Chapter 5

Simulation Models for Solar Photovoltaic Materials

M. Rizwan^{1,*}, Waheed S. Khan², A. Asma³, A. Shehzadi³

¹ School of Physical Sciences, University of the Punjab, Lahore, Pakistan

² Nanobiotechnology Group, National Institute for Biotechnology and Genetic Engineering (NIBGE), Jhang Road, Faisalabad-38000, Pakistan

³ Department of Physics, University of Gujrat, Hafiz Hayat Campus, Gujrat City, Pakistan

*Corresponding Author: rizwan.sps@pu.edu.pk

Abstract

Semiconducting materials have dominated the photovoltaic industry for a long time. The advancement in solar cell technology is significantly influenced by computer modelling, designing and simulations of the semiconductor materials used for the device operation. Different modelling techniques including one, two and three dimensional models had been employed to comprehend the device operation of solar cell and other electronic devices based on semiconductor materials such as silicon and gallium arsenide. The performance of computing power is increasing with the passage of time in order to improve modelling and designing of different semiconductor materials for solar cell devices. In this chapter, different reported semiconductor materials, their standard characteristics and basic history of modelling, standard models used in photovoltaic industry and principles of modelling such as carrier statistics, transitions, band structure and mobility are explained in detail. Different characteristics of semiconductor material like the carrier transportation, carrier statistics, band structure, and heavy doping effect and carrier generations are described with respect to material modelling.

Keywords

Semiconducting Material, Photovoltaic Industry, Band Structure, Carrier Generation, Modelling

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1. Introduction

Accurate and precise modelling of semiconductor devices is a necessity to comprehend semiconductor phenomenon like generation of heat and movement of electrons, impact ionization to make the functions in electronic devices more impeccable. For high field phenomenon the standard drift-diffusion phenomenon cannot be employed since they do not use energy as a dynamic variable. Moreover for the implementation of semiconductors in photovoltaic industry and optoelectronic devices the interactions of EM radiation and carriers is necessary. The general models used for semiconductor modelling used are called hydro dynamical models but they have theoretical drawbacks. A detailed knowledge about the parameters used in solar cells is necessary to understand the device operation of solar cell. In the modern era of knowledge, to comprehend complete device operation of solar cell requires enhancement in the computing power for efficient device operation in accordance with modelling, simulation and optimisation. The characteristics of semiconductor materials are closely related to a solar cell device operation. The semiconductor material characteristics are carrier statistics, transport,

optical properties and recombination methods [1]. The side effects in solar cell device operation are caused due to harmful effects of the radiation that are experimentally observed under heavy doping effects [2].

In solar cell operation a lot of attention is paid to the properties of silicon and germanium that are the basic semiconductor material used in solar cell for energy generation. Various semiconductor fundamental parameters are encountered in photovoltaic applications. The antireflection coating can be utilized in semiconductors by using refractive index information of semiconductors as shown in table 1 [3-7]. Commercially, various computer programs are utilized for the modelling of materials to be used in solar cell operation. Some computer programs for semiconductor modelling are given below[8].

- Personal Computer 1-Dimensional (PC1D) software was established in the Institution of higher education Australia by P.A. Basore and co-workers for solar cell modelling. This 1-Dsimulant is ordinary utilized by public of photovoltaic cell industry[9].
- ATLAS simulation software by SILVACO International is utilized for two and three dimensional modelling of solar cell. A luminous tool that is the computing method is utilized for the ray tracing of response of a solar cell to the light. The monochromatic or multi-spectral sources of light are also utilized in this software[9].
- Another modelling method is MEDICI, it is a 2-D distribution of concentration of carriers and potential of the semiconductor, proposed by TMS (technology modelling associates). Photo generation can also be computed using this model. In a semiconductor device the potential and carrier concentration are computed through modelling technology that associates models in two-dimension via MEDICI. The photon generation can be attributed to multi-tasking spectral sources, which encompass the modern application of optical device [10].

The accessibility of concentration of charge carrier is dealt with certain computing programs. In general, the modelling of solar cells or the modelling of semiconductor devices basically deals with the numerical techniques which can initiates the main principles of discussion [11].

Table 1 The refractive index for common materials [3-7].

Material	Refractive index at	
	$\lambda = 0.589 \mu\text{m}$	$\rho_p \text{ (g cm}^{-3}\text{)}$
Water	1.33-0i	1.00
Silica	1.55-0i	2.66
Ammonium Sulfate	1.53-0i	1.76
Urban aerosol (avg.)	1.56-0.087i	1.7
Hazy aerosol (avg.)	1.96-0.66i	2.0
Clean aerosol (avg.)	1.53-0.015i	1.68

2. History of semiconductor modelling

The developments in the past two decades in the semiconductor industry have led to great interest in material modelling. The quest behind to understand the device operation of silicon based simple devices to high integrated circuits has increased the importance of modelling in the device technology. With each passing day the size of electronic devices is decreasing, while at the same time the structure is getting more complicated. The miniaturization of devices results in complicating the measurement process. Modelling of devices not only leads to better understanding of device operation but also the new device structures. In semiconductor devices, two types of modelling is possible, physical and equivalent models. Physical models explain the physics behind the device operation and equivalent models explain the circuitry. The equivalent models are less practical due to the complexity while the physical models are very significant to comprehend the application of devices.

Physical models are realized through solution of semiconductor equations such as transport equations. Most models utilize the bulk carrier transport equations. The interest in material modelling started about 20 years ago. With time this field has become a well-established industry. Before the availability of wide spread computers, analytical tools were used. Shockley first provided a linear approximation tool that provides basic information regarding device operation but does not give any information regarding optimization. Thus, numerical simulations were introduced to encompass all parameters of device. In the early days, only one dimensional device modelling was used. In 1964, a one dimensional numerical model was used for GaAs.

Around 1969, two dimensional models came on the horizon. These models were used in BJT devices. These two dimensional models however weren't able to explain the 3 dimensional phenomenon in very small devices. Major solid state devices involve three dimensional phenomena such as hot electron generation. Monte Carlo technique for 3-dimensional modelling was introduced in 1966. This technique is used in Si, InP based

devices. With quantum based semiconductor devices, new models are required [12]. All numerical simulations are based on the following principles.

3. Semiconductor band structure

The operation of solar cells have fundamental importance and the main properties of semiconducting materials depends on the band gap which is the difference in valance band and conduction band energy and the structure of crystal is dependent on k-wave vector. The band gap energy and wave vector k is the main parameters that vary with temperature and pressure. The variation in the energy of band gap because of the temperature factor is mathematically designated by Varshni [13],

$$E_g(T) = E_{g0} - \frac{\alpha T^2}{T + \beta} \quad (1)$$

Where T, alpha and beta are the parameters, in which T is absolute temperature. For example for silicon the band gap energy was calculated 1.17eV and constants values are 4.730 and 636 respectively.

The optical transitions in between the band gap produce current through the solar cells. There are different kinds of transition in which two are mentioned here [14]. One is direct transition that occurs, when the net momentum is null from ion-electron transition then that transition is direct, another case is indirect transition in which addition of pair of electron-ion is considered [14, 15]. In indirect transition the phonon is required for the complete transition that is due to thermal quantum lattice vibration.

Semiconductors are of two kinds:

3.1 Direct band gap semiconductors

In direct band gap, when the top of valance band and bottom of conduction band occur at the same k-point of first Brillouin zone, such semiconductors are characterized as direct band gap semiconductors.

3.2 Indirect band gap semiconductor

In case of indirect band gap, the maxima of valance band and the minima of conduction band occur at the different k-point of first Brillouin zone [16], such semiconductors are called as indirect band gap semiconductors.

The direct band gap semi-conductor is stronger than indirect band gap [17] and is considered in case of optical absorption, for example the silicon and gallium arsenide etc. as shown in Figure 1 [18].

Figure 1 For Si, GaAs, InP and InGaAs the optical absorption. Reprinted from Ref. [18] under open access conditions.

4. Semiconductor's carrier statistics

In thermal equilibrium, the two factors, temperature and the electrochemical potential represented by E_f is constant for a given device [19]. The concentration of electron is n and concentration of hole is represented by the p and the product of these concentrations is not dependent on substitution concentration. The law of mass action given by [20],

$$np = n_i^2 = N_c N_v \exp\left(-\frac{E_g}{k_B T}\right) \quad (2)$$

where T is the absolute temperature, k is Boltzmann constant, n_i is the intrinsic concentration of semiconductor of electron and N_c, N_v are the effective density of conduction and valance band [21].

The effective density of states are $N_c N_v$ are given by,

$$\left. \begin{aligned} N_c &= 2 \left(\frac{2\pi m_e k_B T}{h^2} \right)^{3/2} \\ \text{And} \\ N_v &= 2 \left(\frac{2\pi m_h k_B T}{h^2} \right)^{3/2} \end{aligned} \right\} \quad (3)$$

Here, m_e and m_h are the effective masses of electron and holes density of states and h is the planks constant.

The product of electron hole concentration does not obey for operation of solar cell from the equation 2. Differences may lead to transition of electron between different bands or quantum sates that will lead to gradients of the electrochemical potential and temperature and current also runs [17]. Then suitable kinds of carriers are explained for each energy band level to represent by a quasi-Fermi level. However, the quasi-Fermi level of concentration of electron in conduction band may be examined by E_{Fn} , the holes concentration in valance band by E_{Fp} [22].

It is important to explain the potential of electron and holes as given by,

$$\left. \begin{aligned} E_{Fn} &= -q\phi_n \\ E_{Fp} &= -q\phi_p \end{aligned} \right\} \quad (4)$$

The electron and holes carrier concentration terminologies are explained in equation 5 [23-30]. The solar cell operation does obey the above equation in order to explain the quasi-Fermi level of potentials of electron and hole [31].

$$\left. \begin{aligned} N_c \exp\left(\frac{E_{Fn}-E_c}{K_B T}\right) & \quad n_i \exp\left(\frac{q(\psi - \phi_n)}{K_B T}\right) & N_c F_{1/2} \exp\left(\frac{E_{Fn}-E_c}{K_B T}\right) \\ N_v \exp\left(\frac{E_v - E_{Fp}}{K_B T}\right) & \quad n_i \exp\left(\frac{q(\phi_p - \psi)}{K_B T}\right) & N_v F_{1/2} \exp\left(\frac{E_v - E_{Fp}}{K_B T}\right) \end{aligned} \right\} \quad (5)$$

5. Carrier mobility

The current densities of electron and hole are given by [27],

$$\left. \begin{aligned} j_n &= q\mu_n n\varepsilon + qD\nabla_n n \\ j_p &= q\mu_p n\varepsilon - qD\nabla_p n \end{aligned} \right\} \quad (6)$$

In equation 6,

μ_n = The mobility of electrons

μ_p = The mobility of holes

n = Concentration of electrons

p =Hole-concentration

D = Diffusion current for holes and electrons

And

ε = Electric field.

The first terms in equation 6 is due to electric field ε , and second is accountable for diffusion. The drift mobility is ratio of drift velocity by field strength in above equation that explains the weak field. Electron and holes are charge carriers and dependence of impurity substitution on charge carriers is a function of temperature as in form of lesser or higher carriers. If we increase the temperature then the charge carrier concentration also varies according to situation. The Caughey-Thomas [32] is representing the empirical dependencies for case of silicon is given by,

$$\mu = \mu_{min} + \frac{\mu_0}{1 + \left(\frac{N}{N_{ref}}\right)^a} \quad (7)$$

The different charge carrier values are in majority and minority as explained by the various parameters. For example the silicon, the majority carrier mobility and minority carrier mobility values are reported in literature [23, 33-35].

At high concentration, the effect of lattice on the scattering, impurity scattering, carrier-carrier scattering is significant [36].

When the carrier velocity reaches to saturation, there is a low current flow in same direction of electric field, and thus the mobility of carriers accelerates. The mean velocity that is the function of field is described as,

$$v = \frac{\mu_{lf}}{\left(1 + \left(\frac{\mu_{lf} \varepsilon}{v_{sat}}\right)^\beta\right)^{1/\beta}} \quad (8)$$

Here β is parameter of carrier mobility as a low field, for electron its value is 2 and for holes equal to 1, v_{sat} is the velocity at saturation point same for both holes and electrons [37-39].

The saturation velocity is given by,

$$v_{sat} = \frac{2.4 \times 10^7}{1 + 0.8e^{\frac{T}{600}}} \quad (9)$$

In case of gallium arsenide, the information collected for mobility of majority carriers is related to some literature review in [35], the data given is more difficult for numerical or empirical analysis. The mobility of minority carrier as a function of impurities concentration as shown in Figure 2 [40] and Figure 03 [41].

Figure 2 Minority-carrier mobility as a function of temperature [39]. Reprinted from ref. [40] copyright (1995), with permission from AIP Publishing.

Figure 3 Mobility dependence on the doping concentration for gallium arsenide, [41].
Reprinted from ref. [41], copyright (2000), with permission from AIP Publishing.

The silicon and gallium arsenide carrier mobility are a function of electric field and the velocity is such and is given by as follows [34],

$$\mu_n = \frac{\mu_{lf} + v_{sat} \left(\frac{\varepsilon}{\varepsilon_0} \right)^\beta}{\left(1 + \left(\frac{\varepsilon}{\varepsilon_0} \right)^\beta \right)} \quad (10)$$

Where μ_{lf} is represented by the mobility of low field carriers, ε_0 is equal to 4×10^3 V/cm and the parameter beta is equal to 4 for electrons and 1 for holes [1, 33].

The v_{sat} for silicon and gallium arsenide is given by [42],

$$v_{sat} = 11.3 \times 10^6 - 1.2 \times 10^4 T \quad (11)$$

Here, T is represented by absolute temperature.

Indium phosphide the majority carrier mobility is reported in figure 4.

Figure 4 Mobility dependence on the doping concentration for indium phosphide. Reprinted from ref. [41] copyright (2000), with permission from AIP Publishing.

6. Carrier generations by optical absorption

6.1 Band-to-band transitions

In solar cells main function of carrier generation is the light absorption. Consider for the case of planar slab, the photon which move to semiconductor that produces the pairs of electron and hole, $g(x)\delta x$, of thin layer of slab from depth $x \rightarrow x + \delta x$. The generation Function $g(x)$ is given by,

$$g(x) = \alpha(\lambda) \exp\{-\alpha(\lambda)x\}$$

Here, $\alpha(\lambda)$ is represented by absorption coefficient, absorption coefficient as a function of energy is given in figure 5 [43]. The $g(x)$ is a function defined by the ratio of generation rate G to volume that's defined by the above equation

Generation Function = g/A

In above equation A indicated the sample area.

Rajkananand co-workers [19] reported that a fundamental formula for the case of silicon is described by the absorption coefficient,

$$\alpha(T) = \sum_{j=1,2} C_i A_j \left[\frac{\{h\nu - E_{gj}(T) + E_{pi}\}^2}{\{ \exp(E_{pi}(KT)) - 1 \}} + \frac{\{h\nu - E_{gj}(T) - E_{pi}\}^2}{\{1 - \exp(E_{pi}(KT))\}} \right] + A_d \{h\nu - E_{gd}(t)\}^{1/2} \quad (12)$$

Here, $h\nu$ show the photon energy, $E_{g1}(0) = 1.1557\text{eV}$, $E_{g2}(0) = 2.5\text{eV}$ and $E_{gd}(0) = 3.2\text{eV}$ the energies shows that the lowest indirect band gap and lowest direct band gap, respectively. Now, represented by the transverse optical and transverse acoustic phonons of the Debye frequencies $E_{p1} = 1.827 \times 10^{-2}\text{eV}$ and $E_{p2} = 5.773 \times 10^{-2}\text{eV}$, and $C_1 = 5.5$ & $C_2 = 4.0$ and $A_1 = 3.231 \times 10^2\text{cm}^{-1}\text{eV}^{-2}$, $A_2 = 7.237 \times 10^3\text{cm}^{-1}\text{eV}^{-2}$ and $A_1 = 1.052 \times 10^6\text{cm}^{-1}\text{eV}^{-2}$. The band gap is a function of temperature, for example if we change the one parameter second is automatically changed according to our desired requirements. These parameters $\alpha = 7.021 \times 10^{-4}$, eV/k^2 and $\beta = 1180k$ are described by the three band gap energies E_{g1} , E_{g2} and E_{gd} .

Figure 5 For solar cell the absorption coefficient as a function of energy[43]. Reprinted from ref. [43] under the terms of Creative Commons License

6.2 Free-carrier absorption

Electron transition from an initial state to final state upon absorption of photon can happen in a region in the same band due to two parameters one is impurity and other is because of strong interactions within the band. As a result of such transition current is generated by the band-band transition rather than electron hole pair that is produced due to free carrier absorption. The photon energies might be equal to band gap for the case of free carrier absorption rather than absorption coefficient and could be included in form of exponential equation.

The region of high impurity or doping concentration depend on where the band edge is residing in various form of phenomena's.

For the free-carrier concentration uses the PCID model to calculate absorption coefficient and computes on the experimental data:

$$\alpha_{FC} = K_1 n \lambda^a + K_2 p \lambda^b \quad (13)$$

Where, these parameters are described in a, b, K_1 and K_2 in nanometre dimensions. For various parameters such as o mobility of electrons and holes are reported. The free carrier absorption co-efficient a, b, k_1 and k_2 have constant values. For example silicon, gallium arsenide and indium phosphide were reported with their different constant values.

6.3 Heavy doping effects

The electronic properties of semiconducting material exhibit unless impurity density is very high. The depiction of electronic properties is not dependent on the interaction of electron to the isolated impurities. Two impurity bands are formed when the doping concentration are enhanced, one is impurity band and the other is separate from the coulomb wave function due to other doping effects on impurity band [44]. Both bands are combined together and form a merged band that describe the localised states. To describe the semiconductor device operation and the optical parameters, the reasonable interaction in between the electron-electron that gives exchange energy and co-relation energy are discussed.

Band anisotropy and effective masses are utilized to calculate more accurate results for the practical purpose to explain the complex phenomenon of band gap narrowing. Absorption at low temperature data is utilized for the optical measurement of the device operation. The band gap narrowing is represented by the symbol ΔE_g . For the case of n-type material is given by,

$$\Delta E_g = KT \ln \frac{N_D p_0}{n_i^2} \quad (14)$$

Here, p_0 is represented by the concentration of minority holes and N_D represent the doping donor concentration.

From literature review, the values can be compared with experimental work that has been computed from the different phenomena's. Sample is prepared using different material to study the band gap narrowing by the Jain and co-workers [45]. Klaasenet co-workers [46] and its co-worker are working on the device modelling of semiconductor based silicon. By comparing the theoretical corrected values with the experimental data from literature review gives a new estimated value of intrinsic free carrier concentration of the n and p-type of narrowing band as described by Klaasenet and co-workers [46] to single expression,

$$\Delta E_g (meV) = 6.92 \left[\ln \frac{N_{dop}}{1.3 \times 10^{17}} + \sqrt{\left(\ln \frac{N_{dop}}{1.3 \times 10^{17}} \right)^2 + 0.5} \right] \quad (15)$$

Here the doping concentration is shown by N_{dop} .

Lundstrom et al [40] suggested the formula consists of doping concentration for gallium arsenide is empirical data:

$$\Delta E_g = AN_{dop}^{1/3} + K_B T \ln\{F_{1/2}(E_F)\} - E_F \quad (16)$$

Where, the Fermi energy is represented by E_F . The function $F_{1/2}$ given by,

$$A = \begin{cases} 2.55 \times 10^{-8} eV & (p-GaAs) \\ 3.23 \times 10^{-8} eV & (n-GaAs) \end{cases} \quad (17)$$

7. Modelling simulation and analysis

The progress in Nano/microelectronic is rising as in comparison to the fundamental model TCAD, because one is high cost and other is developing long range order of simulation, optimisation and modelling of geometry. Firstly, the real part of components can be classified individually for the whole explanation, and then examine the element of that system at the end and observe the connection between them.

Simulation is a process in which we can solve the problem through some systems of operation without fabrication. And the theoretically simulation guess is more precise, if we accept the idea of approximation. Modelling is basically defined by the process or device, to find out the way to solve the problem, the analysis of the different conception about geometry that can't be measured or calculated exactly. Basic requirements are simulation, analysis and geometry optimisation for modelling. There are two models, one is used for the curves fitting such as known simulation models that are easier than other models for analysis such as described by their physical aspects in qualitative way. The most common example is Monte Carlo method, one of the applications of the models. It is a simulation method use for various functioning in a system. Using this model, we must be aware of the constraints of the appliances for achieving more accurate results. And we must be comparing the results from literature review in theoretical and experimental papers.

Field of electronic devices is progressing, by designing the geometry for various operations using different parameters to obtain more accurate results during manufacturing for tests. In modern era, the simulation process must be much better to obtain the number of iterations. The simulation and analysis gives 40% success roughly. This estimation clearly depends on the model that is used for simulation. Due to scraps and tests, the uncertainty in parameters can't be removed. The quantum effects prevail, due to the scaling factor used is too large for the model. The theoretical resources are less costly as compared to experimental, which sustain the set expectations. Numerical modelling is utilized for large number of calculations.

Conclusion

It is established that among all the techniques, MEDICI is the most efficient technique for solar cell device operation. Since this three dimensional technique encompasses all aspects of device operation and is ideal for devices based on quantum aspects and also for the miniaturization of electronic devices. The decrement in the size of transistor is a huge recurring demand in semiconductor industry, which increase demand in decrement. The material growth for low dimensional devices has been increased highly. We have shown that some models and techniques for computers modelling and simulation agreed well with theoretical and experimental results. Initially two types of models were used, physical and equivalent, but only physical models survived the industry due to their significance and importance in photovoltaic industry. It is essential to apprehend the physics behind the semiconductor devices for their good performance in application by low dimensional material of simulation and modelling using physical models. These results can be practically applied to electronic devices such as circuit-level simulation for various device models such as MOSFETS, BJT-devices. The cell generated photocurrent, current-voltage graph, carrier statistics and series resistance are used for different methods to estimate the simulations. In upcoming years, various advanced modelling techniques such as those based on quantum mechanics are expected that will lead to revolutionary changes in photovoltaic industry.

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