Multiscale Modeling and Simulation of Nano-electronic Devices

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Current challenges in modeling nano devices

Design, manufacture, and operation of electronic devices, such as metal oxide semiconductor field effect transistors (MOSFETs), have been down-scaled to nano scales, due to continuous demand in rising the performance. At nano scales, major challenges of modeling and simulations of these devices include (i) Quantum effects such as electron connement, sourcedrain off state quantum tunneling current, channel barrier tunneling, many body correlations and channelchannel interference, etc; (ii) Geometric interface effects to the device performance; (iii) randomly distributed individual dopants effects.

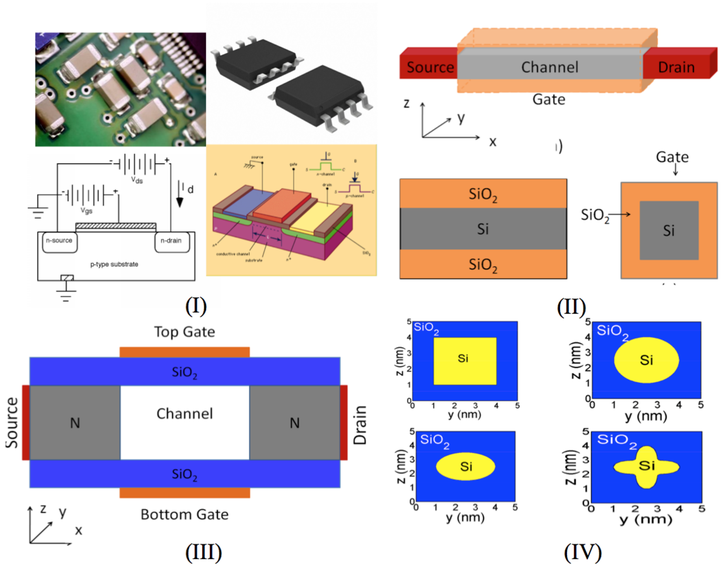

Figure 1: (I) Examples of nano-devices; (II) diagrams of a Four-gate MOSFET; (III) diagram of a DG-MOSFET; (IV) examples of possible material interfaces.

In this project, we proposed a framework model and developed mathematical tools to handle these challenges. Figure 1 displays examples of nano-devices and diagrams of the models we studied: a four-gate MOSFET and a double-gate MOSFET (DG-MOSFET).

Model: framework of total free energy functional

The mathematical model is setup based on a total free energy functional, including dynamics of electrons and system electrostatics:

$$\begin{aligned} G_\Gamma[u,n] = \int \Bigg\{ & \sum_j \frac{\hbar^2 f(E_j-\mu)}{2m(\mathbf{r})}|\nabla\Psi_j(\mathbf{r})|^2 + U_{\text{elec}}[n] + E_{\text{XC}}[n] \\ & + u(\mathbf{r})n_d(\mathbf{r})q + u(\mathbf{r})q\sum_i^{N_a} Z_i\delta(\mathbf{r}-\mathbf{r}_i) - \frac{\epsilon(\mathbf{r})}{2}|\nabla u|^2 \\ & + \lambda\left[n_0 - \sum_j f(E_j-\mu)|\Psi_j(\mathbf{r})|^2\right]\Bigg\} d\mathbf{r}. \end{aligned} \tag{1}$$

which consists of kinetic and potential energies of electrons, and system electrostatic energies on an equal footing. Variables $u(\mathbf{r})$, $n(\mathbf{r})$ are the electrostatics and electron number density, respectively. This model incorporates material interface (Γ), randomly distributed individual dopants ($\delta(\mathbf{r}-\mathbf{r}_i)$) and quantum dynamical electron structures.

Acknowledgement

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Coupled governing equations

A system of coupled governing equations can be derived from the energy functional:

- **Poisson Equation** gives the electrostatics $u(\mathbf{r})$:

$$\frac{\delta G_\Gamma[u,n]}{\delta u} = 0 \Rightarrow -\nabla\cdot(\epsilon(\mathbf{r})\nabla u(\mathbf{r})) = -n(\mathbf{r})q + n_d(\mathbf{r})q + q\sum_i^{N_a} Z_i\delta(\mathbf{r}-\mathbf{r}_i'), \tag{2}$$

- **Generalized Kohn-Sham equation** for wavefunctions $\Psi_j(\mathbf{r})$ of electrons.

$$\frac{\delta G_\Gamma[u,n]}{\delta \Psi^\dagger} = 0 \Rightarrow \left(-\nabla\cdot\frac{\hbar^2}{2m}\nabla + V(\mathbf{r})\right)\Psi_j(\mathbf{r}) = E_j\Psi_j(\mathbf{r}), \tag{3}$$

- **The Self-consistent system:** Equations (2) and (3) are coupled together by relations:

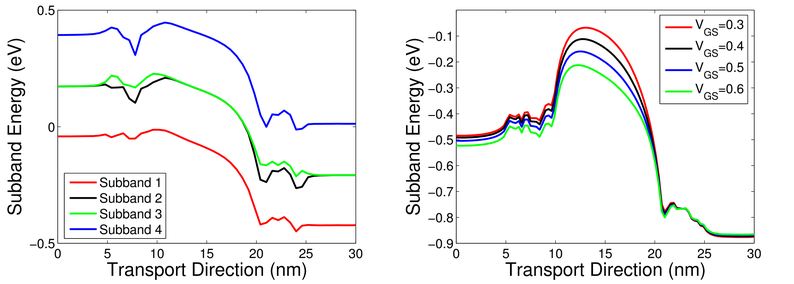
$$n(\mathbf{r}) =< \mathbf{r}|f(H-\mu|\mathbf{r}>= \sum_j |\Psi_j(\mathbf{r})|^2 f(E_j-\mu) \tag{4}$$

$$V(\mathbf{r}) = u(\mathbf{r})(-q) + U_{\text{XC}}[n(\mathbf{r})] + U_{\text{phon}}[n(\mathbf{r})] \tag{5}$$

Highly accurate and effective mathematical algorithms, such as Matched interface and boundary method (MIB), Dirichlet-to-Neumann mapping, or Gummel iteration, are utilzied to handle numerical difficulties of the system.

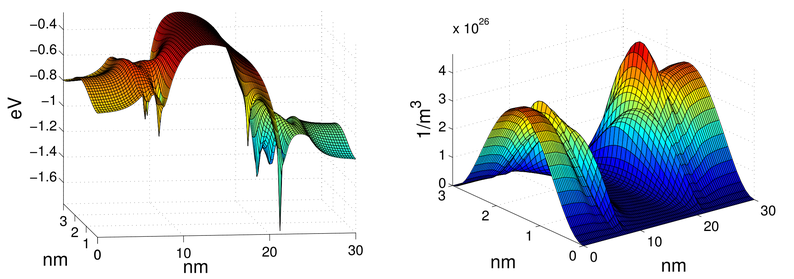
Physical profile of nano-MOSFET

The following figures give basic physical profiles of a four-gate nano-MOSFET with randomly distributed individual dopants, in terms of subband transport energies, system electrostatics and electron density.



(a) Quantized or subband transport energy (b) subband energy under different gate voltages

Figure 2: Subband energies



(a) Potential energy (b) electron density

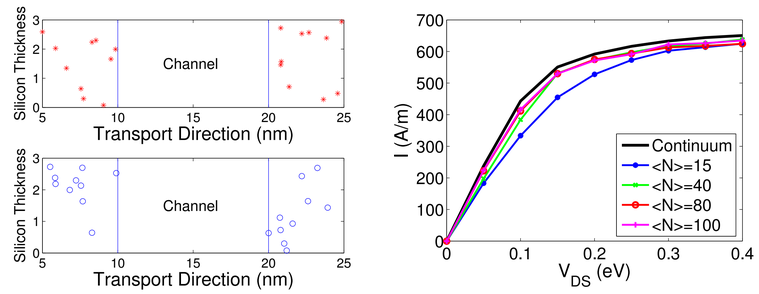
Figure 3: Potential energy and electron density

Conclusion

This work presents mathematical models and computational algorithms for the simulation of nano-scale MOSFETs. A unied two-scale energy functional is introduced to describe the electrons and the continuum electrostatic potential of the nano-electronic device. Quantum dynamics of electron transport, material interface effect and randomly distributed discrete dopants are considered in the model. The current uctuation and voltage threshold lowering effect induced by the discrete dopant model are explored for two types of nano-MOSFET.

Simulation Results

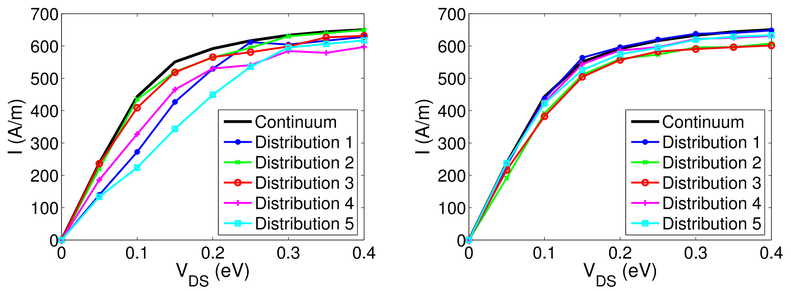
Simulations are carried out for a DG-MOSFET and a four gate-MOSFET, current-voltage (IV) curves are recorded under different source-drain voltages, gate voltages, different numbers and distributions of random dopants.



(a) Random discrete dopants (b) Effect of discrete dopants

Figure 4: Microscopic dopants distributions make macroscopically identical MOSFET different

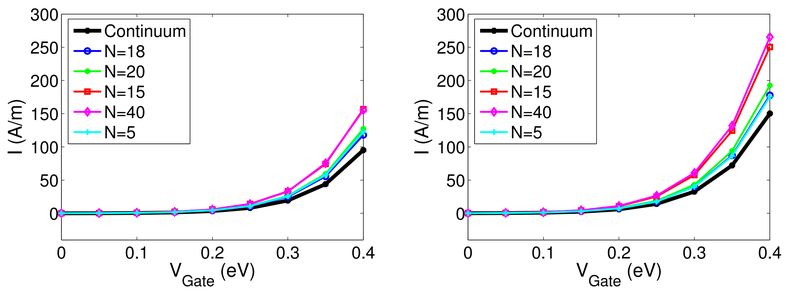
Macroscopically, the individual dopants introduce the uctuation in on-state currents. The above figure displays a configuration of DG-MOSFET with random individual dopants (left), and the averaged current fluctuation effects of different number of individual dopants, comparing to continuum dopant.



(a) 15 individual dopants (b) 80 individual dopants

Figure 5: IV curves of nano-MOSFET with individual and continuum dopants

The above figure shows the IV curves of a four-gate MOSFET with different distributions of same number of individual dopants. Left: 15 dopants, right: 80 dopants.



(a) low source-drain voltage (b) high source-drain voltage

Figure 6: Discrete dopants induced voltage threshold lowering effects

Another interesting aspect of the individual dopants is the lowering effect of the device voltage threshold, this is presented in the above figure.

References

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