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First Self-Consistent Full-Band – 2D Monte Carlo – 2D Poisson Device Solver for Modeling SiGe Heterojunction p-Channel Devices

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Though their necessity is still perhaps few years out, alternative MOSFET structures shown in Fig. 1 appear to deliver the technologies that will scale CMOS further than ever anticipated. Regarding the performance of SiGe p-channel devices, it is necessary to investigate a variety of issues that require atomic scale electronic structure and transport calculations. These include investigations of the role of alloy scattering, the thickness of the cap Si layer, the role of strain-induced interface roughness (that depends upon the temperature growth conditions), the presence of a parallel channel at the interface and how it affects the device performance. To determine the effect of thickness variations, one needs to evaluate the associated fluctuations in the electrostatic potential at the Si/SiGe interface using self-consistent solution of the Poisson equation coupled with the Schrödinger equation which utilizes the effective masses derived from k.p calculations. Another issue is the strain-splitting of the heavy-hole and the light-hole bands and the role played by quantum-mechanical size-quantization effects at the source end of the channel on the overall device performance.

To incorporate band-structure effects like warping, anisotropy and non-parabolicity in the description of carrier transport, our device simulator couples a 2D Poisson solver with a discretized 6×6 k.p Hamiltonian solver that includes the effect of the confining potential and provides the subband structure in the channel region. Strain effects in buried channel strained-SiGe MOSFET simulations are included by employing the 6×6 Bir-Pikus strain Hamiltonian perturbatively. Having calculated the hole band-structure in the contacts (3D) and the subband structure (2D) in the active device region i.e. under the gate self-consistently with the 2D Poisson equation, the quantum mechanical hole density in the channel is then calculated by weighing the sheet density of each subband with the probability density corresponding to that subband along the device depth and then summing over all subbands of each of the six bands. The initialization of carriers in real space is based on the local 3D carrier density for holes in the reservoirs. In the channel region the carriers are assigned to subbands in a probabilistic manner that reflects the contribution to the hole sheet density from different subbands.

We use an Ensemble Monte Carlo (EMC) particle based simulator to handle the transport of holes. After the carriers are initialized, a bias is applied on the drain contact and the Monte Carlo algorithm takes over the hole transport, performing the drift and scattering of carriers. As the simulation time evolves in steps of 0.1 fs, and the carriers drift under the influence of the electric field, the confining potential changes along the channel from the source end to the drain end, and this, in turn, changes the hole subband structure in the channel. As a result, the hole subband structure and subsequently the scattering rates must be updated frequently during the simulation to reflect these changes.

The density of states for 2D confined carriers in the channel for the case of a triangular test potential is shown in Fig. 2; the left panel is for Si inversion layer, while the right panel is indicative of the same for strained SiGe inversion layer.. The drain current enhancement ratio of the strained SiGe MOSFET over the conventional Si MOSFET as a function of the applied drain bias for different gate voltages is shown in the right panel of Fig. 3. At the conference we will discuss the method we have used to eliminate the subband crossings.

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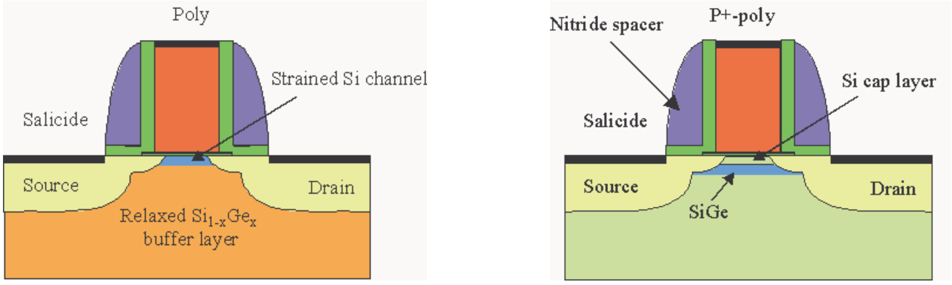

Fig. 1. Alternative device structures in SiGe technology. Left panel - Both pMOS and nMOS enhanced carrier mobility can be achieved. Critical issue is the fabrication of the buffer and strained layers. Doping further degrades the mobility. Right panel – This device structure is used to boost the pMOS behavior by introducing a quantum well beneath the Si layer. The alloy disorder scattering and the parallel transport channel is a problem.

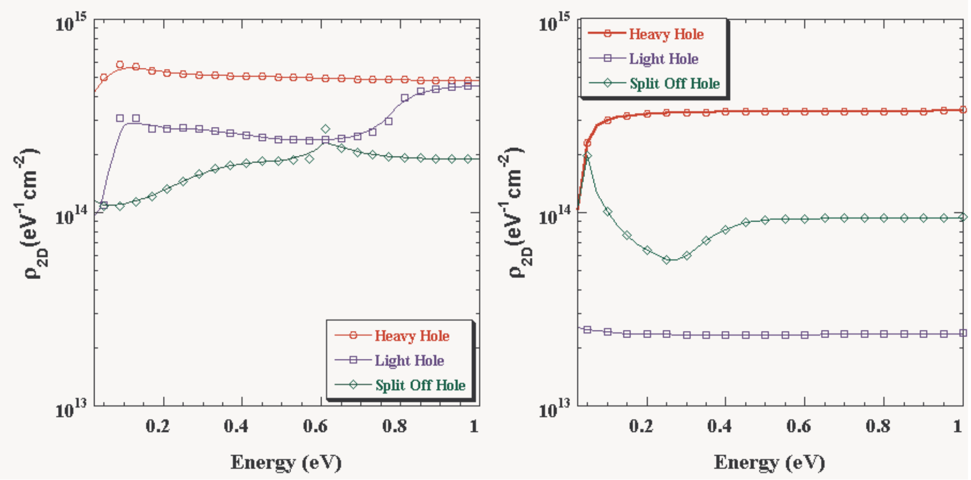

Fig. 2. The density of states for 2D confined carriers in the channel for the case of a triangular test potential; the left panel is for Si inversion layer, and the right panel is indicative of the same for strained SiGe inversion layer. Considering the left panel: (a) The deviation of the 2D density of states obtained by a full band calculation from a regular step-like profile expected out of an effective-mass type approximation is clearly seen in the case of the light hole and split off bands. (b) Subband crossings are seen in the case of light hole and split off subbands, where these subbands cross into higher lying heavy hole subbands, resulting in spikes in the density of states. For the case of the right panel: (c) The heavy and light hole subbands have a clear density of states with no subband crossings, (d) The split off band actually follows the heavy hole subband density of states and there is a subband crossing from split off subband into the heavy hole subband. The crossover then changes shape and the density of states consequently drops and settles down to a constant value at higher energies.

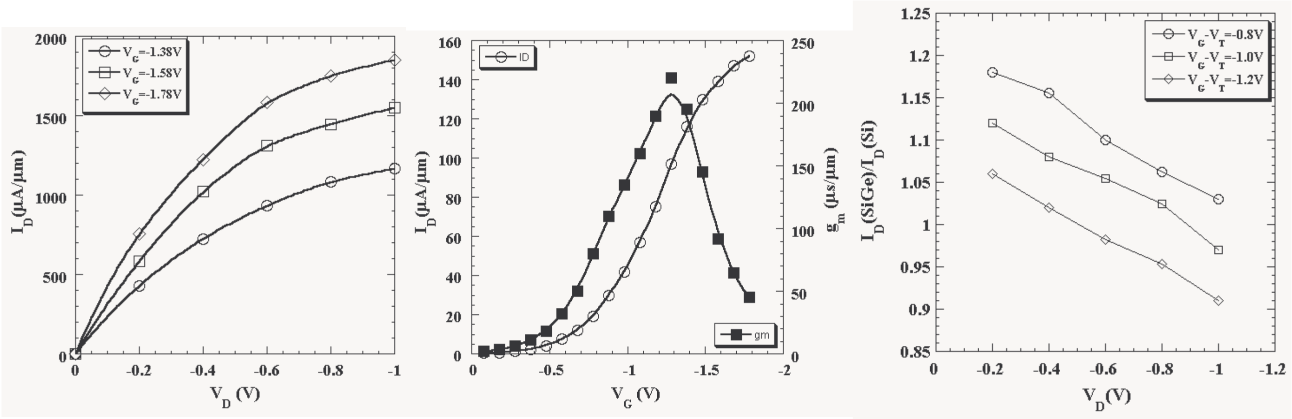

Fig. 3. Left panel - Output characteristics of the 25 nm p-channel strained SiGe MOSFET. Central Panel - Transfer characteristics of the 25 nm p-channel strained SiGe MOSFET. The device exhibits a peak transconductance of ~220µS/µm. Thus, the enhancement in transconductance of the strained SiGe MOSFET over the Si MOSFET is about 26%. Right panel - Drain current enhancement of the strained SiGe MOSFET over the conventional Si MOSFET. It is seen that the SiGe MOSFET clearly performs better than the conventional Si MOSFET at low values of applied drain bias (low field regime) and moderate values of the gate voltage. This is the regime in which the hole mobility enhancement is predicted for device structures using a strained SiGe layer as the active layer for carrier transport.