## Simulation of AC Responses Using Non-Equilibrium Green's Function at Finite Frequencies

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The theory of AC quantum transport has been well established during the last decades. However, there are only a few papers where the AC quantum transport theory is applied to electronic devices [1-3]. Therefore, it is timely to investigate the AC characteristics of a threedimensional nanosheet MOSFET with the AC NEGF method.

A nanosheet MOSFET with a rounded corner is used for the simulation as shown in Fig. 1. The corner radius is assumed to be 2.5 nm. The silicon channel is undoped and the gate length is 10 nm. The source and drain regions are doped with a donor concentration of  $10^{20}$  cm<sup>-3</sup>. The channel direction is [100] and (001) surface is considered. The wavefunction vanishes completely at the silicon-oxide interface. Contacts are considered as semi-infinite leads and the workfunction of the gate contact is 4.3eV. Ballistic transport and effective mass approach are also assumed to simplify the simulation.

In this work, the AC NEGF simulation using the decoupled mode-space approach [4] is tried. To consider the effect of Coulomb interaction, the AC NEGF and Poisson equations are solved self-consistency. The DC and AC NEGF simulation capability has been implemented into our in-house simulator, G-Device. DC NEGF results are shown in Fig.2.

Some of the key equations in the AC NEGF simulation are introduced in Tab. 1 [1-2]. Firstly, the simulation under the zero-frequency limit ( $\omega \rightarrow 0$ ) is implemented. The results are shown in Figs. 3 and 4. The results of transconductance and output resistance from the AC NEGF simulation are consistent with DC NEGF results. The AC electron density under a gate excitation agree well with the DC results by a finite difference. The AC electron density results at finite frequencies with different bias conditions are shown in Fig. 5. As the frequency increases, the electron density along the channel fluctuates.

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$$G_{AC}^{r}(E) = G_{DC}^{r}(E + \hbar\omega)[V_{AC}(\omega) + \Sigma_{AC}^{r}(E + \hbar\omega, E)]G_{DC}^{r}(E), \quad G_{AC}^{a}(E) = G_{DC}^{a}(E + \hbar\omega)[V_{AC}(\omega) + \Sigma_{AC}^{a}(E + \hbar\omega, E)]G_{DC}^{a}(E)$$
(1)

$$\Sigma_{AC}^{\gamma}(E+\hbar\omega,E) = \frac{qv_{ac}}{\hbar\omega} \left[ \Sigma_{DC}^{\gamma}(E+\hbar\omega) - \Sigma_{DC}^{\gamma}(E) \right] \quad (\gamma = r, a, <)$$
<sup>(2)</sup>

$$G_{AC}^{<}(E) = G_{DC}^{r}(E + \hbar\omega)\Sigma_{AC}^{<}(E + \hbar\omega, E)G_{DC}^{r}(E)^{\dagger} + G_{AC}^{r}(E)\Sigma_{DC}^{<}(E)G_{DC}^{r}(E)^{\dagger} + G_{DC}^{r}(E + \hbar\omega)\Sigma_{DC}^{<}(E + \hbar\omega)G_{AC}^{a}(E)$$
(3)

Table.1 AC NEGF equations.





Fig. 1: Nanosheet MOSFET used in this work. The right subfigure shows the cross-section along the channel.

Fig.2: I-V curves of the DC NEGF. The tunneling current curve when gate voltage is 0.5V is shown in the right subfigure.



Fig.3: Transconductance and output resistance curves. Blue solid lines are calculated from the DC NEGF with a small excitation. Symbols are from the AC NEGF results under the zero-frequency limit.



Fig.4: AC electron density according to a gate excitation under the zero-frequency limit. The left subfigure shows the AC electron density at equilibrium. The right one shows a non-equilibrium condition:  $V_{GS} = 0.1V$ ,  $V_{DS} = 0.2V$ .



Fig.5: AC electron density according to a drain excitation at a non-zero frequency ( $0.2 \text{ THz} \sim 16 \text{ THz}$ ). Real and imaginary parts are represented separately. Two subfigures on the left show results at equilibrium. Other subfigures on the right show results for a non-equilibrium condition.