Monte Carlo Hole Mobility Calculations with a First Principles Alloy Scattering Approach

Barry Zorman, Santhosh Krishnan, Dragica Vasileska, Jialei Xu and Mark Van Schilfgaarde
Arizona State University, Tempe, AZ, 85287-5706, USA
email: Barry.Zorman@asu.edu

Continued scaling of semiconductor devices leads to numerous challenges that have to be overcome in order to achieve device behavior that satisfies speed and power constraints. Since a lot of present issues do not have existing solutions like, for example, the choice of the proper high-k dielectric that will reduce gate leakage at the acceptable value and still lead to relatively high inversion layer mobilities, alternative device structures have been sought. Possible alternatives to conventional CMOS devices include silicon-on-insulator devices, dual-gate structures, FinFETs and strained-Si or strained-SiGe devices. The later material system is already been used in the production of high-frequency bipolar junction transistors and is considered as possible alternative to conventional CMOS.

It is now well known that in many heterostructure devices, such as strained SiGe p-MOSFETs, alloy scattering[1] plays a significant role in determining the hole mobility. The strain induced modification of the bandstructure, on the other hand, affects the phonon, surface roughness, Coulomb, and alloy disorder scattering rate, which in turn influences the hole mobilities and, consequently, the device performance. The strain in alloyed SiGe causes 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. Therefore, to properly describe the operation of device structures that utilize strained-Si or strained-SiGe layers, it is necessary (1) to include into the theoretical model the strain modification of the band structure and (2) to properly model alloy disorder scattering. The problem is that there is a big uncertainty on the choice of the alloy scattering parameters[2] used in Monte Carlo models with both effective mass and k·p bandstructures.

To address this issue, we recently developed a method to incorporate alloy scattering into Monte Carlo simulations using first principles density functional theory (DFT) calculations. A statistical model of the alloy is used, and the atomic pseudopotentials include spin-orbit coupling terms. Strain in the alloy and across interfaces is included by lowering the structural energy with Broyden-Fletcher-Goldfarb-Shanno minimization[3] subject to constraints on the atomic forces determined by the strain. Confinement at the SiO_2/Si cap layer is approximated as a hydrogen passivated Si surface. Figure 1 shows part of the valence bandstructure near the Γ point for a strained 1nm SiGe (31.25%) channel capped by silicon. The bandstructure shown was computed on a parallel machine with a 28 Rydberg plane-wave kinetic energy cutoff. Although a self-consistent density functional bandstructure/Monte Carlo/Poisson equation calculation is beyond the reach of current computers, density functional bandstructure calculations can include the gate bias induced self-consistent potential from our effective mass based Monte Carlo/Poisson code. Then, the use of first principles energy dispersion and wave-functions for the calculation of all of the scattering mechanisms eliminates the need to include alloy scattering in the Monte Carlo simulation. The approach we have developed, based on the above idea, is currently being applied to the calculation of the hole transport properties of a small strained SiGe channel pMOSFET structure, and compared to effective mass results.

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[3] Broyden C.G., *J. Inst. Math Appl.,* **6**, 76 (1970); Fletcher R., *J. Comput.,* **13,** 317 (1970); Goldfarb D., *Math. Comp.,* **24**, 23 (1970); Shanno D.F., *Math. Comp.,* **24**, 647 (1970).

A full journal publication of this work will be published in the Journal of Computational Electronics.

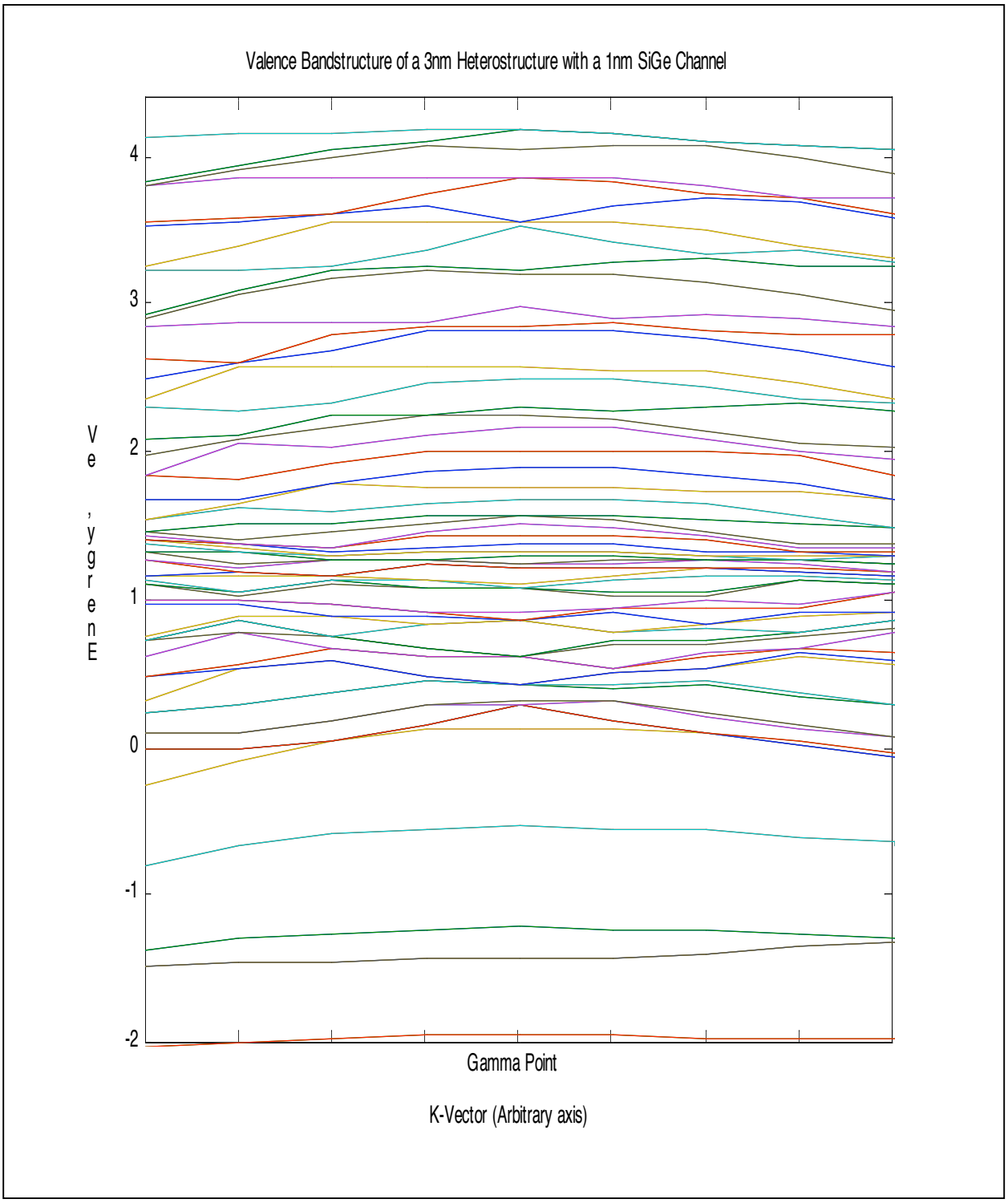

Figure 1: Valence band-structure of a SiGe heterostructure near the Γ point, which shows the effects of strain, alloying, and confinement on the heavy-hole and light-hole bands.

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