

Effect of Ge Mole Fraction on Current, Voltage and Electric Field Characteristics of High Doping Nanoscale Si_{1-x}Ge_x/Si P-N Diode

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Abstract—In this paper, we report the simulation of high doping nanoscale heterojunction diode, particularly Si_{1-x}Ge_x/Si p-n diode, using Cogenda Visual TCAD. In order to gain knowledge on electrical properties of this diode, we exhaustively simulate the effect of Ge mole fraction in SiGe material on current, voltage and electric field characteristics. The simulation covers Ge mole fraction of 0.2 to 0.7 in SiGe material as acceptor and Si material as donor. Both acceptor and donor have concentrations of 10²⁰ per cm³ and areas of 10 × 10 nm². Under forward bias voltage, higher Ge mole fraction will produce higher current. This phenomenon happens due to lower energy band gap at higher Ge mole fraction condition. Besides that, higher Ge mole fraction has lower energy difference between P side and N side of diode. According to the simulation result, Si_{0.8}Ge_{0.2} has energy band gap about 0.8 eV, meanwhile Si_{0.3}Ge_{0.7} has energy band gap about 0.5 eV. Lower energy band gap causes more electrons have enough energy to cross the junction. Meanwhile under reverse bias voltage, high doping nanoscale diode will produce infinitesimal current. At the junction, high doping nanoscale Si_{1-x}Ge_x/Si P-N diode also has lower electric field (measured at the center of diode) at higher Ge mole fraction. Under reverse bias voltage of -2 V, Si_{0.3}Ge_{0.7} has maximum electric field about 5.89 × 10⁶ V/m, meanwhile Si_{0.8}Ge_{0.2} has maximum electric field about 6.17 × 10⁶ V/m. We predict that Ge mole fraction has inversely proportional effect to the maximum electric field value. Therefore, we concluded that Ge mole fraction affects current, voltage and electric field characteristics of high doping nanoscale Si_{1-x}Ge_x/Si P-N diode.

Keywords— SiGe; Si; Ge; mole fraction; current; voltage; electric field; p-n diode; high doping; nanoscale; Cogenda Visual TCAD.

I. INTRODUCTION

Effect of Ge mole fraction of SiGe device on current and voltage has been investigated by some researchers. H. J. Huang *et al.* examined about forward and reverse bias characteristics of selective epitaxial growth SiGe/Si of 1000×1000μm² diode area with different Ge mole fraction. Higher current was obtained at higher Ge mole fraction [1,2]. A. Gupta *et al.* reported that in reverse bias, the junction capacitance of the SiGe diode is considerably less than that of the Silicon diode. Assuming that the difference in permittivity is small, the depletion width of the SiGe diode is therefore larger than that of the Silicon diode [3].

Other research shows that Ge mole fraction of SiGe diode also affect electric field. S. Banerjee *et al.* investigated about electric field profile at different current density of Si/Si_{0.9}Ge_{0.1} heterojunction DDR IMPATT [4]. J.Y. Li and J.C. Sturm observed the effect of Ge fraction on high field band to band tunneling in P⁺-SiGe/N⁺-SiGe junction [5].

SiGe diode fabrication has been conducted by some researchers using various techniques. E.V. Jelenkovic *et al.* demonstrated the formation of SiGe(P⁺)-Si(N) diode fabricated by co-sputtering and post-deposition annealing. SiGe film was deposited and in-situ by RF magnetron co-sputtering on oxidized and bare silicon wafer. Nominal thickness of the film was 20 nm and 500 nm [6]. Another technique to prepare SiGe layer is using chemical vapor deposition [7,8].

Here, we report the effect of Ge mole fraction on current, voltage and electric field characteristics of high doping nanoscale Si_{1-x}Ge_x/Si P-N diode by simulation using Cogenda Visual TCAD, a semiconductor simulator software provides by Cogenda Pte Ltd. Due to the critical thickness constrain caused by Si and Ge lattice mismatch [9], this report will be limited to the Ge mole fraction of 0.7.

II. METHODOLOGY

We simulate the Si_{1-x}Ge_x/Si p-n diode using Cogenda Visual TCAD. As an acceptor (P side), the Si_{1-x}Ge_x has an area of 10 × 10 nm². Similarly to Si, as a donor (N side), has an area of 10 × 10 nm². The simulation of P-N diode is shown in Fig. 1. Both acceptor and donor have concentrations of 10²⁰/cm³. Here we simulate and analyze current, voltage and electric field of Si_{1-x}Ge_x/Si p-n diode with Ge mole fraction from x = 0.2 to 0.7.

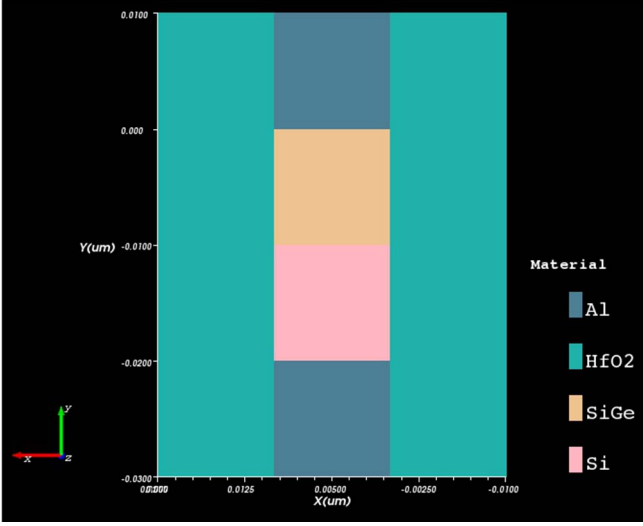


Fig. 1. P-N diode simulation using Cogenda Visual TCAD.

III. RESULT

We simulate current-voltage characteristics of high doping nanoscale $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ P-N diode under forward bias from 0 to 1 V and reverse bias from 0 to -2 V with variation of Ge mole fraction from $x = 0.2$ to 0.7. The results are shown in Fig. 2 and 3.

Under forward bias condition, the Ge mole fraction of $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ P-N diode affects the current. For Ge mole fraction of $x=0.7$, the diode begins to conduct at $V \approx 0.57$ Volt, meanwhile for Ge mole fraction of $x=0.2$, the diode starts to conduct at $V \approx 0.9$ Volt.

Under reverse bias condition, the Ge mole fraction of $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ P-N diode also affects the current. Although it produces infinitesimal current, higher Ge mole fraction will produce higher current.

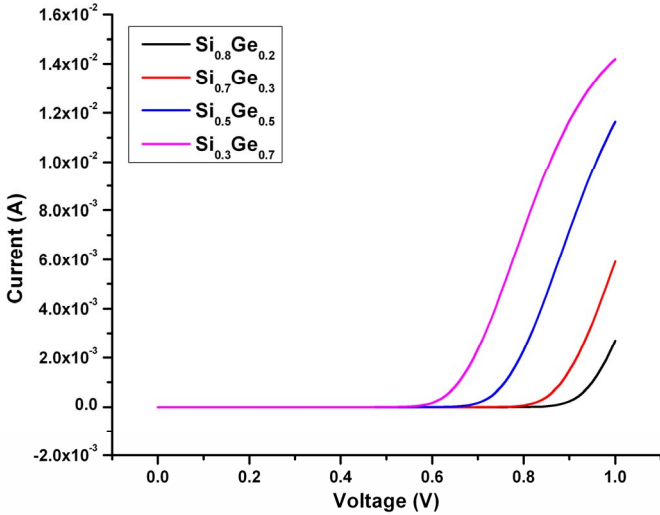


Fig. 2. Current-Voltage characteristic under forward bias.

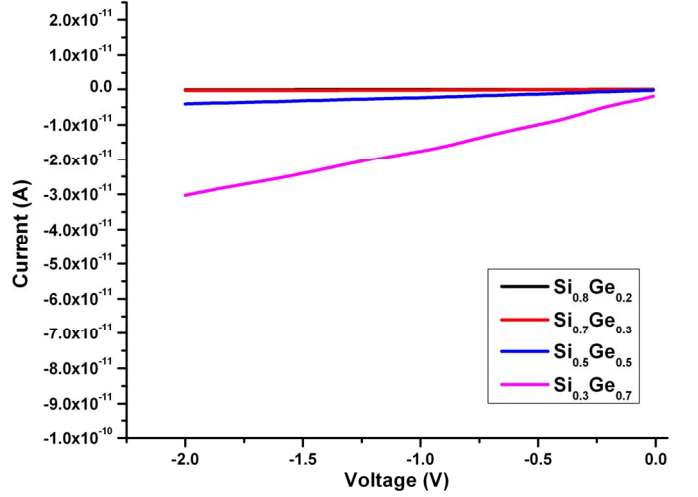


Fig. 3. Current-Voltage characteristic under reverse bias.

From Fig. 2 and Fig. 3, high doping nanoscale $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ P-N diode can be used as a rectifier with higher Ge mole fraction will produce higher current.

We also simulate electric field of high doping nanoscale $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ P-N diode under reverse bias voltage = -2 V with variation of Ge mole fraction from $x = 0.2$ to 0.7. The results are shown in Fig. 4 and Table 1.

As stated in Table I, Ge mole fraction of $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ P-N diode affects the electric field. At the junction, higher Ge mole fraction will produce lower maximum electric field.

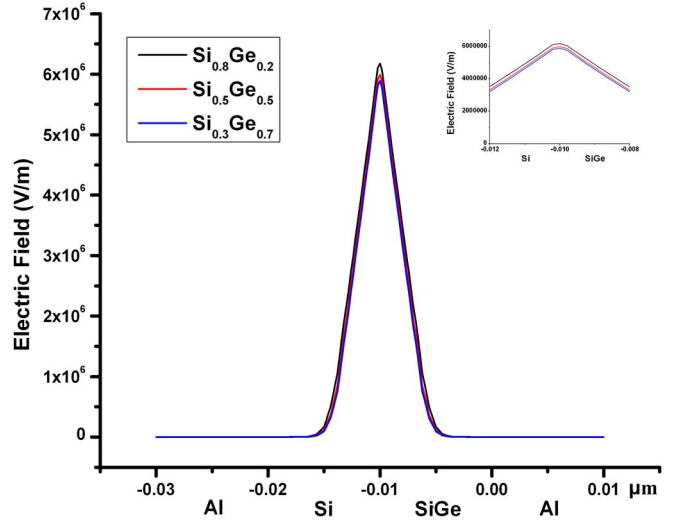


Fig. 4. Electric field characteristic under reverse bias.

TABLE I. GE MOLE FRACTION AND MAXIMUM ELECTRIC FIELD

Ge Mole Fraction	Max. Electric Field (V/m)
$\text{Si}_{0.8}\text{Ge}_{0.2}$	6.17×10^6
$\text{Si}_{0.5}\text{Ge}_{0.5}$	5.99×10^6
$\text{Si}_{0.3}\text{Ge}_{0.7}$	5.89×10^6

IV. DISCUSSION

As shown in Fig. 2 under forward condition, high doping nanoscale $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ P-N diode will provide higher current with higher Ge mole fraction. This is consistent with result obtained by Huang *et al.* [1, 2] and Li *et al.* [5]. As stated by other papers, lower energy band gap achieves at higher Ge mole fraction condition [10-13]. Energy band gap (E_g) is energy difference between the bottom of conduction band (E_c) and the top of valence band (E_v); Hence, lower energy band gap causes more electrons having enough energy to cross the junction from n^+ side to p^+ side. According to Srinivasan *et al.*, increases Ge mole fraction will decrease Kelvin resistance [14]. Therefore, higher Ge mole fraction will produce higher current. Using the result of quantitative data from simulation using Cogenda Visual TCAD, we draw the energy band diagram of high doping nanoscale $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ P-N diode as shown in Fig. 5. Under forward bias voltage = 1 V, for $\text{Si}_{0.3}\text{Ge}_{0.7}$, it has $E_g \approx 0.5$ eV, meanwhile for $\text{Si}_{0.8}\text{Ge}_{0.2}$, it has $E_g \approx 0.8$ eV. Under reverse bias condition, as shown in Fig. 3, high doping nanoscale $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ P-N diode will provide higher leakage current with higher Ge mole fraction. This fact is observed due to lower electric field at the junction of diode with higher Ge mole fraction as shown in Fig. 4 and Table I. This is also consistent with other papers [1, 2]. Using the result of quantitative data from simulation, we draw the energy band diagram of high doping nanoscale $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ P-N diode under reverse bias voltage = -2 V as shown in Fig. 6.

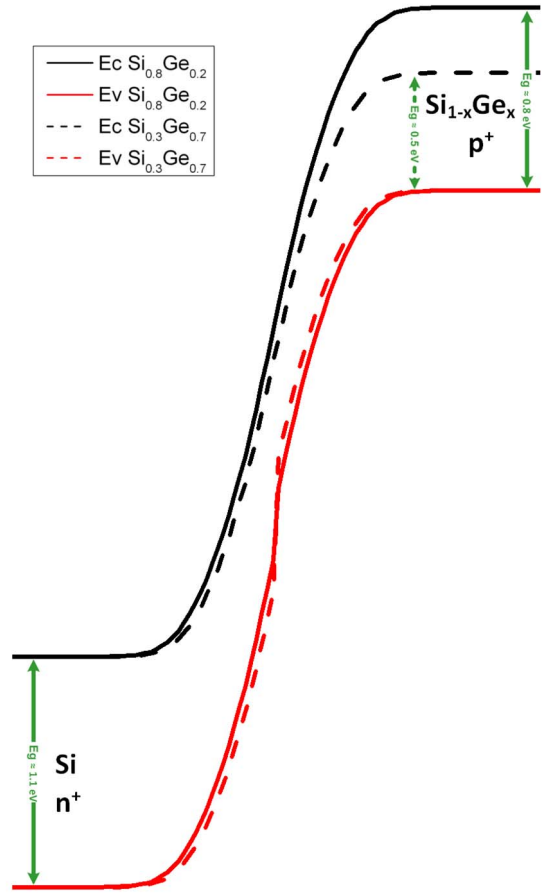


Fig. 6. Energy band diagram under reverse bias.

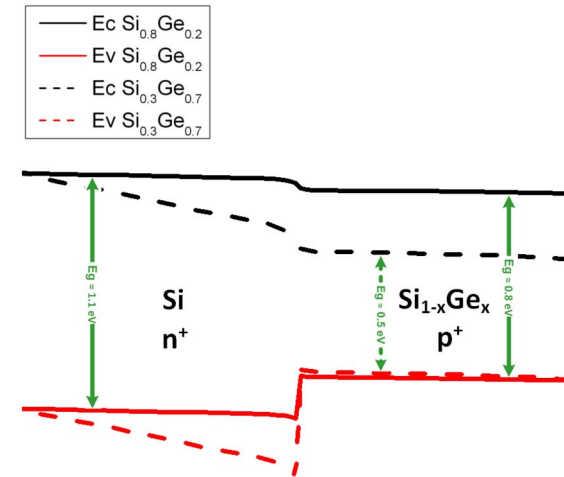


Fig. 5. Energy band diagram under forward bias.

As shown in Fig 4, the maximum electric field has inversely proportional value with Ge mole fraction of high doping nanoscale $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ P-N diode. Higher Ge mole fraction will produce lower electric field peak. This fact is consistent with Banerjee *et al.* [4]. According to quantitative data from simulation using Cogenda Visual TCAD, we predict that Ge mole fraction has linear effect on maximum electric field value of high doping nanoscale $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ P-N diode as shown in Fig. 7. Under reverse bias voltage = -2 V, for $\text{Si}_{0.3}\text{Ge}_{0.7}$, it has maximum electric field $\approx 5.89 \times 10^6$ V/m, meanwhile for $\text{Si}_{0.8}\text{Ge}_{0.2}$, it has maximum electric field $\approx 6.17 \times 10^6$ V/m.

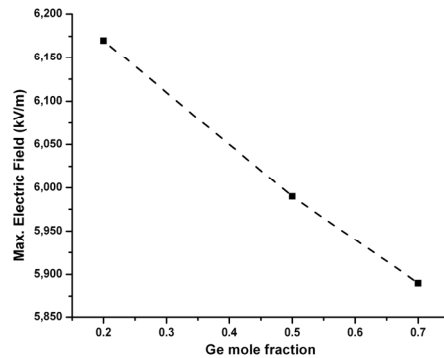


Fig. 7. Effect of Ge mole fraction on maximum electric field.

V. CONCLUSION

We have already simulated the effect of Ge mole fraction from $x=0.2$ to $x=0.7$ in SiGe material on current, voltage and electric field characteristics of high doping nanoscale $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ P-N diode using Cogenda Visual TCAD. It can be concluded that under forward bias voltage, higher Ge mole fraction will produce higher current. This phenomenon happens due to lower energy band gap at higher Ge mole fraction condition. Under reverse bias voltage, the diode will provide higher leakage current with higher Ge mole fraction. This fact is observed due to lower energy band gap at higher Ge mole fraction condition and also lower maximum electric field at the junction of diode with higher Ge mole fraction. We predict that Ge mole fraction has inversely proportional effect to the maximum electric field value of the diode.

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