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Impact of Channel Shape on Carrier Transport Investigated by Ensemble Monte Carlo/Molecular Dynamics Simulation

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Abstract—**Effect of the channel shape on the nano-scale carrier transport is studied by using the ensemble Monte-Carlo - molecular dynamics method (EMC/MD). Carrier transport in hone-shaped asymmetric channels which widen from source to drain sides is simulated by comparing that in the conventional straight channels. The obtained conductance of the horn-shaped channels is larger than that of the straight channel, as a result of the enhancement of the carrier mobility in the hone-shaped channel. This can be attributed to two reasons: the collimation effect of the asymmetric channel peculiar in the quasi-ballistic carrier transport regime, and the suppression of carrier-carrier interaction due to widening of the channel.**

Keywords-component; EMC-MD method, MOSFET, assymetric channel, collimation effect, ballistic transport

I. INTRODUCTION

In the Si CMOS technology, variations between individual device performance is now a serious issue to be solved. The variation arises from the limit of fabrication accuracy such as lithography and the statistical fluctuation in the number and the positions of dopants in each device. In addition, drain current fluctuation in time-scale, i.e. current noise, is getting a serious problem in accordance with the continuous scale-down in the device size and increase in the operation frequency. Shrinkage of the device dimensions leads to the decrease in the number of carriers in the channel. This enhances the discreteness of the carriers, resulting in the increase in the current fluctuation.

As the device size falls below the length of carrier mean free path, the carrier transport mechanism is considered to change into “quasi-ballistic”, in which carriers experience only a small number of phonon scattering events during their motions through channel region [1]. In the quasi-ballistic regime, effect of the interface scattering becomes significant compared to the other scattering mechanism such as carrier-carrier, carrier-impurity, carrier-phonon interaction [2,3]. Therefore, the channel shape is considered to have an impact on the carrier transport. It has been suggested that in mesoscopic system, the carrier motion along the channel can be enhanced by employing an asymmetric shaped channel [4].

In this work, we investigate effect of the channel shape on carrier transport by using the ensemble Monte-Carlo - molecular dynamics (EMC/MD) method [5,6]. We calculated the mean current for various shapes of channel: hone-shaped asymmetric channels which widen from source to drain sides, a reversed-hone shaped channel which narrows from source to drain, and a conventional straight channel.

II. SIMULATION METHOD AND MODEL

The simulation concept of the EMC/MD method is illustrated in Fig. 1. In this method, carriers are treated as classical particles, and their real-space trajectories under the Coulomb point-to-point potentials are calculated by the MD algorithm. The acoustic and optical phonon scattering are taken into account as stochastic changes in the momentum of carriers according to the standard energy-dependent formulations based

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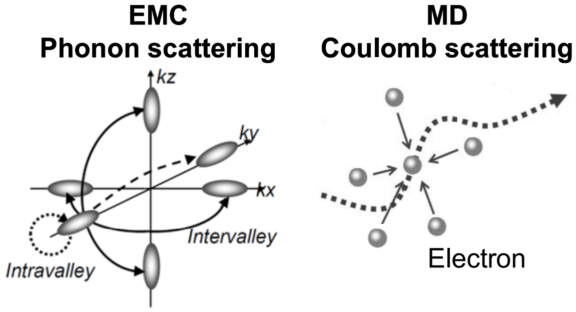

Fig. 1 Concept of the EMC/MD method.

on the Fermi golden-rule-type approach [5] in a bulk band structure. Six equivalent X-valleys of conduction bands are expressed by an ellipsoidal non-parabolic band mode, which is represented as

$$E(1+\alpha E)=\frac{\hbar^2}{2}\left[\frac{(k_x-k_{x0})^2}{m_x}+\frac{(k_y-k_{y0})^2}{m_y}+\frac{(k_z-k_{z0})^2}{m_z}\right], \quad (1)$$

where m_x, m_y, and m_z are effective masses for x, y and z axes, respectively. The two of the effective masses are transverse effective masses: $m_t = 0.19m_0$, where m_0 is the electron rest mass. The other is longitudinal effective mass: $l_l = 0.98m_0$. k_{x0}, k_{y0}, and k_{z0} are the center of X-valley coordinate (wave vector in case that energy takes minimum value). α (= 0.5 eV^{-1}) is a nonparabolicity parameter.

In this simulation, we newly introduced a cylindrical object as a building unit of the side walls of the channel. The cylindrical object is designed to repel carrier electrons isotropically. Various shapes of channel can be easily modeled by piling the cylindrical objects along side interfaces of the channel. The interaction between electrons and the cylindrical objects is described by a repulsive potential as a function of distance r between a carrier electron and the axis of the cylindrical object. The potential function, $V(r)$, is defined as

$$V(r)=V_0\left(\frac{\sigma_{core}}{r-r_{core}}\right)^{\gamma}\cdot\exp\left[\frac{\sigma_{cutoff}}{r-r_{cutoff}}\right], \quad (r<r_{cutoff}), \quad (2)$$

where V_0, γ, σ_{core}, r_{core}, σ_{cutoff}, r_{cutoff} are parameters. r_{core} is the radius of the cylindrical object. Carrier electrons are prohibited to penetrate inside of the cylinder. r_{cutoff} is the cut off distance of the interaction. The parameter values are shown in Fig.2, which are determined so as to describe the barrier at the Si/SiO_2 interface for conduction electrons. The typical value of the conduction band off-set at the Si/SiO_2 interface is about 3eV. Assuming that the interfacial roughness is about 0.35 nm [7], the potential parameters are chosen so as to reach the band off-set within the range of the interfacial roughness from the cut off distance.

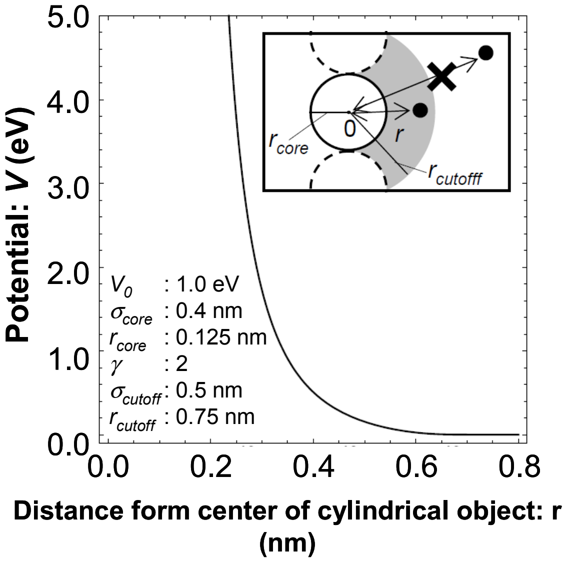

Fig. 2 Potential profiles of a cylindrical particle. The expression of the potential function is described as the equation (2).

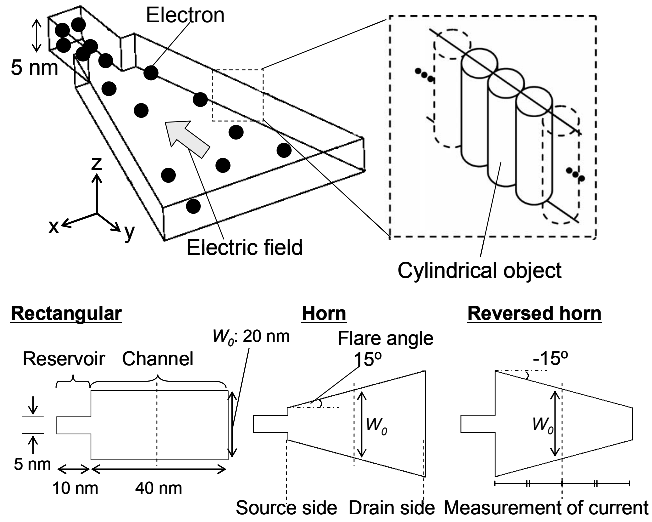

Fig. 3 Simulation model for electron transport in symmetric and asymmetric channels. Cylindrical objects are pilled along the side wall of channel. Current is estimated by counting the number of electrons passing through the cross section at the channel center.

We have examined three models of the intrinsic Si channel as shown Fig. 3. One is a rectangular shape channel which corresponds to a conventional straight channel, and the others are asymmetric, horn and reversed-horn shapes which have flare angle of ±15° through the channel. All models are the same in the channel volume, i.e., the channel resistances are equal to each other if the resistivity is identical. The same number of carriers is included in the channel, so that the carrier density is also identical (9.4×10^{18} cm^{-3}). Carriers are injected from a reservoir connected to the channel as indicated in Fig. 3. The momentum of the carrier at the instance of the injection is stochastically determined according to the Boltzmann distribution at room temperature. A constant electric filed (5 kV/cm) is applied along the channel. The carrier which reaches at the end of the channel is eliminated and a new carrier is generated in the reservoir. Thus, the number of the carriers is kept constant during the simulation. In these conditions, we estimated the current by counting the number of the carriers passing through the cross section at the center of the channel.

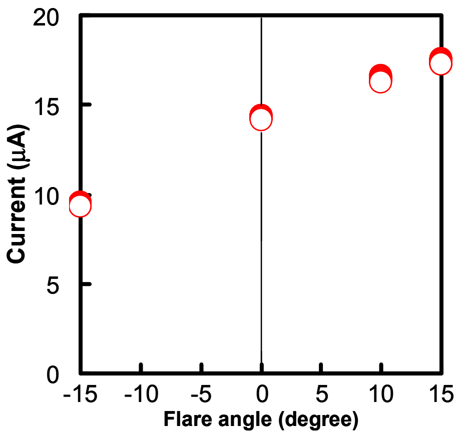

Fig. 4 Flare angle dependency on current. Current increases with increase in the flare angle in the horn channel. On the contrary, current decreases in the reversed horn channel.

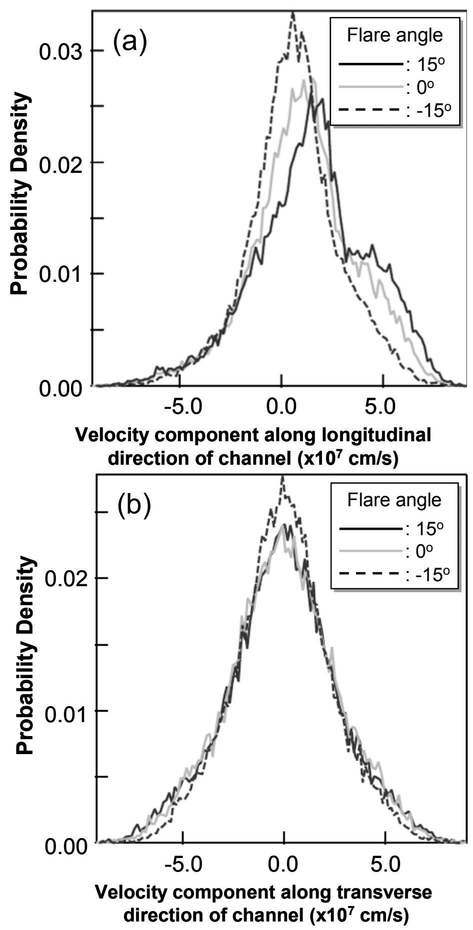

Fig. 5 Histogram of velocity distribution along (a) longitudinal and (b) transverse direction of channel.

III. Results and Discussion

Figure 4 shows flare angle dependency of the mean current. Each plot is calculated by averaging current within each sampling period of 133 ps which corresponds to a sampling frequency of 7.6 GHz. It is clearly shown that the current increases with the flare angle. Contrary, the current decreases in the case of the reversed-horn channel, i.e., negative flare angle. In general, current increases with the carrier density and/or the carrier mobility. Because the number of carriers is kept constant during the present simulations, the result indicates that carrier mobility is enhanced in the horn channel.

Figure 5 shows the distribution of velocity components along longitudinal and transverse directions of the channel, which are calculated from trajectories in the phase space for all electrons in the channel region. In case of the horn channel, the peak of velocity component along the channel direction is shifted to higher side compared to the straight and the reversed-horn channels. In the reversed horn with a flare angle of -15°, the velocity distribution is shifted to lower velocities. Thus, the increase in the mean current in the horn channel can be attributed to the enhancement of the carrier mobility.

Figure 6 shows the two dimensional profiles of velocity component along the longitudinal direction of the channels. Carriers reach maximum velocities at the drain sides of the channels, indicating that carriers are continuously accelerated throughout the channel. In this simulation, the number of carrier-phonon scattering during one passage through the channel is less than 10 times. Thus, the quasi-ballistic carrier transport occurs in the present simulation.

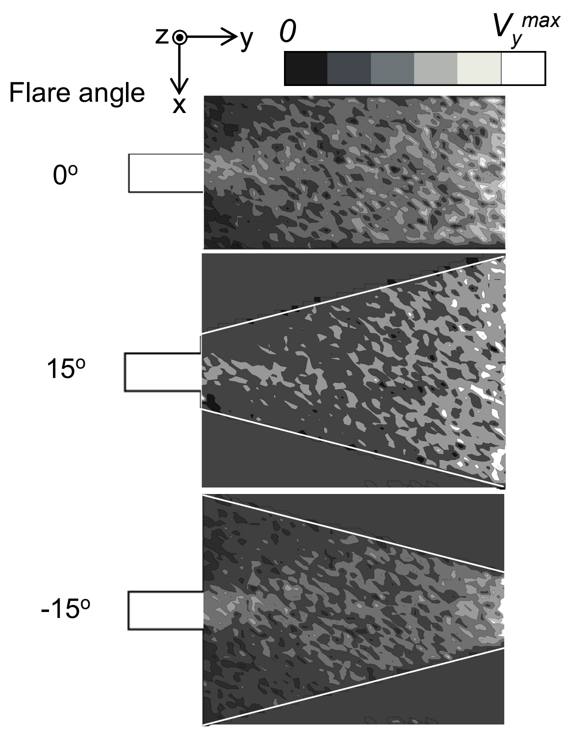

Fig. 6 Time averaged 2D profiles of velocity component along longitudinal direction of channel.

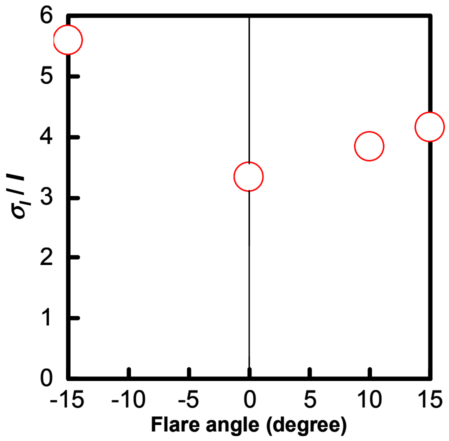

Fig. 7 Flare angle dependency of current fluctuation.

The enhancement of carrier velocities in the horn shaped channel can be attributed to collimation by the interface scattering. Carrier scattering at the interface occurs elastically in the present simulation so that the incidence and reflection angle is identical. Because the interface of the horn shaped channel is tilted from the channel, the longitudinal component of carrier momentum increases by the interface scattering. Thus, the momentum is collimated along the channel direction in the horn geometry.

Another possible reason is the suppression of the carrier-carrier scattering in the horn channel. The drain side of the horn shaped channel is wider than other channel shapes, so that the mean distance between carriers is relatively large. Due to the decrease in the carrier-carrier scattering events, the carrier mobility increases in the horn shaped channel. On the other hand, the narrowing at the source side has little effect on the carrier mobility, because the injected carriers from the small reservoir spread into the channel and cannot reach the side interface for a while. Thus the carrier-carrier scattering probability is mainly depends on the channel width of the drain side.

Figure 7 shows the variation coefficient of the current noise. The current fluctuation is minimized in the straight channel, and increases in both the horn and the reversed-horn channels. The increase in current fluctuation in the horn channel can be explained by the spread of the velocity distribution along longitudinal direction of channel as shown in Fig. 5(a), because the velocity distribution along the transverse direction of the channel is almost the same between the straight and the horn channels, as shown in Fig. 5(b). The enhancement of the current fluctuation in the reversed-horn channel can be explained by the decrease in the mean current.

IV. CONCLUSION

Carrier transports in asymmetric horn shaped channels were studied by the EMC/MD simulation and were compared to that of symmetric straight channel. The conductance of the horn shaped channel is larger than that of the straight channel, as a result of enhancement of the carrier mobility. This can be attributed to the two reasons: the collimation effect of the asymmetric channel peculiar in the quasi-ballistic carrier transport regime, and the suppression of carrier-carrier interaction due to the widening of channel. Current fluctuation in the horn shaped channel is not reduced compared to that in the straight channel in the present simulation. Asymmetric horn shaped channels has an advantage in enhancement of current drivability in nano-scale transistor.

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