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Simulation of Charge Carriers Generation Rate of SiGe Quantum Dot Based Intermediate Band Solar Cell

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Abstract. In this paper, the influence of the utilization of SiGe quantum dot on carrier generation rate for intermediate band solar cell application will be discussed. The simulation performed to calculate the generation rate which is a function of the effective band gap dan the absorption coefficient value of the material has been done with 3 variations of germanium composition and 4 variations of quantum dot size. The performance of SiGe with 50% of Germanium composition will be compared with pure Silicon and pure Germanium while the variations of quantum dot size used are 1nm, 2nm, 3nm and 4nm. Simulation results show that increasing numbers of Germanium atoms within the material combined with larger size of quantum dot leads to higher generation rate and helps broadening the range of photon energy which can contribute on the creation of electron-hole pair. Adding Ge into Si quantum dot is found to be effective to increase the generation rate of electrons and holes.

Keywords: Generation Rate, Quantum dot, SiGe, Solar Cell
PACS: 81.07.Ta, 61.72.uf, 88.40.hj, 72.20.Jv, 42.70.Qs

INTRODUCTION

Silicon-germanium (SiGe) nanostructure has opened new prospects in creating enhanced electronic devices, especially for semiconductor devices. SiGe quantum dot is one form of nano-sized materials whose growth can be done with self-assembled process [1, 2]. There have already been studies on SiGe quantum dot to seek for deeper understanding of this material. In 2002, Tevaarwerk et al used electric force microscopy (EFM) to study the electrical isolation of SiGe quantum dots [3]. In the previous work, a study on the formation of Si/Ge quantum dot [4] and an experiment that confirmed the quantum confinement effect in Si quantum dot with Ge core [5] had also been done. SiGe quantum dot has also been applied in electronic devices such as in solar cells [6], even in optoelectronic devices such as infrared photodetectors and LEDs [1]. In 2010, Lee, Dezsi, and Venkatasubramanian had grown SiGe quantum dot to be applied in thin film solar cell [6]. Fig. 1 shows a sketch of SiGe quantum dot energy band diagram. In this case, SiO_2 acts as the insulator and confines SiGe material. As a nano-scale material, material's effective band gap will change depends on the band gap of bulk material also conduction and valence band offsets which will be formed because the band gap differences between SiGe and SiO_2.

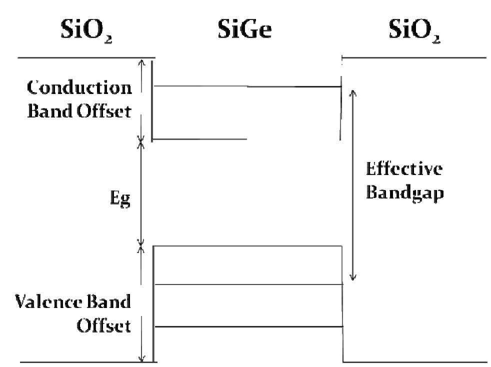

FIGURE 1. Sketch of SiGe quantum dot energy band diagram.

Solar cells were created with the purpose to convert solar energy into power source. This happens when the sun light hits a semiconductor with an amount of energy higher than the energy gap material. The energy will then create a pair of electron and hole. This is when the charge carrier generation occurs. Generated charge carriers will flow and produce

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electrical current. One factor that has limited the conversion efficiency from solar energy into electrical energy in solar cell is that photon with smaller energy cannot contribute on the creation of electrons and holes as free charge carriers. The development of solar cell with the goal of improving efficiency so far has brought us into the third generation solar cell, which is a solar cell with the utilization of quantum structure as its base material.

The utilization of SiGe quantum dot is intended to create intermediate band in solar cell application. Intermediate band solar cell was introduced in 1997 by Luque and Marti who simulated a solar cell with single intermediate band where the maximum efficiency obtained was 63.2% [7]. Furthermore, in 2009, Jenks and Gilmore simulated a solar cell with two intermediate bands with maximum efficiency of 72.8% [8].

Intermediate band solar cell can theoretically help to improve the efficiency of solar cells. Quantum dots that are arranged periodically will form a band in the middle of the forbidden band. The intermediate band in solar cell can be formed as a consequence of the presence of quantum dot bound state in the smaller band gap semiconductor material which is placed between larger band gap semiconductor materials. In intermediate band solar cell, it is important to consider the space between quantum dot. This is to help establish well-placed intermediate band and to prevent symmetry breaking which can result in a failure on the creation of intermediate band [8]. Figure 2 shows the structure of SiGe quantum dot based solar cell.

Intermediate band that formed will become an additional stepping stone for the electrons to excite from the valence band into the conduction band. The purpose of this paper is to investigate the influence of the utilization of SiGe quantum dot on carrier generation rate for intermediate band solar cell application.

CALCULATIONS PERFORMED IN SIMULATION

In this paper, some variations on variables that might affect the properties of SiGe quantum dot were determined. There are 3 variations of Ge composition and 4 variations of quantum dot size that are considered in the simulation. The variations of Ge composition are 0% (pure Silicon), 50% (SiGe), and 100% (pure Germanium) and the variations of quantum dot size are 1nm, 2nm, 3nm and 4nm. The output of this paper is to know the effect of these two variables on the generation rate of SiGe quantum dot.

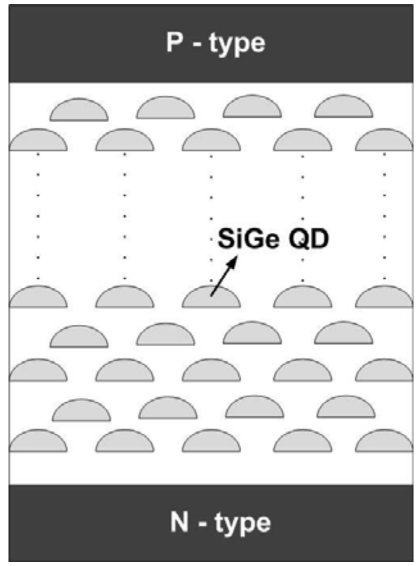

FIGURE 2. SiGe quantum dot based solar cell structure

Once the variations on Ge compositions are determined, the electron affinity can be calculated. The calculation on electron affinity was needed because the depth of conduction band offset and valence band offset are very dependent on the electron affinities of both materials, SiGe quantum dot and SiO_2. The combination between the depth of the offset and the size of quantum dot will affect the space between energy levels within the quantum dot. Eventually, the effective band gap of different dot sizes, which had been determined in the first place, can be calculated.

To be able to find the generation rate, the calculation to find absorption coefficient values needs to be performed beforehand. Absorption coefficient defines the material ability to absorb energy. Every material only absorbs photon with an amount of energy with specific frequency and wavelength. To calculate the absorption coefficient, the formulation is as follow,

$$\alpha(hf) \approx A*(hf - Eg)^{1/2} \qquad (1)$$

where A is a constant with value of $2x10^4$, h is planck's constant, f is photon's frequency, and Eg is material band gap.

Once the absorption coefficient is determined, the generation rate can be calculated with formulation as shown in Eq. (2).

$$G_{th} = \alpha \frac{P_{opt}}{E_{ph} A} \qquad (2)$$

where P_{opt} is the illumination power and E_{ph} is the energy of incoming photon. Generation rate is the number of electrons generated in each unit volume per unit time as a result of photon absorption.

From the equation, generation rate and absorption coefficient are linearly related. Generation is one of the important parameters in solar cell. Generation rate at each photon energy value is different as well at each incoming photon wavelength.

RESULTS

From Fig. 3, the relation of two variables, Ge composition and effective band gap, with the influence of quantum dot size is shown. From the figure, it can be seen that the effective band gap of the material is smaller when there is more Ge composition within the material. Quantum dot size also can be seen affects the effective band gap, where a bigger quantum dot leads to a smaller effective band gap. This shows one of the advantages of using quantum dot where choosing a quantum dot size is intended to obtain an effective band gap value which meets the requirements.

Fig. 4 shows the influence of the presence of Ge composition in Si quantum dot on the generation rate at wavelength range from 400 to 1400 nm. A wider range of wavelength and a higher value of generation rate can be seen as the composition gets bigger. As there is more Germanium in the material, the highest value of generation rate is in a longer wavelength. In Fig. 5, the influence of quantum dot size on the generation rate of SiGe quantum dot is shown. From Fig. 5, the bigger the quantum dot size, the higher the generation rate and the wider the range of wavelength. Both Fig. 4 and Fig. 5 show that the generation rate value is different at different wavelength value.

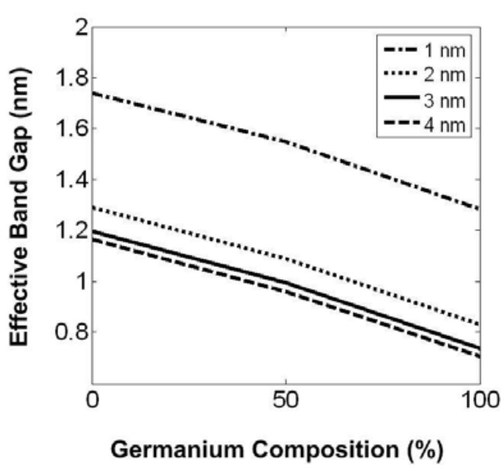

FIGURE 3. Germanium composition effect on SiGe Quantum Dot material effective band gap.

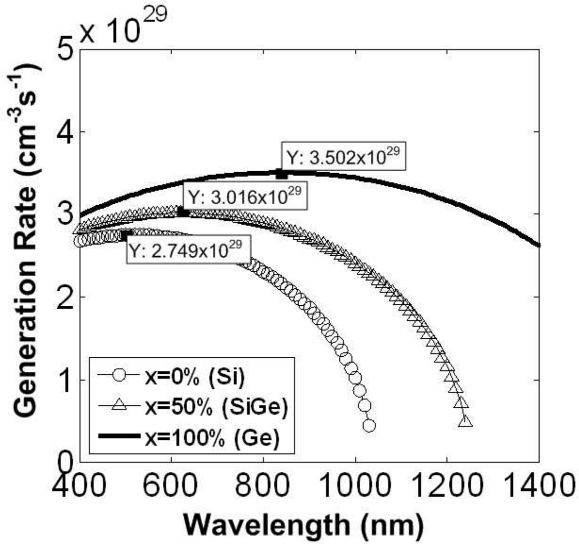

FIGURE 4. Generation rate of Silicon-Germanium quantum dot as a function of wavelength at different Germanium compositions with size of 3 nm

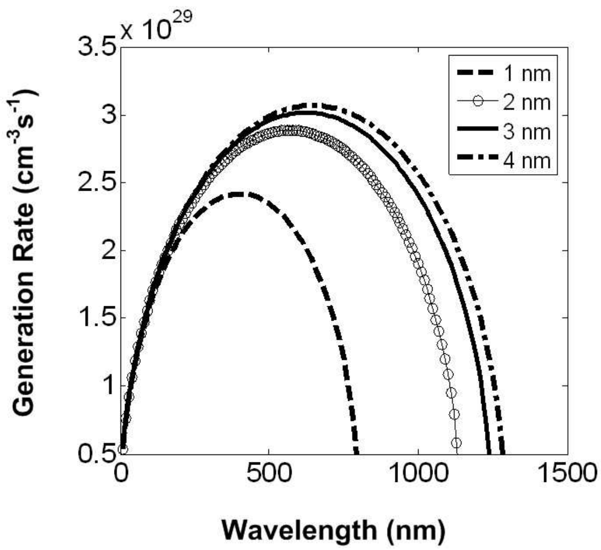

FIGURE 5. Generation rate of Silicon-Germanium quantum dot as a function of wavelength at different quantum dot sizes at 50% Germanium composition

DISCUSSION

The use of SiGe structures on the solar cell was intended to improve the device performance in terms of absorbing part of solar spectrum which in conventional solar cell is usually wasted and maximize the use of incoming solar energy. A combination between Silicon whose band gap is 1.2 nm and Germanium whose band gap is 0.67 nm, will create a material with a band gap between 0.67 to 1.2 nm. It is expected that with the use of this material, the charge carrier generation rate can be higher. By utilizing the near infrared part of the spectrum to create more pairs of electrons and holes, the device current will increase so that overall device efficiency can be increased.

The advantage of using quantum dot is the size adjustment, making it easier for us to obtain an effective band gap needed since changes in size will result in changes in effective band gap of the material. The objective is so that device can absorb the near infrared part of the spectrum can be accomplished by adjusting the size of the quantum dot. As in Fig. 4, differences in size result different effective band gaps. With the knowledge of the size of quantum dot material needed in order to absorb the near infrared part of solar spectrum, our initial objective can be achieved properly.

Fig. 4 shows the influence of the presence of Ge composition in Si quantum dot on the generation rate. A wider range of wavelength and a higher value of generation rate can be seen as the composition gets bigger. As there is more Germanium in the material, the highest value of generation rate is in a longer wavelength, which means that the highest value of generation rate can be obtained with the absorption of lower energy photons.

In Fig. 5, the influence of quantum dot size on the generation rate of SiGe quantum dot is shown. From Fig. 5, the bigger the quantum dot size, the higher the generation rate and the wider the range of wavelength. That means there is also a wider range of photon energy that can contribute to create a pair of electron and hole. For photovoltaic applications, the incident light consists of a combination of many different wavelengths, and therefore the generation rate at each wavelength is different.

From Fig. 4 and Fig 5, the effectiveness of using SiGe were shown. But still, it can be seen in Fig. 4 that pure Ge can give a higher generation rate. In theory, this happens, but experimentally, when pure Ge has a contact with oxide, in this case SiO_2, defects occur and these defects will trap the free electrons resulting on the decreasing of current. Defects on Ge-oxide had been discussed [9,10]. Therefore, the role of Si on the material is still needed since Si interacts better with oxide.

CONCLUSION

The utilization of SiGe quantum dot on intermediate band solar cell in order to achieve a higher generation rate has been simulated. The size of quantum dot is much related to the effective band gap of SiGe quantum dot material as shown in Fig. 3. It can be concluded that an addition of Ge to Silicon quantum dot and a bigger quantum dot size are found to be effective to increase the generation rate of electrons and holes.

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