Simulation of Electron Transport in Si Nano Devices

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It is well recognized that simply scaled Si MOSFETs do not exhibit any performance improvement in deca-nanometer regimes [1]. Nevertheless, the origin of the performance degradation is still unclear and attributed to additional scattering due to impurities and/or the surface-roughness, or parasitic resistance [2]. Very recently, it was pointed out from 2D Monte Carlo (MC) studies that the trend of device performance degradation is remarkably similar to that due to the Coulomb interaction [3-4]. We have recently developed a 3D MC device simulator including the full Coulomb interaction as accurately as possible (Fig.1). As a result, our MC simulator is capable to simultaneously simulate both the correct mobility up to the electron density of 10^{20} cm^{-3} and the collective excitations (plasma waves) for the first time (Fig.2).

Figure 3 features the main results of the present study where the velocity and kinetic energy distributions at the points close to the source and drain contacts (x = 4 and 96 nm) and along the channel in double-gate MOSFETs are shown. Two vertical lines (Right Figure) show the source/channel and channel/drain junctions. There are several features to be noted: 1) Two electron streams in the channel represent quasi-ballistic transport associated with two different effective masses. 2) The velocity and energy distributions coincide at the locations close to the source and drain edges. This implies that quasi-equilibrium is achieved at the contacts and the distribution function is consistent with the boundary condition imposed. 3) The velocity distribution is much broader that than that of 300 K and the degeneracy of electron gas in high-doped source/drain is properly simulated. 4) The effective electron temperature (~ 800K) is even higher than the Fermi energy (~ 60 meV) in source/drain and the potential fluctuations indeed affect the kinetic energy distribution. 5) The velocity distribution near the virtual source in the channel greatly deviates from the thermal-equilibrium. This implies that the “scattering model” associated with the *kT*-layer [5] should be taken with great caution. Figure 4 shows the gate length dependence of transconductance. We find that the device performance degradation is observed around Lg=20 nm due to the long-range part of the Coulomb interaction, consistently with previous 2D MC simulations [3-4]. Since the surface roughness scattering is intentionally eliminated in the present MC simulations, this degradation might represent the intrinsic scaling limit and indicate that the ballistic limit could not be attainable by “simple scaling”. This is also consistent with the previous theoretical prediction based on the boundary layer considerations [6].

In summary, we have shown by our newly developed 3D MC simulations that the Coulomb interaction is indeed a key ingredient to achieve correct simulations in nano-scale devices for the reliable prediction of device properties.

References:

[1] A.Khakifirooz and D.A.Antoniadis, IEEE TED-55, 1391 (2008). [2] A.Cros et al., IEDM Tech.Dig., 663 (2006). [3] M.V.Fischetti *et al.*, Proc.IWCE (2009). [4] M.V.Fischetti and S.E.Laux, J.Appl.Phys., 89, 1205 (2001). [5] M.Lundstrom, IEEE EDL-22, 293 (2001). [6] N.Sano, Phys.Rev.Lett., 93 246803 (2004).

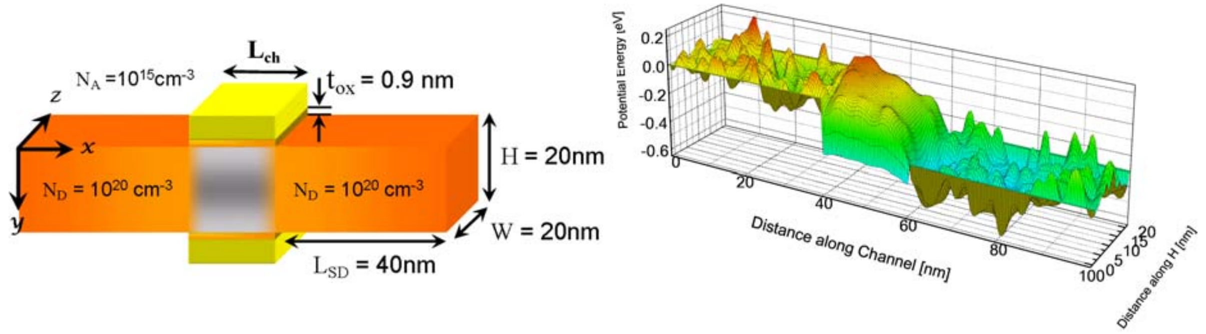

Fig.1. (Left) Schematic picture of double-gate MOSFET structure incorporated into the MC simulations. The gate length is varied from 50 nm down to 5 nm, and we employ the cross-sectional area of 20 x 20 and 10 x 10 nm2 so that the quantum confinement effect is insignificant. **(Right)** Typical output from the MC calculations representing the potential profile in the plane parallel to the gate (L_g=20 nm). The magnitude of potential fluctuations in the source and drain is about 200 meV which is comparable to the energy of plasmon for the electron density of 10^{20} cm^{-3}.

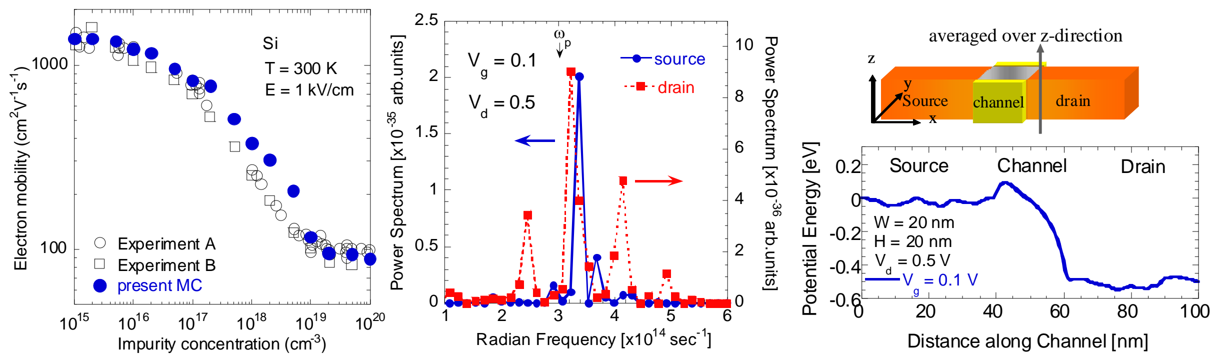

Fig.2. (Left) Impurity density dependence of electron mobility in Si. The present MC could simulate the correct mobility up to 10^{20} cm^{-3}. **(Center)** Power spectrum of potential fluctuations in the source and drain regions under device operation. A clear peak structure (especially in the source) is observed at the plasma frequency. **(Right)** Spatially averaged potential profile along the channel direction. The potential is nearly flat in the source and drain, which implies that quasi-equilibrium is achieved in the MC simulations, consistently with the boundary condition imposed at the source and drain ends.

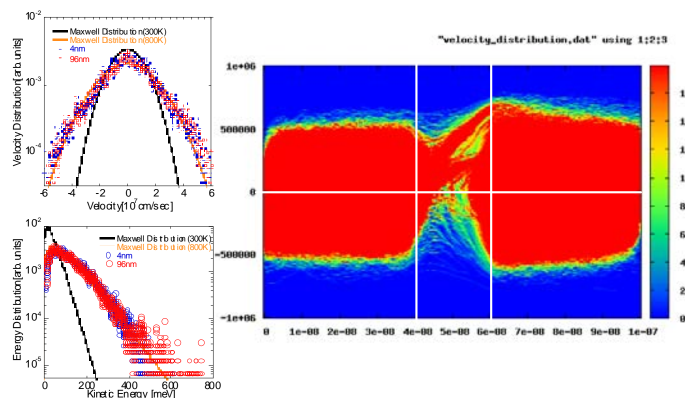

Fig.3. (Left) Velocity and kinetic energy distributions at the location close to the source and drain contacts (x=4 and 96nm). **(Right)** Velocity distribution along the channel. Two vertical (white) lines show the source/channel and channel/drain junctions. Two electron streams in the channel show quasi-ballistic transport associated with the two different effective masses.

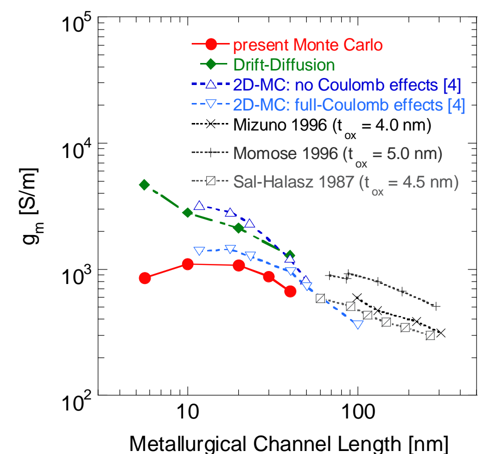

Fig.4. Transconductance as a function of gate length obtained from the present 3D MC (solid circles) and the previous 2D MC [4] (empty triangles) simulations. The experimental results are taken from literature.