Research Article

Analysis of Si/SiGe Heterostructure Solar Cell

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Sunlight is the largest source of carbon-neutral energy. Large amount of energy, about 4.3×10^{20} J/hr (Lewis, 2005), is radiated because of nuclear fusion reaction by sun, but it is unfortunate that it is not exploited to its maximum level. Various photovoltaic researches are ongoing to find low cost, and highly efficient solar cell to fulfil looming energy crisis around the globe. Thin film solar cell along with enhanced absorption property will be the best, so combination of SiGe alloy is considered. The paper presented here consists of a numerical model of Si/Si_{1-x}Ge_x heterostructure solar cell. The research has investigated characteristics such as short circuit current density (J_{sc}), generation rate (G), absorption coefficient (α), and open circuit voltage (V_{oc}) with optimal Ge concentration. The addition of Ge content to Si layer will affect the property of material and can be calculated with the use of Vegard's law. Due to this, short circuit current density increases.

1. Introduction

The development of new energy sources is continuously being enhanced because of the critical situation of the nonrenewable resources. Thus, the renewable energy sources have become a more important contributor to the total energy consumed in the world. Sun provides enormous amounts of energy, powering oceans as well as atmospheric currents and cycle of evaporation. Electricity from solar energy is one of the most unprecedented cost effective methods of electricity production. Japan is leading with 64% electricity production using photovoltaic solar cell as shown in Figure 1. The solar cells have considerably reduced the cost/watt of produced electricity by a factor of 5–10 to compete with fossil and nuclear electricity and by a factor of 25–50 to compete with primary fossil energy [1]. Therefore, solar energy is one of the attractive types of renewable sources of energy replacing fossil fuels due to its profusion. In fact, the demand for solar energy has increased over the past 20 years. The market for PV systems is growing worldwide. In fact, nowadays, solar PV provides around 4800 GW. The sun continuously supplies about 1.2×10^{25} [1] terawatts of energy which is greater than any other renewable or nonrenewable sources of energy. Solar

cell is generally constructed using crystalline silicon (c-Si) which has absolutely low absorption coefficient because of its indirect band structure; therefore, it is less preferable for solar technology. Here alloy of SiGe is considered due to its low energy band gap and increase in absorption coefficient as compared to Si. Figure 2 shows the average solar radiation near Jammu, India. The sun path with respect to its elevation to the surface is shown in blue and the hour curve is represented in red.

In Section 2, the total probability for generation of photon is discussed. Section 3 highlights the modeling parameters of n-on-p junction. Section 4 elaborates the numerical model configuration. Simulation results are presented under Section 5 with simulated data.

2. Probability Analysis

Solar irradiance curves are shown in Figure 3, with top most curve representing solar spectrum outside the earth's atmosphere also known as air mass zero condition (AM0) which reaches the earth's surface directly. Global irradiance is a nonconcentrating system which uses the scattered, diffuse, and ground reflected irradiance. Earth receives more energy

FIGURE 1: Electricity production in world in MW [2].

FIGURE 2: Average solar radiation from June to December [3].

from the sun in just one hour than the world uses in a whole year [4]. The efficiency of solar cell depends on total probability of photon generation in a device.

The distribution of fixed amount of energy depends upon the density of available energy states and the probability of occupying that state. This probability is given by the distribution function, but if in a given energy interval there are more available energy states then that will give a greater weight to the probability for that energy interval.

From Fermi-Dirac distribution function [5] at a certain temperature the probability of electrons that occupy a certain energy level is given by

$$F(E) = \frac{1}{1 + e^{(E-E_F)/kT}}. \quad (1)$$

Probability to find the particular state is defined by Fermi level because it lies in midway between E_c and E_v as shown in Figure 4. Let us consider that the energy distribution

FIGURE 3: Solar spectral irradiance.

FIGURE 4: Band diagram of p-n junction solar cell in darkness and under illumination.

is uniform then the probability of electron presence in conduction band $n(E_c)$ is proportional to

$$e^{-(E_c-E_{FN})/kT}, \quad (2)$$

where E_{FN} is the occupancy of energy in conduction band. The probability of holes present in valance band $p(E_v)$ is proportional to

$$e^{(E_v-E_{FP})/kT}, \quad (3)$$

where E_{FP} is the occupancy of energy in valence band. The total probability for photon generation is proportional to $n(E_c) * p(E_v)$ so from (2) and (3) we get

$$e^{(E_v-E_c)/kT} \cdot e^{(E_{FN}-E_{FP})/kT}, \quad (4)$$

where difference of valance band and conduction band energy is termed as energy band gap E_g and the other exponential part is constant for a given doping.

3. Modeling Parameters

3.1. Dielectric Constant (ϵ_r). The permittivity or relative dielectric constant is an important property of material which

varies with different layers, that is, different mole fraction of Ge, which is generally specified by

$$\epsilon_{r\text{SiGe}} = \epsilon_{r\text{Si}} (1 - X) + \epsilon_{r\text{Ge}} (X), \quad (5)$$

where $\epsilon_{r\text{Si}}$ and $\epsilon_{r\text{Ge}}$ are the relative permittivity of silicon and germanium material, respectively. The mole fraction of Ge is given as X .

3.2. Energy Gap (E_g). Due to the different thickness of Si and Ge alloys the stacked layers are formed which relates to different energy thresholds, absorbing a different band of the solar spectrum over a wide range from silicon (1.12 eV) to germanium (0.66 eV). The energy gap of combination is calculated using Vegard's law:

$$E_{g\text{SiGe}} = E_{g\text{Si}} (1 - X) + E_{g\text{Ge}} (X), \quad (6)$$

where $E_{g\text{Si}}$ and $E_{g\text{Ge}}$ are the energy gap for pure Si and Ge materials. For type-I heterostructure we use the following relation:

$$\Delta E_g = \Delta E_v + \Delta E_c. \quad (7)$$

3.3. States Density. Using Maxwell-Boltzmann approximation in equilibrium state for the carrier concentrations as a function of the Fermi level, carrier concentrations can be represented as [6, 7]

$$p = N_v e^{((E_v - E_F)/kT)}, \quad (8)$$

$$n = N_c e^{((E_F - E_c)/kT)}, \quad (9)$$

where N_c and N_v are the states effective density in the valence and conduction band, respectively. E_F is the Fermi level, E_v and E_c are the valence and conduction band energy level, respectively. T is the temperature and k is the Boltzmann constant.

3.4. Absorption Coefficient. Absorption coefficient calculation is an important factor for analysing solar cell as it decides the fraction of photon absorbed on the surface. In semiconductors it is realized as transferring of energy from photons to electrons due to which electrons transit from valence band to conduction band and create electron-hole pairs. Consider

$$\alpha = \alpha_{\text{Si}} (1 - X) + \alpha_{\text{Ge}} (X), \quad (10)$$

where α_{Si} and α_{Ge} are the absorption coefficient of silicon and germanium material. The absorption coefficients for n-type Si and Ge are taken from [5] and [8], respectively, for the calculation of α_{SiGe} .

4. Model Configuration

The selection of semiconductor for constructing a solar cell should be chosen on the basis of absorption of the solar spectrum, that is, as much as possible. Therefore, a low band

FIGURE 5: Schematic structure of Si/SiGe heterojunction solar cell.

gap is desirable. However, this is counterbalanced by the desire to have a large built-in voltage which requires a larger band gap. Long wavelength response can be enhanced by reducing the band gap and this can be done by incorporating Ge into the SiGe layer.

The model includes the $\text{Si}_{1-x}\text{Ge}_x$ layer where x is the mole fraction of Ge [8]. With the changes in Ge-content, material properties of a Ge-incorporated Si layer change. Vegard's law is used to approximate some material parameters of $\text{Si}_{1-x}\text{Ge}_x$ alloy, for example, diffusion coefficient, relative permittivity, and absorption coefficients for different Ge-content (x). We have considered a typical layer structure of Si/ $\text{Si}_{1-x}\text{Ge}_x$ heterojunction solar cell as shown in Figure 5; it is an n on p model where n-type SiGe layer is responsible for absorption, that is, acting as active base layer. Very thin (~ 5 nm) layer of highly doped n-Si acts as capping layer to increase the luminescence efficiency. This schematic represents a solar cell consisting of front ohmic contact fingers, strip, and indium tin oxide film as an antireflection coating. The back ohmic contact was formed by printing the Al paste on the entire backside of the surface. Indium tin oxide (ITO), a transparent contact layer, and antireflection coating on upper layer of the structure allow the light to travel through this layer. Within the active base layer electron-hole pairs are generated with the incident of suitable wavelength light. These photogenerated holes and electrons are separated out by diffusion and drift process giving rise to the photocurrent.

In dark, drift of thermally generated minority carrier across junction constitutes reverse saturation current and at zero bias it is balanced by small flow of majority carrier in opposite direction; that is, net current is zero. Under illumination, when monochromatic light of wavelength λ is incident and if junction is illuminated by photon with $h\nu \geq E_g$ the number of carriers collected per incident photon at each wavelength [9] is calculated as follows: at a distance x from the surface generation rate (G) is given by

$$G(\lambda, X) = \alpha(\lambda) F(\lambda) [1 - R(\lambda)] e^{-\alpha(\lambda)x}. \quad (11)$$

Here we will consider the case of holes first. From Figure 6, we can observe that coordinate x is directed from n-SiGe to p-Si, and we have assumed origin ($x = 0$) between the n^+ Si capping layer and n-SiGe layer junction, neglecting the thickness of thin capping layer. One-dimensional steady-state continuity equation for holes in n-side under low injection condition can be written as

$$G_p - \frac{p_n - p_{no}}{\tau_p} - \frac{1}{q} \frac{dJ_p}{dx} = 0, \quad (12)$$

where G_p is the generation rate of holes, τ_p is the minority hole recombination life time, p_{no} and p_n are the densities of holes at equilibrium and under illumination, respectively, and J_p is the conduction current density due to holes. The current density equation for holes in n-side excluding the depletion region can be written as

$$J_p = -qD_p \frac{dp_n}{dx}, \quad (13)$$

where D_p refers to diffusion coefficient of holes in the SiGe layer. Each side of junction is doped constantly.

These equations are solved considering generation rate $G(\lambda, x)$ with appropriate boundary conditions to get an expression for the density of holes. At surface ($x = 0$), recombination velocity of holes is S_p and at depletion edge ($x = x_j$) due to the electric field excess carrier density is small [9]. Hence, the wavelength-dependent diffusion current density for holes (J_p) is given as

$$\begin{aligned} J_p(\lambda) &= - \left(\frac{q \times F(\lambda) (1 - R)}{1 - \alpha_{\text{SiGe}}^{-2}(\lambda) L_p^{-2}} \right) \\ &\times \left[\frac{(S_p / \alpha_{\text{SiGe}}(\lambda) D_p) + 1}{(S_p L_p / D_p) \sinh(x_j / L_p) + \cosh(x_j / L_p)} \right. \\ &- \frac{((S_p / \alpha_{\text{SiGe}}(\lambda) D_p) \cosh(x_j / L_p)) e^{-\alpha_{\text{SiGe}}(\lambda) x_j}}{(S_p L_p / D_p) \sinh(x_j / L_p) + \cosh(x_j / L_p)} \\ &- \left. \frac{((1 / \alpha_{\text{SiGe}}(\lambda) L_p) \sinh(x_j / L_p)) e^{-\alpha_{\text{SiGe}}(\lambda) x_j}}{(S_p L_p / D_p) \sinh(x_j / L_p) + \cosh(x_j / L_p)} \right], \quad (14) \end{aligned}$$

where $F(\lambda)$ is the number of incident photons per area per second, R (reflectivity) is the fraction of these photons reflected from surface, and $\alpha_{\text{SiGe}}(\lambda)$ is the absorption coefficient of SiGe layer. $L_p = \sqrt{D_p \tau_p}$ is the diffusion length of minority holes in n-SiGe. Assuming front side of n-on-p junction to be uniform in a lifetime, mobility and doping level at a particular wavelength of this photocurrent would be observed. Similarly, by solving continuity and current density

FIGURE 6: Layer structure of SiGe/Si solar cell.

equations for electron, the diffusion current density due to minority electrons (J_n) in p-Si can be obtained:

$$\begin{aligned} J_n(\lambda) &= - \left(\frac{q \times F(\lambda) (1 - R) e^{-\alpha_{\text{SiGe}}(\lambda) d_{\text{SiGe}} - \alpha_{\text{Si}}(\lambda) w_{\text{Si}}}}{1 - \alpha_{\text{SiGe}}^{-2}(\lambda) L_n^{-2}} \right) \\ &\times \left(1 - \frac{1}{\alpha_{\text{Si}}(\lambda) L_n} \right) \\ &\times \left[\frac{(S_n L_n / D_n) (\cosh(H' / L_n) - e^{-\alpha_{\text{Si}}(\lambda) H'})}{(S_n L_n / D_n) \sinh(H' / L_n) + \cosh(H' / L_n)} \right. \\ &+ \left. \frac{\sinh(H' / L_n) + \alpha_{\text{Si}}(\lambda) e^{-\alpha_{\text{Si}}(\lambda) w_{\text{Si}}}}{(S_n L_n / D_n) \sinh(H' / L_n) + \cosh(H' / L_n)} \right], \quad (15) \end{aligned}$$

where H' as shown in Figure 6 is the p-base neutral region, $\alpha_{\text{Si}}(\lambda)$, L_n , and S_n are the corresponding parameters for electrons in Si-like holes in SiGe.

Some photogeneration currents take place within the depletion region. The electric field in region is high; photogenerated carriers are accelerated out of depletion region before they recombine. Hence, drift current density (J_{dr}) can be expressed as

$$\begin{aligned} J_{\text{dr}}(\lambda) &= qF(\lambda) (1 - R) \\ &\times \left[e^{-\alpha_{\text{SiGe}}(\lambda) x_j} (1 - e^{-\alpha_{\text{SiGe}}(\lambda) w_{\text{SiGe}}}) + e^{-\alpha_{\text{SiGe}}(\lambda) (w_{\text{SiGe}} + x_j)} \right. \\ &\times \left. (1 - e^{-\alpha_{\text{SiGe}}(\lambda) w_{\text{Si}}}) \right], \quad (16) \end{aligned}$$

where w_{SiGe} and w_{Si} are the widths of insertion of the depletion region deep in the n-SiGe and p-Si regions, respectively. J_{dr} in comparison with diffusion component is negligible.

FIGURE 7: Photon generation rate as a function of surface distance.

The calculations are done without considering trapping. Total generated photo current density can be expressed as

$$J(\lambda) = J_p(\lambda) + J_{dr}(\lambda) + J_n(\lambda). \quad (17)$$

By integrating $J(\lambda)$ over full range of solar radiation we obtain total photocurrent:

$$J_{ph} = \int_{\lambda_1}^{\lambda_2} J(\lambda) d\lambda. \quad (18)$$

Total current can be defined as

$$J = J_0 (e^{qv/kT} - 1) - J_{ph}, \quad (19)$$

where J_0 is the saturation current density.

5. Simulation Result

The numerical modeling and simulation is done with MATLAB software using different parametric value [8, 10] as shown in Table 2.

The τ_p is the recombination life time of electron-hole pair in n-type. With the help of numerical solution of above set of equation the solar cell modeling has been performed using the software. For simulation purpose device parameters are required to calculate all properties like mobility of hole/electron, doping, thicknesses, band gap, intrinsic concentration, and so forth; few are provided in Table 2.

5.1. Generation Rate. The number of electrons generated at each point in solar plate due to the absorption of photons is termed as generation rate. The graph is plotted using (11) for two different wavelengths with the help of different parameters from Table 2. The generation rate of SiGe material at different wavelength is shown in Figure 7.

FIGURE 8: SiGe bandgap and saturation current calculation.

The initial operating temperature is fixed to 300 K. The generation rate has been simulated using a numerical model. From observation we can conclude that the light consists of different wavelength; therefore generation rate is different for different wavelength [11]. It is an exponentially decreasing curve throughout the material and the generation is the highest at the surface of the material.

5.2. Band Gap and Saturation Current. The conventional p-n junction solar cell has single bandgap E_g . Photon with energy greater than E_g contributes to the cell output when exposed to the solar spectrum. The wavelength to photon energy conversion, we have used relation,

$$\lambda = \frac{1.24}{hv} \mu\text{m}. \quad (20)$$

The dependence of saturation current density as a function of SiGe band gap $E_{g\text{SiGe}}$ with different Ge content is shown in Figure 8. The saturation current can be calculated using the following formula:

$$I_s = qN_cN_vA \left(\frac{1}{N_A} \sqrt{\frac{D_n}{\tau_n}} + \frac{1}{N_D} \sqrt{\frac{D_p}{\tau_p}} \right) e^{-E_g/kT}, \quad (21)$$

where N_A and N_D stand for density of acceptor and donor atoms. q is the absolute value of the charge of an electron. From Figure 8 it can be noted that smaller E_g in high-Ge concentration SiGe solar cell results in high I_s . To make thin film solar cell which absorbs more than 90% of the sunlight low bandgap materials must be firmly developed [10].

Therefore to adjust the spectral response, germanium a low bandgap material with bandgap 0.66 eV~1.1 eV is chosen. After mixing of germanium in thin film materials, SiGe can significantly adjust the material to proceed towards the low bandgap as a function of Ge mole fraction, as shown in Figure 8, thereby enhancing light absorption rate and ultimately improving the conversion efficiency of new solar cells.

TABLE 1: SiGe parameters at different mole fraction.

Properties	Materials				
	$x = 0$ Si	$x = 0.1$ $\text{Si}_{0.9}\text{Ge}_{0.1}$	$x = 0.2$ $\text{Si}_{0.8}\text{Ge}_{0.2}$	$x = 0.3$ $\text{Si}_{0.7}\text{Ge}_{0.3}$	$x = 1$ Ge
Dielectric constant (ϵ_r)	11.9	12.31	12.72	13.13	16
D_p (m^2/s)	2.458×10^{-4}	2.419×10^{-4}	2.38×10^{-4}	2.341×10^{-4}	2.07×10^{-4}
D_n (m^2/s)	6.986×10^{-4}	7.193×10^{-4}	7.40×10^{-4}	7.60×10^{-4}	9.056×10^{-4}
Energy gap E_g (eV)	1.12	1.074	1.028	0.982	0.66
Effective density of states in valence band, N_v (cm^{-3})	1.04×10^{19}	9.96×10^{18}	9.52×10^{18}	9.08×10^{18}	6×10^{18}
Effective density of states in conduction band, N_c (cm^{-3})	2.8×10^{19}	2.62×10^{19}	2.44×10^{19}	2.27×10^{19}	1.04×10^{19}
Intrinsic carrier concentration (n_i) (cm^{-3})	1.45×10^{10}	2.413×10^{12}	4.81×10^{12}	7.21×10^{12}	2.4×10^{13}

TABLE 2: Parametric value used in simulation.

Parameters	Value
Concentration (SiGe)	$3 \times 10^{25} \text{ m}^{-3}$
Concentration (Si)	$3 \times 10^{22} \text{ m}^{-3}$
Reflectivity (R)	0.9
Device area (A)	$4 \times 10^{-4} \text{ m}^2$
d_{SiGe}	50 nm
d_{Si}	100 nm
τ_p	$1 \times 10^{-8} \text{ s}$

FIGURE 9: Theoretical SiGe absorption coefficient with the different Ge content.

5.3. Absorption Coefficient and Wavelength. With the increase in Ge content along with smaller band gap energy E_g of thin SiGe film, the absorption rate shoots high and more electron hole pair can be generated due to the incident light. Generation of a higher number of electron hole pairs implies higher short circuit current density and efficiency of SiGe solar cell [7].

FIGURE 10: J_{sc} and V_{oc} in the SiGe solar cells with different Ge concentrations.

Figure 9 shows the absorption coefficient as a function of wavelength for the standard global AM1.5 spectrum. According to Figure 9, E_g is varying inside the layer from 1.12 to 0.66 eV as stated in Table 1 for $\text{Si}_{1-x}\text{Ge}_x$ alloy layer structure, which enhanced the photon absorption probability in that layer. Adding Ge to the solar cell, one can reduce the band gap and enhance response over long wavelength [8].

5.4. Current Density J_{sc} . The current density as a function of voltage along with voltage characteristics of solar cell is presented in Figure 10. From the figure, short circuit current of solar cell is the highest current which may be drawn from the solar cell. Due to increase in absorption coefficient of SiGe solar cell its J_{sc} can be increased greatly. After the analysis it is observed that when mole fraction of Ge (X) is 0.15 then the highest J_{sc} 382.5 A/m² is achieved in the solar device. The reason is smaller SiGe bandgap layer which leads to more photon absorption and electron-hole pair generation. Figure 10 compares the J_{sc} and V_{oc} among the different Ge concentrations systemically.

With the increase in Ge concentration, the J_{sc} increases and V_{oc} decrease. This is due to the energy band structure

characteristic of SiGe. It can be observed that there is a drastic increase of the photocurrent J_{sc} [7]. Consider

$$\text{Efficiency} = J_{sc} \times V_{oc} \times FF, \quad (22)$$

where V_{oc} is determined by the properties of the semiconductor and depends on the J_{sc} and J_o . Equation (22) states that efficiency is directly proportional to the product of short current density and open voltage in SiGe solar cell.

6. Conclusions

Sunlight is a source of infinite energy and as days are down solar cell efficiency is approaching theoretical limit. The Ge concentration in the SiGe-based solar cell has been investigated qualitatively by the MATLAB theoretical calculation and simulation. Some parameters which directly affect the efficiency are simulated and taken under consideration for having better efficiency, which can be improved with the convenient Ge addition to the SiGe solar cell; from (22) the most appropriate Ge mole fraction is considered so that the increase in short circuit current density without affecting the open circuit voltage will lead to high efficiency.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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