# Impact of the Ge Content and the Epitaxial Thickness on the Bandgap Shrinkage Induced Leakage Current of Recessed $Si_{1-x}Ge_x$ Source/Drain Junctions

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**Abstract—The purpose of this paper is to evaluate the impact of process-induced stress on the generation current for fully-strained $Si_{1-x}Ge_x$ S/D junctions. The Ge content of the compressively strained SiGe epitaxial layer plays a key role in the tensile stress levels present in the underlying Si substrate. I-V measurements were employed to further investigate the leakage current enhancement due to the stress-induced bandgap narrowing in the Si depletion width when no extended defects are formed. An empirical approach is proposed to describe the Ge content dependence of the bandgap-shrinkage induced leakage current. An increase of the intrinsic carrier concentration as a function of the stress levels in the Si depletion layer adjacent to the S/D region is observed. This increase is consistent with literature values. Moreover, the role of the epi layer thickness in the generation current is also discussed.**

**Index Terms—Area leakage current, bandgap shrinkage, generation current, SiGe Source/Drain junctions, strain engineering,**

## I. Introduction

FOR strained channel pMOSFETs, a uniaxial compressive stress in the channel is induced by a selective epitaxial growth of $Si_{1-x}Ge_x$ in recessed source/drain (S/D) regions [1]. In order to improve the transistor performance, an important factor to consider is the uniaxial stress level in the channel which yields a hole mobility enhancement and boosts the drive current. Higher channel stress levels can be achieved by increasing the Ge content and the epi layer thickness in the S/D regions. However, a major concern when increasing the Ge concentration is the strain relaxation process, often leading to a lower hole mobility enhancement, through the formation of misfit and threading dislocations (Fig. 1), and which significantly degrades the device performance.

The analysis of recessed SiGe S/D-substrate diode characteristics [2,3] is a useful technique to assess the epitaxial quality. The reverse $p^+n$ diode current is a highly sensitive method, on the one hand, to investigate the presence of electrically active defects in the depletion region, which reduce the generation lifetime and enhance the generation current and, on the other, to evaluate the tensile stress in the Si depletion region, which reduces the bandgap and increases the leakage.

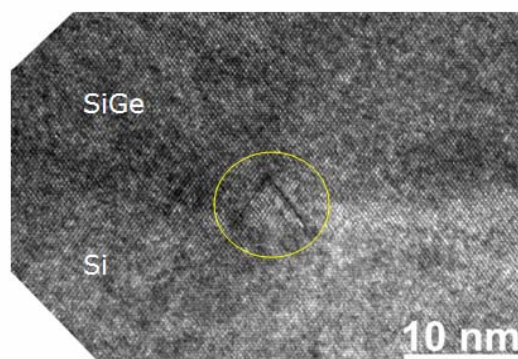



Fig. 1. TEM cross-section of a SiGe/Si interface of a recessed S/D junction. Some extended defects are observed at the interface.

The aim of this work is to investigate the effect of the Ge content and the epitaxial thickness on the bandgap shrinkage-induced leakage current in the regime where no strain-relaxation processes are present.

## II. EXPERIMENTAL

The recessed SiGe S/D junctions were fabricated on 200mm Czochralski silicon wafers. Active diode regions were defined by shallow trench isolation (STI) followed by an n-well implantation. The trenches of the S/D regions were fabricated between 40 and 80 nm etch depth, and were refilled by in-situ highly boron-doped SiGe epitaxial layers with a Ge content of 20% and 30%, using an ASM Epsilon® 2000 reactor. The layers were capped with a 25 nm $Si_{0.8}Ge_{0.2}$ top layer. Dopant activation was achieved using a 1050°C spike anneal. The process was continued with a nickel silicidation of the contacts and a Cu backend. It should be noted that the junction depth is located around the SiGe/Si interface. Therefore, the depletion width will be mainly located in the low-doped region of the junction, which resides in the Si substrate.

The diode I-V characteristics were performed between -2V and 1V at room temperature on four square and rectangular diodes with different perimeter/area (P/A) ratio. The area of the different diodes ranges from 100 to 5000 μm$^2$, while the perimeter varies from 40 to 5200 μm. The perimeter and area leakage current components ($J_P$ and $J_A$, respectively) have been extracted at fixed reverse bias from the slope and intercept of the reverse current density $J_R$ versus perimeter/area ratio plot, given by (1) [4,5]. This approach is valid when corner and parasitic components can be neglected.

$$\frac{I_R}{A} = J_A + \frac{P}{A} J_P \quad (1)$$

A good linear correlation has been observed, emphasizing that the leakage current sources are uniformly distributed across the wafer. The measurements were verified for five different dies per wafer.

No dislocations were detected by Nomarski optical microscopy, showing no evidence of relaxation in the studied samples.

## III. STRESS ANALYSIS

The lattice constants of $Si_{1-x}Ge_x$ alloys are larger than for Si. The difference in the lattice parameter creates a biaxial in-plane compressive stress on the layer and a tensile extension perpendicular to the interface. The biaxial in-plane stress or lattice mismatch stress (σ), is given by the standard elasticity theory as [6]:

$$\sigma = [2G(1+\upsilon)/(1-\upsilon)]\varepsilon \quad (2)$$

where ε is the elastic strain and G is the shear modulus and ν the Poisson ratio of the $Si_{1-x}Ge_x$ epi layer. The mismatch stress σ is proportional to the elastic strain ε, which can be expressed as function of the mismatch strain f, the dislocation density ρ and the active component of the Burger's vector $b_{eff}$ as [7]:

$$|\varepsilon| = f - \rho b_{eff} \quad (3)$$

It should be noticed in (3), that a decrease of the total strain at the $Si_{1-x}Ge_x$/Si interface is expected when plastic relaxation processes take place through the formation of misfit and threading dislocations at the interface and in the epi layer, respectively. Another important parameter to consider is the critical thickness $h_c$ [6,7], at which the relaxation becomes energetically favored.

The interest of this work is focused on the analysis of the impact of the stress on the induced bandgap shrinkage. Therefore, this study will consider only the fully-strained case, where no relaxation occurs. In this case, the misfit parameter associated with a $Si_{1-x}Ge_x$ epi layer on Si describes the elastic strain and can be expressed as [6,7]:

$$f_m(x) = \frac{a_{SiGe} - a_{si}}{a_{Si}} \quad (4)$$

Where $a_{SiGe}$ and $a_{Si}$ are the lattice parameters of $Si_{1-x}Ge_x$ and Si respectively. Vegard's law describes $a_{SiGe}$ as a function of the %Ge content as [6,7]:

$$a_{SiGe} = a_{Si} + \frac{x}{100} \cdot (a_{Ge} - a_{Si}) \quad (5)$$

A more accurate approach, in which is considered the mismatch strain at 300K, is given by [6]:

$$f(x) = 0.041 \, x/100 \quad (6)$$

Using standard values for $Si_{1-x}Ge_x$ alloys (G=64GPa and υ=0.28), high mismatch stress levels are obtained for fully-strained $Si_{1-x}Ge_x$/Si(100) heterostructures (Fig. 2). On the other hand, no impact of the epi layer thickness on the mismatch stress levels is expected for fully-strained $Si_{1-x}Ge_x$ S/D junctions.

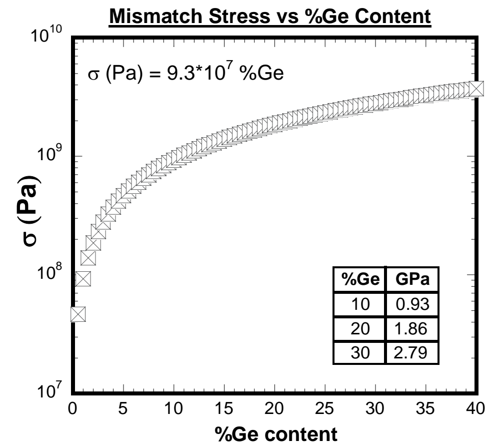



Fig. 2. Predictions of the %Ge content dependence of the mismatch stress for fully-strained $Si_{1-x}Ge_x$/Si(100) heterostructures.

According to elasticity theory [8], the compressive biaxial in-plane stress in the $Si_{1-x}Ge_x$ epitaxial layer will translate into reactive forces on the top of the underlying silicon substrate (Newton's third law) leading to a biaxial tensile stress on top of the bulk silicon. The biaxial tensile stress present in the Si depletion region will be mainly responsible for the induced leakage current. The minimization of the elastic energy will lead to zero strain on the substrate far away of the heterostructure.

## IV. Bandgap Shrinkage Induced Generation Current at 300K

### A. *Theoretical Basis of the p-n Junction Characteristics*

The total area leakage current density $J_A$, can be expressed as the sum of the generation component $J_{gbA}$ and the diffusion component $J_{dA}$:

$$J_A = J_{gbA} + J_{dA} \tag{7}$$

The effect of the diffusion component at room temperature is usually small and can be neglected. Therefore, the reverse current density will be mainly dominated by the generation processes in the depletion region, for junctions that are not too shallow and at 300 K. According to the Shockley-Read-Hall (SRH) theory, the generation current density is given by [9,10]:

$$J_{gbA} = \frac{qn_i W}{\tau_{gSRH}} \tag{8}$$

where q is the elementary charge, $\tau_{gSRH}$ the generation lifetime, W the depletion width, and $n_i$ the intrinsic carrier concentration. The intrinsic carrier concentration is connected with the semiconductor bandgap $E_g$ as [11]:

$$n_i = \sqrt{N_C N_V}\, e^{-E_g/2kT} \tag{9}$$

where $N_C$ and $N_v$ are the effective density of states in the conduction and valence band respectively, and k=8.617 343(15)×$10^{-5}$ eV/K is the Boltzmann constant.

In the next sections, the effect of the stress on the generation current for fully-strained $Si_{1-x}Ge_x$/Si(100) heterostructures will be analyzed assuming no impact of the stress levels on the $\tau_{gSRH}$.

### B. *Stress Effect on the Depletion Width*

The width of the space-charge region W is a function of the built-in junction potential $V_0$ and the junction voltage V as

$$W \propto \sqrt{(V_0 - V)} \tag{10}$$

where $V_0$ is logarithmically dependent on $n_i^{-2}$. Therefore, the W dependence on the stress will be small compared with variations on $n_i$, and can be assumed to first order approximation as a constant.

### C. *Stress Effect on the Intrinsic Carrier Concentration*

No significant variation with biaxial tensile stress of the density of states and of the effective masses of Si is expected [12]. The effect of the stress on the intrinsic carrier concentration $n_i$ can be determined by considering the effects of the stress on the energy band structure. The ratio of densities with and without strain $\gamma(\varepsilon)$ for Si can be expressed as follows (11) [13]:

$$\frac{n_i^2}{n_0^2} = \frac{p_n}{p_0} = \frac{n_p}{n_{p0}} = \frac{1}{6}\left[\exp\left(\frac{\Delta E_{V1}}{kT}\right) + \exp\left(\frac{\Delta E_{V2}}{kT}\right)\right] \times\left[\exp\left(-\frac{\Delta E_{c1}}{kT}\right) + \exp\left(-\frac{\Delta E_{c2}}{kT}\right) + \exp\left(-\frac{\Delta E_{c3}}{kT}\right)\right] = \gamma_v(\varepsilon) \tag{11}$$

where $\Delta E_C$ is the change in the energy minima of the conduction level under stress, and $\Delta E_v$ is the change in the energy on the heavy and light hole valence levels under stress. At high stress levels $\gamma_v$ is linked with the stress as [14]:

$$\gamma_v = C_1 e^{C_2} \tag{12}$$

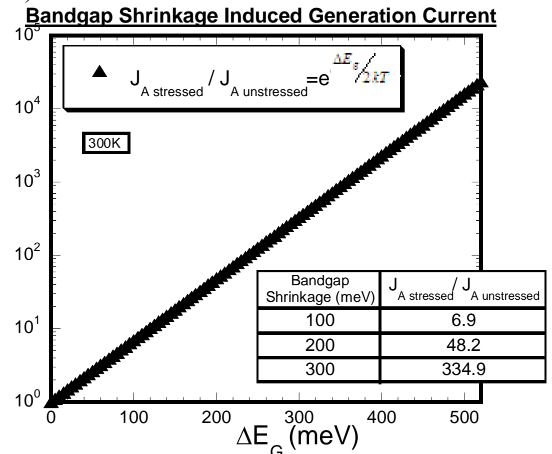
where $C_1$ depends on the stress orientation, and $C_2$ depends on the stress orientation and the stress level. It is well known that hydrostatic strain (dilatation stress) is mainly responsible for the bandgap shrinkage $\Delta E_g$ [15], thus taking into account as first approach that the stress is only affecting the bandgap:

$$C_2 = \frac{\Delta E_g}{kT} \tag{13}$$

Therefore $n_i$ can be described as:

$$n_i = \sqrt{N_C N_V}\, e^{-E_{g0}/2kT} e^{\Delta E_g/2kT} \tag{14}$$

As a result, an increase of the generation current due to the bandgap narrowing by a factor $e^{\Delta Eg/2kT}$ is expected at 300K (Fig. 3).




| Bandgap Shrinkage (meV) | J A stressed / J A unstressed |
|---|---|
| 100 | 6.9 |
| 200 | 48.2 |
| 300 | 334.9 |

Fig. 3. Predictions of the bandgap shrinkage induced generation current for fully-strained $Si_{1-x}Ge_x$/Si(100) heterostructures at 300K.

## V. Results and Discussion

According to the area leakage current density plots of Fig. 4 and Fig. 5, an increase of one decade is observed for every 9% Ge content for fully-strained $Si_{1-x}Ge_x$/Si heterostructures. This observation, consistent with the proposed model, points to the fact that the epi layer thickness has no marked impact on the stress levels in the Si depletion region for the thickness range studied (40-80 nm).

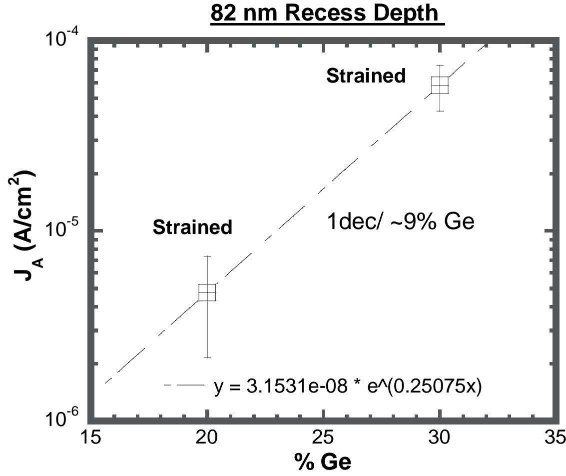



Fig. 4. Area leakage current density at -1V and 300K, for recessed $Si_{1-x}Ge_x$ S/D junctions with 82 nm recess depth. The strain relaxation was evaluated by Nomarski microscopy. An increase of one decade per 9% of Ge content is observed.

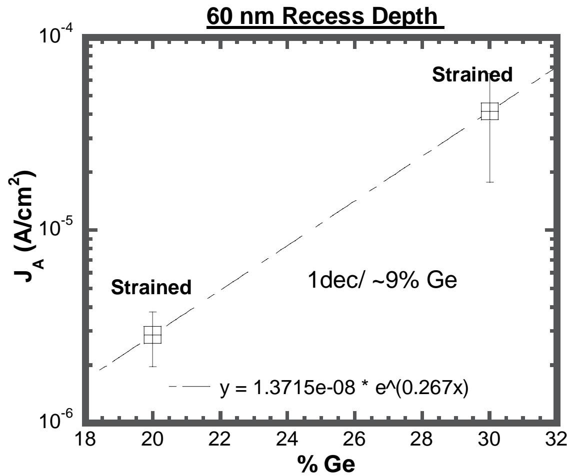



Fig. 5. Area leakage current density at -1V and 300K, for recessed $Si_{1-x}Ge_x$ S/D junctions with 60 nm recess depth. The strain relaxation was evaluated by Nomarski microscopy. An increase of one decade per 9% of Ge content is observed.

The experimental results were obtained from fully-strained $Si_{1-x}Ge_x$ S/D junctions (20<x< 30 with three different recess depths). The exponential dependence observed in Fig. 4 and Fig. 5 enables the extraction of an empirical modeling (15) to quantify the stress-induced bandgap narrowing on the Si depletion width in the regime when no relaxation occurs. An uncertainty of 9.5% is obtained.

$$\Delta E_g = 12.7x \quad \text{meV} \qquad (15)$$

The bandgap narrowing derived for the Si depletion region is 0.14meV/MPa. This value is in perfect agreement with previously reported data [15,16]. As observed in Fig. 6, an increase of more than two and three decades of the generation current is obtained for the splits with 20% and 30% Ge content, respectively.

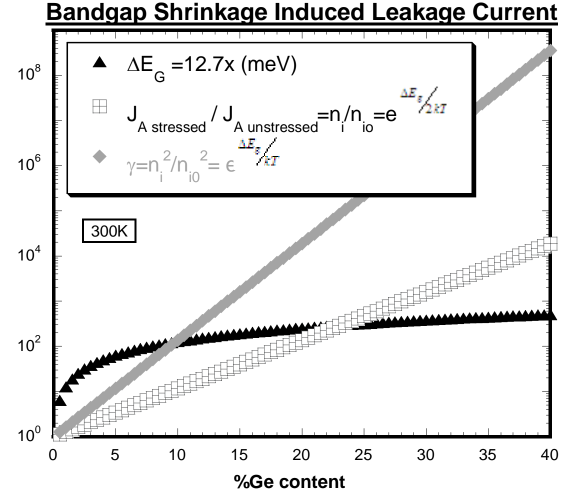



Fig. 6. Bandgap shrinkage induced generation current for fully-strained $Si_{1-x}Ge_x$/Si(100) heterostructures at 300K.

The analysis of the ratio of the minority carrier density with stress to the unstressed carrier density versus stress in Si (Fig. 7) is obtained from (12)-(15). A similar tendency to previously published results is observed [13].

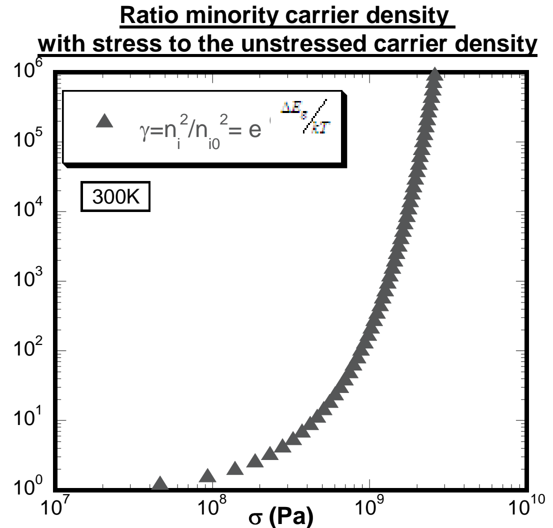



Fig. 7. Ratio of the minority carrier density with stress to the unstressed carrier density for the underlying silicon substrate at 300K as a function of the compressive stress.

## VI. Conclusions

In summary, a one decade increase of the bandgap-shrinkage induced leakage was measured for every 9% of Ge content in the study of fully-strained $Si_{1-x}Ge_x$ S/D junctions. No significant dependence of the epi layer thickness in the

range 40-80 nm on the stress levels of the Si depletion region was observed in the regime where no plastic relaxation occurs. An empirical approach has been developed to quantify the bandgap narrowing due to the tensile stress levels in the Si depletion region. A reduction of 0.14meV/MPa of the Si bandgap was found and is in perfect agreement with literature. Finally, an empirical approach was proposed to describe the Ge content dependence of the bandgap shrinkage induced leakage current.

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