Simulation Study of Quasi-ballistic Transport in Asymmetric DG-MOSFET by Directly Solving Boltzmann Transport Equation

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Abstract—In this work, we simulate double-gate MOSFET using a two-dimensional direct Boltzmann transport equation solver. Simulation results are interpreted by quasi-ballistic theory. It is found that the relation between average carrier velocity at virtual source and back-scattering coefficient needs to be modified due to the over-simplified approximations of the original model. 1D potential profile model also needs to be extended to better determine the kT-layer length. The key expression for back-scattering coefficient is still valid but a field-dependent mean free path is needed to be taken into account.

Index Terms—Boltzmann Transport Equation, Double-gate FETs, Numerical simulation, Quasi-ballistic transport

I. INTRODUCTION

AS the gate length of MOSFETs scaling down to sub-100nm regime, new transport phenomena such as velocity overshooting and quasi-ballistic transport challenged our traditional understanding of MOSFETs [1], [2]. Many works of experiments, simulation and modeling have been conducted to accurately account for the behavior of nanoscale MOSFETs, among which the quasi-ballistic transport model developed by Natori and Lundstrom [3]–[7] has attracted much attention due to its simplicity and abundant physical insight. However, because of the complex nature of carrier transport in nanoscale transistors, controversies regarding to the detail of quasi-ballistic model have been intensively discussed [8]–[10].

On the other hand, multi-gate thin body MOSFETs with gate length around 20nm have been in volume production and MOSFETs with extremely small size and complicated structure are being investigated both theoretically and experimentally. Whether the quasi-ballistic model can accurately describe the behavior of such MOSFETs remains to be seen.

Recently, a lot of work has been done to experimentally justify the validity of the quasi-ballistic model [9], [11] and compact models based on ballistic theory have been established [12]. However, most of these works focused on simple single-gate MOSFETs with relatively long channel length, thus the validity of ballistic model for multi-gate MOSFETs with channel length shorter than 10nm remains a question due to sophisticated 2D electrostatics and strong non-equilibrium transport phenomena.

One possible solution to examine quasi-ballistic transport phenomenon is to use quantum mechanical-based numerical simulation. In nanoscale MOSFETs, dimensionality is reduced due to quantum confinement; and it is possible to solve the Boltzmann transport equation (BTE) directly without using Monte Carlo method [13]–[15]. By directly solving the BTE and coupling it to the Schrödinger equation [16]–[18], the quantum effect can be accounted in a natural way.

To evaluate 2D quasi-ballistic transport in highly-scaled DG-MOSFET and investigate the validity of quasi-ballistic theory in the simulated conditions, we present a numerical study of Si thin body double-gate MOSFETs with very short channel length using a time-dependent multi-subband Boltzmann transport equation solver [19]–[20]. Simulation results and important parameters are examined according to quasi-ballistic theory. The validity of quasi-ballistic model is also discussed.

II. SIMULATION METHOD AND PHYSICAL MODELS

Double-gate n-MOSFETs with different top-gate voltage V_{gt} and back-gate voltage V_{gb} are simulated in this work. Channel length of the simulated device varies from 9nm to 18nm and the effective oxide thickness is 1nm. Source and drain length are both 9.9nm with a doping concentration of $1 \times 10^{20} \text{cm}^{-3}$, channel is undoped and body thickness is 3nm.

We use a time-dependent deterministic Boltzmann transport equation solver [19]–[20] to treat the 2D electron gas. Quantum confinement is taken into account by solving Schrödinger equation at each slice in the confined direction, and 2D Poisson's equation is solved self-consistently with the Schrödinger equation. A finite volume method is used to

discrete the BTE, and a finite difference method is used to solve the Poisson and Schrödinger equation.

Phonon scattering is carefully treated in this simulator [19], [20]. Both intra-valley and inter-valley phonon scattering are included and the effects of such scattering mechanisms are discussed in detail.

Information such as electron distribution function, electron density and velocity profile along the channel can be directly extracted from the simulation results, helping us to investigate the details of transport properties in nanoscale MOSFETs and making it possible to compare between the simulation results and the quasi-ballistic model [5], [7], [12], [21].

Quasi-ballistic model uses several physically-meaningful parameters to characterize scattering processes:

Back-scattering coefficient r is defined as the percentage of carriers that are back-scattered at the top of barrier, which indicates the scattering rate near the virtual source. Detailed analysis [5] states that r is related to the so called "critical length" l_{kT} and the mean free path λ:

$$r = \frac{l_{kT}}{l_{kT}+\lambda} \tag{1}$$

Rigorous definition of l_{kT} and λ can be found in [5], [7]. In quasi-ballistic theory, hot electrons are injected from the virtual source and drift down the potential barrier. Electrons are highly unlikely to return to the source once they experience a potential energy drop that is greater than their kinetic energy. The region corresponding to this potential drop is the so-called critical region, and the length of this region is denoted as l_{kT}. The mean free path λ is the average carrier travelling distance between two individual scattering events, indicating how often a carrier is scattered inside the channel.

The back-scattering coefficient r is defined as the ratio between the negative-directed flux (I^-) and the positive-directed flux (I^+) at the virtual source under high drain bias [7]:

$$r = \frac{I^-}{I^+} \tag{2}$$

which, in our simulation, can be directly extracted by analyzing the positive and negative current flow.

On the other hand, r can also be expressed by the ratio between ballistic injection velocity and the average velocity with scattering, at the virtual source [7]:

$$v_{scat} = \frac{1-r}{1+r} v_{ballistic} \tag{3}$$

So we extracted the back-scattering coefficient r using the above two method to examine the validity of (2) and (3). The result is plotted in Fig.1.
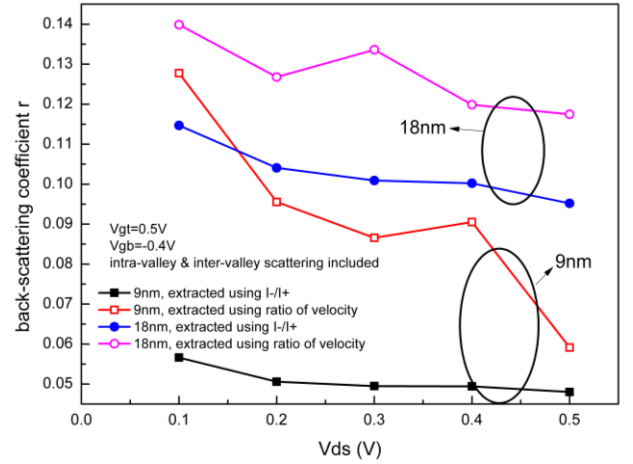

Fig. 1. Back-scattering coefficient extracted using flux ratio (2) and velocity ratio (3).

It is observed that there is a systematic deviation between the two back-scattering coefficients extracted using the different methods mentioned above. Using the original definition (2), we find the back-scattering coefficient r that is systematically smaller than using (3). This deviation is due to two simplified assumptions in (3): First, (3) assumes that scattering does not change the carrier concentration at the top of barrier, i.e. the transistor is perfectly well-tempered so that carrier densities at the top of barrier are the same for ballistic and non-ballistic channels. The second approximation is that the velocity of the positive flux (v^+) is equal to the velocity of the negative flux (v^-). In our simulation, however, the carrier concentration is 4.7% (for L=9nm) and 3.2% (for L=18nm) higher in ballistic channel than in non-ballistic channel due to 2D electrostatics. The ratio v^+/v^- is in the range of 1.1 to 1.2 instead of 1, indicating that slower carriers are more likely to be back-scattered. In the situation where v^+ is not equal to v^-, (3) needs to be modified as $v_{scat} = \frac{1-r}{1+(\frac{v^+}{v^-})r} v_{ballistic}$ [11],[23], to take the influence of v^+/v^- into consideration. Both of the effects are sources of error when computing r, and neglecting either of them will lead to an overestimation of r. This conclusion is consistent with the data in Fig. 1.

In [12], it is proposed that 1D potential profile along the channel region can be approximated by a power function:

$$V(x) = V_{ds} \left(\frac{x}{L'}\right)^{\frac{1}{a}} \tag{4}$$

Where L' is the distance of V_{ds} potential drop and $x=0$ corresponds to the position of virtual source. a is a fitting parameter in the range of 0.66 to 0.75 [12] under different scattering conditions. However, the precise determination of a and L' remains to be difficult. Another problem is that this model does not consider the effect of gate voltage on potential profile.

In reality, what we care about is the potential profile near the virtual source. Region where the potential energy is less than the maximum value by several kT is of less interest to us. Results of simulation show that l_{kT} seldom exceeds half of the

TABLE I
RESULTS OF FITTING PARAMETER A (GATE VOLTAGES ARE V$_{GT}$=0.5V, V$_{GB}$=-0.4V)

Gate length and scattering conditions	Vds (V)	Barrier height (V)	0.5L' (nm)	a
9nm ballistic	0.1	0.0881	4.8	0.4711
	0.5	0.0735	6	0.4105
9nm with scattering	0.1	0.0882	4.8	0.4649
	0.5	0.0737	6	0.4058
18nm ballistic	0.1	0.1156	9.6	0.2904
	0.5	0.1128	10.8	0.2616
18nm with scattering	0.1	0.1118	9.6	0.3032
	0.5	0.1088	10.8	0.2894

gate length under reasonable V_{ds}, thus we could just model the potential profile in the range of 50% V_{ds} drop and the rest of $V(x)$ is of little importance to us. On the other hand, we add a barrier height term (*BH*) in the model to account for the extra potential drop due to the potential barrier near the source side, and we express the modified expression as:

$$V(x) = 0.5[V_{ds} + BH(V_{gs}, V_{ds})]\left(\frac{x}{0.5L'}\right)^{\frac{1}{a}} \quad (5)$$

The definition of *L'* also changes to the length of (*Vds+BH*) potential drop. The above expression better characterizes potential behavior, as shown in fig. 2, because gate-voltage dependence is taken into account, and the barrier-lowering effect is also automatically included in the *BH* term.

Then we extract parameters (*BH* and *L'*) from the simulation results and calculate *a* to examine the validity of (5).

An example of the fitting result is shown in Fig.2. The final results are listed in table 1.
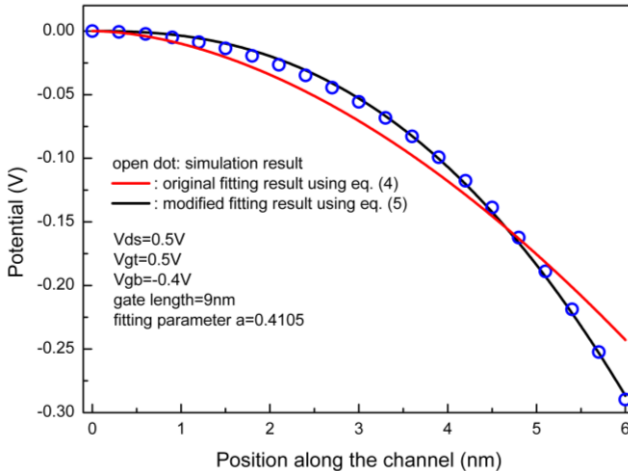

Fig. 2. An example of fitting using (5).

It can be observed that the extracted *a* from simulation is significantly smaller than what the 1D quasi-ballistic model predicts. *a* also varies greatly under different gate length. On the other hand, contrary to the original quasi-ballistic model, we observed that scattering conditions have a negligible impact

on *a* thus we can view *a* as scattering independent. This phenomenon is reasonable as has been mentioned that scattering has little effect on the potential profile. On the other hand, the difference between 1D quasi-ballistic theory and our 2D simulation results may be attributed to the complex 2D electrostatics, consistent with findings in [8], [10].

To compare our simulation results with quasi-ballistic model, the following method is adopted to extract meaningful parameters regarding to quasi-ballistic transport:

1. MOSFETs with identical structure and bias profile are simulated under ballistic and non-ballistic conditions respectively. Then the back-scattering coefficient *r* is extracted from the original flux ratio definition (2).

2. Potential profile along the channel is simulated by solving 2D Poisson's equation and Schrödinger equation self-consistently. The critical length l_{kT} is then extracted from the simulated potential profile.

3. The mean free path λ is finally calculated using (1).
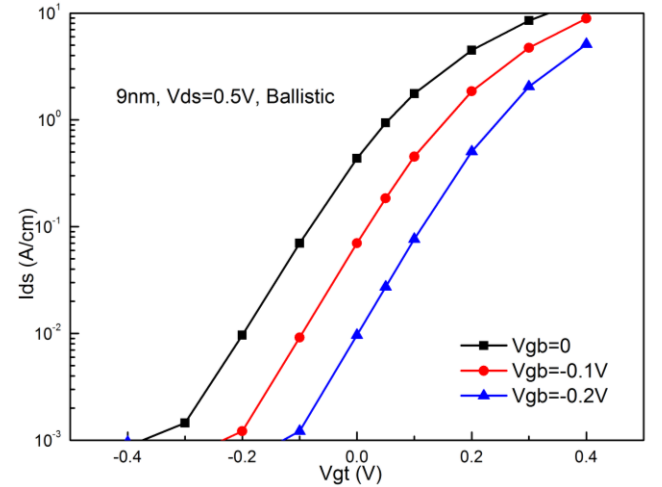
III. RESULT AND DISCUSSION

Fig. 3. Simulated I_{ds}-V_{gt} curve under different V_{gb}.
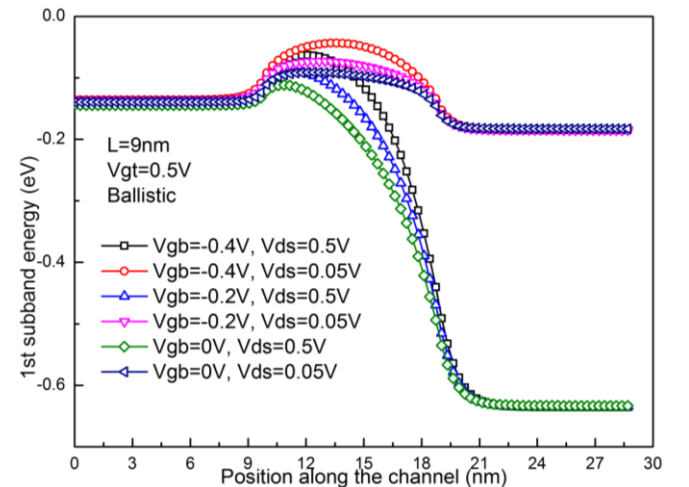

Fig. 4. Simulated potential profile along the channel under differ back-gate voltage.

Fig.3 shows the simulated I_{ds}-V_{gt} curve under different V_{gb}. It is shown that the back-gate voltage can modulate I_{ds} by tuning

the threshold voltage of the top gate. Fig.4 better illustrates this by showing the fact that the barrier height near the source side can be effectively modulated by the back-gate voltage. According to ballistic theory [5], in purely ballistic channel, carrier concentration and average carrier velocity at the top of barrier are determined by the barrier height, regardless of other external voltages such as gate voltage and source-drain voltage. This prediction is confirmed by our simulation shown in Fig.5, which in turn validated our simulation method.
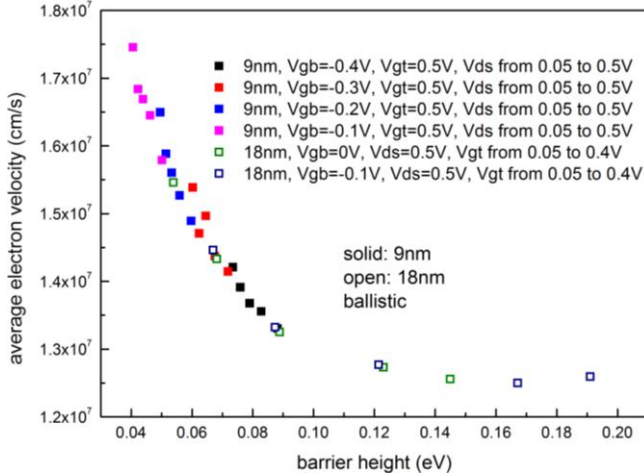

Fig. 5. Average electron velocity at the top of barrier as a function of barrier height.

Scattering modulates both carrier concentration and average velocity at the top of barrier, thus degrading source to drain current. However, under quasi-ballistic model, it is assumed that scattering has little effect on carrier distribution profile even though self-consistent potential profile may change under different scattering conditions. We examine this assumption by showing carrier density vs barrier height in Fig.6. It is confirmed that scattering has negligible effect on carrier concentration, so velocity degradation is the dominant cause for current reduction.
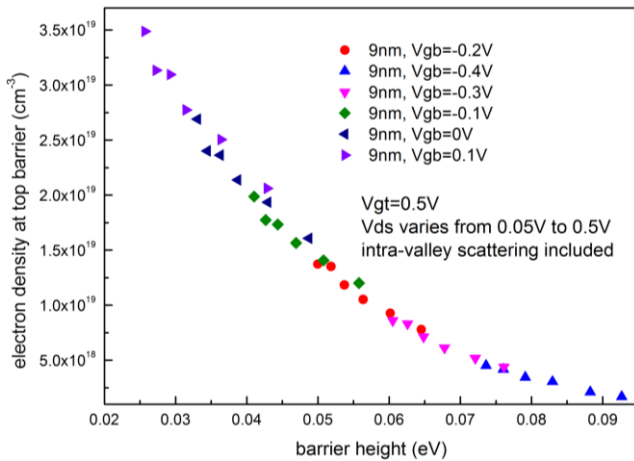

Fig. 6. Carrier density vs barrier height showing that scattering has little effect on electron density distribution.

Equation (1) is a simple expression that relates the back-scattering coefficient r to the critical layer length l_{kT} and low-field mean free path λ. However, the validity of this relation has attracted much attention [8], [22]. We address this

problem by adopting (1) to our simulation results and see whether (1) can correctly describe the back-scattering behavior on the top of barrier in our simulation.

To better elucidate the problem, we simulated cases under different scattering conditions with identical structures and bias. This is done by switching on and off different scattering mechanisms in our simulation program. Using the extraction method mentioned above (l_{kT} is directly extracted from the simulated potential profile), the relation between back-scattering coefficient r and voltage bias is shown in Fig.7. It is clear that r is voltage-dependent, which, according to quasi-ballistic theory, is due to different l_{kT} under different bias conditions.
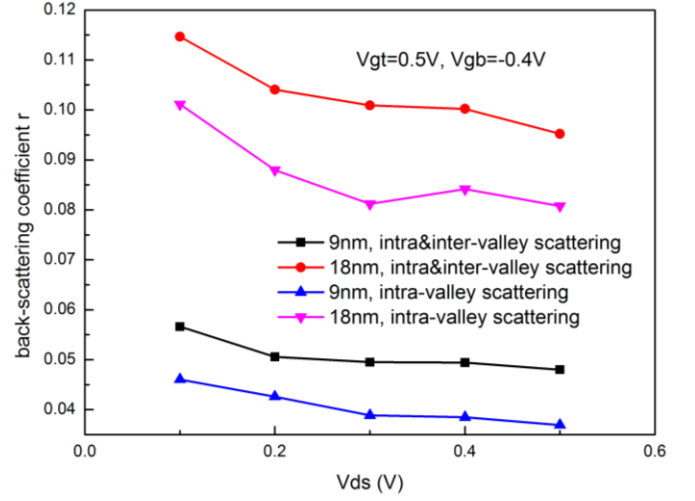

Fig. 7. Back-scattering coefficient r under different gate length and scattering conditions.

However, to quantitatively justify (1), we rewrite (1) as

$$\frac{1}{r} = 1 + \lambda \left(\frac{1}{l_{kT}} \right) \qquad (6)$$

Both mean free path λ and low-field mobility μ characterize the severity of scattering in the channel, and the possible relation between λ and μ has been discussed in [24], [7], [25] but a more rigorous investigation is still needed. In the original quasi-ballistic theory, λ is assumed to be bias and structure independent. If this assumption is true, then $1/r$ and $1/l_{kT}$ should exhibit an exact linear dependence under identical scattering conditions. We examine this assumption by plotting in Fig.8 the $1/r$ vs l_{kT} relation.
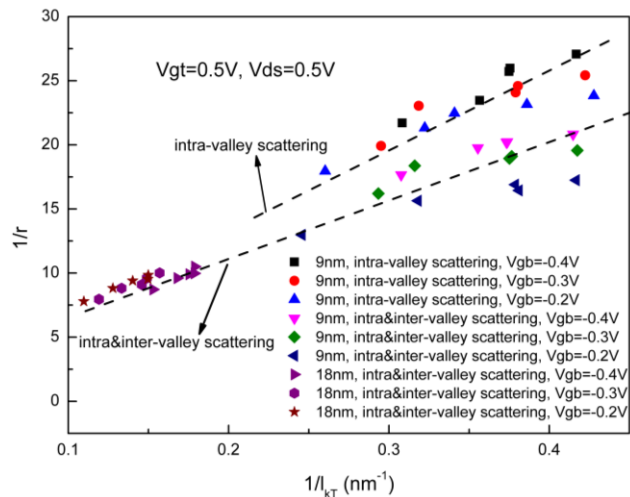
Fig. 8. *1/r* dependence on *1/l_{kT}*, dashed lines indicate the observed linear dependence.

As expected, a linear relation between $1/r$ and $1/l_{kT}$ can be roughly observed so (6) (thus (1)) holds well for devices with relatively long channel (18nm channel length in our case). However, the $1/r$ vs l_{kT} behavior deviates from the ideal linear dependence in short-channel devices and becomes bias-dependent. This leads to the conclusion that the low-field mean free path λ is no longer valid to describe r in short-channel devices, instead, a field-dependent mean free path should be used if we assume that (1) is still valid for very short channel devices. A more detailed observation shows that for 9nm channel length devices, $1/r$ is smaller under V_{gb}=-0.2V than under V_{gb}=-0.4V. This observation is consistent with the conclusion that λ is field-dependent and we may attribute this behavior to the 2D charge distribution difference under different back-gate voltage: scattering is less severe under a back-gate voltage that is more negatively biased.

IV. CONCLUSION

A deterministic simulation of DG MOSFET with different top-gate and back-gate bias is done in this work, and quasi-ballistic theory is adopted to explain the simulation results. The major conclusions are:

1. According to quasi-ballistic theory [5], [7], [12], [21], back-scattering coefficient r can be extracted using either flux ratio method or velocity ratio method. However in our simulation, r extracted from these two different methods are inconsistent with each other, indicating that two basic approximations regarding charge density and velocity in the original theory may no longer be valid in 2D condition.

2. We propose a modification to the original modeling of potential profile [12] to better describe the potential profile along the channel. It is also found that under 2D condition, the fitting parameter a deviates from 1D condition, and the difference is illustrated in the text.

3. The general back-scattering coefficient dependence on l_{kT} and λ is consistent with our simulation result, while a field-dependent mean free path λ is needed to replace the constant low-field mean free path to yield a more precise r.

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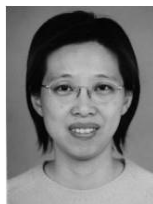
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