Mobility in FDSOI Devices: Monte Carlo and Kubo Greenwood Approaches Compared to NEGF Simulations

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1. Introduction

This paper presents a thorough comparison of mobility calculations in Fully-Depleted Silicon on Insulator (FDSOI) devices. Semi-classical approaches, such as the Kubo-Greenwood (KG) and the multi-subband Monte Carlo (MSMC) methods, are compared to quantum Non-Equilibrium Green's Functions (NEGF) results. All solvers use purely parabolic band structures for electrons with a Si/SiO$_2$ barrier of 3.15 eV and an oxide effective mass of 0.5 m$_0$. The considered scattering mechanisms include phonon and surface roughness (SR). The phonon scattering parameters of Ref [1] and SiO$_2$/Si roughness parameters of Ref. [2] are used in all simulations to guarantee consistent comparisons. The front gate stack of the devices is made of 2 nm of SiO$_2$ and of 2 nm of HfO$_2$. The undoped silicon active layer thickness varies from T_{Si}=2 nm up to T_{Si}=10 nm and the BOX thickness is 25 nm.

2. Scattering time based approaches

Semi-classical approaches such as the Kubo Greenwood and the MSMC have often been used to calculate the mobility in FDSOI devices [1-5]. However a direct comparison between published results is difficult, because either model parameters or SR profiles are different. In this abstract, we provide a comparison between two KG solvers, namely the STM in-House UTOX solver [6] and the commercial SBAND solver [7]. We extended the comparison to the Udine University MSMC solver [1,5].

All solvers treat the interaction with acoustic phonons as an isotropic, elastic mechanism while inter-valley phonon scattering is treated as isotropic with fixed phonon energies. SR scattering is treated as an elastic, anisotropic mechanism within either the Prange-Nee approximation [1,5,7], the generalized Prange-Nee model [2,6], or the Gamiz numerical approach [3,6]. The matrix elements are screened with a scalar Lindhard approach.

3. NEGF

NEGF mobility calculations have been performed with the TB_SIM solver from CEA [8]. We generated periodic random SR samples [4] with width W=20 nm and length L=30 nm (see Figure 1). We then built devices made of these units repeated once, twice (L= 60 nm), and up to three times (L= 90 nm). One nanometer of SiO$_2$ is included in the effective mass Hamiltonians on both sides of the film. The resistance of the devices was next computed in a mode space approach, including electron-phonon scattering. As expected, it is proportional to the length (that is, to the number of units, see Figure 2), allowing for an accurate extraction of the resistance of the SR sample. We finally computed the phonon-limited mobility μ_{PH} in smooth films and extracted an "effective" surface roughness-limited mobility μ_{SR} from Matthiesen's rule. The obtained μ_{SR} is, therefore, the SR mobility to be combined with the phonon mobility to recover the total mobility given by the NEGF calculation. We stress that a direct "surface roughness only" NEGF calculation (no phonons) would bring even lower SR mobilities, as the absence of inelastic pathways for electron scattering strengthens localization. We have verified that the width and length of the SR sample are large enough to limit statistical bias ($\Delta\mu_{SR}/\mu_{PH}$ = 2.5%).

5. Results and Discussion

Figure 3 shows the phonon-limited mobility as a function of the active layer thickness. All solvers are in excellent agreement. We therefore now focus on the SR mobility.

There are two closely related approaches to compute the impact of a local fluctuation of the electrostatic potential due to SR. The former one, derived from the well-known Prange-Nee approximation, regroups SR models described in [1,2,4,5]. The latter approach, originally proposed by F. Gamiz [1,3], consists in a numerical evaluation of the scattering potential. As shown in Figure 4, two independent Poisson-Schrodinger calculations of the electrostatic potential are performed: the first one in the considered device, and a second one on the same device with the front or the back SiO$_2$/Si interface shifted by Δ. Figure 5 shows that the mobility obtained with this numerical approach agrees well with the usual Prange-Nee-based approaches.

Figure 6 compares the SR-limited mobility obtained with the semiclassical methods to the NEGF results. The former solvers, in close agreement one with each other, clearly overestimate the SR-limited mobility with respect to NEGF. This is further emphasized in Figure 7, which shows the SR-limited mobility as a function of T_{SI}. The results of S. Jin [2] have also been reported on this figure. They account for carrier density fluctuations and image charge effects, but are still above NEGF data. In figure 8, the total mobility is compared to measurements [9]. It appears that the widely used set of parameters for phonon [1] and SR [2] leads to mobilities larger than experimental data. Figure 9 shows the mobility obtained with optimized parameters. All phonon deformation potentials have been increased by 20%. Additionally the SR parameter Δ has been increased to 0.67 nm in KG calculations (but not in NEGF).

To conclude, we have shown that semi-classical approaches are in excellent agreement with quantum NEGF simulations for electron-phonon scattering, yet not for SR scattering. This sheds new light on the explanation of mobility degradation in thin films.

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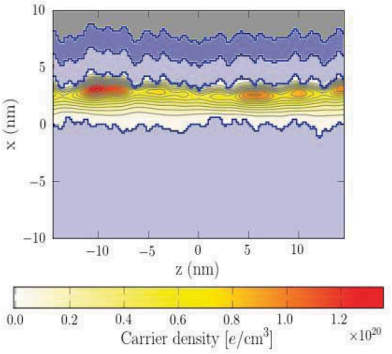

Figure 1 : Carrier density with NEGF in a 4 nm thick FDSOI film. Interface roughness generated with an exponential autocorrelation function (Δ=0.47 nm and Λ=1.3 nm).

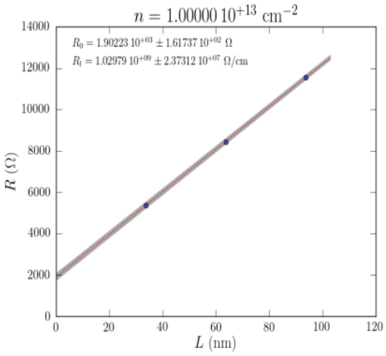

Figure 2 : NEGF resistance of the FDSOI film as a function of length. The slope gives the mobility, while the intercept at L=0 is the quantum “ballistic” resistance.

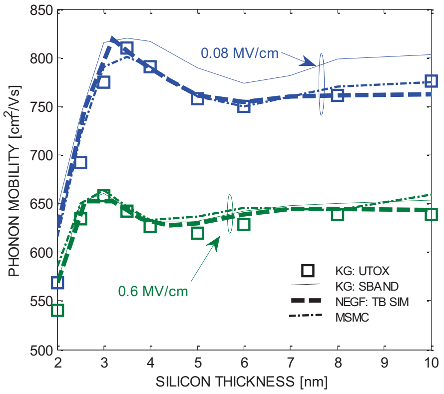

Figure 3 : Comparison of phonon-limited electron mobility in FDSOI devices as a function of active layer thickness. Phonon parameters from [1].

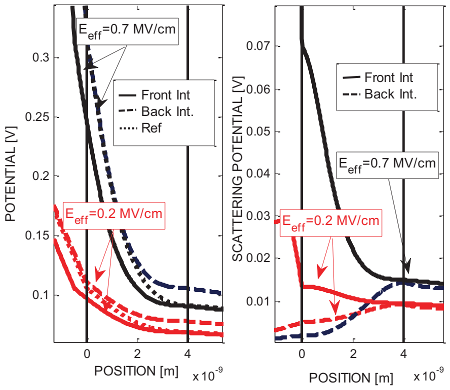

Figure 4 : Electrical potential changes (left) in a 4 nm thick FDSOI device (Ref.) for front and back interface fluctuations (Δ=0.47 nm) and associated scattering potentials (right) defined as the difference between the potential in the reference device and the one in the device with a shifted front or back interface.

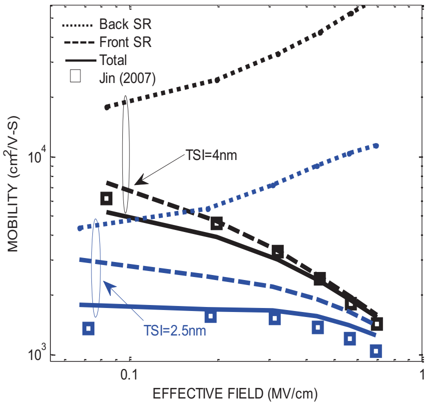

Figure 5 : SR-limited electron mobility calculated with Gamiz [3] approach in FDSOI: Influence of the Back interface roughness and comparison with Jin [2] model (density fluctuation and polarization terms neglected).

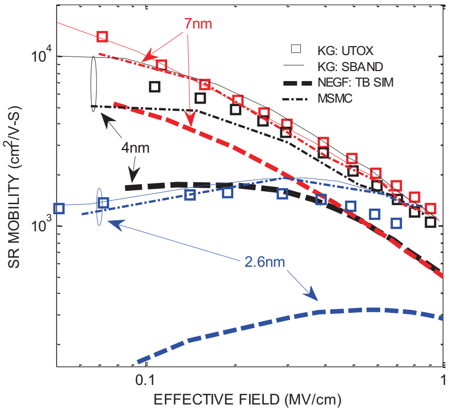

Figure 6 : SR-limited electron mobility for T_{SI}=2.6 nm, 4 nm and 7 nm: scattering time-based methods and NEGF predictions (exponential SR autocorrelation with Δ=0.47 nm; Λ=1.3 nm).

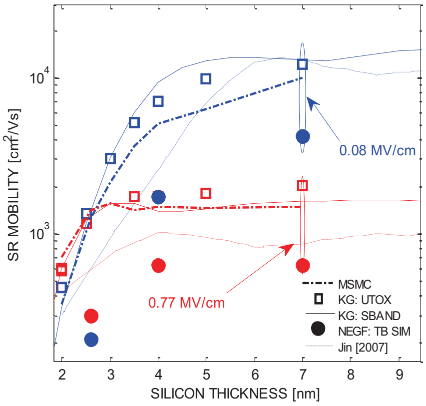

Figure 7 : SR-limited electron mobility vs T_{SI}. Summary of simulation results with present solvers and comparison with S. Jin results [2]. (effective field E_{eff}=0.08 and 0.77 MV/cm; exponential SR autocorrelation with Δ=0.47 nm; Λ=1.3 nm).

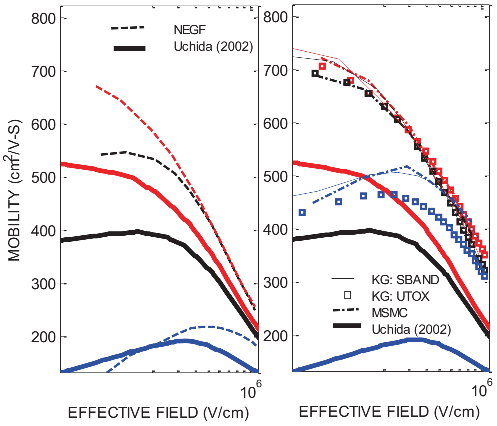

Figure 8 : Total electron mobility in a 2.5 nm, 4 nm and 7 nm FDSOI film calculated with NEGF (left) and scattering time-based methods (right). Comparison with experimental data from K. Uchida [9] (From top-to-bottom: T_{Si}=2.48, 4.3, 7.4 nm).

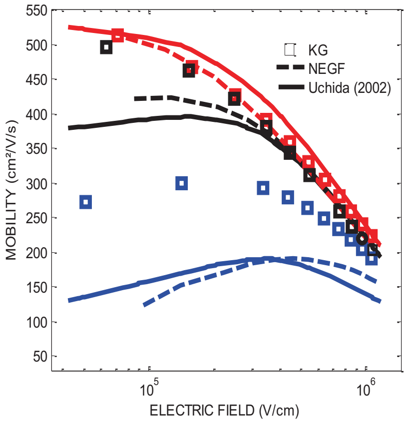

Figure 9 : NEGF with enhanced phonon deformation potentials (+20%) compared to KG results with enhanced phonon (+20%) and SR parameters (Δ=0.67 nm; Λ=1.3 nm).