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Numerical Simulation of $Si_{1-x}Ge_x$ Thin Film Solar Cell Using AMPS - 1D

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Abstract: *Crystalline silicon-germanium ($Si_{1-x}Ge_x$) alloy based single junction solar cells with graded Ge fraction are simulated as intrinsic (i) layer between p-doped and n-doped hydrogenated amorphous Si (a-Si: H) layers. In this paper, I have used the global air mass AM 1.5G (one sun) illumination (1 kW/m^2, 0.32 - 1.3 µm) to calculate the optimum efficiency of single junction solar cells with different band gap energy by varying Ge concentration with the help of one dimension simulation program AMPS-1D that was initially developed at the Pennsylvania State University, USA. Alloys that have a lower band gap can extend infrared response of a silicon cell and hence increase the current generation but simultaneously it will also cause the device to suffer loss in voltage. The enhancement of efficiency with respect to pure Si by incorporating SiGe alloys into thin film single and multilayer structures shows that such loss in voltage overcomes the increase of current within the device of thickness less than 6 µm. The optimum efficiency is obtained by introducing multi (four) i-layers in the step of 25% increasing Ge concentration including a germanium like $Si_{1-x}Ge_x$ layer of 0.90 mole fraction (x) towards the back surface of the device and shows better result to the efficiency with respect to pure Si cell. Multilayer approach of single junction SiGe becomes insignificant in comparison to the pure Si as i-layer for device thickness greater than about 6 µm. The whole range of Ge concentrations, p-layer thicknesses from 1 – 100 nm and surface recombination velocities from 10 – 10^7 cm.s^{-1} are explored. In the simulation, the current density-voltage (J-V) characteristics are performed by varying Ge concentration and the quantum efficiency by varying total device thickness from 1 to 60 µm.*
Keywords: *AMPS-1D simulation, conversion efficiency, SiGe thin film, solar cell, quantum efficiency.*

I. Introduction

Solar energy can be used for multipurpose from among the various renewable energy sources especially for solar cell. In future solar cell will take much important role in daily life for new generation at the edge of finishing of conventional energy sources. Characteristic properties and abundances of silicon and germanium inspire humankind to invent efficient solar cell. The thin film processing is one of the technologies to make such cells with high efficiency, consuming less material, low process temperature and providing the capability of large-area production [1, 2]. However, enhancement of efficiency in Si solar cell is one of the methods to introduce a lower band gap material into the device. Germanium is such lower band gap material to absorb the infrared wave in solar spectrum in addition to the efficient front surface light trapping of the cell and hence increase the photo generation. Also Si and Ge are completely miscible in all respects like lattice matching, vapour pressure etc. to construct graded solar cell of multi-layer structures [3].

Healy and Green have studied bulk devices using low Ge concentrations (x) using from 0 to 28% of Si-Ge alloys [4]. Ruiz et al [5] have looked at mono crystalline devices and have determined the absorption coefficients for photon energies of 0.6 to 1.5 eV and have concluded that a Ge concentration of 50% is optimal for bulk devices. Chirstoffel et al [6] have modeled the bulk hetero-structures using germanium concentrations about 30% with alloy layer of 10 to 40 µm and have predicted an efficiency gain of up to 0.7% without the use of light trapping. Kochier et al [7] have used PC1D (a one-dimensional circuit simulation package) to simulate the effect of incorporating a layer of $Si_{1-x}Ge_x$ alloy into the multilayer structure and have shown the optimal efficiency for high Ge concentration. Researchers have been performed much work on $Si_{1-x}Ge_x$ alloy based solar cells. However, improvement in the efficiency of the thin film based solar cells is a challenge for them.

II. Simulation Model with AMPS-1D

The theoretical calculations carried out using AMPS-1D (Analysis of Microelectronic and Photonic Structures) for the analysis were based on Poisson's equation and the first-principle continuity equations of electrons and holes [8] and used to analyze the carriers transport behavior of semiconductor electronic and optoelectronic device structures including solar cells.

In one dimension case, Poisson's equation is written as;

$$\frac{d}{dX}\left(-\varepsilon(X)\frac{d\Psi}{dX}\right) = q * [p(X) - n(X) + N_D^+(X) - N_A^-(X) + p_t(X) - n_t(X)] \quad (1)$$

where, the electrostatic potential Ψ, the free electron n , free hole p , trapped electron n_t, and trapped hole p_t as well as the ionized donor-like doping N_D^+ and ionized acceptor-like doping N_A^- concentrations are all functions of the position co-ordinate X. Here, ε is the permittivity and q is the magnitude of charge of an electron. The continuity equations for the free electrons and holes in the delocalized (band) states of the conduction band and valence band, respectively, have the forms:

for electron ; $$\frac{1}{q}\left(\frac{dJ_n}{dX}\right) = -G_{op}(X) + R(X) \quad (2)$$

and for hole; $$\frac{1}{q}\left(\frac{dJ_p}{dX}\right) = G_{op}(X) - R(X) \quad (3)$$

where J_n and J_p are, respectively, the electron and hole current densities. The term R(X) is the net recombination rate resulting from direct band-to-band recombination and indirect Shockley-Read-Hall (SRH) recombination through gap (localized) states and the term $G_{op}(X)$ is the optical generation rate as a function of X due to externally imposed illumination.

The AMPS-1D can operate in two distinct modes: the density of state (DOS) mode or the lifetime mode. The DOS mode allows the definition of multiple defect states using densities, energy distribution, and capture cross-sections. The lifetime model does not allow the said recombination processes, where inputs are given in the form of carrier life times, which are assumed constant, independent of light and voltage bias. In this paper, a combination of crystalline Si and Ge semiconductors as intrinsic layers is employed to design a multi-stacked hetero layer solar cell using the DOS mode.

III. Modeling Parameters

Band gap (E_g) : The stacked layers are formed by different band gaps of SiGe alloys which can be tailored from 1.12 eV to 0.66 eV. Sant et al [9] have developed two equations by nonlinear spline and polynomial interpolation methods in which one allows the fundamental band gap to be calculated for germanium contents of less than 85% and another greater than 85%. The common understanding is that the band structure of $Si_{1-x}Ge_x$ alloys changes from silicon like to germanium like at a Ge percentage of around 85%. This change shows itself as a rapid decrease in band gap of the alloys between 85 and 100%. The developed energy gap equations by Sant et al with Ge mole fraction (x) in $Si_{1-x}Ge_x$ alloy are as follows

$$E_g\,(eV) = 1.106 - 0.454x + 0.208x^2 \ldots\ldots \quad \text{for} \quad x < 0.85 \quad (4)$$
$$= 2.089 - 1.498x + 0.066x^2 \ldots\ldots \quad \text{for} \quad x > 0.85 \quad (5)$$

Absorption coefficient (α): Efficiency of solar cell depends on some factors including absorption coefficient that plays a significant role as a function of energies of incident photons, band gap and phonon for indirect transition. Braunstein et al [10] have shown the two-step phonon assisted transition for indirect band gap semiconductor materials where both energy and momentum are conserved and the corresponding absorption coefficient for SiGe solar cell can be determined from the following expression of Macfarlane and Robert as

$$\alpha\,(cm^{-1}) = A\left[\frac{(h\gamma - E_g - \bar{E}_{ph})^2}{1-\exp(-\bar{E}_{ph}|kT)} + \frac{(h\gamma - E_g + \bar{E}_{ph})^2}{\exp(-\bar{E}_{ph}|kT)-1}\right] \quad (6)$$

where, hγ and $\bar{E}_{ph}$ are, respectively, the energy of incident photon and average energy of all contributed phonon and A be the average weighing factor of the absorption coefficient. The first and second term in the right hand side of above equation represents the phonon assisted emission and absorption process, respectively. For SiGe alloys A and $\bar{E}_{ph}$ are taken as 3200 and 50 meV, respectively [11]. Also other parametric equations as a function of x are given by

Electron affinity (χ) : in eV $$\chi(x) = 4.05(1-x) + 4.0x\ ^* \quad (7)$$

Electron mobility (μ_n): in cm^2/V-s $$\mu_n(x) = 1500(1-x) + 3900x\ ^* \quad (8)$$

Hole mobility (μ_p): in cm^2/V-s $$\mu_p(x) = 450(1-x) + 1900x\ ^* \quad (9)$$

The * marked equations are obtained from the linear approximation of the corresponding parameters of Si and Ge.

Relative permittivity ($\boldsymbol{\varepsilon_r}$)[12]: The relative permittivity or dielectric constant is a measure of optical properties of SiGe alloy layers and is given by the following relation as a function of x

$$\varepsilon_r(x) = 11.8 + 4.2x \quad (10)$$

Effective density of states $(\mathbf{N_C}, \mathbf{N_V})$ **:** The electron and hole concentration in conduction and valence band in a semiconductor can be written, respectively, as

$$n = N_C e^{\frac{(E_f - E_c)}{kT}}, \text{and} \quad p = N_V e^{\frac{(E_v - E_f)}{kT}} \quad (11)$$

where, N_C , E_c and N_V , E_v are the effective density of states and mobility edges in the conduction and valence band, respectively. E_f is the Fermi level at absolute temperature T and k be the Boltzmann constant. The data of intrinsic concentration (n_i) of $Si_{1-x}Ge_x$ solar cell for all Ge mole fractions has been taken from the graphical representation by Kochier et al [7] from where N_C can be calculated by knowing N_V [12], n_i and putting the value of E_g from equations (4) and (5) in the following two relations, respectively.

$$N_V\ (cm^{-3}) = [0.6x + 1.04(1-x)] \times 10^{19} \quad (12)$$

, and $$n_i^2(cm^{-6}) = np = N_C N_V e^{-E_g/kT} \quad (13)$$

IV. Cell Structures

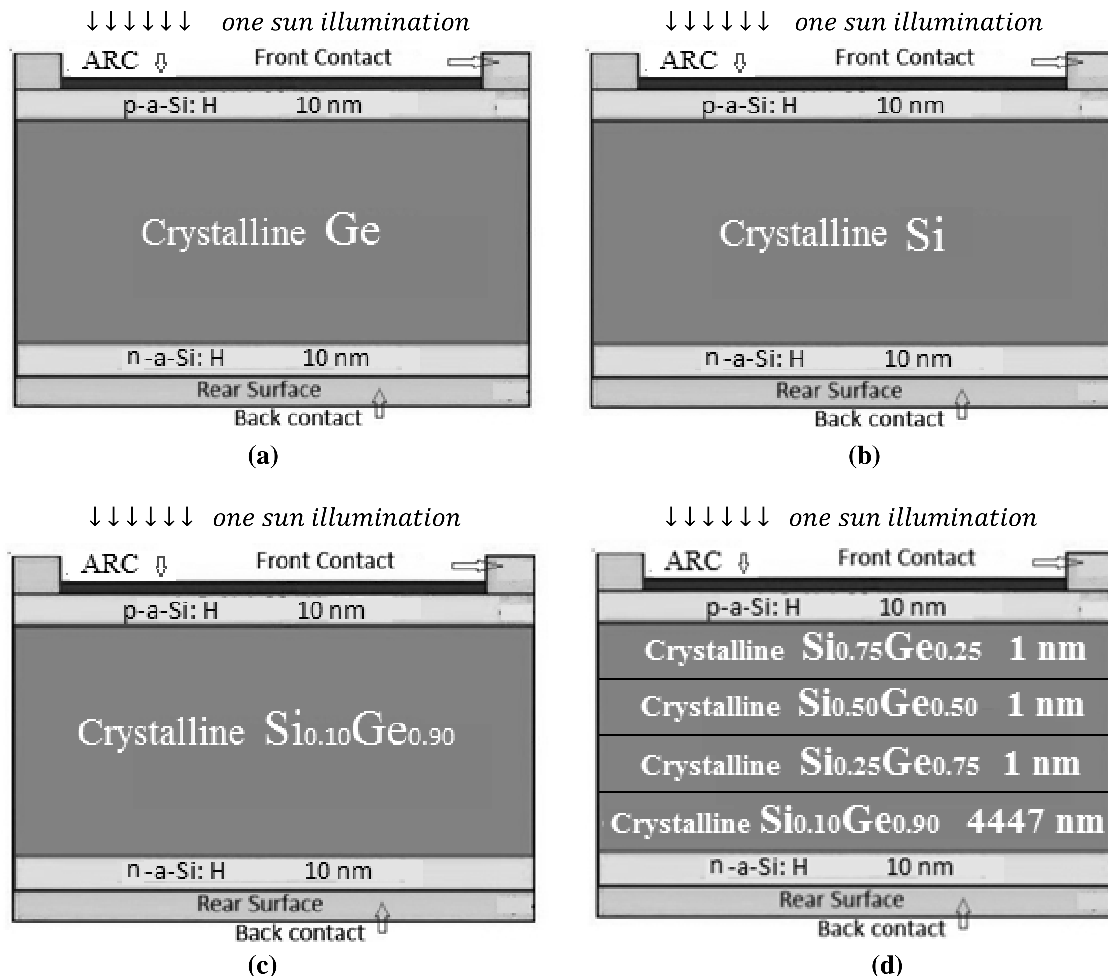


Figure 1: Schematic diagram of single junction solar cell structures with i-layer crystalline (a) Ge, (b) Si, (c) $Si_{0.10}Ge_{0.90}$, and (d) multi Si_xGe_{1-x} layers for the total device thickness of 4.47 µm.

V. Parameters for the $Si_{1-x}Ge_x$ Solar Cells

Table: Model parameters used in the simulation for **(a)** p-layer a-Si: H, **(b)** n-layer a-Si: H and for crystalline i-layers of **(c)** Ge, **(d)** Si, **(e)** $Si_{0.75}Ge_{0.25}$, **(f)** $Si_{0.50}Ge_{0.50}$, **(g)** $Si_{0.25}Ge_{0.75}$ and **(h)** $Si_{0.10}Ge_{0.90}$.

*Energy gap for p-a-Si: H and n-a-Si: H layers are taken same from intrinsic a-Si: H [13].

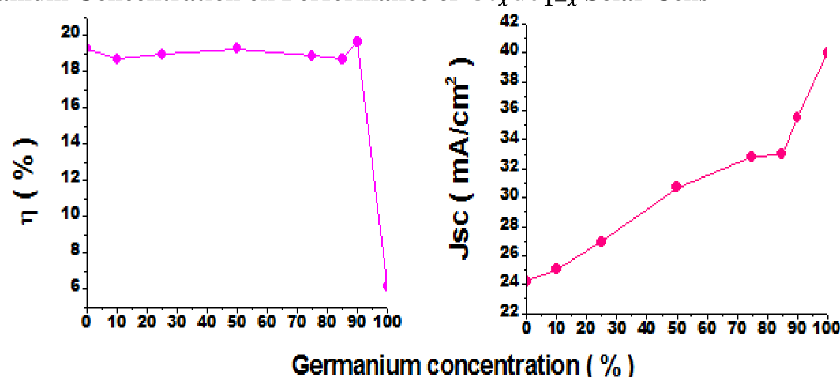
Parameters	Numerical values for							
	(a)	**(b)**	**(c)**	**(d)**	**(e)**	**(f)**	**(g)**	**(h)**
Dielectric constant	11.9	11.9	16	11.8	12.85	13.9	14.95	15.58
Energy gap (eV)	1.72*(**1.82**)	1.72	0.66	1.12	1.01	0.93	0.88	0.87
Mobility of electron (cm^2/V-s)	10	20	3900	1500	2100	2700	3300	3660
Mobility of hole (cm^2/V-s)	1	2	1900	450	812.5	1175	1537.5	1755
Intrinsic carrier concentration, n_i (cm^{-3})	-	-	2.40×10^{13}	1.0×10^{10}	8.70×10^{10}	4.20×10^{11}	1.33×10^{12}	2.75×10^{12}
Effective density of states in conduction band, N_c (cm^{-3})	2.5×10^{20}	2.5×10^{20}	1.02×10^{19}	5.73×10^{19}	5.08×10^{19}	7.65×10^{19}	1.37×10^{20}	3.41×10^{20}
Effective density of states in valence band, N_v (cm^{-3})	1.5×10^{20}	1×10^{20}	6.0×10^{18}	1.04×10^{19}	9.30×10^{18}	8.20×10^{18}	7.10×10^{18}	6.44×10^{18}
Acceptor /Donor concentration (cm^{-3})	3×10^{19}/	/1×10^{19}	-	-	-	-	-	-
Electron affinity (eV)	3.8	3.8	4.0	4.05	4.04	4.03	4.01	4.0

VI. Results and Discussions

In this paper, several Si_xGe_{1-x} single junction solar cells are designed by varying germanium concentrations from $0-100\%$ of intrinsic (i) layer between doped p-type and n-type hydrogenated amorphous Si (a-Si:H). The photo-generated short-circuit current density (J_{SC}) and the open-circuit voltage (V_{OC}) of each structure under $AM\ 1.5G$ (one sun) illumination (1kW/m^2, 0.32 - 1.30 μm) of photon flux from ASTM G173-03 [14] are simulated for different cell thickness varying from 1 to 60 μm. The fill factor (FF) in conjunction with V_{OC} and J_{SC} determines the maximum power $(V_{mp}J_{mp})$ per m^2 from the solar cell which is defined as the ratio of the product of V_{mp} $and\ J_{mp}$ to the product of V_{OC} and J_{SC} of the cell i.e. $FF = \frac{V_{mp}J_{mp}}{V_{oc}J_{sc}}$ and in addition, the conversion efficiency (η) $= \frac{V_{mp}\ J_{mp}}{P_{in}}$, where P_{in} be the incident power of photon per m^2 on the solar cell.

Fig. 2 shows the variation of performances $(\eta, J_{SC}, V_{OC}$ and $FF)$ as a function of Ge concentration of i-layer of thickness of 4.45 μm between 10 nm of each p-a-Si:H and n-a-Si:H layers of the cell (Fig. 1). It is observed that V_{oc} decreases with decrease of band gap (E_g) as the germanium concentration increases. But this decrease is quite small compared to the increase of J_{sc} leading to an overall optimum increase in η (19.68%) at 90% concentration of Ge corresponding to E_g of 0.79 eV relative to pure Si solar cell. This leading performance of efficiency for thin film SiGe alloy based solar cell continues to device thickness of about 6 μm (Fig. 3) and then it becomes insignificant compared to the efficiency of crystalline Si cell. Similarly the FF decreases very slowly with increase of germanium concentration and a sharp drop is observed at pure Ge. It is also observed that except short-circuit current, the other parameters (η, V_{OC} $and\ FF$) of pure Ge are not promising and therefore is not suitable for single junction solar cell applications. Another notable observation is that from 85% Ge concentration, the performances of $Si_{1-x}Ge_x$ alloys have changed significantly from silicon like to germanium like.

Effect of Germanium Concentration on Performance of Si_xGe_{1-x} Solar Cells



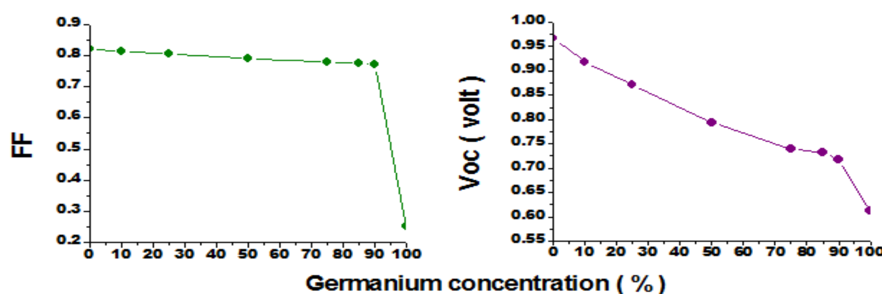


Figure 2: Variations of η and J_{SC}; V_{OC} and FF as a function of germanium concentration.

A comparison of efficiency with i-layer thickness from 1 – 60 µm for crystalline Si, $Si_{0.10}Ge_{0.90}$ and multi (four) $Si_{1-x}Ge_x$ alloy layers is shown in Fig. 3. It is observed that the η of single junction SiGe alloy based thin film device (fig. 1c) of 0.90 Ge concentration and multi layer device (fig. 1d) predominate (e.g., by 1.29% at 1µm device thickness) with respect to pure Si for cell thickness less than 6.37 µm and after that they change their dominancy leading to high efficiency for crystalline Si as absorbing layer. It is also shown from Fig. 3 that the solar cell for multi (four) i-layers, the efficiency curve almost merges the curve of single i-layer cell of 90% Ge concentration. When the model parameters within first bracket in Table are taken by remaining other parameters same, then the dominancy of the efficiency (e.g., by 1.21% at 1µm) for SiGe alloy (fig. 1d) remains within the same device thickness ($\sim 6.37\ \mu m$) compare to pure Si.

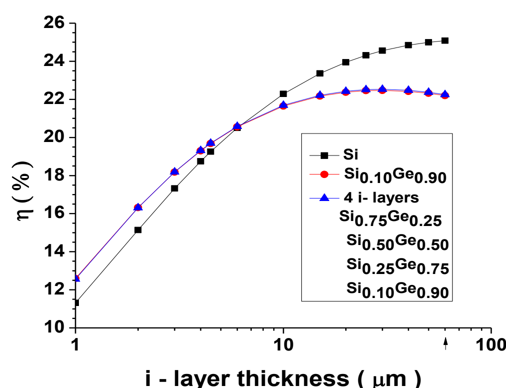


Figure 3: Comparison of efficiency with i-layer thickness for Si, $Si_{0.10}Ge_{0.90}$ and $Si_{1-x}Ge_x$ alloys (four i-layers) in thin film solar cells.

J-V Characteristics of the Solar Cells

Fig. 4 shows the current density (J) – voltage (V) characteristics of Si, Ge and $Si_{1-x}Ge_x$ solar cells for total device thickness of 4.47 µm. It is observed that the curve for Ge cell shows higher J_{SC} that is a common property of low band gap material with significantly low V_{OC} and hence lesser efficiency and fill factor than Si and $Si_{0.10}Ge_{0.90}$ solar cells. The J_{sc} and V_{oc} of SiGe cells compromise between those for Ge and Si cells and ultimately give optimum η (19.70%), for multi (four) i-layers of Ge concentration varying from 25 to 90% as shown in the figure 1 (d).

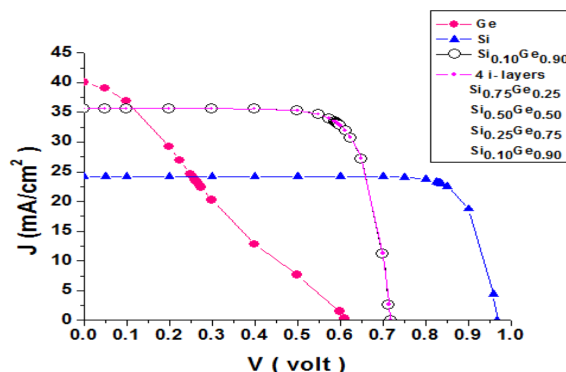


Figure 4: J-V characteristics of Ge, Si and $Si_{1-x}Ge_x$ alloys for i-layer(s) as a parameter of Ge concentration in thin film of 4.47 µm device thickness.

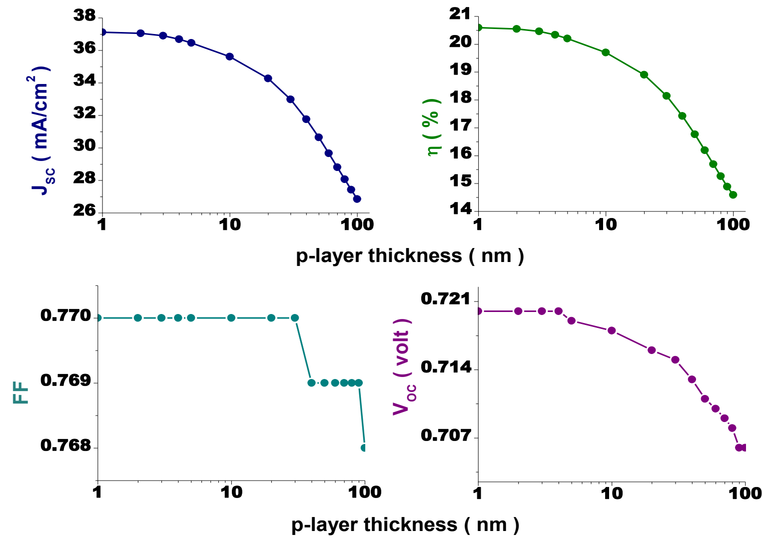


Figure 5: Variations of J_{SC} and η ; FF and V_{OC} as a function of p-layer thickness.

Fig. 5 shows the variation of performances with thickness of p-layer (a-Si: H) for $Si_{1-x}Ge_x$ solar cell. The J_{sc} and V_{oc} values decrease with increase of thickness (p-layer) resulting the decrease of efficiency. This decrease is due to the enhancement of opportunity and time of photo generated carriers to recombine at surface and in bulk as thickness increases before reaching into i-layer. Thus for fabrication of solar cell, in general, the thickness of p-layer should be taken small so that maximum amount of incident light will reach the absorbing layer.

Fig. 6 shows the variation of performances as a function of surface recombination velocity (SRV) from 10 to 10^7 cm/s by setting remaining parameters as constant for $Si_{0.10}Ge_{0.90}$ solar cell. In surface recombination J_{sc} will be largely affected, and high recombination rates at the top surface have particularly detrimental impact on the short circuit current, because top surface also corresponds to the highest generation region of carriers in the solar cell and this impact can be shown in fig. 6 (a). When surface recombination increases then the carrier starts to recombine at the defect surface which reduces the cell performance. Here the V_{oc} remains almost constant and the FF increases as shown in fig. 6(b) for germanium like $Si_{1-x}Ge_x$ cell with the increase of surface recombination by showing maximum efficiency at SRV of 10^3 cm/s. The η value as shown in fig. 6(c) increases sharply for lower SRV as fast as FF and then decreases without changing V_{oc} and FF due to the decrement of short circuit current for surface recombination.

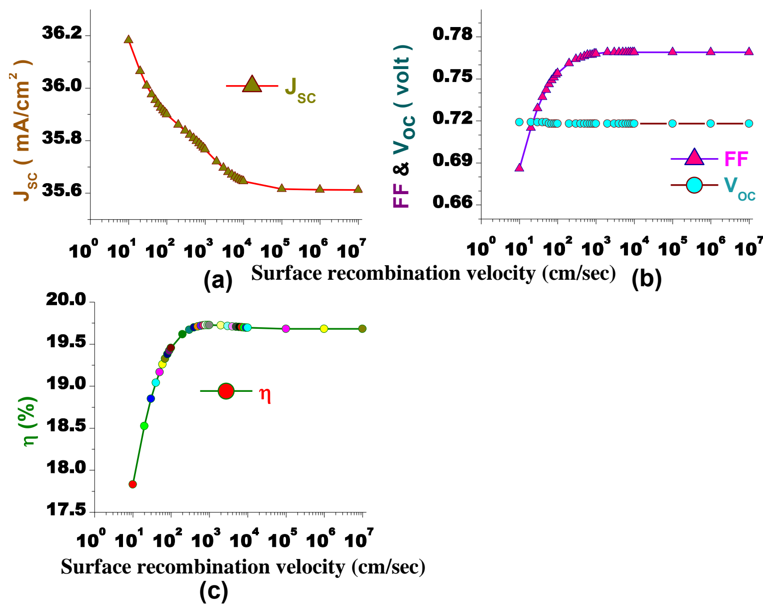
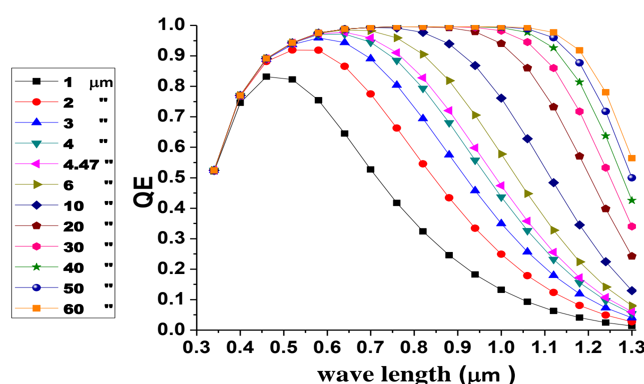


Figure 6: Variations of (a) J_{SC} , (b) FF & V_{OC} and (c) η , as a function of surface recombination.

Quantum Efficiency as a function of Cell Thickness

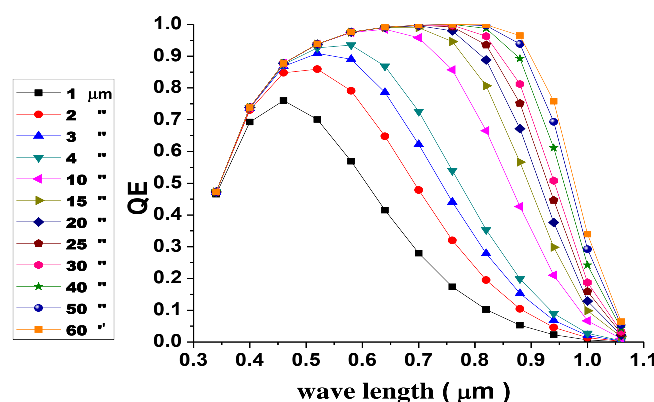
The term quantum efficiency (QE) of the solar cell is defined as the ratio of the number of minority carriers collected by the cell to the number of photons of a given energy incident on the cell. If all photons of certain energy are absorbed and the resulting minority carriers are collected, then the quantum efficiency at that particular energy is unity. The quantum efficiency for photons with energy below the band gap is zero.

Fig. 7(a) shows the QE spectra of the $Si_{1-x}Ge_x$ cell (x of 0.90) as a parameter of device thickness (1–60 μm) by varying i-layer thickness for high SRV of 1.0×10^7 $cm.s^{-1}$ of electrons and holes at the front and back surfaces of the device. It can be observed that for higher thickness, the cell shows broader QE spectra due to the absorption of more photons which improves the overall efficiency (Fig. 8) of the device. The QE spectra for higher thicknesses of the cell, are not only broader but also closer, reveal the no significant change of the curves and hence in the conversion efficiencies exceeding the cell thickness of about 30 μm. In addition, the QE is about 99% for complete absorption of incident photon for wave length (λ) range from 0.66 to 1.1 μm by using efficient anti reflecting coating (ARC) on the front surface of the cell. There are also sharp decrements of QE for lower and higher λ in solar spectrum, respectively, due to front surface recombination and rear surface recombination as well as small absorptions of photons near the band edge (λ~1.30 μm).



(a)

Similarly, the QE spectra for Si solar cell are shown in fig. 7(b) that explains the low efficiency of the cell corresponding to small quantum efficiency in comparison with SiGe cell for device thickness lower than 6.37 μm. As an example for 1 μm of device thickness, the optimum QE of Si and SiGe (fig. 7a) cells are, respectively, 0.76 and 0.83 for λ of 4597 Å. Therefore, the blue (shorter λ) to infrared response of SiGe is more than pure Si that increases the current generation and hence in the overall conversion efficiency for such smaller device thickness.



(b)

Figure 7 QE spectra of solar cells (a) $Si_{0.10}Ge_{0.90}$ and (b) Si as i-layer for different device thickness shows that higher thickness absorbs more photons which improves the overall efficiency of the cells.

Open Circuit Voltage, Fill Factor, Short Circuit Current and Efficiency as a function of Cell Thickness

Fig. 8 shows the variation of the V_{OC}, FF and J_{SC} including η as a function of $Si_{0.10}Ge_{0.90}$ cell thickness. It indicates that below 6 μm thickness, the cell shows the very sharp decrease in the J_{SC} compare to moderate and slight increase of V_{OC} and FF, respectively, and therefore decrease in the η.

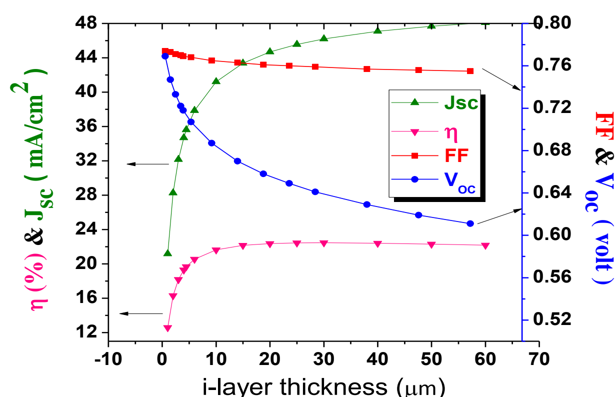


Figure 8: Variations of η , J_{SC} and FF, V_{OC} as a function of device thickness.

VII. Conclusion

The optimum performance of the $Si_{1-x}Ge_x$ single junction solar cell is simulated by AMPS-1D to study the dependence on germanium concentration, absorber layer thickness, p-layer thickness and on surface recombination. The best performance for single i-layer SiGe cell is verified at Ge concentration of 90% for thin film of device thickness below 6.37 μm. Optimum efficiency is obtained as 19.70% for multi (four) i-layers of $Si_{1-x}Ge_x$ cell compare to the results of 19.68% and 19.25%, respectively, for single i-layer germanium like $Si_{0.10}Ge_{0.90}$ cell and for pure Si cell at 4.47 μm device thickness. Another important conclusion is that SiGe cells are significant only for thin film of device thickness less than about 6 μm compare to pure Si and after that only pure Si is sufficient to make high efficient cells as absorbing layer. This work also looks that only for 1 nm thickness of p-layer of amorphous hydrogenated Si and for surface recombination velocity of 10^3 cm-s^{-1} of electrons and holes, the cells show optimum efficiency and for multi i-layers cell it is 20.589% for high surface recombination velocity ($\sim 10^7$ cm.s^{-1}). It is also observed that the conversion efficiency increases until the device thickness reaches at around 30 μm for $Si_{0.10}Ge_{0.90}$ cell and 60 μm for Si cell. There are also very sharp increase of J_{sc} compare to small decrease of V_{oc} with thickness and hence increase in the efficiency below the device thickness of 6 μm.

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