Atomistic Analysis of Electrical Performance of Highly Scaled $Si_{1-x}Ge_x$ p-FinFETs

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Abstract— **SiGe alloy is already being used in the semiconducting industry for inducing strain on Si channel pMOS devices in order to enhance performance. In addition, it is well known that Ge exhibits a higher bulk hole mobility as compared to Si due to lighter hole effective mass. However, increasing Ge concentration in SiGe alloy and inducing compressive strain in the <110> channel orientation both of which increase the mobility and ON state performance, cause a reduction in the band gap value of the semiconducting channel. We show, using atomistic simulations, the possibility of using the effect of quantum confinement in highly scaled 3D FinFETs for reasonably high band gap values while retaining high Ge concentration and high uniaxial strain for better ON performance.**

Keywords- 3D FinFETs; quantum confinement; strain; SiGe alloy; hole conduction; tight binding; atomisitc band structure; injection velocity.

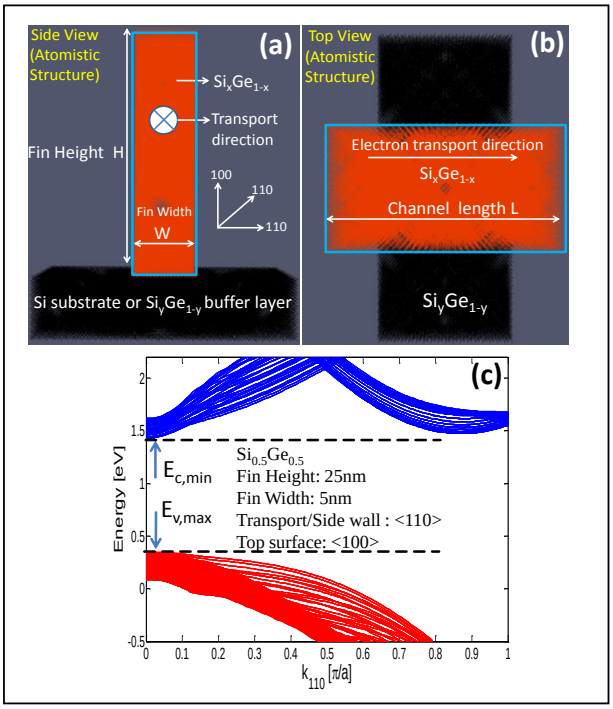
I. INTRODUCTION

SiGe is already being used in the semiconducting industry for inducing strain on Si channel pMOS devices in order to enhance performance. In addition, it is well known that Ge exhibits a higher bulk hole mobility as compared to Si due to lighter hole effective mass [1,2]. Transistors with SiGe alloy channels of various Ge concentrations have also been studied experimentally and show better hole mobility values [3]. It is also generally accepted that FinFETs (Fig.1) provide an attractive alternative for the planar CMOS technology due to better short channel effects (SCEs). Transistor miniaturization in the near future is entering highly scaled dimensions where atomic granularity becomes more and more important and as such, modeling of these devices requires atomistic approaches.

Figure 1. $Si_{1-x}Ge_x$ Fin structures. (a) Shows the side view of the $Si_{1-x}Ge_x$ Fin on top of a layer which can be pure Si substrate or a $Si_{1-y}Ge_y$ buffer layer. (b) Top view. The atomic lattice is assumed periodic along the <110> transport direction, while the width, *W*, varies between 3 to 8 nm and the height *H*, is 25 nm. Significant quantum confinement effects in this paper are predominately determined by the *W* rather than *H* (*W*<<*H*). (c) Shows an example of band structure calculations which are used throughout this paper for obtaining band gap and injection velocity values.

Appropriate atomistic modeling of such devices would contain methods of calculating the band structure and using such band structure calculations to model the electrical characteristics of transistors based on quantum transport models that are also atomistic. Effects such as quantum confinement or tunneling are inherent part of these models.

Here we use semi-empirical tight binding based Hamiltonians for electronic band structure calculations embedded in the atomistic simulator NEMO5 [5]. We then use the Non-Equilibrium Green's Function formalism for ballistic injection velocity calculation which is a measure of ON performance of transistors. We present simulation results on band gap and injection velocities for 3D FinFET devices employing SiGe alloys with 0-100% Ge concentrations (Fig.1).



II. PROBLEM STATEMENT, STRUCTURES AND THE COMPUTATIONAL FRAMEWORK

The height and width of the Fin (Fig.1) are designated as *H* and *W* respectively. The atomic lattice is assumed periodic in the transport <110> direction. This assumption should give valid performance trends for channel lengths of interest in this paper that are longer than 15 nm [5]. Fin widths vary between 3 to 8 nm in this paper while the height is 25 nm. The $Si_{1-x}Ge_x$ Fin structure stands on top of a layer which can be Si substrate or a $Si_{1-y}Ge_y$ buffer layer with different Ge concentrations from the Fin itself. There can be lattice mismatch between the Fin and the layer underneath (Fig.1) which then creates strain in the Fin. Throughout this paper we assume a uniaxially dominated [7] strain along the transport <110> direction wherever strain is present. The side and top surfaces are defined by the <110> and <100> directions respectively. While the Fin height of 25 nm used in this paper does not cause any significant quantum confinement, such affects are associated with Fin widths and cause changes in the band structure (Fig.1c) of the $Si_{1-x}Ge_x$ Fins. These in turn do affect parameters for the device electrical characteristics such as band gap E_g and injection velocity v_{inj}. The significant quantum confinement effects that will be shown in this paper are predominately determined by the *W* rather than *H* since *W*<<*H*.

Fig.1c Shows an example ($Si_{0.5}Ge_{0.5}$) of band structure calculations which are used throughout this paper for obtaining band gap and injection velocity values later on. The underlying fully atomisitic model we use is based on the 20 orbital $sp^3d^5s^*$ (including spin-orbit coupling) tight binding (TB) based band structure calculations [4,5] in the Virtual Crystal Approximation (VCA).

The rest of the paper follows by presenting the effect of confinement on the band gap of SiGe FinFETs followed by adding the effect of strain on the quantum confined structures concluding by a camparison of injection velocity, v_{inj} and band gap, E_g, for various strain values while varying the Ge concentraion between 0-100% in the ultra scaled FinFETs.

III. EFFECT OF QUANTUM CONFINEMENT ON BANDGAP

Figures 2a, b show the band-edge/gap values for various Fin widths as the Ge concentration is varied. Bulk values are also provided for comparison and reference purposes. First thing to note is that the model captures the well known shift in the conduction band minimum ($E_{c,min}$) from the X-valley of Si to L-valley of Ge quite well which occurs around 85% Ge. This is evident from both Fig.2a and Fig.2b. While a sharp drop in the band gap (E_g) occurs for the bulk values once ~85% Ge is reached, the confined structures suffer less of a drop. Moreover, it can be observed that as the width is decreased, the slope of the drop in E_g is also reduced for 0<x<1. This is important for device electrical characteristics because high concentration of Ge is desirable for higher mobility while higher band gap values are desirable for lower

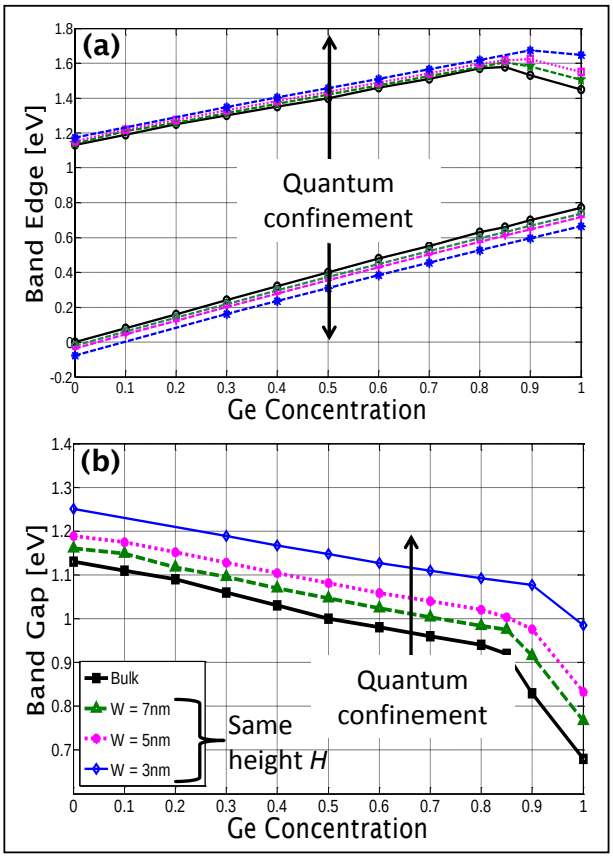


Figure 2. Effect of Ge mole fraction and quantum confinement on band edges and band gap of $Si_{1-x}Ge_x$ FinFETs for 0<*x*<1. The bulk values are also provided for comparison and reference purposes. (a) Conduction ($E_{c,min}$) and valence ($E_{v,max}$) band edges are shown. The lowest $E_{c,min}$ and highest $E_{v,max}$ belong to bulk $Si_{1-x}Ge_x$. Band edges are pushed away from each other for more and more confined dimensions. (b) Band gap value are shown for various widths. There is no strain present in these simulations. The effect of quantum confinement on band gap can be as large as 300meV as compared to bulk Ge in the case of *w* = 3nm Fins. This can be of significant importance especially for high Ge concentrations where the bulk band gap values become small but the confined values are noticeably larger. (Note that if strain is present, it is generally underestood that the band gap values will become even smaller.)

OFF state leakage currents. Once strain is added, E_g would drop even further. But we will show that such degrading effects can be offset by quantum confinement effects that can be seen in Fig.2. This way, the device will benefit from high Ge concentration, high strain values and reasonable band gaps as we will show later on in this paper. In Fig.2 we have shown various widths in the range of 3-8 nm. For the rest of the paper, we will focus on 4nm only noting that there is nothing fundamental about this value. We have chosen this value as an example to draw attention to possible device design scenarios which otherwise might have been overlooked if various effects we consider here had not been incorporated simultaneously.

In the next section we analyze the effect of various strain magnitudes for the highly scaled Fin dimension of 4nm width

by calculating the change in the band gap value E_g. The injection velocity, v_{inj}, will be incorporated in the analysis later on in order to obtain a qualitative understanding of quantum confinement, strain and Ge concentration on electrical characteristics of 3D p-FinFETs.

IV. Combined Effect of Strain and Quantum Confinement on $Si_{1-x}Ge_x$ FinFETs Band Gap

While Fig.2 focused on the effect of quantum confinement, in Fig.3 we have added the effect of strain to the Fin structures. Note that the strain tensor we have used has a dominant uniaxial characteristic which appears reasonable based on the recent modeling and experimental work [6]. It is generally well known that higher strain reduces the band gap. Experiment of Lang et al. [7] showed the sharp drop of the band gap as the Ge concentration (x) of a biaxially strained $Si_{1-x}Ge_x$ layer on top of a Si substrate is increased due to the increased lattice mismatch. In Fig.3 we show a case with differences in 3 aspects:

- The strain tensor we use is dominated by its uniaxial compressive component.
- Highly scaled Fin structures are being studied here. There are significant quantum confinement (QC) effects present due to small Fin widths (3-8 nm in this paper and (8, 4) nm in the Fig.3.). It is evident from Fig.3b that the QC effects can be large enough to completely offset the effect of strain on reducing E_g while still retaining high concentration Ge and high strain (1% which corresponds to more than 1GPa "stress"). We use stress in quotation marks since the tensor transformation from strain to stress can result in non- uniaxial components. Never the less the dominant one is the uniaxial component in the transport <110> direction which is desired for increased mobility. Here, the GPa value is reported for having a rough estimate of the magnitude of compressive stress in units of Pa rather than dimensionless strain percentages.
- The mismatch between the Fin and the layer underneath is kept constant as the concentration of Ge in the $Si_{1-x}Ge_x$ Fin is increased. One way to achieve this is to simultaneously change the Ge concentration in both the $Si_{1-x}Ge_x$ Fin and the $Si_{1-y}Ge_y$ buffer layer so that there is always a constant lattice mismatch (e.g. 25% or 50%) between the two. This keeps E_g from dropping sharply while still retaining reasonably high strain values.

Figures 3a,b show the band-gap values for 8nm and 4nm widths respectively where we have also added the effect of 1% strain. Three curves are shown: bulk values with no strain for reference purposes. Quantum confined values for the Fin dimensions of H=25nm and W=8nm (a), 4nm (b) and lastly, strained values for the same Fin dimensions are also included. It is imperative to note that the strain is kept fixed at 1% for all

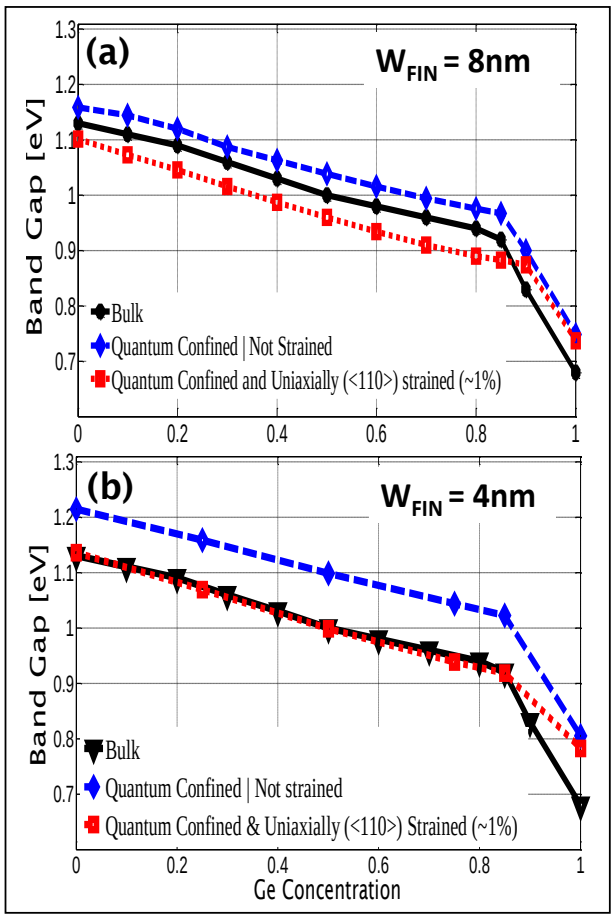


Figure 3. Combined effect of fixed uniaxial strain and quantum confinement for two different Fin widths: 8nm and 4 nm. (a) Three curves are shown: bulk values for reference purposes, quantum confined values for the Fin dimensions of H=25nm and w=8nm and strained values for the same Fin dimensions. It is imperative to note that the strain is kept fixed at 1% for all Ge concentrations which corresponds to ~25% of lattice mismatch between the $Si_{1-x}Ge_x$ Fin and $Si_{1-y}Ge_y$ buffer layer (which could be pure Si for $Si_{0.75}Ge_{0.25}$ Fin). This can be achieved by *simultaneously* changing the concentration of both the $Si_{1-x}Ge_x$ Fin and the $Si_{1-y}Ge_y$ under layer. (b) Bulk, quantum confined and strain quantum confined values are shown for Fin width of 4nm. It is evident from the figure that with a significant strain of 1% (~1.5GPa), quantum confinement effects can keep the band gap values at reasonable levels even for high concentration of Ge.

Ge concentrations which corresponds to ~25% of lattice mismatch between the $Si_{1-x}Ge_x$ Fin and $Si_{1-y}Ge_y$ buffer layer (which could be pure Si for $Si_{0.75}Ge_{0.25}$ Fin). While the 8nm Fin width suffers lower band gap values than bulk because of strain, at 4nm Fin width, the quantum confinement is such that even at about 1% strain, E_g can be equal or larger than bulk. This is promising for increasing performance while keeping leakage manageable.

V. Dependence of Band Gap and Injection Velocity as a Function of Ge Concentration, Quantum Confinement and Strain

To analyze the electrical characteristics, the following quantities are calculated for a 25nm by 4nm device. The simulations have been performed while keeping the inversion charge Q_{inv} constant and about ~1e13/cm^2. (Here, the charge per-unit-length is scaled by the perimeter $2H+W$). Assuming high drain bias, inversion charge is [6-8] calculated as $(N \text{ or } P)_{inv} = q\int DOS(E)\, f_s dE$ where $DOS(E)$ is the density of states while saturation current is obtained via $I_{ds} = \left(q^2/h\right)\int M(E)\, f_s dE$ where M(E) is the number of modes. Injection velocity can readily be calculated using $v_{inv} = I_{ds}/\left(N_{inv} \text{ or } P_{inv}\right)$. Figure 4 shows the dependence of injection velocity and band gap on Ge concentration, quantum confinement and strain. The Fin dimensions are the same for Fig.4a,b,c with H=25nm and W=4nm. The amount of strain is varied from 0 (Fig.4a) to 1% (Fig.4b) to 2% (Fig.4c). In each figure, we simultaneously show the dependence of band gap and injection velocity on the Ge concentration. More analysis is certainly needed to properly analyze the OFF state leakage currents. Our results raise the possibility of using high concentration of Ge and high strain while retaining reasonable band gap values due to high quantum confinement. This can potentially result in the possibility of using high Ge concentration and high strain for SiGe FinFETs for better mobility and ON state performance without sacrificing I_{on} to I_{OFF} ratio.

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Figure 4. v_{inj} and E_g dependence on Ge concentration, quantum confinement and strain. The Fin dimensions are the same for Fig.4a,b,c with H=25nm and W=4nm. The amount of strain is varied from 0 (Fig.4a) to 1% (Fig.4b) to 2% (Fig.4c). In each figure, we simultaneously show the dependence of band gap and injection velocity on the Ge concentration. While more analysis is certainly need especially to properly analyze the OFF state leakge currents, these figures suggest the possibility of using high concentration of Ge, high strain while retaining reasonable band gap values because of high quantum confinement. This can potentially result in the possiblity of using high Ge concentration and high strain for SiGe FinFETs for better mobility and ON state performance without sacrificing I_{on} to I_{OFF} ratio.