure 11 presents GaAs based crystalline solar cell characteristics under illumination \( J=f(V) \) against output voltage for different values of uniform recombination centers concentration: \( N_r = 0, 5.10^{12}, 10^3, 10^{14} \text{ and } 5.10^{15} \text{cm}^{-3} \). The energy of mid-gap recombination centers is \( E_r = 0.71 \text{eV} \) [17]. Electrons capture cross-section \( \sigma_e = 10^{-14} \text{cm}^{-2} \) [17]. Holes capture cross-section \( \sigma_p = 10^{-15} \text{cm}^{-2} \) [17]. Here also, we remark that recombination centers concentration has a minor effect on short-circuit current density \( J_{sc} \). However, increasing recombination centers concentration implies an important decrease of open-circuit voltage and also causes an appreciable reduction of maximum power point coordinates (see figure 12).

**Figure 11.** GaAs based thin-film crystalline solar cell characteristics \( J=f(V) \) under real solar spectrum illumination corresponding to AM1.5 air mass for different concentrations of recombination centers.

**Figure 12.** GaAs based thin-film crystalline solar cell power density characteristics \( P=f(V) \) under real solar spectrum illumination corresponding to AM1.5 air mass for different concentrations of recombination centers.

6. Conclusion
In conclusion, analytical and numerical resolutions of second order non-linear non-homogeneous coupled equations governing the variations of electrostatic potential, electrons and holes densities as well as occupied deep-level traps density (or recombination centers density) throughout one-dimensional GaAs based crystalline thin-film solar cell, was performed according to finite difference approach using Maple computer algebra software. Special attention was given to the effects due to the existence of deep-levels in the middle of the gap. In this way, we have shown that the presence of deep-level traps or recombination centers has a minor influence on short-circuit current density. However, the existence of these traps (or centers) leads, via Shockley-Read-Hall process, to an important decrease of open circuit voltage and to a noticeable drop of maximum power point coordinates as well as solar cell photovoltaic conversion efficiency.

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