Monte Carlo Transport Calculations of Strained SiGe Heterostructures from Ab-Initio Band-structures

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ABSTRACT

We present an *ab-initio* band-structure procedure that can be applied for holes in Monte Carlo simulations of transistors with strained alloyed channels.

Keywords: Monte Carlo, Device Simulation, Ab-Initio, Alloys

1 INTRODUCTION

For many heterostructure devices, such as strained SiGe p-MOSFETs, alloy scattering [1, 2] plays a role in determining the hole mobility, along with phonon, surface roughness, and Coulomb scattering. Surface roughness scattering can be reduced by including a Si buffer layer between the SiGe channel and the gate. The strain in alloyed SiGe causes a splitting of the heavy hole and light hole bands, and enhances hole mobility by lowering the effective mass at the top of the valence band in comparison to unstrained bulk silicon. Alloy scattering, on the other hand, lowers the hole mobility. All of these factors affect device performance; therefore, to properly describe the operation of device structures that utilize strained-SiGe layers it is necessary to include into the theoretical model the strain modification of the band-structure and to properly model alloy disorder scattering. One problem is that there is a big uncertainty on the choice of the alloy scattering parameters [1] used in Monte Carlo models with both effective mass and k·p band-structures.

To address this issue, we have been developing a method to incorporate alloy scattering into Monte Carlo simulations using first principles density functional theory (DFT) calculations. If the effects of the alloy are included in the band-structure and matrix elements used for phonon scattering and other scattering processes, then explicit random number generated alloy scattering can be eliminated as a Monte Carlo scattering process. First principles electronic structure calculations offer a way to include the effects of alloy disorder, strain, spin-orbit coupling, heterostructure offsets, the gate bias induced potential, and quantum confinement into the band-structure and into scattering matrix elements.

The rest of the paper is organized as follows: Section two describes the steps involved for including *ab-initio* band-structures into a Monte Carlo device simulation. Section three presents the DFT band-structure methodology used to describe a heterostructure with an alloyed channel component. Section four presents preliminary band-structure calculations; and the final section presents a summary.

2 METHODOLOGY TO INCLUDE *AB-INITIO* BAND-STRUCTURES INTO A MONTE CARLO CODE

Two of us have developed a code for Monte Carlo simulation of Si and strained SiGe pMOSFETs with a self-consistent effective mass Schrödinger/Poisson solver for holes[3]. First principles band-structure calculations are computationally time consuming for a fully self –consistent Monte Carlo calculation; however band-structure and scattering cross sections using ab-initio calculations can be placed into existing Monte Carlo device simulation codes with the following steps: First, a self-consistent Schrödinger/Poisson calculation is done for a given set of source, gate, and drain biases using an effective mass or k·p Schrödinger solver for the holes. This produces a Hartree potential for the holes.

In the second step, first principles band-structure calculations are done for holes (in the valence band) including the potential from step one. For the SiGe pMOSFET that we are considering, this can be done in slices along the depth of the device, shown as the dashed line in figure 1.

In the third step, the *ab-initio* energy band-structure and *ab-initio* wave-function based scattering rates are used in the full device Monte Carlo algorithm where holes are scattered randomly and the device currents are tabulated. If a periodic supercell geometry and a plane-wave basis are used for the *ab-initio* band-structures, the scattering matrix elements need to include momentum changes by reciprocal-lattice vectors along the confinement direction, as in the case of superlattices. The use of first principles energy dispersion and wave-functions for the calculation of all of the other scattering mechanisms eliminates the need to

include alloy scattering in the Monte Carlo simulation. In both steps two and three above, perturbation theory and interpolation can be used to compensate for limitations in the number of time consuming first principles calculations.

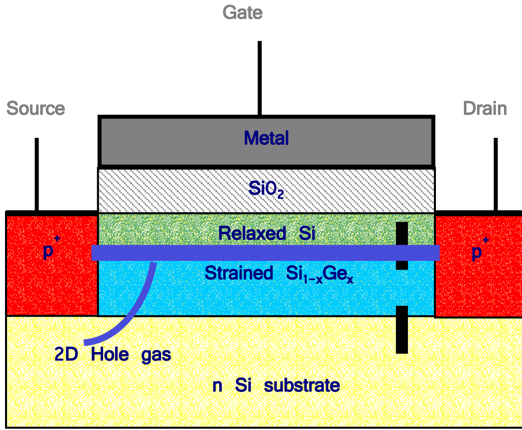

Figure 1: Strained SiGe p type MOSFET. The quantization of 2D hole states is calculated along the dash line.

3 BAND-STRUCTURE METHOD

The hole electronic structure calculations are done with a plane-wave supercell method and the local density approximation (LDA) [4]. The Teter Pade parameterization of the LDA exchange-correlation is used [5]. Calculation times are reduced by performing one k-point calculation per processor on a parallel computer.

Relativistic Hartwigsen-Goedecker-Hutter pseudo-potentials [6] are used for the inclusion of spin-orbit coupling.

Confinement by Silicon Dioxide and termination of the substrate is currently modeled by passivation with hydrogen in a vacuum; though, explicit Silicon Dioxide interfaces may be added in future calculations.

Special "quasirandom" cell structures are used to model the alloy [7, 8]. The neighbor pair correlation function values of a Special Quasirandom Structure are optimized to closely match those of a perfectly random alloy. Fahy and Greer have suggested that the atomic distribution of atoms for alloys grown in layers may deviate from a perfect alloy; and their work presents an alternative model of the alloy [9].

Strain in the alloy and across interfaces is included by lowering the structural energy with Broyden-Fletcher-Goldfarb-Shanno minimization [10] subject to constraints on the atomic forces determined by the strain.

Ref	$m^{(100)}_{hh}$	$m^{(100)}_{Lh}$	$m^{(111)}_{hh}$	$m^{(111)}_{lh}$	$m^{(110)}_{hh}$	$m^{(110)}_{lh}$	m_{so}
This Work	0.26	0.19	0.65	0.16	0.57	0.15	0.18 0.20 0.225
[11] Theory	0.26	0.18	0.67	0.13	0.54	0.14	0.22
[12] Exp.							0.234
[13, 14] Exp.	0.46 0.46	0.171 0.171	0.56 0.57	0.160 0.157	0.53 0.53	0.163 0.163	

Table 1: Bulk Si DFT effective masses in comparison to Ref. [11] and experimental values from references [12-14]
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4 BAND-STRUCTURE RESULTS

Here, the results of preliminary test case band-structure calculations are presented. It is known that computations at the LDA approximation can yield unreliable effective masses for semiconductors without corrections to the excited states [15, 16]. Table 1 shows that the effective masses of bulk Silicon computed with the method of section three reasonably match experimental results, at least in most of directions of k-space that were examined.

Figures 2 and 3 show the top valence bands for a confined 3nm Si slab and a confined (1nmSi/ 1nm SiGe/ 1nm Si) heterostructure respectively. The SiGe alloy layer, strained by biaxial compression, is 31.25% germanium. The energy drop of the top valance band for the SiGe heterostructure with the magnitude of the k-vector is slightly larger (though clearly less than a factor of two) than the drop for the pure Silicon structure. The bands in the SiGe heterostructure are broadened by the presence of alloy disorder, which can be seen in the changing line type.

Figure 4 shows a charge density isosurface for the third from the top valence band eigenstate at k=0 of a (1nm Si/ 1nm strained SiGe/ 4nm Si) heterostructure with no gate potential applied. Even without a bias potential, the charge density for states at the top of the valence band has a higher concentration near the SiGe well region than the 4nm Si substrate layer.

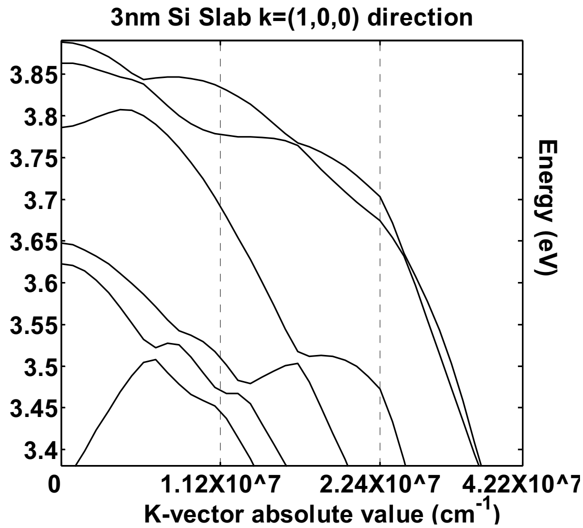

Figure 2: Valence band-structure along the K=(1,0,0) direction for a 3nm Si slab using a rectangular prism unit cell with the long axis in the third direction. A 20.2 Rydberg plane-wave cutoff was used for the calculations of Figs. 2-4. Vertical dashed lines are for reference.

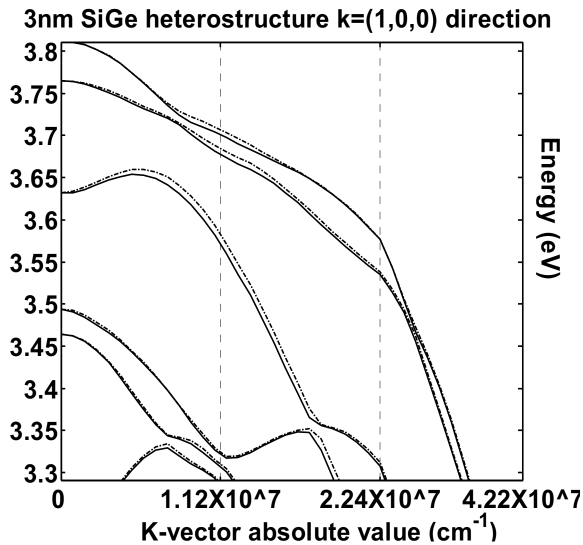

Figure 3: Top of the valence band for a 3nm confined SiGe heterostructure in the same direction as Figure 2. Broadening between solid and dashed curves indicates alloy disorder. Vertical dashed lines are for reference.

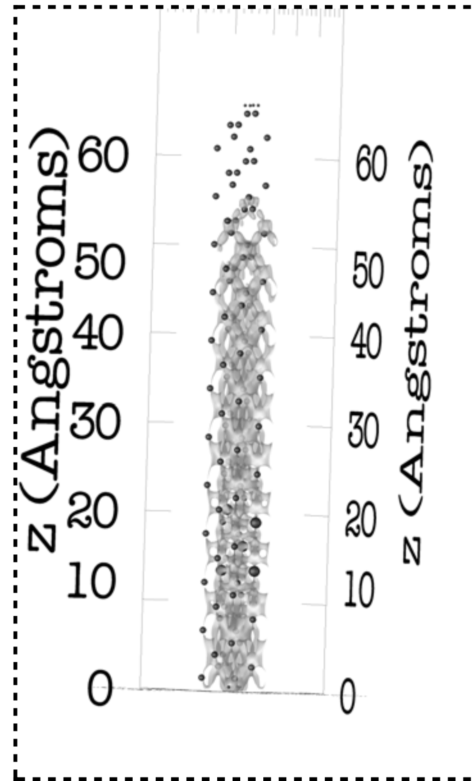

Figure 4: Electron density isosurface (in gray) of a valence band state for a 6nm Si/Strained SiGe/Si heterostructure. The largest size spheres in the 10-20 Angstrom range on the z-axis represent Ge atoms. The four smallest spheres at the top are Hydrogen atoms; while all other spheres are Silicon atoms.

5 SUMMARY

We have proposed a method of including *ab-initio* band-structures for holes in Monte Carlo simulations of strained SiGe channel devices that can incorporate the effects of alloy disorder, strain, spin-orbit coupling, heterostructure offsets, the gate bias induced potential, and quantum confinement. We compared *ab-initio* band-structure calculations for a 3nm heterostructure of (Si/Strained SiGe) to a similar Silicon structure and found some valence band broadening due to the alloy. A full implementation of the proposed Monte Carlo simulations for a device will be presented in future publications and the conference poster session.

Band-structure results were obtained through the use of the ABINIT code, a common project of the Universite Catholique de Louvain, Corning Incorporated, and other contributors (http://www.abinit.org). Some of the calculations were performed on the National Science Foundation Terascale Computing System at the Pittsburgh Supercomputer Center.

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