Low-Field Mobility in Strained Silicon with 'Full Band' Monte Carlo Simulation using k.p and EPM Bandstructure

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***Abstract*-Recent works have shown that accurate band-structure for strained silicon can be obtained using full-zone k.p method [1]. In this paper we have performed full-band Monte Carlo transport simulations in strained silicon using k.p band structure [1], and we have compared to simulations performed using the well-benchmarked EPM band structure [2][3][4].**

I. Introduction

Shrinking of MOSFET device dimensions such as the gate length and the gate oxide thickness is an essential component in CMOS to achieve ITRS requirements. However, conventional scaling down of MOSFET's channel length is declining as the benefit of physical and economic limits are approached. Novel solutions are increasingly being used in MOSFET channel engineering. Strained silicon layer on relaxed $Si_{1-y}Ge_y$ buffer is a typical technique used to improve electrical MOSFET's device performance, due to its enhanced carrier mobility [5]. Many fundamental carrier transport properties of the strained semiconductors are governed by the structure of the energy band. Carriers transport modeling in strained silicon such as the 'full band' Monte Carlo (MC) solution, requires accurate knowledge of the band structure (within 0.01 eV or better). Over the three past decades, the EPM with spin-orbit corrections has proven to be extremely successful in calculating the electronic band structure of relaxed and strained silicon [3][4]. Since, this method has been used in MC simulation, and enables the description of strained silicon [2][6][7]. Recent achievements using 'full zone' k.p methods also give accurate description of the band structure (BS) of strained silicon [1]. In this work, we have performed MC simulations (using MC++ [13]) of silicon bulk mobility as a function of biaxial strain using respectively k.p BS and EPM BS.

II. Electronic Band Structure Analysis

The BS for relaxed bulk silicon and biaxially strained silicon layer on cubic Ge buffer are shown in Fig. 1. Simulations have been performed using local EPM including spin orbit correction [3] and the k.p method described in Ref. [1]. The k.p fitting parameters and the deformation potentials of the Bir and Pickus correction were obtained from a least-square optimization on non-local ab-initio GW calculation [1]. For relaxed structure, we found that the difference in band energies values between k.p method and EPM is typically less than 0.01 eV for the principal band-gaps, and under 0.1 eV at other high symmetry points. In case of biaxially strained silicon on cubic [001]-oriented SiGe buffer, the longitudinal strain is defined by: $\varepsilon_{xx} = \varepsilon_{yy} = a_{\parallel} / a_0 - 1$, where a_0 and $a_{\parallel}$ stand respec-

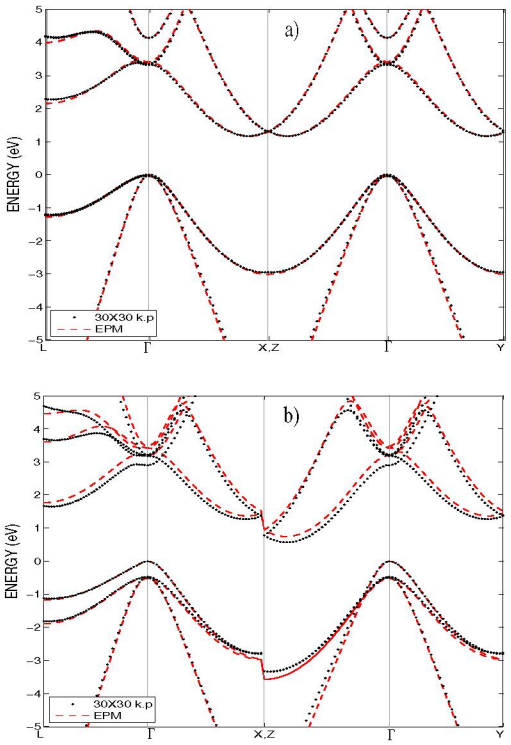

Figure 1: EPM and k.p band structure along various directions; a) relaxed Silicon, b) biaxially strained Silicon on cubic [001]-oriented Ge buffer.

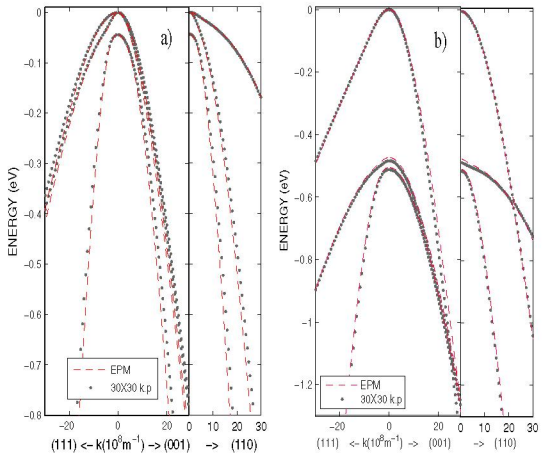

Figure 2: EPM and k.p dispersion relation in the near-Γ region ; a) relaxed Silicon, b) biaxially strained Silicon on cubic [001]-oriented Ge buffer.

tively for the relaxed and the distorted lattice parameter [8]. Using continuum elasticity theory, the perpendicular strain component $\varepsilon_{zz} = -2C_{12}/C_{11} \cdot \varepsilon_{xx}$ can be calculated from the elastic constants (C11=165.8 GPa and C12=63.9 GPa). Due to crystal symmetry lowering by biaxial-strain, the Conduction Bands (CB) Δ-valleys are split into two Δ4 and a Δ2 valleys, and the Valence Bands (VB) degenerated levels at Γ are removed (see Fig. 2). We found out excellent agreement between k.p and EPM results. The splitting deformation potential at Γ for VB (b=-2.35 eV) and at CB minima (Ξ^{Δ}_{u}=8.47 eV) are consistent with the experimental data [9]. One notes nevertheless a slightly different hydrostatic deformation potential for Conduction Band (CB) (Ξ^{Δ}_{d}=1.1 eV) that can be seen in Fig. 1. Unlike to EPM, the k.p Hamiltonian is only a 30×30 matrix, which is computationally far more efficient than EPM (we estimate that the computational time ratio between k.p and EPM can be as large as ~50). In this paper, we show that for 'full band' MC purpose, 'full zone' k.p method gives consistent results with the EPM.

III. Monte Carlo Analysis

Accurate descriptions of the BS curvatures in the neighboring of the CB and VB extrema are key features for transport modeling in strained Silicon. Indeed, transport properties in strained materials are not only governed by the band offsets, but also significantly depend on the curvature masses. Moreover, the DOS and the average carrier scattering rates are obtained from an integration over the BZ [10] and are also very sensitive to the accuracy of the band structure model. For illustration, we show in Fig. 3 the carrier-phonon scattering rates obtained using the procedure described in Ref. [10] using respectively the k.p method and EPM. We used the fitting parameters sets of Ref. [11] for the VB and of Ref. [10] for the CB together with the empirical phonon dispersion relation of Ref. [10]. As seen, the hole-phonon scattering rates are identical for both models. The slight differences for the electron-phonon scattering rates (observable at higher energy) come from the slight difference in BS at high energy. Indeed, the k.p methods, fitted an ab initio GW BS [1], includes non-local effects which are not accounted for in the purely local EPM of Ref. [3]. Although the differencies are small (< 5 %), this can also be seen in the high field (F=300 kV.cm^{-3}) electron distribution function shown in Fig. 4. One notes that at higher energy, the difference (visible in log-scale in the subplot) have a different origin and can be inferred from missing (220) bands in the thirty-level k.p model [1]. This latter difference that occurs at high energy (> 5 eV) only have a small impact on the present bulk mobility calculation.

In a practical way, the BS is computed on a dense set of points in the first BZ (typically 9000 points). The density of states (DOS) and the carrier scattering rates are obtained from the previous calculation following the procedure described in Ref. [13] and stored in memory to speed up calculation of the final state after a scattering event. The scattering mechanism included in the present MC simulation were elastic acoustic phonon scattering and inelastic optical phonon scattering. This is a realistic approximation for phonon-limited bulk mobility in low doped silicon (< 1e18 cm^{-3}). Phonon scattering for electrons and holes have been calibrated to reproduce a large variety of experiments including strain dependent mobility in MOSFET devices [13].

Simulations of bulk mobility in biaxially strained silicon are shown in Fig. 5 for electrons (a) and for holes (b) for a large set of compressive and tensile strain values (up to 4%). MC simulations using respectively k.p and EPM BS were performed at 300 K with an electric field of 2 kV.cm^{-1} along the [001]-direction. As can be seen, the

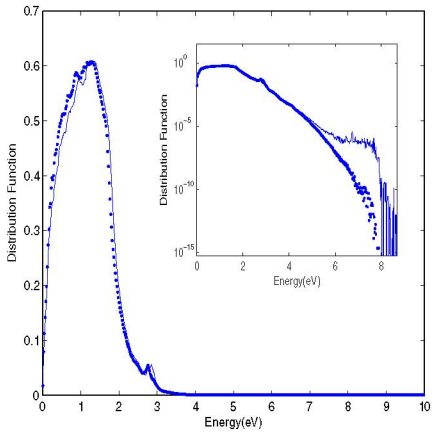

Figure 3: High field electron distribution function at 300 K (F=300 kV.cm^{-1}). Results obtained with k.p (line) and EPM (dots) band structure.

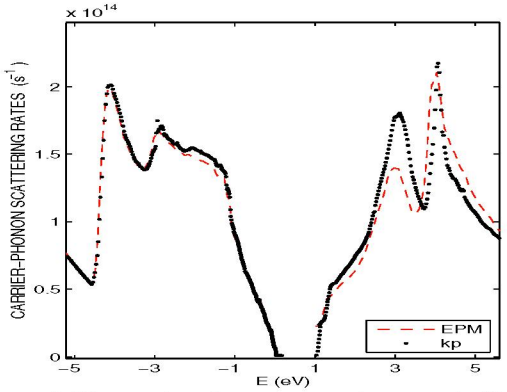

Figure 4: The carrier-phonon scattering rates in Si: Comparison between results obtained using the present 30-level k.p model and EPM model for the band energy calculation (see text for details).

electron in-plane mobility sharply increases with applied strain while the out-plane mobility decreases when a tensile strain is applied. Our results are consistent with simulations of Refs. [2][14][7], however as reported in [2], the in-plane mobility increase depends on the intervalley deformation potential model used for the simulation. Experimental data have reported values at 1% biaxial strain ranging from 2300cm^2/V sec. [12] up to (or even exceeding) 3000 cm^2/V sec. [15]. For holes, the in-plane and the out-plane mobilities increase with applied stain (independently of the sign of the strain). One notes a larger absolute hole mobility increase in Refs. [2] and [6] in which it has been found (in 1.5% biaxially strained Si) to increase respectively by a factor of 9.1 and 4.9 (instead of 3 in the present calculation). The main causes of hole mobility enhancement are the degeneracy removal of the VB at Γ and the reduction of the conduction masses. The difference observed for hole mobility could also be due to the different hole-phonon scattering time approximations used by authors. Unfortunately, to our knowledge no experimental hole bulk mobility measurements in silicon have addressed such a large values of biaxial strain. Indeed, layers subject to such a high strain can only be grown up to very small thicknesses, in which quantization effects occurs and impact the mobility.

IV. Conclusion

We have performed comparison between 'full band' MC simulation of low-field mobility in strained silicon using k.p and EPM banstructures. We have shown that few differences are observable when the computationally more efficient k.p BS is used for the motion and the derived quantities (DOS and scattering rates). We have compared our results to other theoretical works, and we have shown that although similar behaviour, the absolute value for the bulk mobility increase vs. strain is different. We shall view this point as an open problem. Further work along that line is in progress in particular to better estimate the phonon scattering contribution to the low-field mobility.

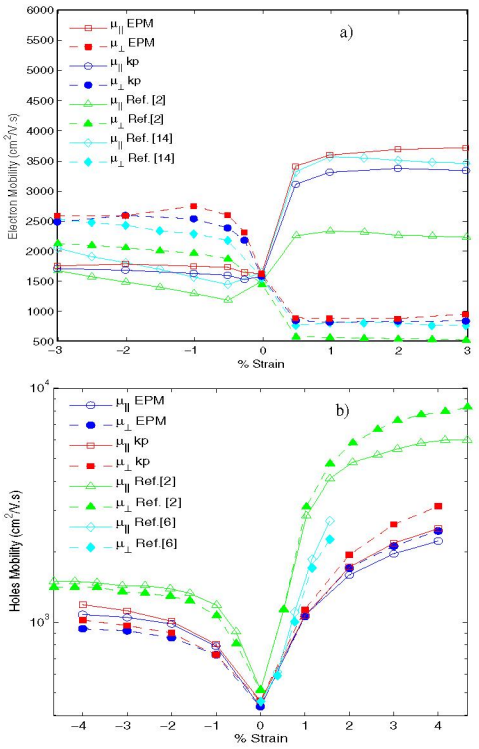

Figure 5: a) Electron and b) holes Bulk Mobility as a function of applied strain. Calculation obtained with the present 'full band' Monte Carlo simulator using k.p and EPM band structure. Comparison with Refs. [2], [6] and [14].

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