

Enhanced Hole Drift Velocity in Sub-0.1 μm Si Devices Caused by Anisotropic Velocity Overshoot.

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1. Abstract

We performed for the first time full band Monte Carlo simulations of anisotropic hole transport in sub-0.1 μm Si devices. We found from this simulation of 0.05 μm channel p-i-p diodes that the hole drift velocity in the channel with the orientation of $\langle 100 \rangle$ with respect to crystallographic direction is enhanced by the velocity overshoot effect, and that the average velocity in the middle of the channel is 25 % higher than for a diode in $\langle 110 \rangle$ direction at room temperature. These results suggest that the current drive capability of sub-0.1 μm pMOSFETs could be optimized by choosing the channel orientation in the $\langle 100 \rangle$ direction.

2. Introduction

Because the valence band of Si, especially the heavy hole band, has a strongly warped shape (Fig. 1), the steady-state drift velocity of holes has anisotropic character in a high electric field (Fig. 2) [1,2]. Although high field hole transport is an important subject to analyze sub-0.1 μm pMOSFETs, there have been few papers concerning this, and they had not discussed about the anisotropic transport [3,4]. We already reported Monte Carlo simulations of anisotropic transient hole transport in bulk Si for homogeneous fields. We had demonstrated that the transient velocity in an electric field applied in $\langle 100 \rangle$ direction showed a larger overshoot effect compared to fields in $\langle 110 \rangle$ and $\langle 111 \rangle$ direction (Fig.3) [5]. It seemed likely that there would be a similar enhancement of the anisotropic overshoot in deep-submicron devices. In this paper, we performed for the first time the simulation of a sub-0.1 μm diode with channels in $\langle 100 \rangle$ and $\langle 110 \rangle$ direction to investigate the anisotropic hole velocity overshoot effect for a non-homogeneous electric field.

3. Model

We applied our full band Monte Carlo device simulator FALCON [6] to perform simulations of a one dimensional diode. The scattering mechanisms we considered were acoustic and non-polar optical phonon scatterings and impact ionization. We employed the inelastic model for acoustic phonon scattering which was proposed by Fischetti et al. [7]. In order to save CPU time, we did not include an ionized impurity scattering, as we assumed that this type of scattering would not be important for high energy hole transport. The deformation potential parameters of acoustic and optical phonons were determined by the curves of measured drift-velocity against the electric field [1,2] for a wide range of lattice temperatures. We obtained good indications for those directional dependence at 77, 200 and 300 K, as shown in Fig. 2. Using determined parameters we obtained a saturation velocity of $10.6 \times 10^6 \text{ cm/s}$ when the applied field of 300 kV/cm was oriented in $\langle 100 \rangle$ direction. We obtained an anisotropic velocity overshoot in the homogeneous field of 100kV/cm, as shown in Fig. 3.

The simulated diode had a p-i-p structure in which a non-doped channel is sandwiched between p-type source and drain regions, which were abruptly doped to $1 \times 10^{19} \text{ cm}^{-3}$, as shown in Fig. 4. The device orientation was defined by setting the vector \vec{r} parallel to the $\langle 100 \rangle$ and $\langle 110 \rangle$ direction. The channel length (L) was varied from 0.5 to 0.05 μm . The applied voltage (Vd) was -0.5 V for 0.05 μm diode and was varied in such a way as to keep Vd/L constant. The simulation was performed for a period of 20 ps in time steps of 1 fs and the used particle number was about 20000. To maintain accuracy for a long channel diode, the multiple refresh method [8] was

employed.

4. Results and Discussion

Fig. 5 shows the calculated profile of the electric field in the $0.5\mu\text{m}$ and $0.05\mu\text{m}$ diodes. The shapes of these profiles are almost equal due to the scaling of the applied voltage and the field strength in the middle of the channel under these conditions was about 100kV/cm for diodes of all sizes. These profiles show little difference between the diodes in $\langle 100 \rangle$ and $\langle 110 \rangle$ direction.

Figs. 6 (a) and (b) show the calculated hole velocity profiles for the $0.5\mu\text{m}$ and $0.05\mu\text{m}$ diodes with channel orientations of $\langle 100 \rangle$ and $\langle 110 \rangle$. It can be seen that for devices of both sizes, the hole velocities in the diodes in $\langle 100 \rangle$ direction are higher than for those in $\langle 110 \rangle$ direction, and that the anisotropy becomes larger with the decrease of the channel length. To clarify whether this behavior with respect to the anisotropy was due to the steady state character or the overshoot phenomena, we plotted the local hole velocity as a function of the local electric field in the channel region. We then compared these graphs with the anisotropy in the graphs of the drift velocity against electric field for bulk steady states in Figs. 6 (c) and (d). We found that the hole velocity for the $0.05\mu\text{m}$ diode was enhanced, while that for the $0.5\mu\text{m}$ diode remained almost the same as for the bulk steady state in the high field region. Note that the enhancement of hole velocity for the $0.05\mu\text{m}$ $\langle 100 \rangle$ diode is larger than that of the $0.05\mu\text{m}$ $\langle 110 \rangle$ diode.

Fig. 7 shows the corresponding local hole energies. For the longer channel diodes, the electric field dependence of the local hole energy is almost similar as for the average hole energy in bulk steady state. This means that for the $0.5\mu\text{m}$ channel, the energy distribution of the holes is not very different from that for the steady state in the homogeneous field. Consequently, the anisotropy of hole velocity was caused by the bulk steady state character. On the other hand, the local hole energies in the $0.05\mu\text{m}$ diodes were much lower than those in bulk steady state. In the homogeneous field, the energy of the transient state, in which the hole velocity reaches its peak value, was also lower than that for the steady state, as shown in Fig. 3. This can be attributed to the change of the electric field, which is too steep that holes would be able to complete energy relaxation, and the hole temperature in the channel stays low in spite of their high drift velocity. It can therefore be concluded that the velocity enhancement in the $0.05\mu\text{m}$ $\langle 100 \rangle$ diode was caused by the anisotropic velocity overshoot effect and the velocity

of $\langle 110 \rangle$ diode was not enhanced in the same way as for the bulk velocity overshoot. Fig. 8 shows the hole velocity in the middle of the channel as a function of the channel length. The hole velocity in the $0.05\mu\text{m}$ diode in $\langle 100 \rangle$ direction becomes larger with the decrease of channel length because of the velocity overshoot enhancement, while the field strength in the middle of the channel is almost equal for all size of diodes. From these results it can be concluded that not only the strength but also the steepness of the electric field variation are important factors for the velocity overshoot effect in sub- $0.1\mu\text{m}$ device. For example, the hole drift velocity is 25 % higher for the $0.05\mu\text{m}$ diode in $\langle 100 \rangle$ direction than that for the diode in $\langle 110 \rangle$ direction.

5. Conclusions

We performed for the first time full band Monte Carlo simulations of anisotropic hole transport and examined the enhancement of the drift velocity in sub- $0.1\mu\text{m}$ diodes with the channel in $\langle 100 \rangle$ direction. Our results show that the improvement in hole velocity for the $0.05\mu\text{m}$ diode is caused by an anisotropic velocity overshoot effect which is as much as 25% higher compared to the diodes in $\langle 110 \rangle$ direction.

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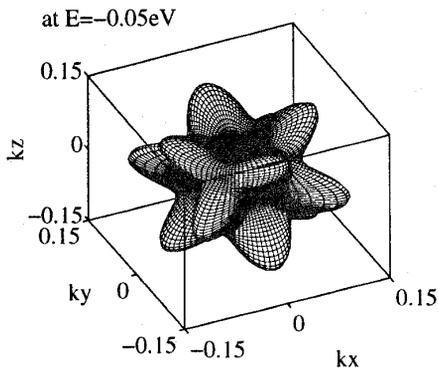


Figure 1: Anisotropic isoenergy surface of Si heavy hole band at a hole energy $E = -0.05$ eV.

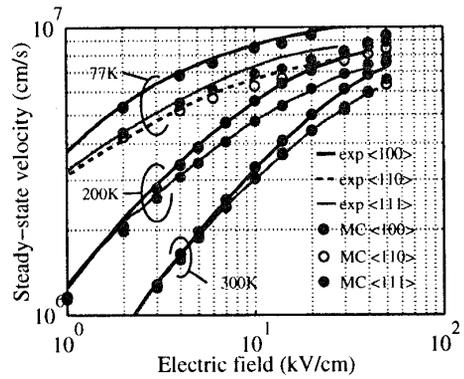


Figure 2: Steady state hole drift velocity as a function of electric field in bulk Si. The lines are based on experimental data reported by Canali et al. [1,2].

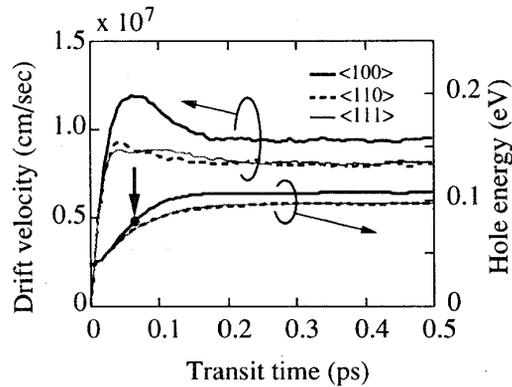


Figure 3: Transient drift velocity and average energy of holes as a function of transit time. 100 kV/cm were applied to the $\langle 100 \rangle$, $\langle 110 \rangle$, and $\langle 111 \rangle$ crystallographic axes in the Si bulk. The closed circle denotes the average energy for $\langle 100 \rangle$ when the drift velocity reaches its peak value.

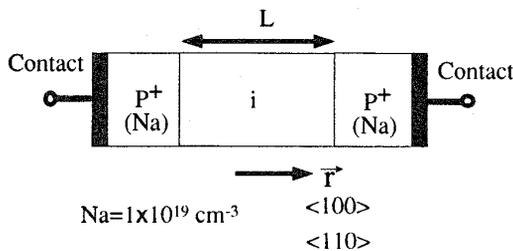


Figure 4: Calculated p-i-p diode structure. The orientation of the diode is defined by setting the vector \vec{r} parallel to the $\langle 100 \rangle$, $\langle 110 \rangle$, or $\langle 111 \rangle$ direction.

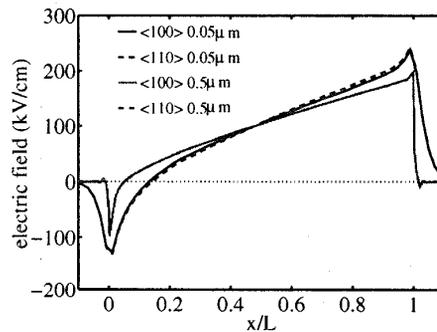


Figure 5: Electric field profile for $L = 0.5$ and $0.05 \mu\text{m}$ diode. The solid and dashed lines stand for the diodes in $\langle 100 \rangle$ and $\langle 110 \rangle$ direction, respectively.

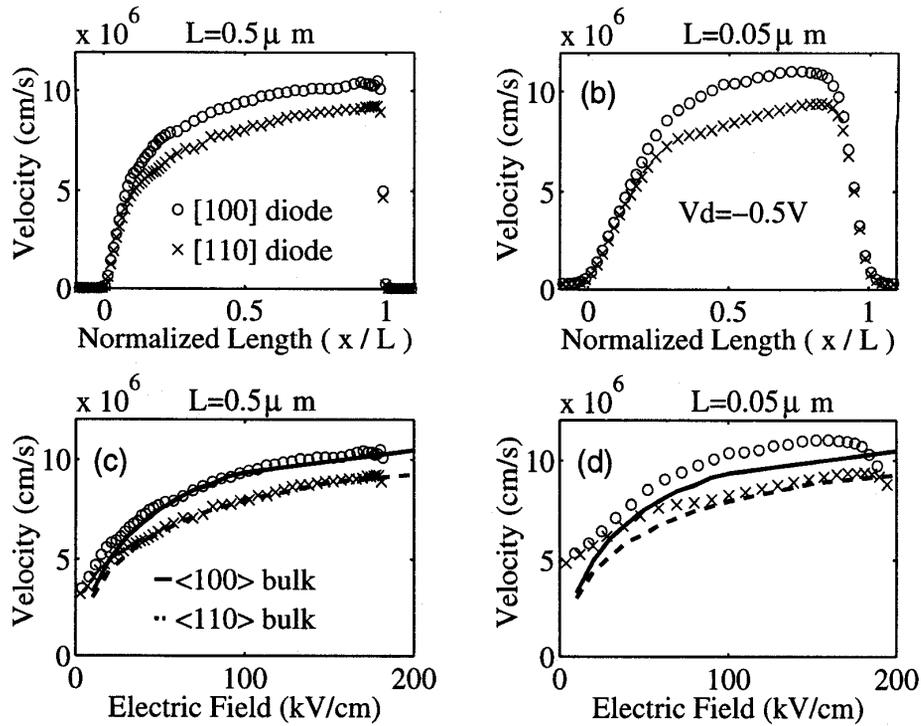


Figure 6: Comparison of the local hole velocities for diodes in $\langle 100 \rangle$ and $\langle 110 \rangle$ direction at 300K. (a) and (b) show the local hole velocity profiles in $0.5 \mu\text{m}$ and $0.05 \mu\text{m}$ diodes. (c) and (d) show the local electric field dependence of the velocity corresponding to the cases depicted in (a) and (b), respectively. The solid and dashed lines denote the average hole velocity in bulk steady state when an electric field is applied in $\langle 100 \rangle$ and $\langle 110 \rangle$ direction.

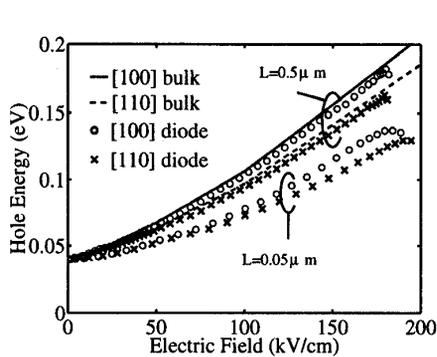


Figure 7: Local hole energy as a function of the local electric field in the channel of $0.5 \mu\text{m}$ and $0.05 \mu\text{m}$ diodes. The solid and dashed lines denote the average hole energy in bulk steady state when an electric field is applied in $\langle 100 \rangle$ and $\langle 110 \rangle$ direction, respectively.

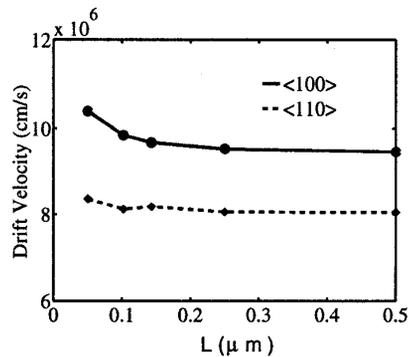


Figure 8: Hole drift velocity in the middle of the channel as a function of channel length. The solid and dashed lines stand for the diodes in $\langle 100 \rangle$ and $\langle 110 \rangle$ direction, respectively.