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# Quantum Simulation of Nanoscale Metal/Insulator Tunnel Transistors

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As the feature sizes of the conventional metal-oxide-semiconductor field effect transistor continue to shrink into the nanometer regime, physical and technological problems such as short-channel effects and dopant fluctuations are emerging. As a solution to the problem, a non-silicon-based metal/insulator tunnel transistor (MITT), where an insulator used as the channel material is sandwiched between metal source and drain electrodes (Fig. 1), has been proposed.[1,2] Since the transport mainly occurs by tunneling through the tunnel barriers that are formed at the metal/insulator interfaces, the short-channel effects can be entirely eliminated. Also, the non-semiconductor system offers several advantages in fabrication processes.

Previous studies on MITT have been done with some approximations to the full quantum solution. In this work, ballistic and diffusive quantum transport in the nano-scale tunnel transistor were calculated using the nonequilibrium Green's function (NEGF) method. The drain current is obtained by using the Landauer-Büttiker formula:

$$I(V) = \frac{2e}{h} \int T(E,V)\,[f_l(E) - f_r(E)]\,dE, \qquad (1)$$

where $f_l(E)$ and $f_r(E)$ are the distribution functions in the source and drain electrodes, respectively. Within the NEGF formalism, the transmission coefficient $T(E,V)$ is written as

$$T(E,V) = Tr[\Gamma_l G \Gamma_r G_d^\dagger], \qquad (2)$$

where $G = [E - H - \Sigma_l - \Sigma_r]^{-1}$, $\Gamma_{l,r} = i(\Sigma_l, r - \Sigma_l, r^\dagger)$, and $H$ is the Hamiltonian for the device region and $\Sigma_{l,r}$ are self-energies for the source($l$) and drain($r$) electrodes.

The Laplace's equation

$$\nabla^2 \phi = 0 \qquad (3)$$

was numerically solved to obtain the potential profile in the channel and oxide regions, while the Poisson's equation with classical charge densities were solved in the substrate region.

We have employed both the coupled-mode space approach and the uncoupled-mode space approach to solve the Green's function numerically and calculate the current. The influence of diffusive scattering on ballistic current has been considered by so called the "Buttiker probe model" where the overall degree of the scattering effects can be adjusted by a parameter which is physically linked to the channel mobility.[3] The overall simulation procedure is shown in Fig. 2.

We have investigated the device characteristics of MITT by varying the device parameters such as the channel length, channel mobility, gate oxide dielectric constant and tunnel barrier height. Firstly, we have found that the channel length can be reduced to down to about 10 nm without loss in on-current, but below about 10 nm, the increase in the tunneling component of the current makes the off-current behavior quite poor, as shown in Fig. 3. Secondly, the device characteristics are improved if the ratio of the gate-insulator dielectric constant $\epsilon_g$ to the channel-insulator dielectric constant $\epsilon_t$ is increased: for $\epsilon_g/\epsilon_t = 3$, the on-off current ratio is improved by a factor of 10 compared with the case of $\epsilon_g/\epsilon_t = 1/3$. See Fig. 4. Thirdly, as the tunnel barrier height becomes higher, on-current becomes almost exponentially small but off-current behavior improves, which leads us to conclude that the optimal barrier height should to be 0.3 $\sim$ 0.5 eV. Fourthly, we have considered the diffusive scattering by using the simple Buttiker probe model and assessed its effect on the ballistic results (Fig. 5). It can be seen in the figure that for the channel mobility $\mu = 100\text{cm}^2/\text{V}\cdot\text{s}$ (which corresponds to the electrons' mean free path of $\sim$ 10 nm), the current is reduced by about 30%. Lastly, negative differential resistance due to resonant tunneling can be observed in the MITT if a double-barrier like potential profile is formed within the channel. Fig. 6 show that the peak location shifts as the gate voltage is varied, opening up the possibility that MITT can be used as a resonant tunneling transistor.

In summary, we have performed ballistic and diffusive quantum simulation of the nanoscale metal/insulator tunnel transistor, and analyzed its device characteristics.

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[3] R. Venugopal, M. Paulsson, S. Goasguen, S. Datta, and M. S. Lundstrom, J. of Appl. Phys. Vol. 93 (2003), pp. 5613-5625

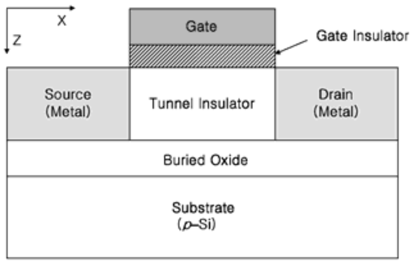


FIG. 1. Simulated Device.

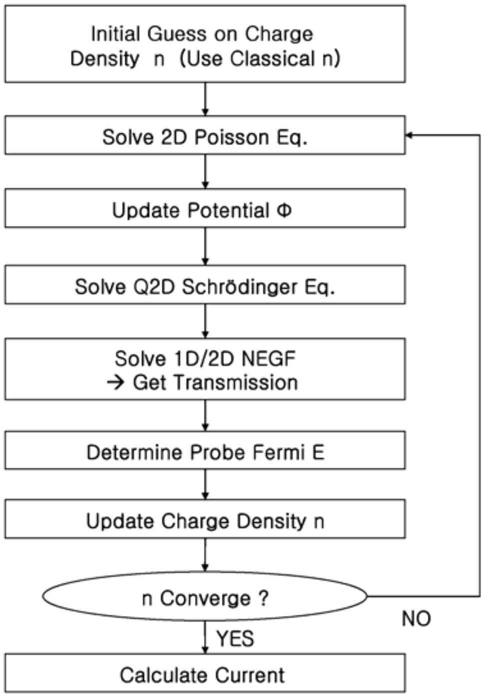


FIG. 2. Flowchart.

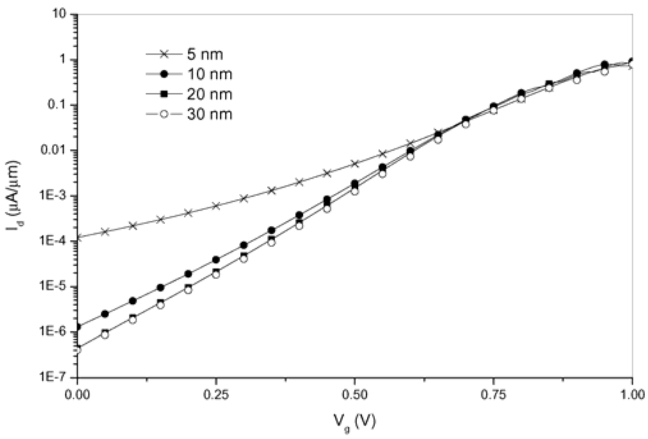


FIG. 3. $I_d$ versus $V_g$ characteristics at $V_d$ = 0.5 V for different channel lengths. The channel depth is 5nm, the barrier height is 0.5 eV, and calculations were done at room temperature (same for subsequent graphs).

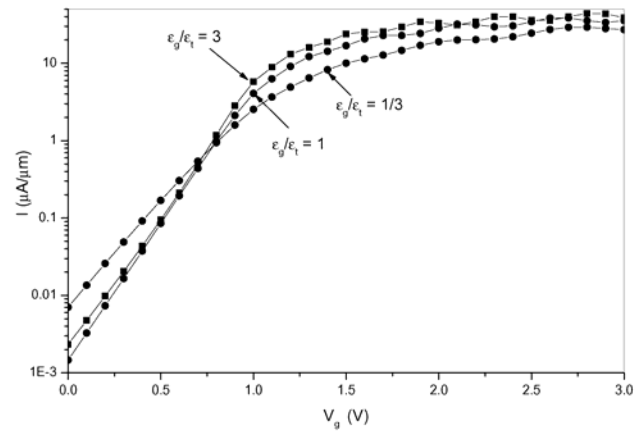


FIG. 4. $I_d$ versus $V_g$ characteristics at $V_d = 0.5$ V and $L =$ 10 nm for different values of the ratio of $\epsilon_g/\epsilon_t$.

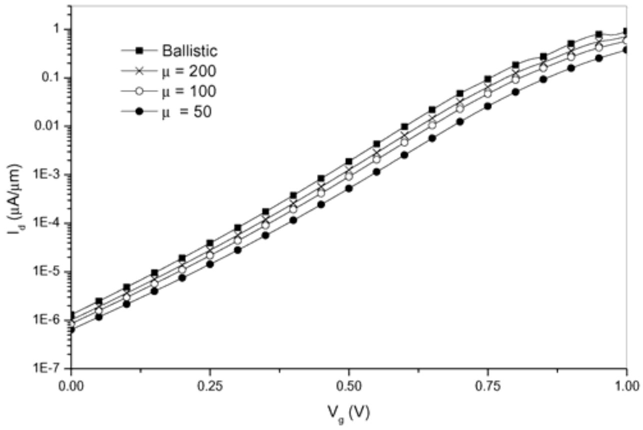


FIG. 5. $I_d$ versus $V_g$ characteristics at $V_d = 0.5$ V and $L = 10$ nm for different values of mobility $\mu$. The unit of $\mu$ is $\mathrm{cm}^2/\mathrm{V}\cdot\mathrm{s}$.

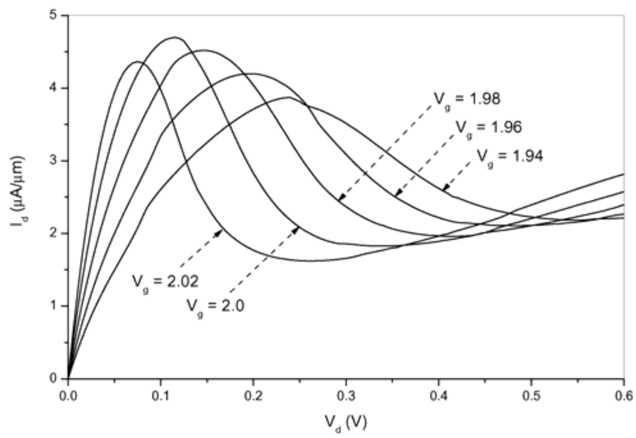


FIG. 6. The negative differential resistance behavior of MITT at room temperature. $L = 10$ nm and $\mu = 100$ $\mathrm{cm}^2/\mathrm{V}\cdot\mathrm{s}$ .