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Effect of the compositional distribution on the photovoltaic power conversion of SiGe solar cells

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Abstract

Theoretical investigation on the photovoltaic power conversion of SiGe solar cells was carried out focusing on the impact of the compositional distribution. The absorption coefficient and the intrinsic carrier concentration were assumed to be macroscopically uniform parameters controlled by the compositional distribution. Under an assumption with finite minority carrier diffusion length, solar cell based on SiGe was revealed to have power conversion superior to that based on Si in a limited compositional window on the Si-rich side. In the window, the increase in the photocurrent density overcompensates the decrease in the voltage, and controls the overall conversion efficiency. The width of the window was greatly affected by the compositional distribution in SiGe. A comparison was made with experiments to support the existence of such a compositional window.

Keywords: SiGe; Compositional distribution

1. Introduction

The maximum conversion efficiency of a solar cell based on a semiconductor single pn junction can be predicted by the band gap energy as shown by Shockley and Queisser (SQ) [1]. In their theory, the optimum band gap energy is approximately 1.4 eV under air mass (AM) 1.5 spectral irradiation. This is a consequence of the basic assumptions which follow: First, the probability of collection of the solar light with energy higher than the band gap was assumed to be unity, which requires an infinite thickness of the absorber or absorption coefficient. Second, all the photogenerated carriers were assumed to contribute to the output current, which requires infinite diffusion length for the minority carriers. If these assumptions are violated, the optimum band gap energy is obviously not the same as the SQ prediction [2].

In fact, Pan et al. have recently reported superior conversion efficiency for solar cells based on multicrystalline (mc)-SiGe with compositional distribution [3] compared with those based on mc-Si [4]. The band gap of Si, which is the most dominant starting material of commercial solar cells, is 1.1 eV, and the incorporation of Ge results in decrease in the band gap [5,6]. Therefore, in the framework of the SQ prediction, the introduction of Ge to mc-Si gives a decrease in the power conversion, which is not consistent with their experimental results. To account for this discrepancy, we have recently reported a simple calculation for the conversion efficiency of mc-SiGe solar cells with large compositional distribution, and showed that Si-rich mc-SiGe solar cells could surpass mc-Si ones when the diffusion length is finite [7]. However, the assumed compositional distribution, which is the dispersion of pure-Ge in a Si matrix, is far from a realistic one.

In this paper, we carried out theoretical investigation on the photovoltaic power conversion of SiGe employing a more realistic compositional distribution. The performance of the SiGe solar cells was calculated by solving one-dimensional steady-state continuity equation under AM1.5 by assuming macroscopically uniform absorption coefficient and intrinsic carrier concentration controlled by the

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compositional distribution. The existence of a compositional window, where the SiGe solar cells can surpass the Si solar cell, was confirmed. The window was found to be strongly dependent on the minority carrier diffusion length and the degree of the compositional distribution.

2. Model for calculations

The detailed description of the model used in this study was reported in Ref. [7]. The fundamental idea and the difference in parameters used for numerical calculations are described below. In order to introduce the effect of the compositional distribution in SiGe with average Ge composition of x, the volume fraction of the $Si_{1-y}Ge_y$ crystal, $P(y)$, is introduced where $P(y)$ satisfies

$$\int P(y)\,dy = 1 \tag{1}$$

and the average Ge composition, x, can be expressed as

$$x = \int yP(y)\,dy. \tag{2}$$

Furthermore, the absorption coefficient, β and the intrinsic carrier concentration, N_i are treated as macroscopically uniform parameters, and they are assumed to be expressed as

$$\beta = \int \alpha(y)P(y)\,dy \tag{3}$$

and

$$N_i = \int N(y)P(y)\,dy, \tag{4}$$

where $\alpha(y)$, $N(y)$ are the absorption coefficient and the intrinsic carrier concentration of bulk $Si_{1-y}Ge_y$.

To investigate the average Ge composition dependence, $P(y)$ was treated as nonzero only for $y = 0$ and 1 in Ref. [7]. This means that mc-SiGe consists of the dispersion of pure-Ge in Si-matrix, which is not realistic in mc-SiGe grown by the directional solidification in a crucible. Although this assumption is useful for rough estimation of the effect of the average composition, it is not useful to discuss the impact of the compositional fluctuation, Δx, at a given average Ge composition. Therefore, in this study, $P(y)$ is treated as nonzero for $y = 0$ and z ($z = 0.10$, 0.20, 0.30, 0.50, 0.75). This set of z was chosen due to the available absorption spectra in the literature [8].

It is noted that our model does not treat real geometry of Si and Ge in the crystal, but we consider "virtually homogeneous SiGe" whose macroscopic properties such as absorption coefficient and intrinsic carrier concentration are determined by Eqs. (3) and (4). Generally speaking, two- or three-dimensional transport equations are necessary to treat nonuniform material by defining the geometry of the nonuniformity. However, our simple model to treat nonuniform material as virtually homogeneous material with modified physical properties permits to use one-dimensional transport equation, which gives us a rough idea how the compositional fluctuation affects the performance of solar cells.

Fig. 1 shows a comparison of calculated absorption spectra, β, of mc-SiGe with a fixed average Ge composition of 0.05 using z of 0.10, 0.50, and 0.75. It is seen that the increase in z results the increase in the absorption coefficient and the decrease in the band gap energy. Therefore, photocurrent density is expected to increase by increasing z if the introduction of the compositional distribution does not reduce the diffusion length of minority carriers.

The solar cell was assumed to consist of a single pn junction formed in a p-type substrate with an abrupt doping profile [9]. The one-dimensional steady-state continuity equations were solved for p-type and n-type regions using boundary conditions, where the excess minority carrier goes to zero at the both edges of the depletion layer. By this process, electron and hole photocurrents collected at the depletion edge can be obtained. In addition, all the carriers generated in the depletion layer are assumed to contribute to the current by the assistance of the built-in electric field. The total photocurrent at a given wavelength was therefore obtained as the summation of the three components. The calculation was carried out with AM 1.5 illumination. The diffusion length of minority carriers was assumed to be independent of z. The integration over the range of wavelengths gives the short-circuit photocurrent density (J_{sc}). The saturation current of the diode (J_o) was calculated from the spatial distribution of minority carriers without illumination, and the open-circuit voltage (V_{oc}) was obtained by assuming the ideal diode as

$$V_{oc} = \frac{k_B T}{q} \ln\left(1 + \frac{J_{sc}}{J_o}\right). \tag{5}$$

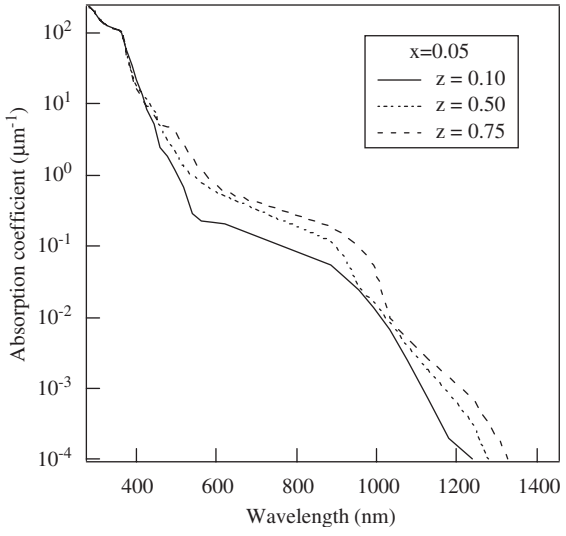

Fig. 1. Calculated absorption spectra of SiGe with an average Ge composition of 0.05 using z of 0.10, 0.50, and 0.75.

The conversion efficiency and fill factor were then calculated by obtaining the operation voltage to maximize the output power.

3. Calculated results and discussion

3.1. Short-circuit current density

Fig. 2 shows the calculated photocurrent density per unit bandwidth for $Si_{0.95}Ge_{0.05}$ solar cells with different z of 0.10, 0.50, and 0.75 using parameters listed in Table 1. The diffusion length of minority electrons was fixed to be 100 μm and assumed to be independent of z. Because of this assumption, the increase in the absorption coefficient originating from the increase of z directly leads to the increase in the photocurrent. This is well illustrated in the enhanced response in the longer wavelength, which improves J_{sc}.

To see the impact of the diffusion length of electrons and the average Ge composition on J_{sc}, calculated results were displayed in Fig. 3 as contour plots for different z of (a) 0.10 and (b) 0.75. As is expected, J_{sc} increases monotonically with increasing diffusion length at a given average Ge composition. The effect of the diffusion length is seen to become larger with decreasing diffusion length as illustrated by the dense contours. Furthermore, J_{sc} is seen to increase with increasing average Ge composition at a given diffusion length reflecting the increased absorption coefficient. It should be remarked that the contour line of a given J_{sc} in Fig. 3(b) is strongly dependent on the average Ge composition, while the dependence is not significant in Fig. 3(a). This originates from the difference in the onset of the response, and can be explained in terms of the red shift of the band gap with increasing z for a given average Ge composition.

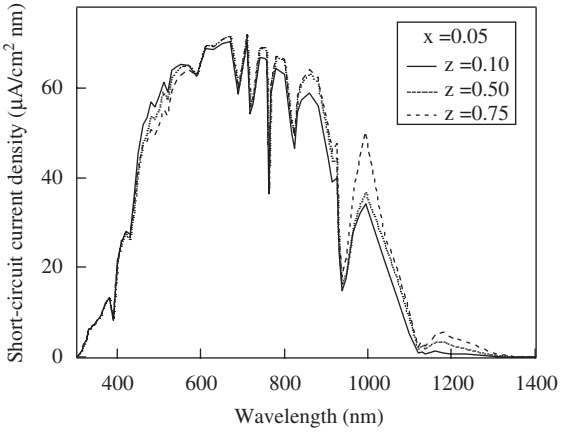

Fig. 2. Comparison of calculated short-circuit current density per unit bandwidth for the SiGe solar cells with an average Ge composition of 0.05 using z of 0.10, 0.50, and 0.75.

Table 1
List of parameters used for the calculations

Donor concentration (cm^{-3})	1×10^{19}
Acceptor concentration (cm^{-3})	1×10^{16}
Surface recombination velocity (cm/s)	1×10^{3}
Back-surface recombination velocity (cm/s)	1×10^{3}
Diffusion coefficient of electrons ($\mu m^2/s$)	2×10^{8}
Diffusion coefficient of holes ($\mu m^2/s$)	4×10^{9}
Diffusion length of electrons (μm)	1–150
Diffusion length of holes (μm)	100
Wafer thickness (μm)	300
Depth of a pn junction (μm)	0.5

3.2. Open-circuit voltage

Fig. 4 shows the contour plots of the calculated V_{oc} as a function of the diffusion length and the average Ge composition for z of (a) 0.10 and (b) 0.75. As a general tendency, the increase in the average Ge composition and the decrease in the diffusion length causes the decrease in V_{oc}. The increase in the intrinsic carrier concentration resulting from the reduction of the band gap and the decrease in J_{sc} explain this phenomenon. It is clearly seen that the contour line for z of 0.75 is steeper than that of 0.10. This is a consequence that the intrinsic carrier concentration becomes larger with increasing z for a given average Ge composition. Therefore, careful attention must be paid for the choice of z. Although the increase in z would be beneficial in terms of the absorption if this could not affect the carrier transport, it could negatively affect V_{oc} through the increase in the intrinsic carrier concentration.

3.3. Overall conversion efficiency

The calculated overall conversion efficiency was shown in contour plots in Fig. 5 for z of (a) 0.10 and (b) 0.75. It is seen that the increase in the diffusion length for a given average Ge composition results in the improvement in the conversion efficiency. On the other hand, the dependence on the average Ge composition is not straightforward. When the diffusion length is large, the contour line has a positive slope with respect to the average Ge composition, indicating that the introduction of Ge is not beneficial for the performance in the solar cell. However, with decreasing diffusion length, the contour line has a negative slope especially when the average Ge composition is small. This indicates the appearance of the compositional window where the introduction of Ge to Si improves the conversion efficiency of the solar cell.

Fig. 6 illustrates the compositional window where the introduction of Ge is advantageous for improvement in the conversion efficiency for z of (a) 0.10 and (b) 0.75. It is seen that the introduction of Ge results in the decrease in the conversion efficiency when the diffusion length is high. This result is consistent with the SQ prediction, and is a consequence of the fact that the decrease in V_{oc} controls the overall efficiency. Since the assumed carrier diffusion length is large enough to collect most of photogenerated carriers, the advantage of increased photocurrent will be lost. This situation could be

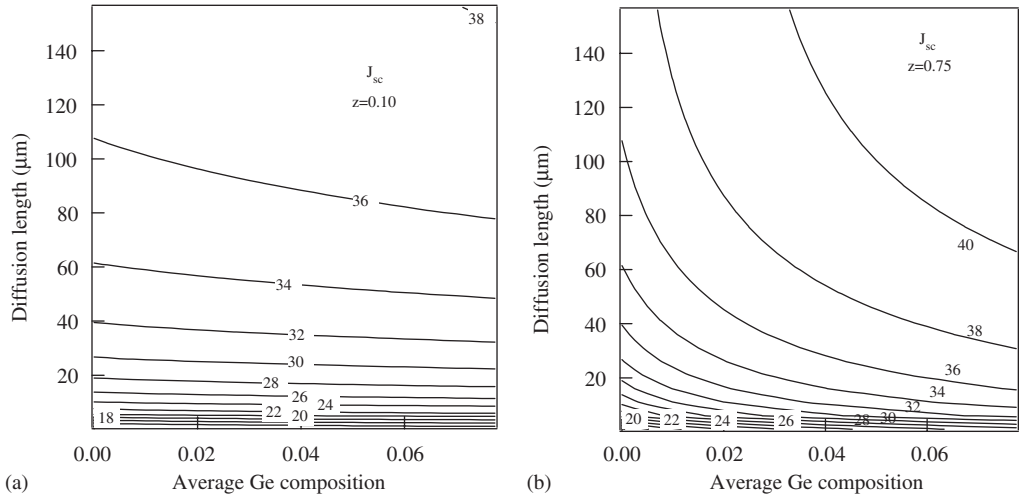

Fig. 3. Contour plots of the calculated short-circuit current density as a function of the diffusion length of minority electrons and the average Ge composition for z of (a) 0.10 and (b) 0.75. The label is shown in the unit of mA/cm^2.

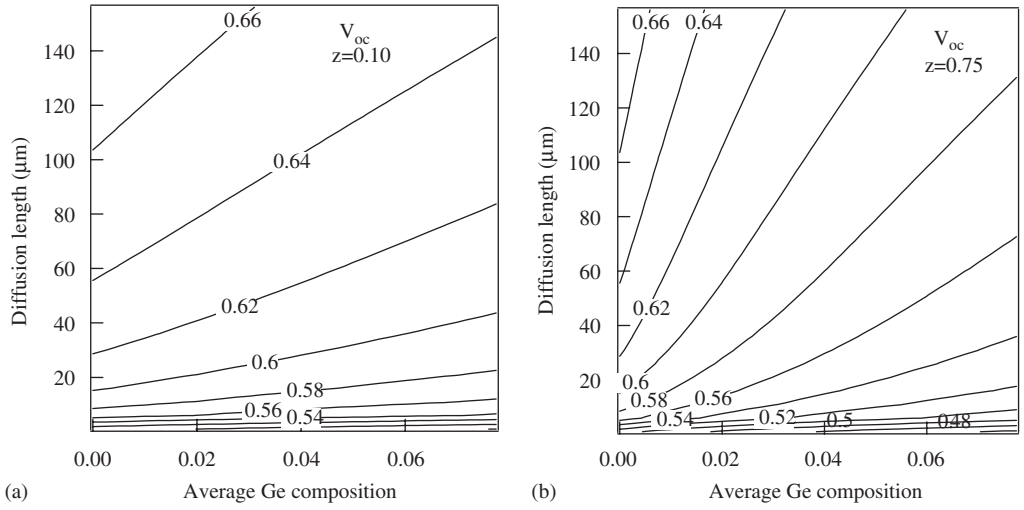

Fig. 4. Contour plots of the calculated open-circuit voltage as a function of the diffusion length of minority electrons and the average Ge composition for z of (a) 0.10 and (b) 0.75. The label is shown in the unit of V.

changed if we violate the assumption of SQ more markedly by decreasing minority carrier diffusion length. With decreasing diffusion length, the relative increase in J_{sc} due to the introduction of Ge becomes more significant. As a consequence, the increase in J_{sc} gives more impact than the decrease in V_{oc} on the overall conversion efficiency. This leads to the appearance of a compositional window where the conversion efficiency of a solar cell based on SiGe can surpass that based on Si. The window is seen to become wider with increasing z due to the increase in the absorption coefficient.

It should be remarked that the line in Fig. 6 was drawn under the assumption that the introduction of Ge does not affect the carrier transport. In fact, the introduction of Ge might cause carrier localization and/or give additional alloy scattering, which could decrease the diffusion length of minority carriers. In this case, the advantageous compositional window will become narrower.

4. Comparison with experiments

The calculated results are compared with the experimental results recently reported by Pan et al. [4] Their material was grown by directional solidification from the SiGe melt in a small crucible with a diameter of 70 mm coated with Si_3N_4, and processed into solar cells by a simple technique, which includes the emitter formation by thermal diffusion of P, deposition of ITO film for antireflection coating, printing, and firing of Ag and Al pastes for contact formation. No light trapping by texturing the surface was done. Due to the small size of the crucible, the measured carrier lifetime was not long and on the order of a few μs, which corresponds to a diffusion length of a few tens of microns.

Fig. 7 compares calculated results with experimentally obtained conversion efficiency. The experimental results are shown in solid circles, and the calculated results are

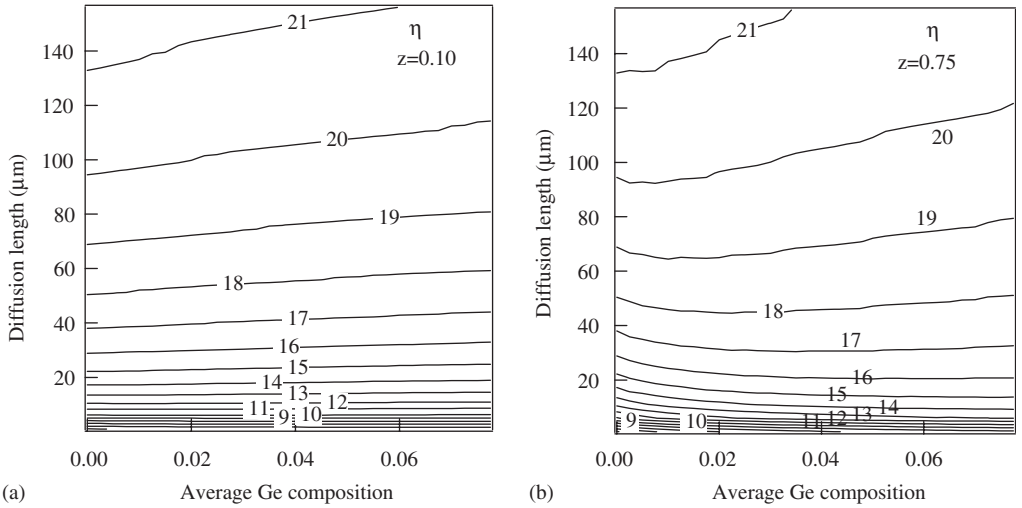

Fig. 5. Contour plots of the conversion efficiency of the solar cell based on SiGe with compostional distribution as a function of the diffusion length of minority electrons and the average Ge composition for z of (a) 0.10 and (b) 0.75. The label is shown in the unit of %.

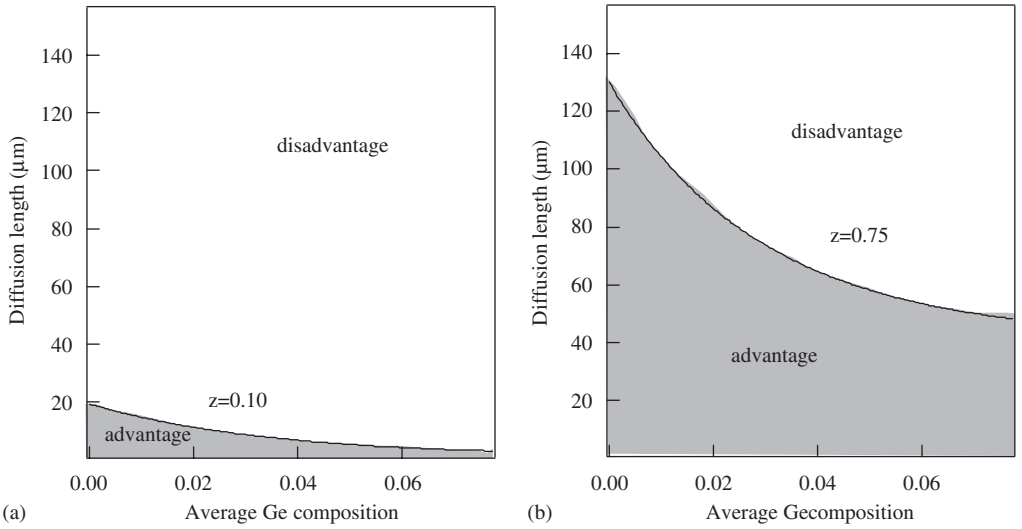

Fig. 6. Compositional window where the conversion efficiency of the solar cell based on SiGe can surpass that of the solar cell based on Si for z of (a) 0.10 and (b) 0.75.

shown for different z. The tendency of the experimental results are reproduced well especially when z is larger than 0.50. Although the experimentally measured compositional distribution does not contain regions with such high Ge composition [10], the internal light scattering due to the modulation of the refractive index and/or the decrease in the band gap due to the built-in strain would enhance the absorption coefficient effectively and compensate for this inconsistency. Importantly, the existence of the compositional window where the conversion efficiency of a solar cell based on SiGe can surpass that based on Si was confirmed both theoretically and experimentally.

Finally, it should be remarked that the addition of a small amount of Ge is considered to be beneficial not only for bulk material with short diffusion lengths but for thin films since the reduction of the absorber thickness would be equivalent to the decrease in the diffusion length. If we consider the situation that the insufficient Si feed stock might limit the rapid growth of photovoltaic industry, the use of thin film Si solar cells with a dispersion of a small amount of Ge might be promising in the future.

5. Summary

We carried out a theoretical investigation on the photovoltaic power conversion of SiGe solar cells with compositional distribution. The effect of the compositional distribution was included in the absorption coefficient and the intrinsic carrier concentration. The existence of a compositional window, where the conversion efficiency of the solar cell based on SiGe can surpass that of the solar cell based on Si, was revealed by solving the steady-state

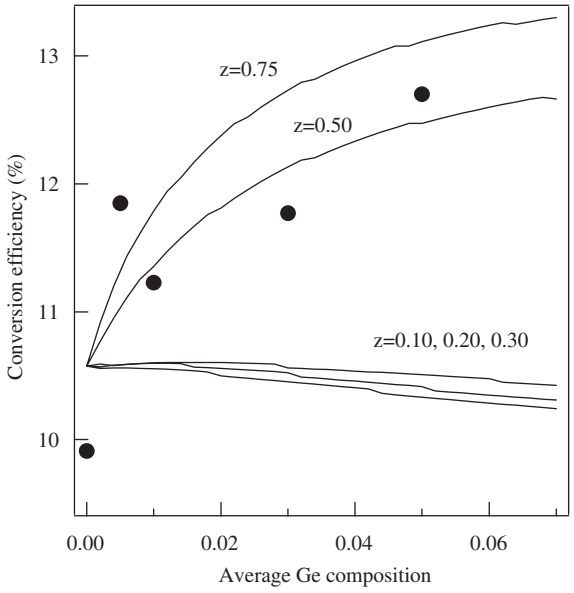

Fig. 7. Comparison of the calculated and experimentally obtained conversion efficiency of the solar cells based on SiGe with compositional distribution.

continuity equation under solar light illumination. This window appears only when the diffusion length is assumed to be finite. The width of such a window was shown to be affected by the degree of the compositional distribution.

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