Effective Monte Carlo Simulator of Hole Transport in SiGe alloys

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It has been found that, with respect to the Negative Bias Temperature Instability (NBTI) effect, p-type silicon-germanium transistors have greater reliability than conventional p-type silicon devices [1]. It has also been shown that holes have higher mobility in SiGe alloys compared to pure silicon [2]. Because of that, it is expected that silicon-germanium alloys will replace pure silicon in the active channel region of the transistor. In this work, an Ensemble Monte Carlo (EMC) transport simulator is presented for simulation of hole transport in SiGe alloys.

In our theoretical model, to simulate the dynamics of holes in the SiGe alloys, the scattering mechanisms due to lattice vibrations [3] and alloy disorder [4], and an effective mass description are used. The nonparabolicity and the warping effect of the heavy-hole and light-hole bands were considered in their dispersion relation [5], while the split-off band was described as parabolic and spherical. The parameters of the dispersion relation were extracted by fitting the expression to the band structure calculated by the Empirical Pseudopotential Method.

The mobility of holes for a range of SiGe alloys was calculated at 300K at low electric field. The simulation mobility results agree well with the experimental data and with a more computationally expensive theoretical model [7] (Fig. 1). The profile of the mobility curve vs. Ge content suggests that the effect of each scattering mechanism on the mobility depends on the Ge content. The high occupancy of the heavy-hole band in high Ge content alloys (Fig. 2) suggests that for high Ge content the interband scattering is reduced. For high Ge content, the intraband alloy disorder scattering rate in the heavy-hole band is lower than for low Ge content (Fig. 3). For holes in the heavy-hole band with energy higher than the thermal energy at 300K, the phonon intraband scattering rates decreases as the Ge content increase (Fig. 4).

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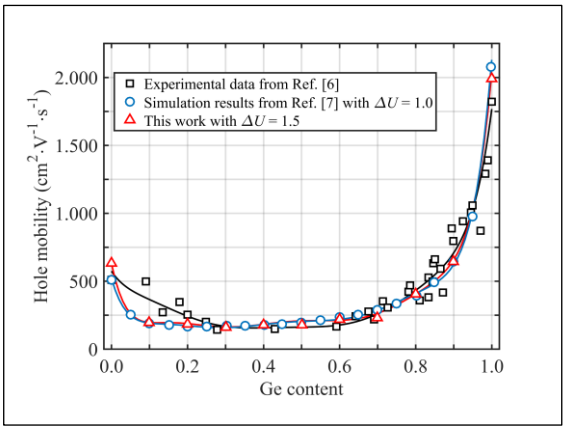

Fig.1: Comparison of the hole mobility in $Si_{1-x}Ge_x$ alloys versus germanium content. The alloy scattering potential used in the in-house simulator is equal to 1.5. The interpolated lines are a guide to the eye.

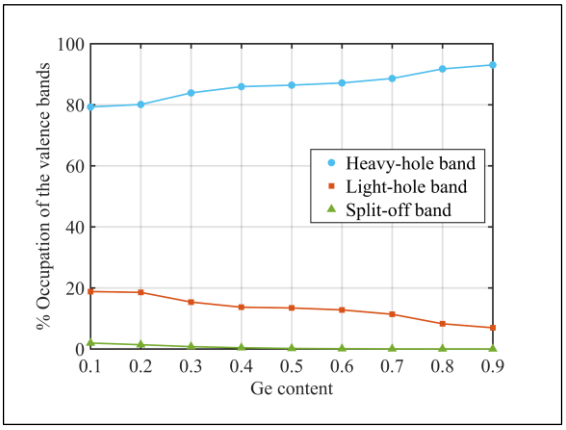

Fig.2: Occupation of heavy-hole band, light-hole band and split-off band versus Ge content. The lines are guide to the eye. This suggests that the interband scattering is reduced as the Ge content increases.

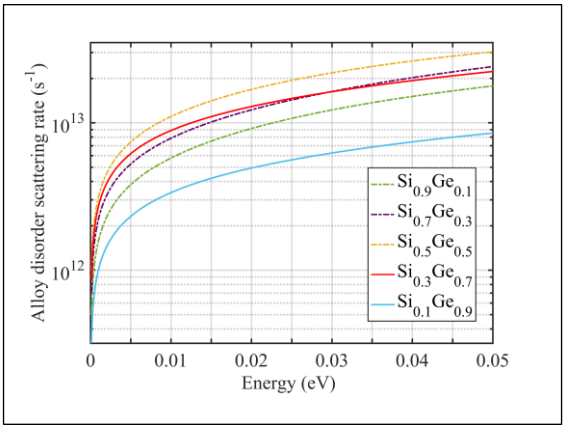

Fig.3: Alloy disorder scattering rate of $Si_{0.9}Ge_{0.1}$, $Si_{0.7}Ge_{0.3}$, $Si_{0.5}Ge_{0.5}$, $Si_{0.3}Ge_{0.7}$ and $Si_{0.1}Ge_{0.9}$. The alloy disorder scattering rates reaches its maximum value for $Si_{0.5}Ge_{0.5}$ and then decreases to reach its minimum value for $Si_{0.1}Ge_{0.9}$.

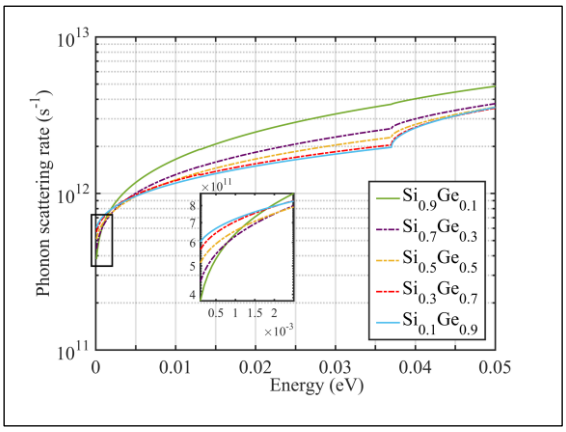

Fig.4: Phonon scattering rate of $Si_{0.9}Ge_{0.1}$, $Si_{0.7}Ge_{0.3}$, $Si_{0.5}Ge_{0.5}$, $Si_{0.3}Ge_{0.7}$ and $Si_{0.1}Ge_{0.9}$. The extremely low energy is depicted in zoom where the total scattering rate increases with the Ge content. For values of energy higher than the thermal energy at 300K, the total phonon scattering rates become smaller as the Ge content increases.

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