Numerical Modeling of Silicon/Germanium (Si/Ge) Superlattice Solar Cells

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Abstract: - Crystalline silicon (Si) is one of the most widely used materials for solar photovoltaic (PV) cells. Nevertheless, its absorption at the low energy (Infrared, IR) and near-infrared regions is weaker than the visible light. These limitations can be overcome by employing germanium (Ge) material to enhance the absorption of solar photons, particularly for the red and near-infrared range. The strategy is to improve the infrared absorption spectrum of Si/Ge solar solar cell by arranging the silicon and germanium materials in superlattice (multilayer) structures where more lights can be absorbed by the solar cell which will increase its efficiency. In this paper, PC1D solar cell modeling software has been used to simulate and analyze the effects of the germanium thickness on the silicon/germanium superlattice (multilayer) solar cell. The performance between the conventional Si solar cell and Si/Ge superlattice solar cell is examined as well. The total thickness is limited to 1µm of both Si and Si/Ge superlattice solar cells. The simulation result shows that the efficiency of 10.16% (V_{OC} = 0.4521V, I_{SC} = 3.337A, FF =0.6734) is achieved with 0.2µm-Ge and 0.2µm-Si window layer, and 0.6µm-Si absorber layer.

Key-Words: - Silicon, germanium, solar cell, multilayer, superlattice Si/Ge, PC1D.

1 Introduction

Solar cells based on crystalline silicon-germanium alloys (SiGe) or multiple bandgap materials have gained much interest in recent years [1]–[5]. Germanium has a great potential application in solar cells due to its capability to absorb photons in low energy. The higher efficiencies can be expected by developing multiple bandgap material due to higher currents yielded from a lower bandgap.

The lattice mismatch about 4.2% between crystalline Silicon (Si) and Germanium (Ge) can be solved by using graded Ge composition layers [6], symmetrically strained Si/Ge superlattices [7], or a SiGe three dimensional(3D) growth mode also known as Stranski–Krastanov (S–K) growth [8].

In this paper, the numerical modeling for Si/Ge quantum well superlattice (multilayer) has been performed using solar cells simulation software PC1D version 5.9. Numerical modeling is a tool to investigate the performance of the designed solar cell as well as examine its practicality.

Superlattice structure has the ability to increase the material's resistance to shearing effects. This resistance can withstand high stresses compared to the conventional materials. Another advantage of this structure is its ability to produce new varieties of semiconductors.

2 Theories

The ideal characteristics of most solar cells can be specified by solving the basic equations of semiconductor physics such as the Poisson's equation, current density equation and continuity equations [9].

2.1 Poisson's Equation

Poisson's equation is the first equation in the system with broad utility in electrostatics. The expression of the Poisson's equation is one of Maxwell's equations and a differentiated form of Gauss's Law which the divergence of the electric field is proportional to the space charge density, ρ.

$$\frac{d\xi}{dx} = \frac{\rho}{\varepsilon} \tag{1}$$

where, ε represents the material's permittivity.

2.2 Current Density Equations

Current density is an essential equation to the design electrical and electronic systems. It is a measure of

the density of flow of a conserved charge and defined as a vector whose magnitude is the current per cross-sectional area. The following expressions show the equations for the total current densities of electrons and holes, J_e and J_h, respectively.

$$J_e = q\mu_e n\xi + qD_e \frac{dn}{dx} \qquad (2)$$

$$J_h = q\mu_h p\xi - qD_h \frac{dp}{dx} \qquad (3)$$

where n is the electron density in the conduction band, p the density of valence band holes, ξ is an electric field, and q is the electronic charge. μ_e and μ_h are electron and hole mobilities whilst D_e and D_h are the electron and hole diffusion coefficients, respectively.

2.3 Continuity Equations

The continuity equation states that a change in electron/hole density over time is due to the differences between the entering and exiting flux of electrons/holes plus the generation and minus the recombination.

$$\frac{1}{q}\frac{dJ_e}{dx} = U - G \qquad (4)$$

$$\frac{1}{q}\frac{dJ_h}{dx} = -(U - G) \qquad (5)$$

where, G denotes the net generation which is induced by the external action, and U is the net recombination rate. The net increasing rate must be zero in steady state conditions.

3 Thin Film Solar Cells Simulation

Feutch [10] recommended that the built-in potential of a heterojunction can be greater than a homojunction made from a smaller bandgap material and as a result, the dark saturation current can be smaller [5]. Germanium (Ge) with the higher bandgap material is a way to decrease the V_{OC}. Ge has the potential to absorb infrared (IR) light whose absorption coefficient is high whilst the Si is expected to be very good for a short wavelength response absorption.

The simulations for both solar cells are performed to analyze their characteristics. Fig. 1 illustrates the schematic of Si and Si/Ge superlattice solar cells model separately that consists of a 100cm^2 solar cell device area, comprises of series and shunt resistances as well as a pyramid textured shallow diffused emitter. The front reflectance across the solar spectrum is set to 10%.
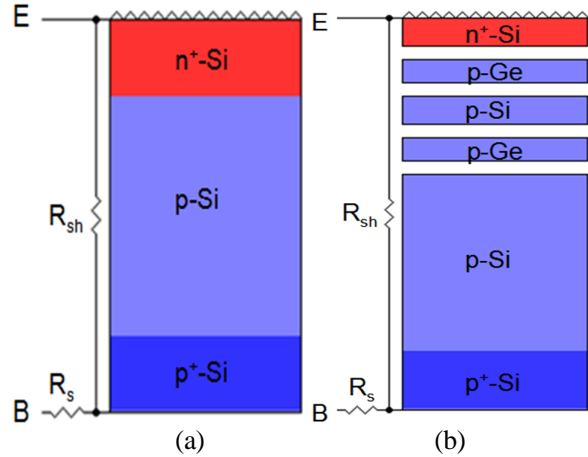

Fig. 1. Device schematic used for PC1D simulation (a) Si solar cell (b) Si/Ge superlattice solar cell

Table 1: Material parameters used in Si solar cell simulation

Solar Cell Structure	Thickness (nm)	Doping Concentration (cm^{-3})
n$^+$-Si	100	1×10^{20}
p-Si	800	1×10^{16}
p$^+$-Si	100	1×10^{20}

Table 2: Material parameters used in Si/Ge superlattice solar cell simulation

Solar Cell Structure	Thickness (nm)	Doping Concentration (cm^{-3})
n$^+$-Si	100	1×10^{20}
p-Ge	10 – 100	1×10^{16}
p-Si	100	1×10^{16}
p-Ge	10 – 100	1×10^{16}
p-Si	680-500	1×10^{16}
p$^+$-Si	100	1×10^{20}

In this simulation, germanium's thickness is increased from 10nm to 100nm based on the step size of 10nm to keep its thickness on the nanoscale (quantum well). In addition, the thickness of the silicon substrate is reduced by 20nm whilst germanium's thickness is increased to maintain the total thickness of the solar cell in 1μm.

The several parameters of both solar cell models are tabulated in Table 1 and Table 2 individually. The front and rear surface recombination velocities are 1×10^6cm/s and 1×10^5cm/s, respectively.

4 Results and Discussions

Fig. 2 depicts the detailed effects of Germanium layer that has been increased from 10nm to 100nm on the cell parameters such as V_{OC}, J_{SC}, FF and η from PC1D simulation.

It can be clearly seen from Fig. 2 that the Ge insertion shows J_{SC} has increased according to the increasing of Ge layer thickness but with a slight decrease in V_{OC}. There is also a slight fluctuation in FF, which is within the range of 0.6733 and 0.6845 due to the series resistance. However, it will increase when this series resistance is reduced and vice versa. It can also be seen that the V_{OC} decreases with a decreasing bandgap by employing germanium material to the cell. As for the cell's efficiency, it increases with an increased thickness in Ge layer due to an additional photocurrent resulting from the increased values in J_{SC}.

On the contrary, the solar cell output parameters (V_{OC}, J_{SC}, FF and η) of the conventional Si solar cell remain constant at 0.5811V, 14mA/cm^2, 0.7024 and 5.714% respectively due to the absence of germanium material in the solar cell. The V_{OC} of the Si is greater than Si/Ge because the absence of germanium material tends to lower the recombination rate in the semiconductor. As a result, the higher V_{OC} is achieved. However, the light harvesting (J_{SC}) of the Si is less than Si/Ge superlattice due to the trade-off between V_{OC} and J_{SC}. The higher FF of the Si device structure is obtained due to FF depends on the value of V_{OC}. The FF increases with the increasing of V_{OC} and vice versa. As expected, the efficiency of the Si semiconductor is less than Si/Ge semiconductor because the Ge is capable to absorb photons with low energy at solar spectrum to produce additional photocurrent.

It can also be observed from Fig. 3 that the quantum efficiency is much affected with the increasing of the Ge layer thickness when the wavelength exceeds 606nm. The Ge film thickness of 100nm (quantum well) with efficiency of 10.16% (V_{OC} = 0.4521V, J_{SC} = 33.37mA/cm^2, FF = 0.6735) showed a better result for Si/Ge superlattice solar cell fabrication.

Fig. 4 depicts the comparison of the quantum efficiency between Si and Si/Ge with Ge thickness of 100nm whereby it shows that 100nm thick of Ge layer has achieved the best result than the Si/Ge superlattice. It can clearly be observed from Fig. 4 that the Si solar cell is only capable to absorb the visible light where the maximum absorption is only 75.7% at 462nm and a weak absorption at near IR range about 25.58% (750nm) to 1.6% (1000nm).
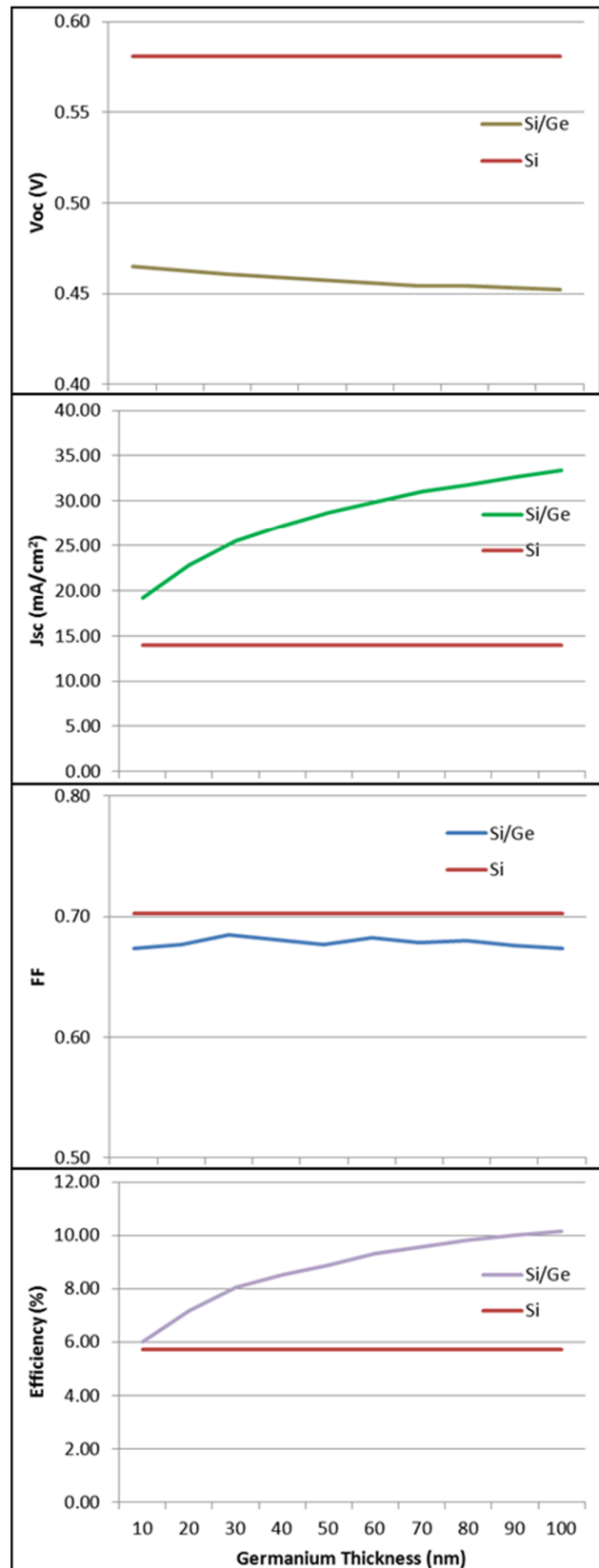

Fig. 2. Effects of Ge thickness on solar cell characteristics.
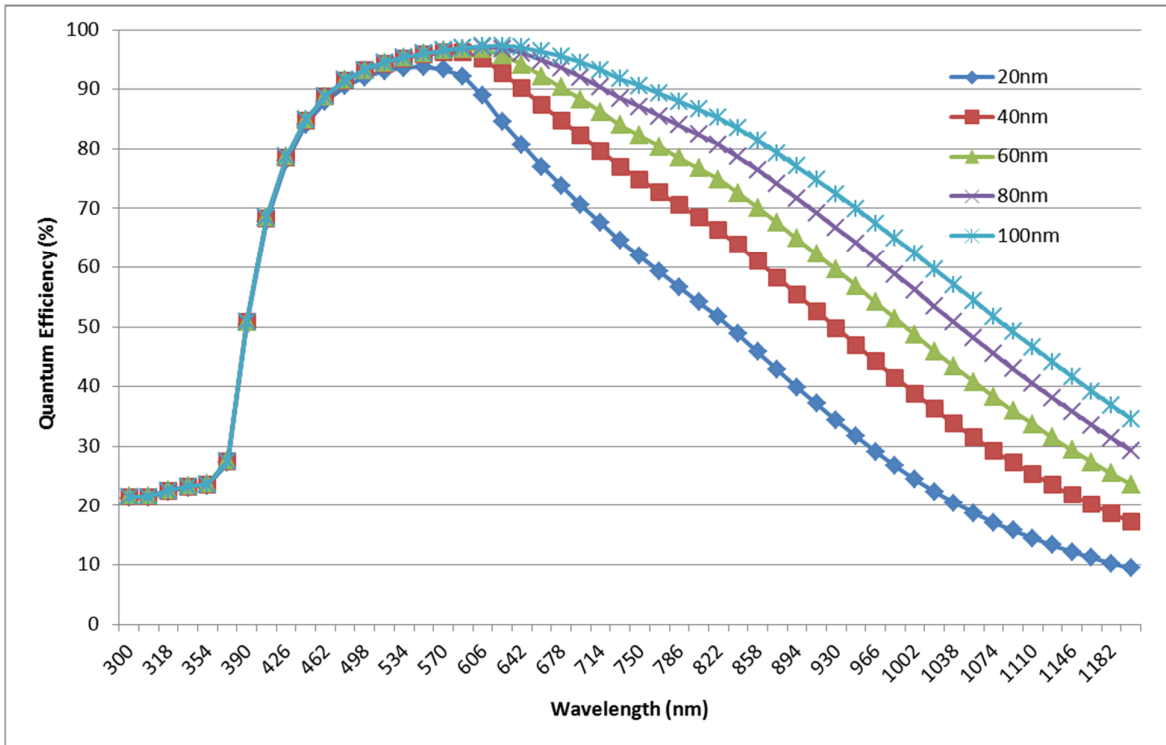
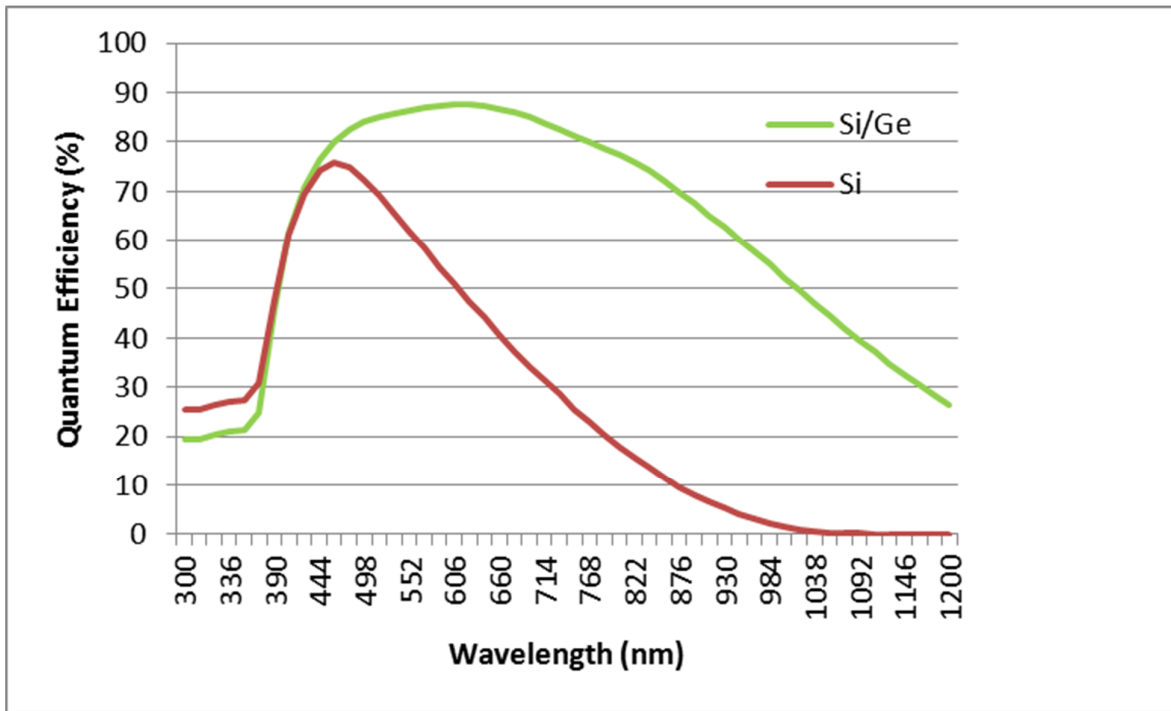Fig. 3.   Effect of Ge thickness on quantum efficiency.

Fig. 4.   Quantum efficiency comparison between the Si and Si/Ge superlattice solar cells.

In contrast, the Si/Ge superlattice solar cell is superior with the ability not only to absorb 90% of photons energy at near IR range but also across the entire IR range – 81.27% at 750nm to 52.31% (1000nm) that clearly improved the properties of Si material.

5 Conclusion

In summary, as the simulations result indicated, a highly efficient 10.16% (V_{OC} = 0.4521V, J_{SC} = 33.37mA/cm^2, FF = 0.6735) Si/Ge superlattice solar cell has been obtained from the numerical analysis with Ge layers thickness of 0.1μm. The Ge employment in thin film solar cells can lead to a significant efficiency improvement if it is employed carefully with pure Si.

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