Theoretical Investigation Of Performance In Uniaxially- and Biaxially-Strained Si, SiGe and Ge Double-Gate p-MOSFETs

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Abstract

Using the Non-local Empirical Pseudopotential method (bandstructure), Full-Band Monte-Carlo Simulations (transport), 1-D Poisson-Schrodinger (electrostatics) and detailed Band-To-Band-Tunneling (BTBT) (including bandstructure and quantum effects) simulations, the effect of uniaxial- and biaxial-strain, band-structure, mobility, effective masses, density of states, channel orientation and high-field transport on the drive current, off-state leakage and switching delay in nano-scale, Si, SiGe and Ge, p-MOS DGFETs is thoroughly and systematically investigated.

Introduction

Currently, uniaxial compressively strained Si is the dominant technology for high performance p-MOSFETs and increasing the strain provides a viable solution to scaling [1,2]. However, looking into future nanoscale p-MOSFETs, it is important to examine novel higher mobility channel materials, like Ge, strained-SiGe or strained-Ge, which may perform better than even very highly strained-Si [3]-[8]. Previous work has attempted to explain the transport in uni-axially strained MOSFETs through simple bandstructure and mobility calculations. However, as we scale MOSFETs down to very short channel lengths, the effect of the high-field transport, density of states (DOS), bandstructure, mobility and effective mass, in determining the eventual current drive needs a thorough and detailed investigation. Further, strain modifies the bandstructure [9] and dramatically changes the BTBT limited off-state leakage [12-13]. In this work, the bandstructures were calculated using the non-local Empirical Pseudopotential method including spi-orbit interactions [10]. Full-Band Monte-Carlo Simulations were used to evaluate the transport [11]. A 1-D Poisson-Schrodinger solver and detailed BTBT simulations (including direct and indirect transitions) were used to calculate the electrostatics and the off-state leakage. We systematically compare and benchmark nano-scale (Ts=5nm, Lg=15nm) DG p-FETs, with different high mobility channel materials (Si, SiGe and Ge), in terms of their important performance metrics - Drive Current, Intrinsic Delay and Off-state Leakage. Two standard channel directions, [100] and [110], on the (001) surface are considered.

Biaxial Strain

Channel Materials and Strain:

We have looked at all possible biaxial strained Si(1-x)Ge(x) alloys grown on relaxed Si(1-y)Ge(y) virtual substrates. A common terminology used in this paper for biaxial strain is a channel material (x,y), where x denotes the Ge content in the channel material and y denotes the Ge content in an imaginary relaxed (r) substrate to which the channel is strained (s). E.g. (0.3,0) is a s-SiGe channel (30% Ge content), compressively strained to an underlying r-Si substrate. (0,0.6) is a s-Si channel, tensile strained to a r-SiGe (60% Ge) substrate.

Effective mass, DOS and Bandgap:

Fig 1(a) and 1(b) show the conductivity effective mass in the x, y and z directions with Ge content (biaxial strain). There is a very rapid reduction in the effective mass of (1,0) s-Ge in the xy-plane, while still remaining quite high in the z-direction. (0,1) s-Si does not exhibit a strong change in the effective mass in the xy-plane and shows a larger reduction in the z-direction. The DOS for all the biaxially strained materials is about an order of magnitude lower than r-Si (Fig.2). The bandgap for (0,1) s-Si and (1,0) s-Ge drops very sharply to ~0.4eV (Fig. 3). For r-Ge the lowest valley is L- with the □- point just ~0.15eV higher. Strain causes the X-valley to rapidly decrease to ~0.5eVand the □-point to increase >1.1eV (Fig. 4).

Low-field Mobility and Velocity-Field curves:

We find a very dramatic increase in mobility with biaxial strain (Fig. 5). The mobility in (1,0) s-Ge is ~25X higher, for (0,1) s-Si ~10X higher and for r-Ge ~4X higher, than r-Si. This is due to a combination of smaller mass and lower scattering due to removal of band degeneracy. Application of biaxial strain, does not greatly affect the high-field transport but it changes the slope of the velocity field curve in the low-field, due to the higher mobility (Fig. 6).

Drive Current, Delay and Off-State Leakage:

Clearly, the highest drive currents are obtained in (1,0) s-Ge

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(Fig. 7). Even though, s-Si has much higher (~2.5X) low-field mobility, r-Ge performs better because of its lower transport mass and higher DOS. The low-field mobility is very high (>10X) in some of these materials but the drive current enhancement is much smaller (~2X) because the transport is still strongly dominated by high-field transport. The intrinsic delay (Fig. 8) still tracks the ON-current closely. The minimum possible (BTBT limited) off-state leakage achievable is shown in Fig. 9. Due to its extremely small bandgap, (0,1) s-Si exhibits a very large leakage. Strained-Ge shows an optimum leakage at ~1.3% (1,0.6). With strain, due to the increase in the □-valley the leakage reduces but due to the rapid reduction in the X-valley, the leakage again increases.

Uniaxial Strain

Channel Materials and Strain:

We have looked at uniaxially strained, Si and Ge MOSFETs on a (001) wafer with channel direction along [100] and [110]. Both tensile and compressive stresses from –5GPa to +5GPa were considered. The uniaxial stress was along the channel direction.

Effective mass, DOS and Bandgap:

The effective masses are shown in Fig. 10. Along [100] Si, the effective mass reduces slightly for both tensile and compressive in all directions. Along Si [110], compressive stress rapidly decreases the mass in the transport direction (x) while greatly increasing the mass in the width direction (y), leading to a high density of states (Fig. 11). For Ge, compressive stress allows a rapid decrease in transport mass and along [110] it behaves similar to Si, allowing a simultaneous increase in the DOS. As seen in Fig. 12, the reduction in bandgap for compressive uniaxial stress along [100] is much larger than along [110]. The relative positions of all the different valleys for Si [110], Ge [100] and Ge 110] are shown in Fig. 13 (a), (b) and (c). The lowest valley for Si is always X-, and for Ge [110] it is L-. However, for Ge [100], the lowest valley shifts from L- to X- for large values of stress, due to the rapid reduction in the X-valley bandgap. For compressive stress in Ge, the □-valley bandgap increases, while for tensile it sharply reduces.

Low-field Mobility and Velocity-Field curves:

The mobility for [100] Ge is the highest along the channel direction, due to its lower mass and removal of band degeneracy (Fig. 14). The mobility is ~2X larger than [110] Ge and ~7X larger than [110] Si. The velocity-field curves are shown in Fig. 15 (a) and (b) (compressive and tensile stress). Ge [110] shows a larger velocity compared to Ge [100]. The velocity for compressive Si [110] is extremely large and exhibits stationary velocity overshoot under bulk conditions.

Drive current, Delay and Off-State Leakage:

From Fig. 16, we find that the large velocity overshoot in compressive Si [110] leads to very high drive currents. The higher mobility of Ge [100] and the higher velocity of Ge [110] compensate, leading to very similar drive currents, which are the highest among all the channels considered. The intrinsic delay for Si [110] is very low (Fig. 17) and nearly equal to Ge because of its greatly enhanced high-field transport. The minimum off-state leakage in compressive Ge [110] is an order of magnitude lower than Ge [100] because of its larger L- and □-valley bandgaps (Fig. 18). Si [110] shows the lowest leakage, (100X lower than Ge), due to of its large indirect X-valley bandgap.

Conclusion

The role of strain, channel orientation, bandstructure, DOS, effective mass, bandgap, mobility and velocity in determining the performance in nanoscale pMOSFETs is examined. For biaxial strain, 1.3% (1,0.6) s-Ge provides the best trade-off between lower leakage (<10nA) and drive current enhancement / delay reduction (~2.5X). For uniaxial strain, mainly due to the large stationary velocity gain, anisotropic effective mass and large bandgap, Si [110] strained compressively to -5GPa performs the best in terms of drive current enhancement / delay reduction (~3X) and low off-state leakage (<1nA).

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Acknowledgements

This work was sponsored by MARCO Materials, Structures and Devices Focus Center (MSD), Initiative for Nanoscale Materials and Processes (INMP) and an Intel Fellowship.

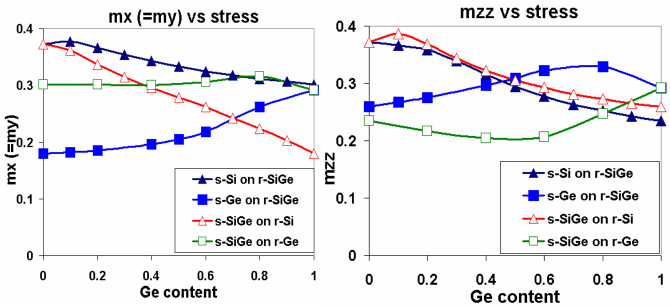

Fig1 (a) and (b): Effective mass in the x, y and z directions with Ge content (biaxial strain). Strained-Ge shows a strong reduction in the mass in the x and y direction compared to the z-direction. The trend is reversed for biaxially strained-Si.

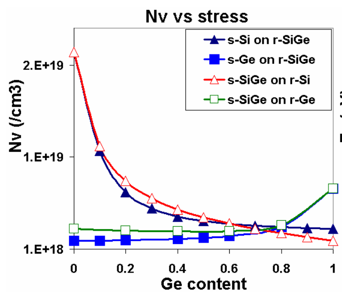

Fig2: Strain drastically reduces the DOS compared to relaxed Si. Relaxed Ge has a higher DOS than (0,1) s-Si.

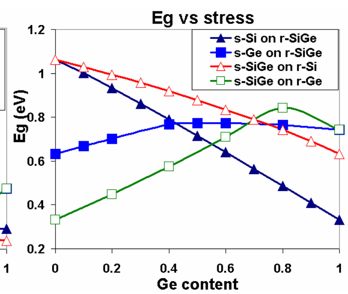

Fig3: The bandgap rapidly decreases as a function of biaxial strain for both Si and Ge. The decrease is faster for Si.

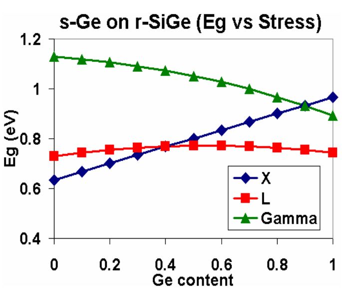

Fig.4: Various valleys and bandgap for biaxial strained-Ge. The X-to-L crossover occurs at high levels of strain. The Γ-valley bandgap increases with compressive strain.

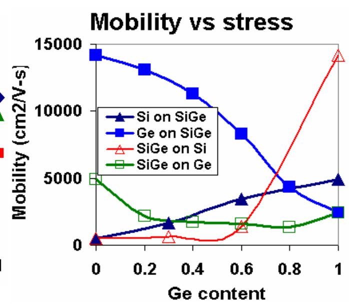

Fig.5: Mobility for s-Ge is 25X higher, for s-Si is 10X higher and for r-Ge is 4X higher than relaxed Si due to lower mass and valley splitting.

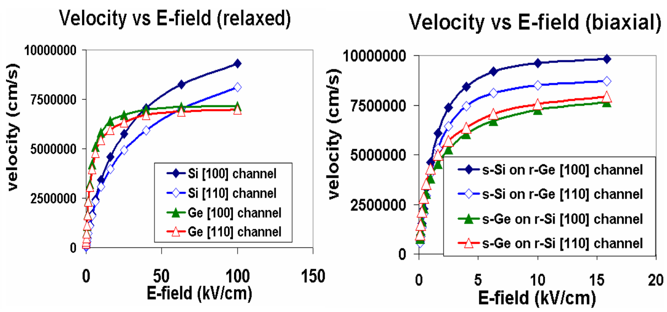

Fig.6: Biaxial strain does not significantly alter the high-field transport properties, but changes the slope of the velocity-field curve in the low-field regime, due to the higher mobility. Higher velocity is obtained along the [100] channel direction for Si and Ge.

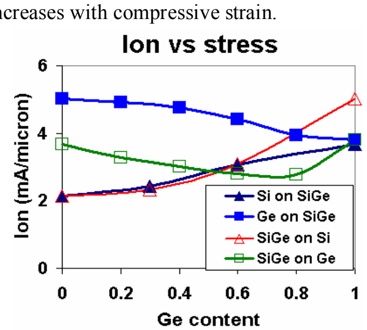

Fig.7: Drive current enhancements are largest for compressive biaxially s-Ge. Relaxed Ge shows higher drive than biaxially s-Si due to lower transport mass and higher DOS. Enhancements are much smaller compared to mobility in nanoscale FETs.

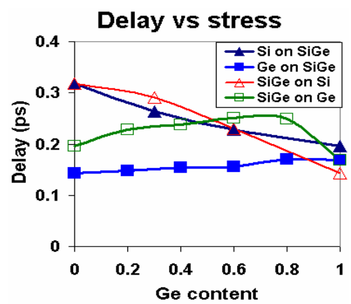

Fig.8: The intrinsic delay still tracks the drive current trends quite closely for biaxially strained materials.

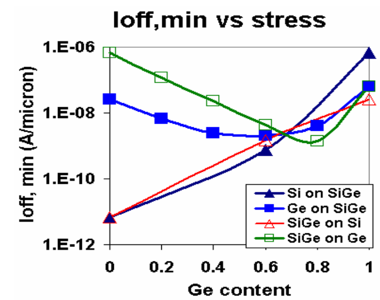

Fig.9: The minimum achievable (BTBT limited) off-state leakage is worst for s-Si, due to its small bandgap. Ge shows an initial reduction in leakage with strain due to the increase in the direct Γ-valley bandgap.

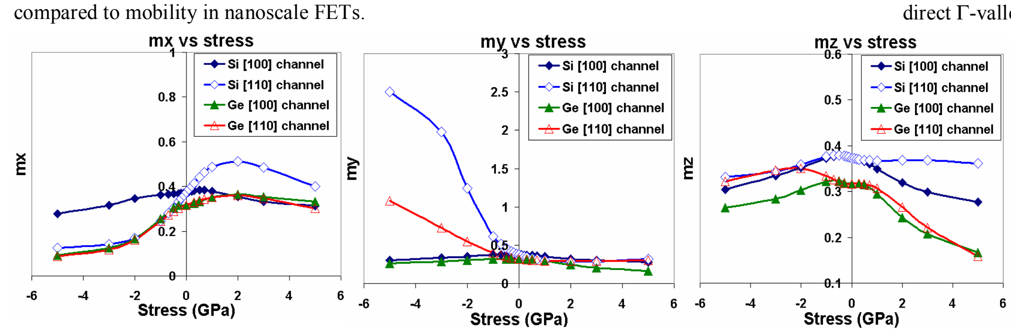

Fig.10 (a), (b) and (c): The effective mass for Si and Ge as a function of uniaxial strain. Si [100] and Ge[100] show a reduction in mx and my with uniaxial stress. The reduction in Ge [100] along x is stronger. Si [110] and Ge [110] show a rapid reduction in mass along the channel and simultaneous increase in the width direction, with applied compressive stress. The z-direction mass is not strongly perturbed for compressive stress.

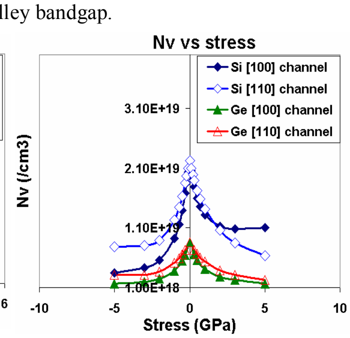

Fig.11: The DOS is larger for the Si and Ge[110] direction compared to [100] direction due to the strong anisotropic nature of the mx and my.

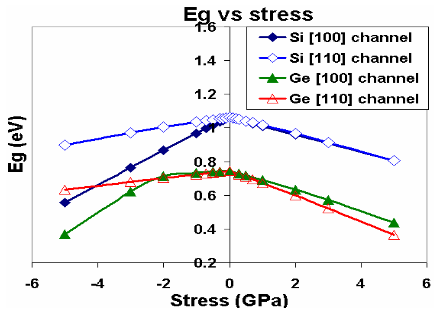

Fig.12: The bandgap reduction for compressive stress along [100] is much larger than [110] for Si and Ge.

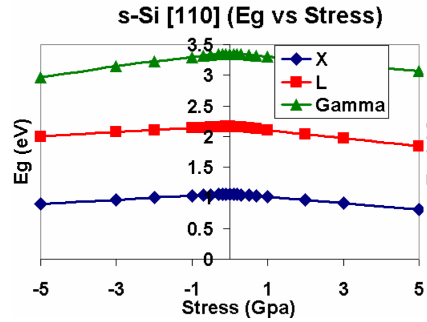

Fig.13 (a): The lowest valley for Si is always X- and the bandgap is relatively large even for large [110] uniaxial stress.

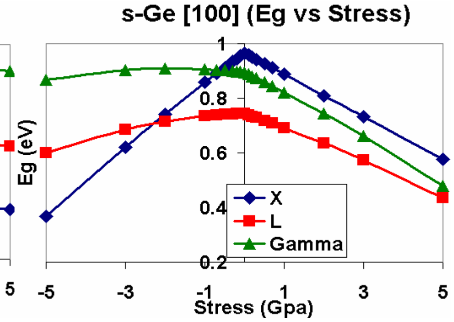

Fig.13 (b): The bandgap is strongly affected by stress for Ge [100]. The lowest valley shifts to X- at high levels of strain.

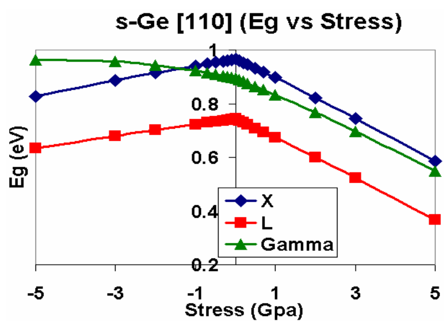

Fig.13 (c): The lowest valley for Ge [110] is always L- and the bandgap is relatively large even for large [110] uniaxial stress. The Γ- valley increases with compressive stress.

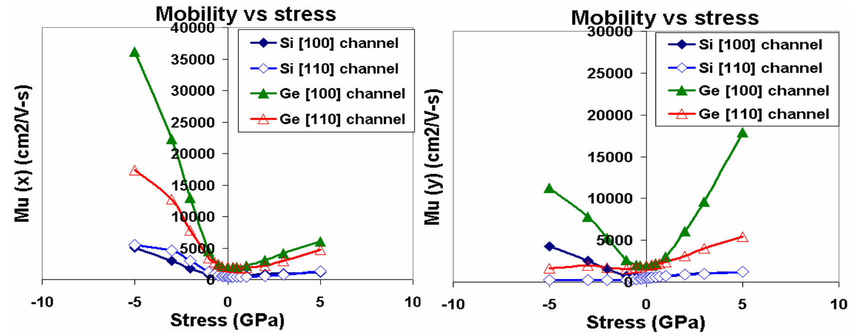

Fig.14 (a) and (b): The low-field mobility vs uniaxial stress for Si and Ge. Mobility is greatly enhanced along the channel for Ge [100] due to the low effective mass, reduced scattering and valley splitting. The anisotropy in the effective mass is reflected in the mobility for [110] direction.

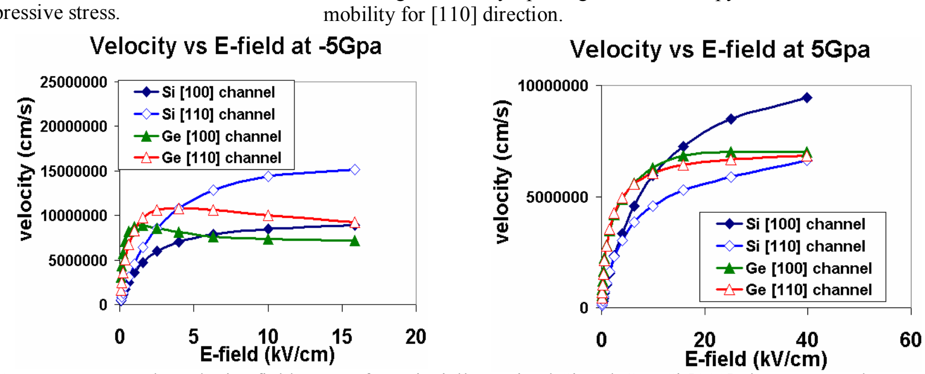

Fig.15 (a) and (b): The velocity-field curves for uniaxially strained Si and Ge. Si [110] shows a very large stationary velocity gain for uniaxial compressive stress under bulk conditions. The high field transport for Ge [110] is also greatly enhanced with uniaxial compressive stress.

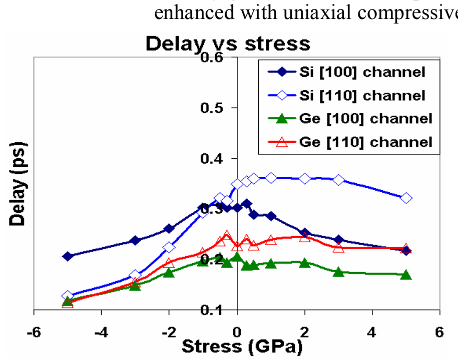

Fig.17: The delay for uniaxially strained Si[110], Ge [100] and Ge[110] are all very low due to their excellent transport properties. The delay tracks the drive current quite well.

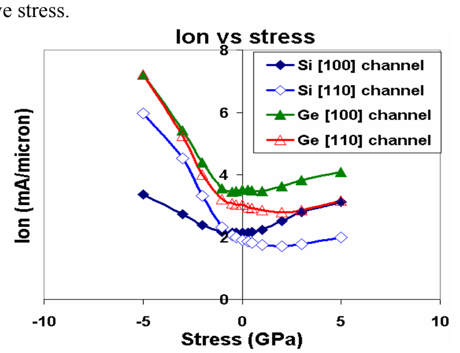

Fig.16: The drive current for Ge [100] and Ge[110] under uniaxial compressive stress is greatly enhanced (3.5X). Si[110] also shows very high drive current (2.5X) due to enhanced high field transport and strongly anisotropic effective mass.

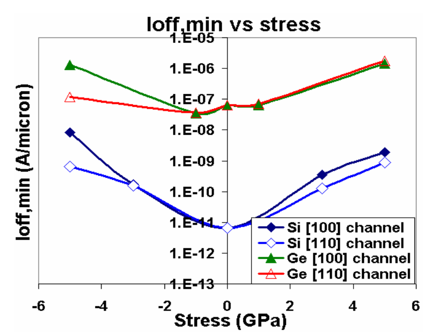

Fig.18: The minimum achievable off-state leakage for [110] under compressive stress is lower than [100] for Si and Ge because of the larger bandgap. Si [110] shows the lowest leakage.