Modeling and Optimization of High Efficiency Silicon Solar Cell by Using Step Graded $\text{Si}_0.7\text{Ge}_{0.3}$ Layer with Phonon Energy Variation

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Abstract- Using Si$_{1-x}$Ge$_x$ in silicon-based solar cell, which has lower bandgap (Eg) value than silicon, a cell can achieve higher efficiency compared to a conventional Si solar cell. Additionally, Si$_{1-x}$Ge$_x$ layer will improve energy absorption in silicon solar cell, extend its response into infrared region and increase current generation. Performance silicon solar cell using step graded index with 30% content of silicon germanium (Si$_0.7$Ge$_{0.3}$) have bigger efficiency than using step graded with other germanium content. In this paper, silicon solar using step graded Si$_0.7$Ge$_{0.3}$ was simulated using PC1D. The efficiency is then calculated by varying its phonon energy value. The phonon constitute the third particle that involving in photon absorption process (absorption and emission of phonon). Then, we investigated influence of phonon change to performance of silicon solar cell by using step graded Si$_0.7$Ge$_{0.3}$. Efficiency as high as 27.16% can be obtained at optimum thickness of the step graded Si$_0.7$Ge$_{0.3}$, and low value of phonon energy.

Keywords—Phonon, Si$_{1-x}$Ge$_x$ alloy, Absorption coefficient

I. INTRODUCTION

Silicon as solar cell substrate material constitute the most used in solar cell devices. This is because that silicon is cheaper, abundance and not hazardous. However, silicon solar weakly absorb light (photon). Some experts have made a lot of research to overcome this weakness. One way is using Si$_{1-x}$Ge$_x$ layer that can improve efficiency on silicon solar cell.

It has been shown that by using alloy material (Si$_{1-x}$Ge$_x$ alloy) in silicon solar cell modifies material’s characteristic and bandgap (Eg). This alloy is also a lattice match with the substrate [1]. Hence, by using Si$_{1-x}$Ge$_x$ alloy, this solar cell can extend the spectrum of light that being absorbed. This silicon, normally, can only absorb visible spectrum. This paper emphasizes on studying the influence of phonon energy to efficiency of silicon solar cell by using step graded Si$_0.7$Ge$_{0.3}$ to get optimal efficiency.

II. MODELLING WITH PC1D VERSION 5.8

In modelling the solar cell device, the model device uses Si$_{1-x}$Ge$_x$ alloy, the most important parameters needed to model alloys are the fundamental bandgap (Eg), the intrinsic concentration ($n_i$) and the absorption coefficient ($\alpha$) plus the direct and indirect bandgap[2]. In this simulation is focus toward parameter of absorption coefficient (intrinsic absorption).

A. Modeling Parameter

Parameters, used in this simulation, are consistent with the ones published by ar cell by Poespawati et al [3]. Using mol fraction of $x = 30\%$ for Si$_{1-x}$Ge$_x$ alloy, it has been shown that higher performance can be obtained compared to other mol fractions.

For this simulation, the absorption coefficient was taken from PC1D (one-dimensional simulation package) internal model. PC1D has two method of calculating photogeneration for device. First, an internal model, which calculate the absorption coefficient using equation involving the four direct and indirect bandgaps[1]. This calculation has been used by Healy and Green [4]. The second one, using of an external file of absorption coefficient versus wavelength such as has been used by Christoffel et al[5].

Absorption of light that happen in semiconductor material, basically divide in two process, that is, direct-band-gap semiconductor and indirect-band-gap semiconductor. Both direct-band-gap and indirect-band-gap semiconductor are model that used in PC1D. Which for direct-band-gap semiconductor, energy transition for photon with higher energy from energy of direct bandgap is given by:[6]

$$\alpha(hf) = A - (hf - E_g)^{1/2}$$  \hspace{1cm} (1)

where $A^*$ is a constant having numerical value of $2 \times 10^4$, $\alpha$ is absorption coefficient as function of photon energy ($hf$) and $E_g$ is bandgap energy.
Whereas for *indirect-band-gap semiconductor*, energy transition process from valence band to conduction band involving not only photons and electrons but also a third particle, a phonon. Characteristic of phonon have opposite characteristic with photon, phonon have low energy but relatively high momentum. Hence, the minimum photon energy required to excite an electron from valence band to conduction band is:[6]

\[ hf = Eg - Ep \]  

(2)

where \( E_p \) is the energy of an absorbed phonon with the required momentum.

At *indirect-band-gap semiconductor*, the absorption of photon involve two step process are phonon emission or absorption. An analysis of the theoretical value of the absorption coefficient gives the results [6]:

\[ \alpha_a(hf) = \frac{A(hf - Eg + Ep)^2}{\exp(Ep/kT) - 1} \]  

(3)

for a transition involving phonon absorption, and

\[ \alpha_e(hf) = \frac{A(hf - Eg - Ep)}{1 - \exp(-Ep/kT)} \]  

(4)

For one involving phonon emission. Since both phonon emission and absorption are possible \( hf > Eg + Ep \), the absorption coefficient is then [6]:

\[ \alpha(hf) = \alpha_a(hf) + \alpha_e(hf) \]  

(5)

### B. Phonon

In physics, phonons is a quantized mode of vibration in a rigid crystal lattice, such as the atomic lattice of a solid. The study of phonons is an important part of solid state physics, because phonons play an important role in many of the physical properties of solids, such as the thermal conductivity and the electrical conductivity[7].

In real solids, there are two types of phonons: "acoustic" phonons and "optical" phonons. Acoustic phonon related to dominant heat carrier in insulators and technologically important semiconductor. Whereas, optical phonon strongly influence optical properties of semiconductor[8]. In particular, the properties of long-wavelength phonons gives rise to sound in solids, hence the name phonon.

As we mentioned in indirect-band-gap semiconductor above, energy that absorbed by phonon require momentum (p). For all practical purpose, a phonon acts as if it carries a momentum p, which is sometimes called the crystal momentum. Therefore, if transition of energy undergo higher momentum also energy that absorbed by phonon is bigger. This matter can be seen from f Hamiltonian equation: [7].

\[ H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2} me\omega \sum_{\langle i|j|\omega \rangle} (x_i - x_j)^2 \]  

(6)

with

\[ p = \hbar k \]  

(7)

where \( p \) is crystal momentum, \( k \) is wave vector of phonon, \( x_i \) is position from for the \( i \)th atom, and \( m \) is mass. From hamiltonian equation, energy of phonon is influenced by kinetic energy (p) and potential energy(x).

In Hamiltonian equation, We introduce a set of N "normal coordinates" \( Q_k \), defined as the discrete Fourier transforms of the \( x_n \), and N "conjugate momenta" \( p \) defined as the Fourier transforms of the \( p_n \)[7]:

\[ x_j = \frac{1}{\sqrt{N}} \sum_{n=-N}^{N} Q_k e^{ikn} \]  

(8)

\[ p_j = \frac{1}{\sqrt{N}} \sum_{n=-N}^{N} \Pi_k e^{-ikn} \]  

(9)

with the quantity \( k_n \) will turn out to be the wave number of the phonon, i.e. \( 2\pi \) divided by the wavelength. It takes on quantized values, because the number of atoms is finite. The form of the quantization depends on the choice of boundary conditions. we impose periodic boundary conditions, defining the \( (N+1) \)th atom as equivalent to the first atom. Physically, this corresponds to joining the chain at its ends. The resulting quantization is:

\[ k_n = \frac{2n\pi}{Na} \]  

(10)

For \( n=0, \pm 1, \pm 2, \pm 3, \ldots, \pm N \), a is lattice spacing.

From equation of (8) and (9), according to Bloch Theory can be represented by[8]:

\[ e^{iNk.a} = e^{2\pi iN_j x_i} = 1 \]  

(11)

With

\[ x_i = m_j / N_j \]  

(12)

above equation can be know that position each atom influenced by atom mass and conjugate momentum.
According Bloch theory acknowledge that wave vector value of phonon are\[^9\]:

\[
k = \sum_{i=1}^{3} \frac{m_i}{N_i} b_i
\]

and the volume \(\Delta k\) of \(k\)-space per \(k\) adlah:

\[
\Delta k = \frac{1}{N} b_1 \cdot (b_2 \times b_3)
\]

assumption the number of allowed \(k\)-vectors in the primitive cell of the reciprocal lattice is equal to the number of cells in the crystal.\[^9\].

Performance of semiconductor (solar cell) strongly influenced by temperature. The total number of phonons in a system that vibrates (crystal) is related to the temperature of the system. At higher temperatures, vibration of an object is stronger and the number of phonons larger. As every phonon carries a quantum of vibrational energy, this means that energy which absorbed since energy transition process from valence band to conduction band will be higher.

**C. Device Structure Modeled**

The structure, which has been modelled in PC1D, is shown in Fig 1. This structure consists of 5 layer. The first layer is n-type silicon, layer 2 to 4 are n-type step graded \(\text{Si}_{0.7}\text{Ge}_{0.3}\) alloy that formed from three step graded are layer 2 is \(\text{Si}_{0.7}\text{Ge}_{0.3}\), layer 3 is \(\text{Si}_{0.8}\text{Ge}_{0.2}\) and layer 4 is \(\text{Si}_{0.725}\text{Ge}_{0.075}\). Whereas, layer 5 is p-type silicon. The total device thickness is 30 \(\mu\)m with each thickness for n-type silicon is 0,2448 \(\mu\)m, step graded \(\text{Si}_{0.7}\text{Ge}_{0.3}\) is 1 \(\mu\)m (3 nm for \(\text{Si}_{0.7}\text{Ge}_{0.3}\) layer , 987 nm for \(\text{Si}_{0.8}\text{Ge}_{0.2}\) layer and 10 nm for \(\text{Si}_{0.725}\text{Ge}_{0.075}\) layer ), n-type silicon layer is 28, 7552 \(\mu\)m. This device structure has been used by Poespawati et al\[^1\].

**III. RESULT AND DISCUSSION**

At previous section has been explained how transition of energy involving not only photon and electron, but also the third particle, a phonon. Energy of phonons are energy that absorbed at transition of energy process with required momentum. Energy of phonon (Ep) constitute a parameter that related to absorption coefficient in PC1D modeling. In PC1D modeling, Ep refer the parameter for intrinsic absorption (indirect gaps), which Ep have two type: Ep1 and Ep2. Both Ep1 and Ep2 are energy that involving at absorption of photon by two step process involving phonon emission or absorption.

This simulation was committed three variation energy of phonon value are Ep1 constant (Ep2 change), Ep2 constant (Ep1 change), Ep1 and Ep2 change respectively. The whole variation was used for all step graded \(\text{Si}_{0.7}\text{Ge}_{0.3}\) layer, with kind of variation are layer 2 change (layer 3&4 constant), layer 2&3 change (layer 4 constant), layer 2,3&4 change, layer 3 change (layer 2&4 constant) and layer 4 change (layer 2&3 constant).

In this simulation is obtained Short circuit current (Isc), open circuit voltage (Voc) and efficiency of reference are 5.403 Ampere, 0.5721Volts and 25.4157% respectively. The reference value based at simulation results that has been published by Poespawati et al\[^1\], without changing phonon energy value (Ep1 and Ep2).

The simulation results can be seen in Fig 2, 3, 4, 5 and 6. In Fig 2, 3 and 4 the change of phonon energy for layer 2 (layer 3&4 constant) undergo not significant the change of efficiency. Layer 2&3 change (layer 4 constant) undergo the change of efficiency significantly compared with layer 2 change (layer 3&4 constant). And For layer 2, 3 and 4 change undergo the change of efficiency significantly compared with layer 2 change (layer 3&4 constant), but not significant compared with layer 2&3 change (layer 4 constant).

**Fig 2. Ep2 (mEV) versus Efficiency (%), with Ep1 constant (18.26 mEV) for layer 2 change (layer 3&4 constant), Layer 2&3 change (layer 4 constant) and layer 2, 3 and 4 change**
For comparison layer 2&3 change (layer 4 constant) with layer 2,3&4. As we can see both layer 2&3 change (layer 4 constant) with layer 2,3&4 are mostly same in the change of efficiency. But in Fig 5 and Fig 6, we can see that for layer 3 change (layer 2&4 constant) undergo the change of efficiency compared with layer 4 change (layer 2&3 constant), which layer 4 change (layer 2&3 constant) are mostly same with layer 2 change (layer 3&4 constant).

From all simulation result, we can see the change of phonon energy at layer 3 change (layer 2&4 constant) with the thickness 987 nm significantly undergo the change of efficiency compare the other layer. Therefore, the change of efficiency with the change of phonon energy is influence by the thickness of layer. Which each thickness of layer are 3 nm for layer 2, 987 nm for layer 3 and 10 nm for layer 4. The change of efficiency that significant enough at layer 3 (987 nm) constitute the effect from the thickness of layer, where with higher thickness also will cause higher volume $\Delta k$. So with the variation of phonon energy from the smallest to the biggest value of phonon energy will be significant like that we can see in Fig 2, 3, 4, 5 and 6. From the whole simulation that has been done, we can see that the smaller phonon energy will result the higher efficiency. With smaller phonon energy will get higher absorption coefficient, so will affect the efficiency of solar cell.

IV. CONCLUSION

The performance of silicon solar cell by using step graded $Si_0.7Ge_{0.3}$ will be optimal with smaller phonon energy. From the simulation result indicates that the variation of phonon energy influenced by the thickness of layer. This simulation is obtained the significant change of efficiency at layer 3 (thickness 987 nm). The optimal efficiency that obtained is 27.16 % for layer 2, 3 and 4 change with Ep1 and Ep2 also change respectively.

REFERENCE


[1] Natalita M Nursam, “Optimalisasi Desain dan Analisa Terhadap Alas Ga0.85Ge0.15/GaAs heteroface homojunction thin-film solar cell”, Skripsi FTUI, 2004


