Monte Carlo simulation study of the impact of strain and substrate orientation on hole mobility in Germanium

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Abstract. The use of alternative channel materials to maintain device performance with scaling for CMOS technology is an active area of research, with Germanium offering an extremely attractive possibility for pMOSFETs in CMOS. In this paper we use full band Monte Carlo transport simulations to investigate the impact of substrate orientation and biaxial strain on hole mobility in bulk Germanium helping to establish a preferential substrate channel orientation that can maximize carrier mobility for these devices.

1. Introduction
Performance boosters such as process induced strain and the introduction of high-k/metal gate stacks that help CMOS technology to deliver continuous performance improvement [1] may yield diminishing returns with future scaling. The investigation of Germanium (Ge) as an alternative channel material and potential technology booster has experienced a revived impetus, especially for p-channel MOSFETs [2] where higher carrier mobility and drive current compared to conventional CMOS devices have already been successfully demonstrated [3]. This has so far eluded Ge n-channel development, with a number of possible reasons proposed [3,4], though recent progress has been reported [5]. The already superior hole mobility of Ge as compared to Silicon (Si) can be improved further by employing strain and exploiting different substrate and channel orientations.

2. Simulation Methodology
Here we investigate the Ge hole mobility enhancement due to biaxial strain from a relaxed Si$_{1-x}$Ge$_x$ buffer layer, with three major substrate orientations: (001), (110) and (111), along with a variety of channel orientations. The fraction of Si in the substrate varies from zero (a Ge substrate) up to 0.6 in steps of 0.1. Fractions of Si above 0.6 are not considered, as they would prove problematic to fabricate with the critical thickness becoming impractical for use. The relationship of applied strain, $\varepsilon$, to Ge content in the buffer, $x$, is given by $\varepsilon = a_{\text{Ge}} / a_{\text{Si}, \text{Gr}} - 1$ where $a_{\text{Ge}}$ and $a_{\text{Si}, \text{Gr}}$ are the lattice constants for the channel and substrate respectively. The relevant values for this study are given in Table 1. In all cases the material is assumed to be undoped.
Table 1. Relationship between Ge content of the SiGe layer and the applied strain.

| Substrate | Strain |
|-----------|--------|
| Ge        | 0%     |
| Si$_{0.1}$Ge$_{0.9}$ | 0.44% |
| Si$_{0.2}$Ge$_{0.8}$ | 0.89% |
| Si$_{0.3}$Ge$_{0.7}$ | 1.33% |
| Si$_{0.4}$Ge$_{0.6}$ | 1.74% |
| Si$_{0.5}$Ge$_{0.5}$ | 2.17% |
| Si$_{0.6}$Ge$_{0.4}$ | 2.59% |

To conduct our study we have employed an ensemble Monte Carlo (MC) technique, encompassing all the major scattering mechanisms [6] though only scattering from acoustic (longitudinal and transverse modes) and optical phonons is included for these bulk-undoped calculations, with parameters calibrated to match the experimentally measured low field mobility and velocity at 220K and 300K. The full bandstructure is obtained using 6-band k•p calculation [7]. Particular care is taken to ensure that the applied electric field in the case of mobility simulations is small enough to avoid undesirable carrier heating [8].

The strain modification of the bandstructure plays an important part in the investigation of the hole mobility in these conditions. The strain removes the underlying 3-fold symmetry and changes the orientation of the iso-energy surfaces [9], as shown in Figure 1 and Figure 2.
This also strongly affects the effective mass and the density of states (DoS), and these are two of the fundamental mechanisms that lead to mobility enhancement. A spherically averaged DoS mass is used in the calculation of the scattering rates, as in [10], and this is plotted in Figure 3 for the heavy (HH) and light hole (LH) bands and for each substrate orientation considered here at 40 meV. The DoS mass progressive decreases for the HH band and levels out towards the maximum level of strain applied in this study. The other significant effect associated with the application of strain to the Ge layer is the energy separation between the normally degenerate HH and LH bands, as illustrated in Figure 4. The consequence of this is that the interband scattering from both the phonon mechanisms is greatly reduced which further leads to a reduction in the occupancy of the light hole band.

While these aspects explain the overall trend of mobility enhancement with strain, they provide little indication of orientation dependence, especially with respect to the channel.

Figure 3. Variation of DoS mass in the HH and LH bands for all 3 substrates in this study.

Figure 4. Variation with strain of the energy separation between the HH and LH bands.

3. Results and Discussion

Figure 5 summarises the results of our simulations – only two channel directions were selected for the (001) substrate orientation, as the ⟨010⟩ direction is identical to the ⟨100⟩ direction. We found that the best potential channel orientation is a ⟨-110⟩ orientation on a (110) substrate in terms of mobility. This is consistent with a previously published study, concerning double gate Ge pMOSFETs [11] where only one level of strain is considered. A significant anisotropy is also observed for the (110) substrate that is not present for the other two.

The energy dispersion relations for the (110) substrate orientation are shown in Figure 6 and provide the best indication of the cause of this directional preference as the strain most significantly impacts upon the shape of the $E$-$k$ relationship for the ⟨-110⟩ ⟨110⟩ channel-substrate direction.

As devices approach the ballistic limit, an important issue for determining device performance is the injection velocity from the virtual-source end of the channel and the corresponding backscattering
These issues are currently being investigated. Here special care must be taken to correctly model the ionized impurity scattering, including the effects of the dynamic screening, which plays an increasingly important role for holes. Appropriate modeling of interface roughness scattering is additionally an area of interest for hole transport in Ge inversion layers.

Figure 6. Energy-momentum dispersion relations for the 3 channel orientations on the (110) substrate. The (-110) direction shows the most dramatic reaction to the application of strain that accompanies the superior mobility enhancement observed for this orientation.

4. Conclusions

We have studied the impact of orientation and biaxial strain on hole mobility in bulk Ge using full-band MC transport simulations calibrated to experimental data. The change of effective mass and the separation in energy between the HH and LH bands resulting from the application of strain causes a continual mobility increase irrespective of orientation. However, we find that a (-110) channel direction on a (110) substrate offers the greatest increase in overall mobility due to the dramatic impact that strain has on the energy-momentum relationship. Further considerations necessary to model scaled pMOS devices are also presented.

References

[1] Watling J R, Brown A R, Ferrari G, Barker J R, Bersuker G, Zeitzoff P, and Asenov A 2008 J. Comp. Theoret. Nanoscience 5 1072–88
[2] Nicholas G, Jaeger B D, Brunco D P, Zimmerman P, Eneman G, Martens K, Meuris M, and Heyns M M 2007 IEEE Trans. El. Dev. 54 2503–11
[3] Kuzum D, Petha A, Krishnamohan T, Oshima Y, Sun Y, McVittie J P, Pianetta P A, McIntyre P C, and Saraswat K C 2007 IEDM Tech. Dig. 723–726
[4] Lieten R R, Degroote S, Kuijk M, and Borghs G 2008 Appl. Phys. Lett. 92 022106
[5] Tsipas P and Dimoulas A 2009 Appl. Phys. Lett. 94 012114
[6] Wiley J D 1971 Phys. Rev. B 4 2485-93
[7] Dijkstra J E and Wenckebach W T 1997 J. Appl. Phys. 81 1259–63
[8] Ottaviani G, Canali F, Nava F, and Kittel C 1955 Phys. Rev. 98 368–384
[9] Rideau D, Feraille M, Ciampolini L, Minondo M, Tavernier C, and Jaouen H 2006 Phys. Rev. B 74 1-20
[10] Fischetti M V and Laux S E 1996 J. Appl. Phys. 80 2234–52
[11] Krishnamohan T, Kim D, Dinh T V, Pham A, Meinerzhagen B, Jungemann C, and Saraswat K 2008 IEDM Tech. Dig. 899-902
[12] Lundstrom M S 1997 IEEE Elec. Dev. Let. 18 361-3

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