MONTE CARLO SIMULATION OF THE ELECTRON MOBILITY IN STRAINED SILICON

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The SiGe/Si material system is recently a subject of increased research interest, since it provides beneficial band structure and transport properties due to strain. Monte Carlo method is used for analyzing these properties. Special focus is put on the description of the anisotropic majority/minority electron mobility in strained Si layers as a function of doping, electric field, and material composition.

Keywords: Monte Carlo simulation, electron mobility, strained Silicon

1. INTRODUCTION

The influence of strain on the intrinsic mobility of Si was first investigated in the early 1950s [1, 2]. The idea came to life again in the 1990s when it was first demonstrated that n-MOSFETs on strained substrates exhibit as much as 70% higher effective mobility than those on unstrained substrates [3]. Since then, the semiconductor industry has adopted several different technologies to introduce strain in the channels of MOS devices. For the CMOS technology, although the SiGe channel has been used to enhance the performance of PMOS transistors, it leads to a lack of improvement for the complementary NMOS transistors. The replacement of the channel material by strained Si, which utilizes an underlying relaxed SiGe [001] substrate for its functioning, renders a solution to the problem since it leads to enhancement of both the electron and hole mobilities. In order to investigate and design strained Si transistors, it is necessary to properly model the carrier mobilities in these devices.

2. SIMULATION RESULTS

Monte Carlo simulation which accounts for alloy scattering and the splitting of the anisotropic conduction band valleys due to strain in combination with an accurate ionized impurity scattering model, allowed us to obtain results for the low-field electron mobility in strained Si (SSi) for the complete range of donor and acceptor concentrations and Ge contents *y* in the $Si_{1-y}Ge_y$ buffer layer. The results obtained have been verified against experimental data which are available in the form of piezo-resistance coefficients. Fig. 1 (left) shows the in-plane (parallel) and the out-of-plane (perpendicular) minority electron mobility in strained Si as a function of the Ge content *y* in the $Si_{1-y}Ge_y$ buffer at 300 K for different acceptor doping concentrations.

The mobility obtained from piezo-resistance coefficients, which exhibits a linear increase for low strain levels [2, 4], is shown for comparison.

The difference between majority and minority electron mobilities [5] is a known phenomenon caused by effects such as degeneracy and the different screening behavior of electrons and holes in the semiconductor. An analytical model which describes this effect based on Monte Carlo simulation data is given in [6]. Fig. 1 (right) demonstrates a good match between the analytical model, our Monte Carlo simulation data, and measurements from [5, 7, 8, 9] for Si at 300 K. We use the same functional form to fit the doping dependence of the parallel and the perpendicular mobility in strained Si [10]. Fig. 1 (right) compares Monte Carlo simulation data with the model for the extreme case of strained Si on Ge.

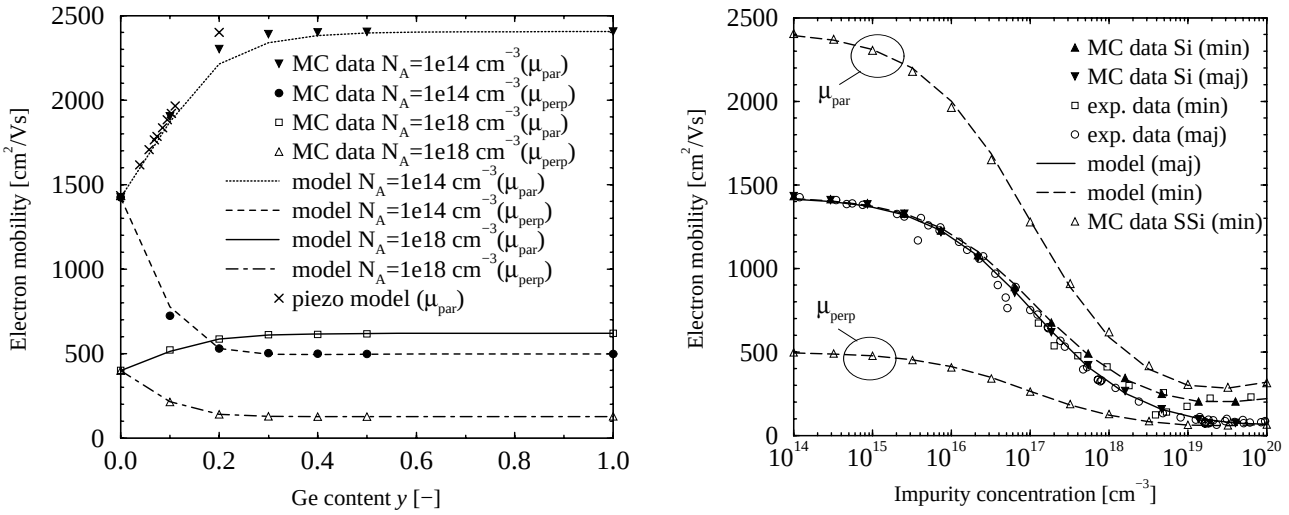

Figure 1. Parallel and perpendicular minority electron mobilities in strained Si as a function of the Ge content *y* in the $Si_{1-y}Ge_y$ [001] buffer layer for different acceptor doping concentrations (left). Comparison between Monte Carlo simulation data and experimental data for the majority and minority electron mobility in Si as a function of doping concentration; Parallel and perpendicular minority mobility in strained Si on Ge (right).

Fig. 2 shows the doping dependence of the in-plane minority and majority electron mobility components in strained Si layers for different Ge contents in the underlying SiGe for [001] orientation of the substrate. The solid lines depict the results as obtained from the analytical model, while the symbols indicate the Monte Carlo simulation results. As can be seen, the model reproduces the increase in minority electron mobility for high doping concentrations for all strain levels, when compared to majority electron mobility.

Fig. 3 (left) presents the velocity-field characteristics for unstrained and strained Si for [100] field direction as obtained from MC simulations. The simulation results agree well with measured data [11, 12] and other Monte Carlo simulation data [13, 14, 15]. Fig. 3 (right) shows the velocity-field characteristics as obtained from MC

simulations for biaxially strained Si grown on a relaxed SiGe substrate for different Ge contents and electric field along the in-plane [100] and out-of-plane [001] direction, respectively. The total velocity increases with strain for a field along the [100] direction and it decreases for a field along the [001] direction. For the in-plane electric field [100] the electron velocity exhibits a region of small negative differential mobility, typical for III-V semiconductor materials.

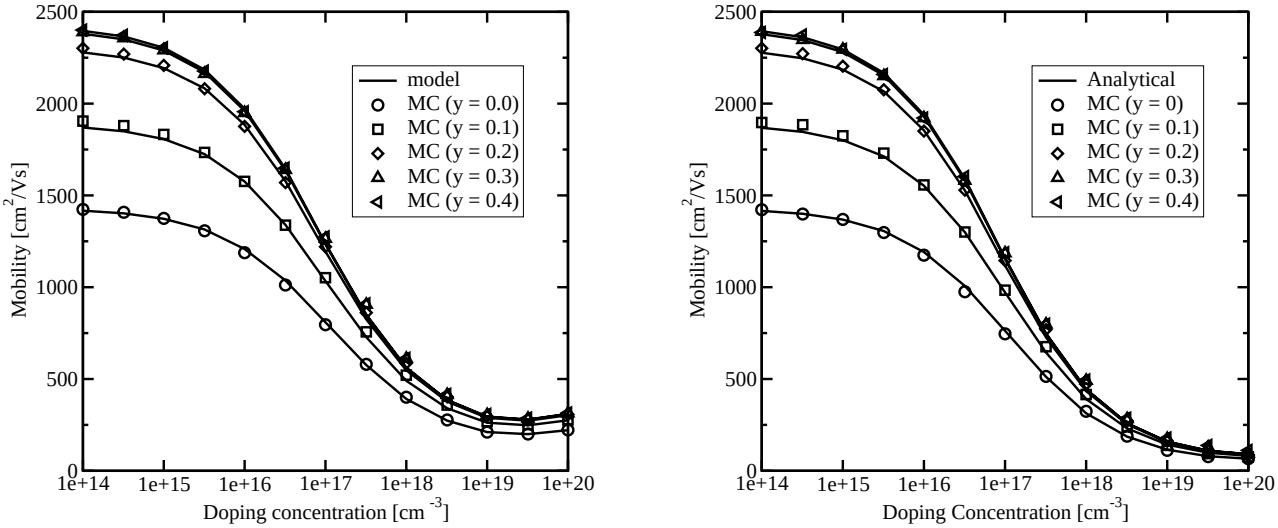

Figure 2. Doping dependence of the in-plane minority (left) and majority (right) electron mobility in strained Si calculated for different Ge contents in SiGe [001] substrate.

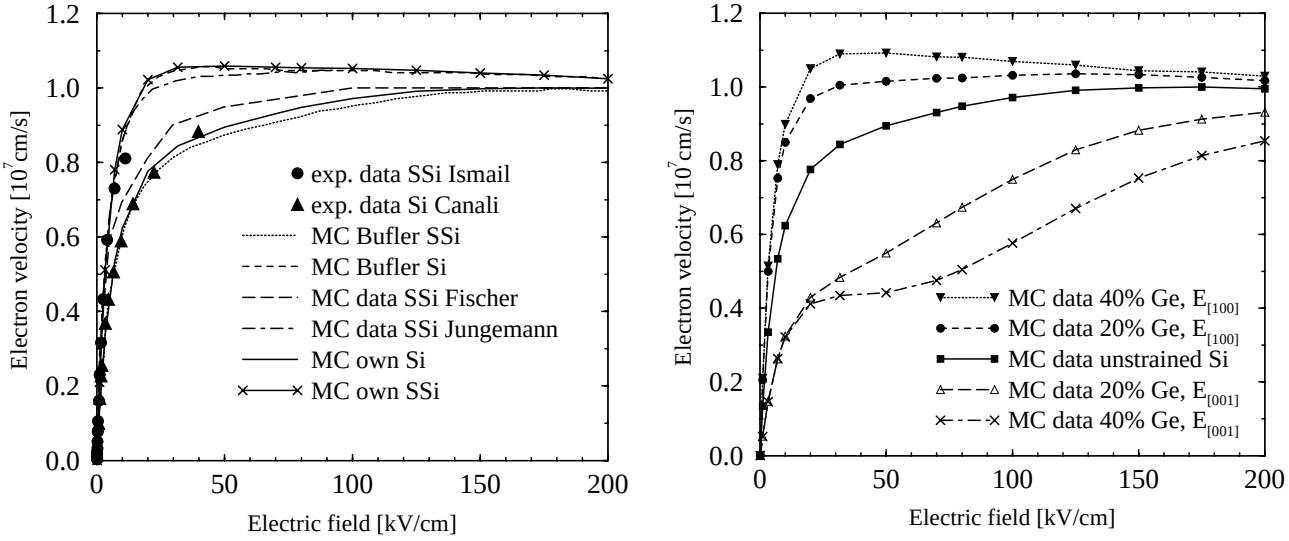

Figure 3. Electron velocity vs. electric field characteristics. Unstrained and strained Si on $Si_{0.7}Ge_{0.3}$ for [100] field direction (left). Strained Si on SiGe with Ge content as a parameter for field along [100] and [001] directions (right).

3. CONCLUSION

We present results from Monte Carlo simulations of strained Si on SiGe [001] substrates. Electron mobilities are obtained for different conditions of doping, strain (substrate mole fractions), and electric field. The results are verified against measurements and other Monte Carlo simulation data. TCAD simulation tools need correct models of the strained Si/SiGe material system, especially with respect to carrier transport. Experimental data remain a basic input for verification of analytical TCAD models. However, Monte Carlo simulation data with confirmed accuracy can deliver information which is still experimentally missing.

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