

# *a-Si/c-Si<sub>1-x</sub>Ge<sub>x</sub>/c-Si Heterojunction Solar Cells*

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**Abstract**— The performance and material quality requirements of thin film a-Si/c-Si<sub>1-x</sub>Ge<sub>x</sub>/Si heterojunction solar cells are investigated by modeling and simulation. The effects of Ge content, Si<sub>1-x</sub>Ge<sub>x</sub> thickness, Si<sub>1-x</sub>Ge<sub>x</sub> lifetime and a-Si/c-Si<sub>1-x</sub>Ge<sub>x</sub> interfacial quality have been studied. The simulations predict that Si<sub>1-x</sub>Ge<sub>x</sub> based thin film solar cells provide a significant increase in solar cell output current for Ge fractions larger than 30%, due to the narrower band-gap and increased absorption. In addition, the efficiency of thin (2μm) Si<sub>1-x</sub>Ge<sub>x</sub> solar cells surpasses that of Si for minority carrier lifetimes larger than 0.5μs. For these 2μm thin layers, simulations predict reduced material quality requirements for Si<sub>1-x</sub>Ge<sub>x</sub> cells, with a clear performance advantage relative to Si based solar cells.

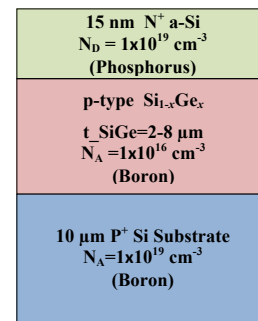
**Keywords**- Solar, Heterojunction, SiGe, Lifetime, Efficiency, thin film

## I. INTRODUCTION

Thin film epitaxial solar cell technology is a very attractive way to help reduce the material consumption cost associated with today's Si wafer based solar cells. These epitaxial layers can be grown at low temperatures with high quality on low-cost substrates [1]. Using single crystal material will improve the efficiency relative to amorphous and poly-silicon solar cells due to the improved material quality. This improved efficiency will add a significant cost benefit [1]. Another way to increase efficiency is to incorporate a semiconductor with a smaller band-gap such as Si<sub>1-x</sub>Ge<sub>x</sub>, in order to absorb more of the solar spectrum, especially in thin layers [2-3]. Si<sub>1-x</sub>Ge<sub>x</sub> based epitaxial layers can be grown at lower temperatures compared to epitaxial Si layers, while maintaining a high crystalline quality. In addition, a heterojunction emitter based solar cell (HIT) can be used to increase the open circuit voltage ( $V_{oc}$ ) in Si cells [4]. Recently, Alberi *et al.* fabricated and simulated a-Si(p<sup>+</sup>)/c-Si(n<sup>-</sup>)/c-Si(n<sup>+</sup>) solar cells in an investigation of the material quality requirements [5]. This HIT cell design can be extended to Si<sub>1-x</sub>Ge<sub>x</sub> based cells to increase the  $V_{oc}$  that is reduced due to its smaller bandgap. In this work, we investigate the use of epitaxial Si<sub>1-x</sub>Ge<sub>x</sub> layers in a HIT cell structure using an a-Si emitter. The key design parameters of a-Si(n<sup>+</sup>)/c-Si<sub>1-x</sub>Ge<sub>x</sub>(p)/c-Si(p<sup>+</sup>) solar cells are studied by modeling and simulation. We investigate the effect of Ge content, Si<sub>1-x</sub>Ge<sub>x</sub> thickness, Si<sub>1-x</sub>Ge<sub>x</sub> lifetime and a-Si/c-Si<sub>1-x</sub>Ge<sub>x</sub> interfacial quality on the performance of the thin film solar cell. Understanding the Si<sub>1-x</sub>Ge<sub>x</sub> material quality needed as a function of heterostructure layer design will determine the suitability of the material and various structures, and hence TCAD simulations can play a vital role in the design process.

## A. Structure

Figure 1 shows the basic structure of the heterojunction solar cell simulated using the Synopsys<sup>TM</sup> TCAD tools [6]. The structure is a stack of 15 nm n-type ( $1 \times 10^{19} \text{ cm}^{-3}$ ) a-Si, followed by a p-type ( $1 \times 10^{16} \text{ cm}^{-3}$ ) Si<sub>1-x</sub>Ge<sub>x</sub> layer and finally a 10 μm p-type ( $1 \times 10^{19} \text{ cm}^{-3}$ ) Si substrate. The p-type Si substrate serves as the back contact, and does not contribute significantly to the carrier generation. For practical applications, a low cost mechanical carrier, such as glass or ceramics, is meant to be used instead of p-type Si substrate, albeit at the expense of material quality.



**Figure 1. Cross-section of the simulated a-Si/c-Si<sub>1-x</sub>Ge<sub>x</sub>/c-Si heterojunction solar cell (layer thicknesses not to scale).**

## B. Physics Based Model for TCAD Simulation

The Transfer Matrix Method (TMM) from Synopsis Device was used to simulate a solar spectrum of AM1.5G. In order to simulate the solar cell in Figure 1, optical parameters must be used for all materials. The wavelength-dependent complex refractive index, for a-Si, Si and Si<sub>1-x</sub>Ge<sub>x</sub> was utilized from published data [7-8]. Complex refractive index is defined as  $n + i \cdot \kappa$ , where  $n$  is refractive index and  $\kappa$  is the extinction coefficient directly proportional to the absorption coefficient of a material. Figure 2 shows extinction coefficient  $\kappa$  as a function of wavelength for different Ge percentages. The bandgap for relaxed Si<sub>1-x</sub>Ge<sub>x</sub> layers is taken from Braunstien *et al.* [9]. For Si<sub>0.5</sub>Ge<sub>0.5</sub>, the bandgap reduces to 0.9eV from 1.16eV for Si. In addition, a conduction band offset ( $E_c$ ) of 0.15eV between a-Si/Si<sub>1-x</sub>Ge<sub>x</sub> is used [10]. The band-diagram near the a-Si/Si<sub>0.5</sub>Ge<sub>0.5</sub> interface for  $V=0$  is shown in Figure 3. It also should be noted that the electron/hole mobility of the Si<sub>1-x</sub>Ge<sub>x</sub> layer is set to be equal to that in Si in these simulations. Finally, the minority carrier lifetime ( $\tau$ ) of the Si<sub>1-x</sub>Ge<sub>x</sub> layer is treated as a parameter by modifying  $\tau_{max}$  for holes and electrons in the Shockley Read Hall (SRH) Scharfetter recombination model [11].

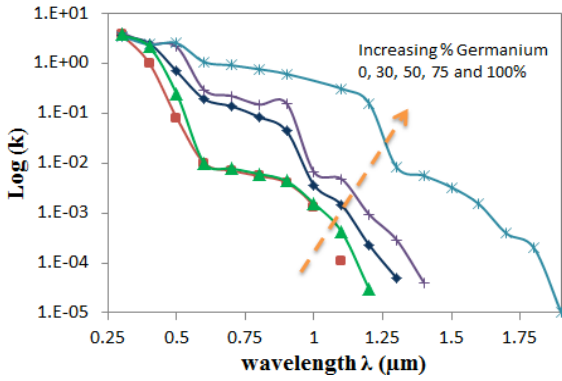


Figure 2. Extinction coefficient ( $\kappa$ ) values for  $c\text{-Si}_{1-x}\text{Ge}_x$  vs. wavelength, for various Ge percentages [8].

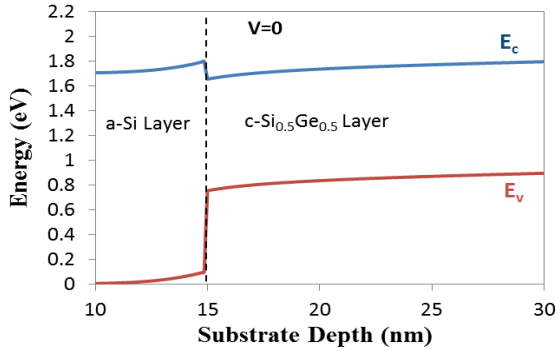


Figure 3. Band diagram between  $a\text{-Si}/c\text{-Si}_{0.5}\text{Ge}_{0.5}$

### C. Results

Figure 4 shows simulated  $V_{oc}$  as a function of the minority carrier lifetime ( $\tau_n$  and  $\tau_p$ ) of a 2  $\mu\text{m}$ -thick  $\text{Si}_{0.5}\text{Ge}_{0.5}$  layer comparing an  $a\text{-Si}$  emitter to a  $\text{Si}_{0.5}\text{Ge}_{0.5}$  emitter. The small bandgap  $\text{Si}_{0.5}\text{Ge}_{0.5}$  (0.9 eV) will increase the generation leakage of the diode and thus reduce  $V_{oc}$  significantly. By using  $a\text{-Si}$  with a bandgap of 1.7 eV as the  $n$ -type region of the  $p\text{-n}$  diode, an additional barrier is created which reduces the concentration of thermally generated carriers that reach the contact. As a result, this heterojunction diode will reduce the reverse leakage thus increasing  $V_{oc}$  of the solar cell, as in a HIT  $c\text{-Si}$  cell [4]. It should be noted, as in the HIT-cell, the additional barrier will reduce the number of optically generated carriers that reach the contacts. However, since the magnitude of optically generated carriers is so large, the effect on the photocurrent is small.

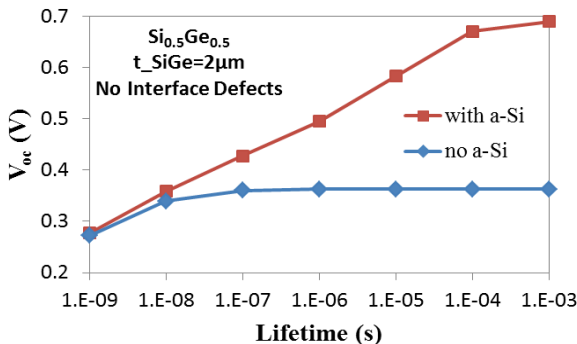


Figure 4.  $V_{oc}$  vs.  $\text{Si}_{0.5}\text{Ge}_{0.5}$  lifetime comparing the heterojunction  $a\text{-Si}/c\text{-Si}_{0.5}\text{Ge}_{0.5}$  solar cell to a homojunction  $\text{Si}_{0.5}\text{Ge}_{0.5}$  solar cell.

Figure 5 shows  $V_{oc}$  versus the minority carrier lifetime for different Ge percentages for a 2  $\mu\text{m}$ -thick  $\text{Si}_{1-x}\text{Ge}_x$  layer. The  $V_{oc}$  can be recovered to the pure Si case ( $\sim 0.6\text{V}$ ) for a minority carrier lifetime of  $\sim 0.1\text{ms}$  in the  $\text{Si}_{0.5}\text{Ge}_{0.5}$ .

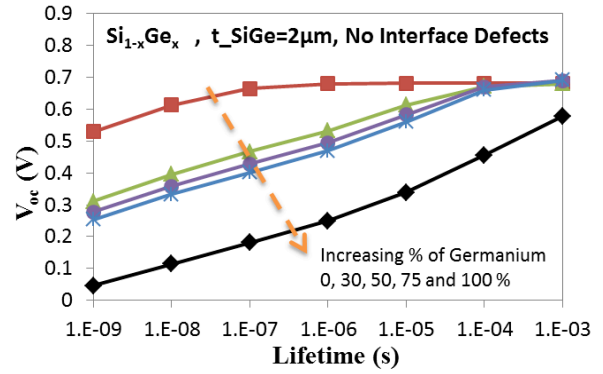


Figure 5.  $V_{oc}$  vs.  $\text{Si}_{1-x}\text{Ge}_x$  lifetime for a heterojunction  $a\text{-Si}/c\text{-Si}_{1-x}\text{Ge}_x/c\text{-Si}$  solar cell for increasing Ge percentage.

By using a smaller band-gap thin-film material, more of the solar optical spectrum is utilized and the short circuit current ( $J_{sc}$ ) increases. Figure 6 shows the increase in  $J_{sc}$  with increasing Ge concentration for a 1  $\mu\text{s}$  lifetime, which might be expected for a CVD grown epitaxial  $\text{Si}_{1-x}\text{Ge}_x$  grown on silicon with a graded buffer layer.  $J_{sc}$  increases significantly for Ge contents above 30%, reaching a peak value of  $\sim 30\text{ mA/cm}^2$  for 75% Ge. There is slight decrease in current for 100% Ge due to increase in recombination due to much smaller bandgap of 0.67eV. Also for Ge content larger than 75%,  $J_{sc}$  does not change with thickness. This is due to the fact there is a large increase in absorption near the junction as seen in Figure 2 from the extinction coefficient.

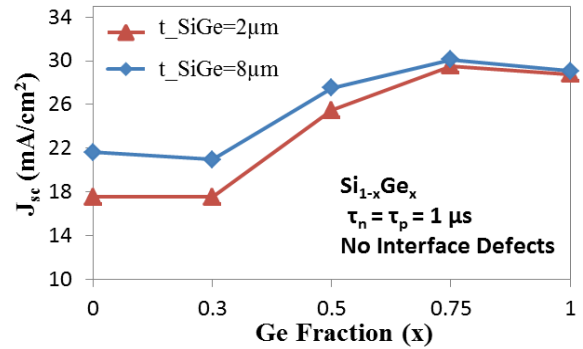


Figure 6.  $J_{sc}$  vs. Ge % for the  $a\text{-Si}/c\text{-Si}_{1-x}\text{Ge}_x/c\text{-Si}$  solar cell. The  $\text{SiGe}$  thickness is 2 and 8  $\mu\text{m}$ , the lifetime is set to  $1\mu\text{s}$  and  $S=0$ .

The efficiency of the solar cell is a strong function of the material quality, i.e. the carrier lifetime. Figure 7 plots the efficiency vs. minority carrier lifetime for the 8  $\mu\text{m}$ -thick  $\text{Si}_{1-x}\text{Ge}_x$  layer. The graph shows that if the material quality is very poor with a low lifetime, the efficiency does not depend on the Ge percentage significantly. This is directly related to  $V_{oc}$  since for low lifetimes the diode leakage current will increase. Conversely, if the lifetime is very high, above 50  $\mu\text{s}$ ,  $c\text{-Si}_{1-x}\text{Ge}_x$  can overtake Si in terms of efficiency for Ge percentages 50% and 75%. Figure 8 plots the efficiency vs. minority carrier

lifetime for 2  $\mu\text{m}$ -thick  $\text{Si}_{1-x}\text{Ge}_x$ . For the 2 $\mu\text{m}$ -thick case, the  $\text{Si}_{1-x}\text{Ge}_x$  efficiency surpasses that of Si for lifetimes larger than 0.5 $\mu\text{s}$  and for Ge percentages 50% and 75%. This illustrates that the material quality requirement is less stringent for thinner cells and highlights the potential advantage  $\text{Si}_{1-x}\text{Ge}_x$  for this application.

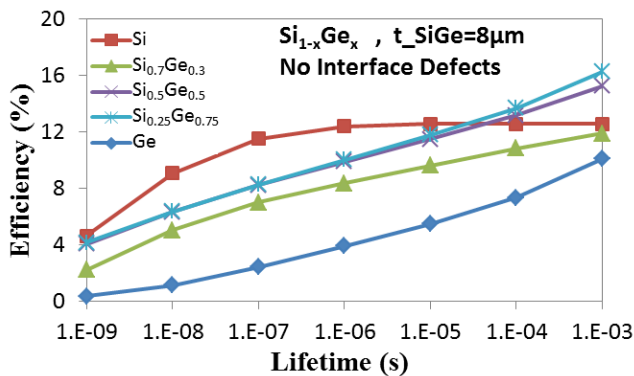


Figure 7. Efficiency (%) vs.  $\text{Si}_{1-x}\text{Ge}_x$  lifetime for an 8  $\mu\text{m}$  heterojunction a-Si/c-Si $_{1-x}\text{Ge}_x$ /c-Si solar cell for increasing Ge percentage.

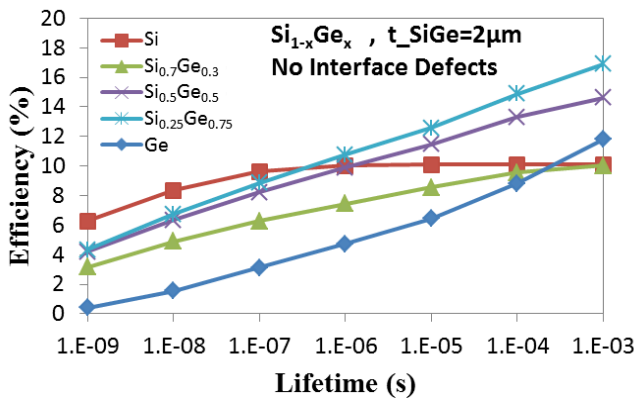


Figure 8. Efficiency (%) vs.  $\text{Si}_{1-x}\text{Ge}_x$  lifetime for a 2  $\mu\text{m}$  heterojunction a-Si/c-Si $_{1-x}\text{Ge}_x$ /c-Si solar cell for increasing Ge percentage.

In addition to bulk recombination, the a-Si/c-Si $_{1-x}\text{Ge}_x$  interface will have a non-zero surface recombination velocity due to interface traps. These interface traps are likely located in the midgap of a-Si and Si. The effect of the traps can be simulated by increasing the surface recombination velocity at the a-Si/c-Si $_{1-x}\text{Ge}_x$  interface. Figure 9 shows  $V_{oc}$  vs. surface recombination velocity for different c-Si $_{0.5}\text{Ge}_{0.5}$  lifetimes. The curves show the  $V_{oc}$  does not change with increased surface recombination velocity at the a-Si/Si $_{0.5}\text{Ge}_{0.5}$  interface for minority carrier lifetimes of 1 to 100ns. For lifetimes larger than 100ns,  $V_{oc}$  starts to decrease with increasing recombination velocity. This indicates the interface defects are now contributing to the dark current.

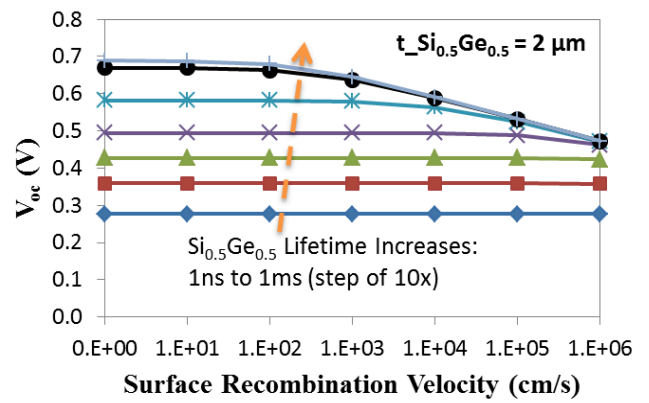


Figure 9.  $V_{oc}$  vs. a-Si/Si $_{1-x}\text{Ge}_x$  surface recombination velocity for a heterojunction a-Si/c-Si $_{0.5}\text{Ge}_{0.5}$ /c-Si solar cell for increasing lifetime of c-Si $_{0.5}\text{Ge}_{0.5}$  layers.

Figure 10 plots light J-V characteristics under 1 sun in AM1.5G for increasing surface recombination velocity with a minority carrier lifetime of 1ms. In this case, interface defects will dominate the diode reverse leakage current. In addition, the short circuit current ( $J_{sc}$ ) is independent of surface recombination velocity and is strictly a function of optical generation. This is due to the fact that the magnitude of optically generated current is significantly larger than the concentration of carriers that are generated/recombined due to the interface defects. On the contrary, the dark current is significantly affected by generation/recombination at the interface, due to the small magnitude of the current. These results indicate that care is needed to optimize both the c-Si $_{1-x}\text{Ge}_x$  material quality and the a-Si/c-Si $_{1-x}\text{Ge}_x$  interface for this solar application.

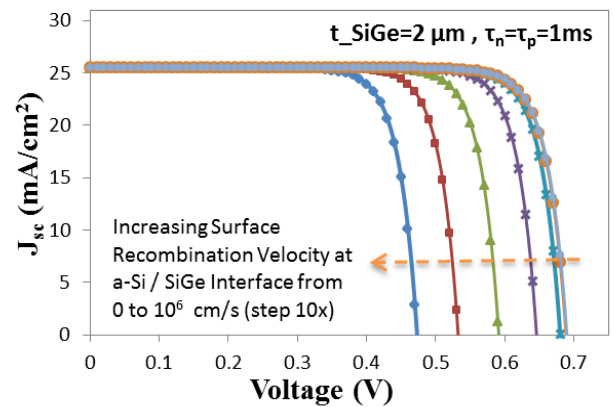


Figure 10: IV curves for a-Si/c-Si $_{0.5}\text{Ge}_{0.5}$ /c-Si solar cell with increasing surface recombination velocity at the a-Si/Si $_{0.5}\text{Ge}_{0.5}$  interface.

## SUMMARY

Heterojunction a-Si/c-Si<sub>1-x</sub>Ge<sub>x</sub>/c-Si solar cells were studied by TCAD. The smaller bandgap of c-Si<sub>1-x</sub>Ge<sub>x</sub> provides an increase in the optically generated current. The loss in  $V_{oc}$  can be recovered by using a c-Si<sub>1-x</sub>Ge<sub>x</sub> layer of high quality combined with a large bandgap a-Si emitter with a low defect interface to c-Si<sub>1-x</sub>Ge<sub>x</sub>. Moreover, the results predict that a-Si/c-Si<sub>1-x</sub>Ge<sub>x</sub>/c-Si solar cells can provide a clear performance advantage to c-Si based cells for sufficiently thin films.

## ACKNOWLEDGMENT

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