Effect of Mobile Space Charge in Si/Si$_{0.9}$Ge$_{0.1}$ Heterojunction Double Drift Impart Oscillator at W-Band Window Frequency

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Abstract : *Studies on mobile space charge effect in the depletion layer of heterojunction Si/Si$_{0.9}$Ge$_{0.1}$ IMPATT diode (p$^+$pnn$^+$ structure with p$^+$ = Si$_{1-x}$Ge$_x$, p = Si$_{1-x}$Ge$_x$, n = Si and n$^+$ = Si; mole fraction x = 0.1) has been simulated at 94 GHz window frequency. The simulation study based on drift-diffusion model for the study of DC, high frequency and negative resistivity properties of the device at different bias current densities has been carried out. The maximum DC-to-millimeter wave conversion efficiency of 14.82% is obtained at a bias current density of 0.7 × 10^8 A/m^2. Si/Si$_{1-x}$Ge$_x$ DDR Impatts is found to give peak negative conductance at about 92 GHz (close to 94 GHz design window frequency) for a bias current density of 0.7 × 10^8 A/m^2. The device performance degrades with mobile space charge effect at bias current densities exceeding 2.0 × 10^8 A/m^2. Hence bias current density up to 2 × 10^8 A/m^2 may be considered as the limit to realize high efficiency with high power from the device.*
Keywords: *Conversion efficiency, Heterojunction, Impatt diode, Millimeter wave, Space charge.*

I. Introduction

IMPATT (Impact Ionization and Avalanche Transit Time) diodes are the powerful solid state source of microwaves and millimeter waves operating at a wide range of frequency spectrum starting from X-Band to sub-millimeter wave region. Now-a-days Impatt devices are very efficient and highly suitable source in fulfilling the ever increasing communication needs owing to its vast operating frequency range, greater conversion efficiency and higher output power. Over the past few years significant progress in technology has led to the development of Impatt oscillators at frequencies from 30 to 300 GHz.

Silicon (Si) is the most popular choice in the global semiconductor market as their manufacturing cost is low but the driving force behind today's growth in high speed optical networking and inexpensive, light weight personal communication devices is definitely silicon-germanium (SiGe). The technology derived from SiGe increases operating speed, reduces electronic noise, lowers power consumption, supports higher levels of integration and thus facilitates design of more functional components on a chip. The substantial performance has rapidly pulled up SiGe as the perfect material choice for both wireless integrated circuits (ICs) and low-power radio frequency (RF) chips. As per expectation, the number of SiGe based applications will explode with time. SiGe heterojunction is a revolutionary technology in which the electrical properties of silicon are augmented with that of germanium. As such, SiGe offers a bridge between low cost, low power, low frequency silicon chips and high cost, high power, high frequency chips made from class III-V semiconductor materials such as GaAs and InP. SiGe technology also maintains the key advantages of the state-of-the-art silicon processing. As silicon and germanium have similar chemical and physical properties, SiGe processing is relatively simple unlike the manufacture of other high-speed semiconductors made of two or more materials. SiGe semiconductors have much higher speed than simple silicon based chip. Using SiGe technology IC manufacturers can reengineer the band gap of silicon for higher performance, producing a heterojunction system that is compatible with silicon technology. SiGe is used for the for the fabrication of Heterojunction Bipolar Transistors (HBTs), Bipolar complementary MOS (BiCMOS), Modulation Doped Field Effect Transistors (MODFETs) and Infrared Photoconductors operating into the millimeter wave frequency spectrum thereby making Si$_{1-x}$Ge$_x$ a viable material for microwave and millimeter wave source and related circuit applications.

Heterostructure IMPATT and MITATT (Mixed Ionization Tunneling and Avalanche Transit Time) reported in recent times are capable of enhancing their efficiency by localizing the avalanche zone [1-7]. Moreover Si$_{1-x}$Ge$_x$ with Si has come up as a technologically important material combination for both electronic and opto-electronic devices [8-12]. Luy et al [13] in Daimler Chrysler have fabricated Si$_{1-x}$Ge$_x$ (for x=0.6) heterostructure MITATT based on Si and have obtained 25mW of power with a conversion efficiency of 1.03% at 103 GHz. Mishra et al [14] assumed that the hole ionization rate in SiGe is higher than electron ionization rate and has proposed a single-sided (Si/Si$_{1-x}$Ge$_x$) heterostructure MITATT for x=0.5. Many researchers have used the Monte Carlo based ionization rate data for IMPATT/MITATT. According to all of these results the

ionization rate of holes in SiGe is higher than the electron ionization rate. Recent experimental results obtained by Lee et al [15], theoretical results obtained by Yeom et al [16] and other research groups [17,18] clearly indicate that the ionization rate (α) to the hole ionization rate (β) varies from 0.3 to 3.3; the composition of x in Si$_{1-x}$Ge$_x$ varying from 0.08 to 1.0, with $\alpha/\beta = 1$ at x=0.45. The potential application of Si/Si$_{1-x}$Ge$_x$ based IMPATTs / MITATTs has aroused great interest among the author to study the effect of mobile space charge on the millimeter wave properties of the device.

II.   Design Procedure And Method Of Simulation

The Si/Si$_{1-x}$Ge$_x$ heterojunction DDR Impatt diode comprises of both n$^+$ and n layers of Si, both p and p$^+$ layers of Si$_{1-x}$Ge$_x$ and mole fraction x = 0.1. The variation of band gap with Ge mole fraction x for unstrained Si$_{1-x}$Ge$_x$ is given by E$_g$(x) = 1.12 – 0.46x. The schematic structure, doping profile and electric field profile of the heterojunction DDR Impatt diode are depicted in Fig. 1. The ionization rate data are taken from Lee et. al. [15], carrier saturation drift velocities are evaluated by the full-band model in the undoped Si$_{1-x}$Ge$_x$ as a function of Ge content from Thomber [19] and the other material parameters for Si$_{1-x}$Ge$_x$ are taken from data reported elsewhere [20-22]. The parameters for Si are taken from data reported elsewhere [22-24]. The material parameters used for the present study are enlisted in Table-1.

Computer simulation method based on drift-diffusion model is used for to compute the properties of the heterojunction Si/Si$_{1-x}$Ge$_x$ diode. The total width of the diode active region is selected as 900 nm for Si/Si$_{1-x}$Ge$_x$ heterostructure DDR Impatt diode. A symmetrical diode structure has been considered both with respect to doping and material distribution. To obtain device performance at 94 GHz, the background doping concentration and the corresponding depletion layer width are simultaneously designed. For an optimal punch through field profile of the diode the doping concentration is considered equal throughout the active region of the diode and is determined to be 4.5×10^{22} m^{-3} for Si/Si$_{1-x}$Ge$_x$ heterostructure and 6.3×10^{22} m^{-3} for Si. The diode area is taken to be 10^{-10} m^2.

The DC-to-mm wave conversion efficiency of the Impatt diode is calculated from Scharfetter – Gummel [25] semi empirical formula

$$\eta = (2m'/\pi) \ [V_D/(V_A + V_D)] \times 100\% \tag{1}$$

$$= (2m'/\pi) \ (V_D/V_B) \times 100\% \tag{2}$$

Where RF voltage modulation m$'$ is taken to be 50% in our present analysis. V$_D$ is the drift zone voltage drop, V$_B$ is the breakdown voltage and V$_A$ is the avalanche voltage taken from the point where J$_{diff}$(x)/J$_0$ become 0.95. Thus for the optimization of the diodes, the doping concentration is chosen to realize an optimum punch through factor. The dc bias current density is varied from 0.5×10^8 Am^{-2} to 5×10^8 Am^{-2} and variations of avalanche voltage, breakdown voltage and the conversion efficiency for the heterojunction DDR diode is obtained. The analytic process is repeated for several dc bias current densities and the effect of mobile space charge is observed. The results of the simulation of DC analysis are taken as input parameters for the simulation of high frequency properties of Si/Si$_{1-x}$Ge$_x$ Impatt diode. The range of frequencies exhibiting negative conductance of the diode can easily be computed by Gummel-Blue method [26]. From the dc field and current profiles, the spatially dependent ionization rates that appear in the Gummel-Blue equations are evaluated and fed as input data for the small signal analysis. The edges of the depletion layer of the diode, which are fixed by the dc analysis, are taken as the starting and end points for the small signal analysis. The admittance plot (G-B plot) is carried out at bias current density generating the highest conversion efficiency and the negative resistivity profiles are obtained for different values of DC bias current density. At the resonant frequency of oscillation, the maximum power output P$_{RF}$ from the device can be obtained from the following expression,

$$P_{RF} = V^2_{RF} \ (G_p) \ A/2 \tag{3}$$

where V$_{RF}$ is the amplitude of the RF swing and is taken as V$_B$/2, assuming 50% modulation of the breakdown voltage V$_B$. G$_p$ is the diode negative conductance at the operating frequency and A is the area of the diode, taken as 10^{-10} m^2.
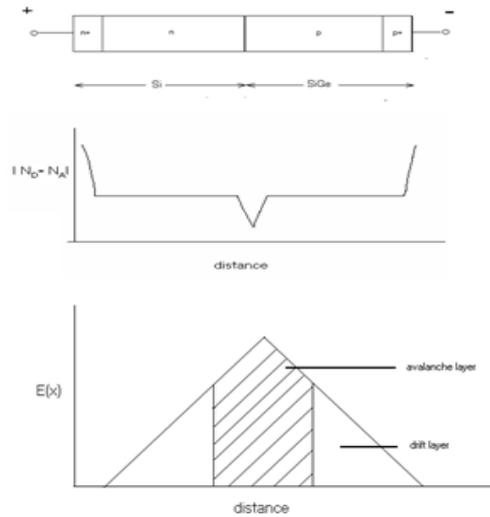
Fig. 1: Structure of Si/Si$_{1-x}$Ge$_x$ heterojunction DDR Impatt diode with its doping profile and Electric Field Profile

TABLE- 1: MATERIAL PARAMETERS FOR Si AND si$_{1-x}$ge$_x$

Parameters	Si	Si$_{1-x}$Ge$_x$
A$_n$ (10^8 m^{-1})	0.62	3.65
b$_n$ (10^8 Vm^{-1})	1.08	0.99
A$_p$ (10^8 m^{-1})	2.00	6.44
b$_p$ (10^8 Vm^{-1})	1.97	1.57
Ah$_n$ (10^8 m^{-1})	0.50	3.65
bh$_n$ (10^8 V m^{-1})	0.99	0.99
Ah$_p$ (10^8 m^{-1})	0.56	6.44
bh$_p$ (10^8 V m^{-1})	1.32	1.57
v$_{sp}$ (10^5 ms^{-1})	0.76	0.70
v$_{sp}$ (10^5 ms^{-1})	1.00	0.72
μ$_n$ (m^2 V^{-1} s^{-1})	0.135	0.055
μ$_p$ (m^2 V^{-1} s^{-1})	0.048	0.051
ε (10^{-09} Fm^{-1})	0.104	0.109

A$_n$, A$_p$, b$_n$, b$_p$	:	Ionization coefficient of electrons and holes resp. at low fields
Ah$_n$, Ah$_p$, bh$_n$, bh$_p$	:	Ionization coefficient of electrons and holes resp. at high fields
v$_{sn}$,v$_{sp}$	:	Saturation drift velocity of electrons and holes respectively
μ$_n$,μ$_p$	:	Mobility of electrons and holes respectively

TABLE- 2: DC PROPERTIES OF Si / Si$_{1-x}$Ge$_x$ DDR IMPATT FOR VARIOUS VALUES OF CURRENT DENSITY (J)

Parameters	J = 0.5 × 10^8 Am^{-2}	J = 0.7 × 10^8 Am^{-2}	J = 2 × 10^8 Am^{-2}	J = 3 × 10^8 Am^{-2}	J = 4 × 10^8 Am^{-2}	J = 5 × 10^8 Am^{-2}
E$_m$ (× 10^8 Vm^{-1})	0.3212	0.3212	0.3212	0.318	0.316	0.313
X$_0$ (nm)	-0.186	-0.0256	-0.69	-0.964	-0.116	-0.132
W$_{An}$ (μm)	0.166	0.17	0.204	0.246	0.295	0.343
W$_{Ap}$ (μm)	0.147	0.145	0.145	0.147	0.146	0.152
W$_n$ (μm)	0.4482	0.4482	0.4482	0.4482	0.4482	0.4482
W$_p$ (μm)	0.4498	0.4498	0.4498	0.4498	0.4498	0.4498
B$_v$ (V)	15.82	16.09	17.1	17.72	18.25	18.64
B$_a$ (V)	8.55	8.6	9.42	10.4	11.44	12.61
η(%)	14.63	14.82	14.30	13.15	11.88	10.3

E$_m$, X$_0$	:	Magnitude and location of electric field maximum.
W$_{An}$, W$_{Ap}$	:	Avalanche region width of n- and p-region respectively
W$_n$, W$_p$	:	Depletion layer width of n- and p-region respectively
B$_v$,B$_a$	:	Breakdown voltage and Voltage drop across the avalanche region resp.

TABLE – 3: HIGH FREQUENCY PROPERTIES OF Si/ Si$_{1-x}$Ge$_x$ DDR IMPATT DIODE

Parameters	J = 0.5 × 10^8 Am^{-2}	J = 0.7 × 10^8 Am^{-2}	J = 2 × 10^8 Am^{-2}
Operating frequency (GHz)	87	94	133
Value of the n-side maxima of resistance (Ωm)	-0.0177	-0.0180	-0.170
Value of the p-side maxima of resistance (Ωm)	-0.0281	-0.0241	-0.182
Position of the n-side maxima of resistance (× 10^{-7} m)	0.8600	1.780	2.26
Position of the p-side maxima of resistance (× 10^{-7} m)	6.46	7.5	9.00
Conductance (× 10^8 Sm^2)	-0.63	-1.51	-18.83
Susceptance (× 10^8 Sm^2)	5.80	6.62	10.79
Estimated Output Power (W)	0.197	0.489	6.88
Quality Factor Q = |B| / |G|	9.20	4.38	0.57

III.   Results And Discussions

The structure, doping profile and the variation of electric field with distance of Si/Si$_{1-x}$Ge$_x$ heterojunction DDR impatt diode is depicted in Fig. 1. The various DC parameters of Si/Si$_{1-x}$Ge$_x$ DDR impatt for different values of bias current density are noted in Table-2 while Table-3 gives the high frequency properties of Si/Si$_{1-x}$Ge$_x$ DDR impatt. Simulation studies have been done for proper understanding of the DC and high frequency properties of the Impatt diode as analytical methods do not provide accurate information. Small signal analysis has been carried out as it provides insight into the mm-wave properties.

The plots of electric field profile of Si/Si$_{1-x}$Ge$_x$ heterojunction impatt at various bias current densities are plotted in Fig. 2. The electric field profile at higher values of bias current densities are observed to exhibit appreciable distortion owing to the influence of space charge effect. The peak electric field E$_m$ at the p-n junction is seen to decrease with increase in bias current density.

The extension of avalanche zone can be estimated from the J$_{diff}$(x)/J$_0$ profile of DDR impatt diode at various bias current densities as depicted in Fig. 3. The figure reflects that the avalanche zone of Si/Si$_{1-x}$Ge$_x$ impatt is very narrow and from Table-2 is also seen that the avalanche zone width increases as bias current density increases owing to the pronounced effect of mobile space charge in the depletion layer of the device.

The breakdown voltage increases with input bias current density for DDR structure clearly indicating a space charge induced positive resistance in the device. The breakdown voltage characteristics are plotted in Fig. 4. It is also interesting to note from Table-2 that the avalanche zone does not extends equally on n and p layers of the DDR heterojunction diode.

The DC-to-millimeter wave conversion efficiency (η) increases very slowly at lower range of current density and attain a maximum value of η=14.82% for Si/Si$_{1-x}$Ge$_x$ heterojunction DDR impatt at a bias current density of 0.7×10^8 A/m^2 as depicted in Fig. 5. Thus it is very much evident that the space charge limitation of the performance is very much pronounced for heterojunction impatts.

The various parameters needed to study the high frequency properties of Si/Si$_{1-x}$Ge$_x$ heterojunction impatt diode are enlisted in Table-3. The real and imaginary parts of the diode admittance are computed for various DC current densities and for different frequencies to obtain conductance vs. susceptance (G-B) plot. The G-B plot of flat profile DDR heterojunction impatt diode at a bias current density of 0.7×10^8 A/m^2 is depicted in Fig. 6. The optimum frequency for peak negative conductance and the avalanche frequency at which G becomes negative is obtained from G-B plot. The plot reflects peak negative conductance at about 92 GHz which is very close to the design frequency of 94 GHz. The Q-factor obtained at optimum bias current density is 4.38. The negative resistivity profiles are shown in Fig. 7.
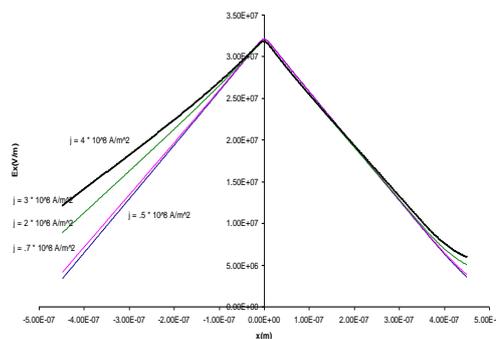

Fig. 2: Electric Field profile of Si/Si$_{1-x}$Ge$_x$ heterojunction DDR Impatt diode at different current densities
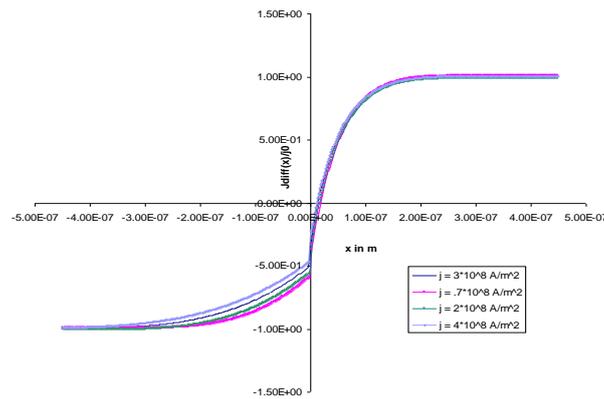
Fig. 3: J$_{\text{diff}(x)}$ / J$_0$ profile of Si/Si$_{1-x}$Ge$_x$ heterojunction DDR Impatt diode at different current densities
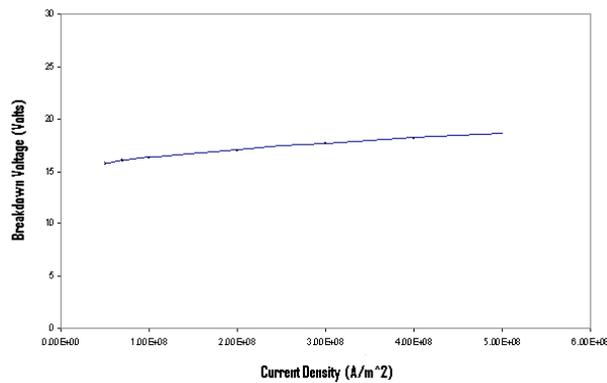

Fig. 4: Breakdown voltage of Si/Si$_{1-x}$Ge$_x$ heterojunction DDR Impatt diode at different current densities
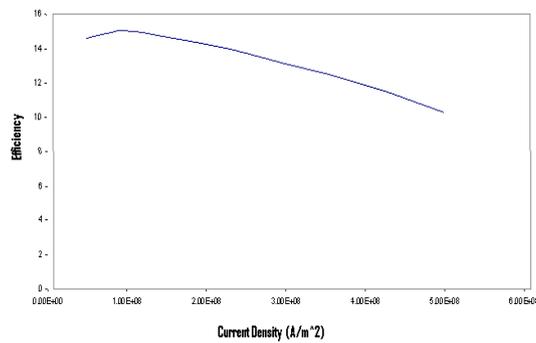

Fig. 5: Efficiency plot of Si/Si$_{1-x}$Ge$_x$ heterojunction DDR Impatt diode at different current densities
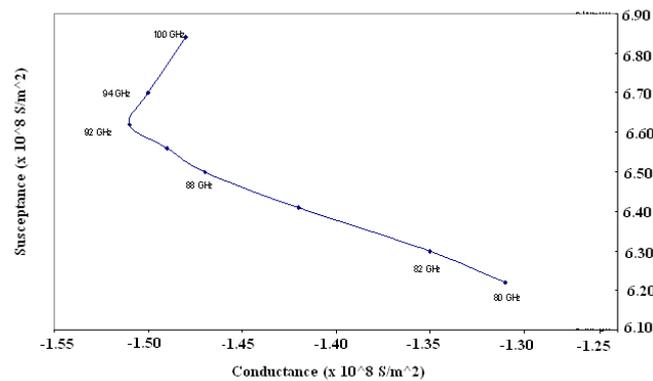

Fig. 6: G-B plot of Si/Si$_{1-x}$Ge$_x$ heterojunction DDR Impatt diode at J = 0.7 x 10^8 A/m^2
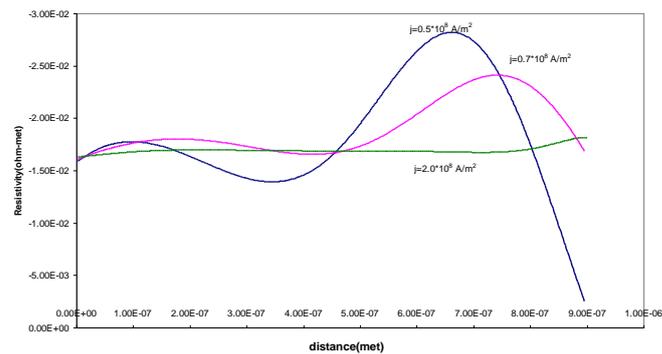
Fig. 7: Negative resistivity profiles of Si/Si$_{1-x}$Ge$_x$ heterojunction DDR Impatt diode at different current densities

IV.   Conclusion

The simulated results reveal that Impatt diode based on Si/Si$_{1-x}$Ge$_x$ heterojunction produces high efficiency and high output power. The breakdown voltage for Si/Si$_{1-x}$Ge$_x$ Impatt is found to be small and hence the input power is less but owing to greater efficiency the overall estimated output power is large. It is also possible to generate negative resistance in the millimeter wave frequency band in the unstrained Si/Si$_{1-x}$Ge$_x$ DDR Impatt diodes for value of mole fraction x = 0.1. The new structure exhibits high negative conductance, low quality factor and high value of negative resistance. Thus the simulated results are very encouraging, promising and indicates clearly the possibility of designing and fabricating Impatt diodes based on totally new material, i.e., unstrained Si/Si$_{1-x}$Ge$_x$ as the base material, suitable for operation at millimeter wave domain. The bias current density may be limited up to 2×10^8 A/m^2 to realize high efficiency with high power from Si/Si$_{1-x}$Ge$_x$ heterojunction DDR Impatt devices as above that the device performance degrades owing to the effect of mobile space charge.

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