PCCP

Cite this: *Phys. Chem. Chem. Phys.*, 2011, **13**, 14365–14369

www.rsc.org/pccp

PAPER

Multiscale quantum mechanics/electromagnetics simulation for electronic devices

ChiYung Yam,[a] Lingyi Meng,[a] GuanHua Chen,*[a] Quan Chen[b] and Ngai Wong*[b]

Received 15th March 2011, Accepted 13th May 2011
DOI: 10.1039/c1cp20766k

The continuous downsizing of modern electronic devices implies the increasing importance of quantum phenomena. As the feature sizes of transistors inch towards 10 nanometer, simulations including quantum effects and atomistic details are inevitable. Here we report a novel hybrid quantum mechanics and electromagnetics (QM/EM) method to model individual electronic components at the nanoscale. QM and EM models are solved in different regions of the system in a self-consistent manner. As a demostration, we study a carbon nanotube based electronic device embedded in a silicon block. Good agreement is obtained between simulation by QM/EM method and full QM treatment of the entire system.

1 Introduction

Developments in the semiconductor industry alter the way we communicate, entertain, transport and work. The need for more and more computing power fosters the continuous miniaturization of semiconductor microelectronics which crams proportional amounts of transistors in the same silicon space. According to the Moore's Law, the number of transistors that can be placed inexpensively on an integrated circuit has doubled approximately every two years. While the trend has continued since the transistor was first integrated into a silicon chip about half a century ago, further miniaturization faces physical limits in conventional semiconductor technology. As the feature sizes of the transistors are trending smaller and smaller to 10 nm, the quantum effects and atomistic details play an important role which cannot be neglected. This implies the current operation principles, structures and designs may no longer work. Moreover, fabrication and measurement of nanoscale electronic devices are extremely expensive and time consuming.

Modeling has been playing a vital role in the evolvement of today's semiconductor industry.[1,2] Its importance grows with the increasing complexity of integrated circuit designs. Compact models are indispensable tools for both circuit design and simulation. Being an integrated component of Electronic Design Automation (EDA) tools, compact models can be constructed through physics interpretation, model reduction techniques, or curve fitting to the experimental data. Among the physical models, the majority are based on classical continuum model which was generally successful because of the macroscopic lattice structure and large electron wavelength. Description of electronic transport in nanoscopic devices, however, requires quantum mechanical model including full atomistic details. Continuum model such as effective mass approximation (EMA) breaks down and electronic structure has to be taken into account explicitly. Moreover, many of the effective parameters used in EMA are not known for this length scale. Thus, conventional compact models are no longer appropriate for circuit design at 10 nm scale.

In recent years, nonequilibrium Green's function (NEGF) technique[3] enjoys popularity in the context of quantum transport. Combining with density functional theory (DFT), research on electronic transport through semiconductor device or individual molecules has revealed various interesting quantum phenomena which is not accessible through classical models. Whereas the industrial applications of molecular electronics stay out of reach in the moment, feature size of transistors is entering the quantum regime in few years' time. Simulation models beyond classical continuum models is highly desirable to provide a correct physical description. This paper presents a novel multiscale quantum mechanics and electromagnetics (QM/EM) method without sacrificing physics like other classical continuum models. In analogy with the hybrid quantum mechanics/molecular mechanics (QM/MM)[4] approach which is widely used to study the chemical processes in biological systems in the field of computational chemistry, QM/EM method combines the accuracy of QM and efficiency of EM method. While QM method provides accurate treatment of the system, simulations on entire transistor which take the full atomistic structure into account are numerically demanding. In QM/EM method, the entire system is partitioned into QM and EM regions. To increase efficiency, we adopt the density functional tight binding (DFTB) method,[5,6]

[a] *Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong. E-mail: ghc@everest.hku.hk*
[b] *Department of Electrical and Electronic Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong. E-mail: nwong@eee.hku.hk*

an approximated DFT method. The combined NEGF + DFTB[7] method is applied to simulate the active device region where the electron scattering process takes place, the remaining including interconnects and substrate are modeled using Maxwell's equation together with semi-classical drift-diffusion equation, and simulated *via* computational EM solvers.[8–12] QM and EM calculations are linked by means of boundary condition between the two regions and are solved iteratively until self-consistency is achieved.

The present paper is organized as follows. In Section 2, we briefly review the DFTB method and its NEGF extension for quantum transport. The coupled electromagnetics semiconductor method is also presented. The section ends with the description of the multiscale QM/EM approach to electronic device simulations. Simulations on a carbon nanotube based electronic device embedded in a silicon block is given in Section 3 followed by a brief summary in Section 4.

2 Methodology

2.1 DFTB method

As an approximate DFT method, DFTB method[5,6] constructs a non-orthogonal tight-binding (TB)-like representation of the single-particle wavefunctions. The total energy is given by,

$$E_{\text{tot}} = \sum_{i=1}^{\text{occ}} \langle \psi_i | \hat{H}_0 | \psi_i \rangle + E_{\text{XC}}[n_0] - \int V_{\text{XC}}[n_0, \vec{r}] n_0(\vec{r}) d\vec{r} - \frac{1}{2} \int \int \frac{n_0(\vec{r}) n_0(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r} d\vec{r}' + \frac{1}{2} \int \int \left[\frac{1}{|\vec{r} - \vec{r}'|} + \frac{\delta^2 E_{\text{XC}}}{\delta n(\vec{r}) \delta n(\vec{r}')} \Big|_{n=n_0} \right] \delta n(\vec{r}) \delta n(\vec{r}') d\vec{r} d\vec{r}' \quad (1)$$

where $\hat{H}_0$ is the Hamiltonian of the reference system, n_0 and δn are the reference electron density and the change of electron density, respectively. $\hat{H}_0$ matrix is calculated based on a two-center approximation and the matrix elements are tabulated together with the overlap matrix elements with respect to the interatomic distance. The second to fourth terms in the right hand side (RHS) of eqn (1) depend only on the n_0 and constitute the repulsive energy. The last term in eqn (1) is approximated by the interaction between the Mülliken charges Δq_a on each atom,

$$E_{\text{2nd}} = \frac{1}{2} \sum_{a,b} \gamma_{ab} \Delta q_a \Delta q_b \quad (2)$$

where γ_{ab} are parameters giving a measure of electron-electron interaction and decay reciprocally with the distance between atoms a and b. The Fock matrix in DFTB can be obtained through the derivative of the total energy with respect to the density matrix as

$$H_{\mu\nu} = \langle \phi_\mu | \hat{H}_0 | \phi_\nu \rangle + \frac{1}{2} S_{\mu\nu} \sum_c (\gamma_{ac} + \gamma_{bc}) \Delta q_c, \quad \forall \mu \in a, \nu \in b, \quad (3)$$

where $S_{\mu\nu}$ is the overlap matrix, ϕ_μ and ϕ_ν are the basis functions. The second term in eqn (3) accounts for contributions from the changes of electron density with respect to n_0 and needs to be determined self-consistently.

2.2 NEGF extension for open systems

For a semi-infinite system under study as shown in Fig. 1, the total energy is not well-defined, variational principle thus no longer holds for such systems. The DFTB method has to be generalized to treat open systems out of equilibrium. The Hamiltonian takes the general form,

$$H_{\mu\nu} = \langle \phi_\mu | \hat{H}_0 | \phi_\nu \rangle + \delta V_{\mu\nu}[\Delta q_a] \quad (4)$$

where the second term accounts for the Hartree and exchange–correlation potential due to the change of electron density. For an electronic device shown in Fig. 1, the electrostatic potential in the left and right leads is set by the applied voltage, and potential in the device region is computed from the Poisson equation,

$$\nabla^2 \delta V(\mathbf{r}) = 4\pi \delta n(\mathbf{r}) \quad (5)$$

under these boundary conditions. For isolated systems, the electrostatic potential tends to zero at infinity and the contribution to the Fock matrix reduces to the second term in RHS of eqn (3). The density matrix[13] is computed as,

$$\sigma_{\mu\nu} = -\frac{i}{2\pi} \int G^<_{\mu\nu}(E) dE \quad (6)$$

where $G^<$ is the electron-electron correlation matrix which gives the spectral density of occupied states, represented on the atomic basis. It is expressed as,

$$G^<(E) = G^r(E) \Sigma^<(E) G^a(E)$$
$$G^{a\dagger}(E) = G^r(E) = [ES - H + \Sigma^r(E)]^{-1} \quad (7)$$

where G^r,G^a are the retarded, advanced Green's functions, respectively. $\Sigma^<$,Σ^r are the lesser and retarded self-energies, respectively. Eqn (5) and (6) are solved self-consistently and the current flowing through the electronic device can be evaluated *via* the Landauer formula,[14,15]

$$I(V) = \frac{2e^2}{h} \int_{-\infty}^{\infty} T(E, V)[f^L(E) - f^R(E)] dE \quad (8)$$

where f is the Fermi function, and $T(E,V)$ is the transmission coefficient at energy E under bias voltage V. The transmission coefficient is related to Green's functions by

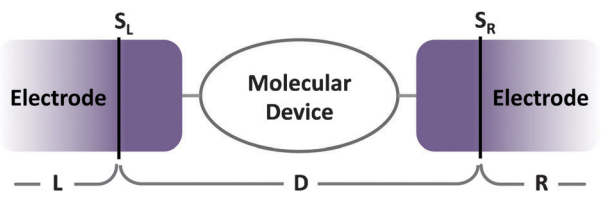

Fig. 1 Schematic diagram of an electronic device. L and R are semi-infinite leads connected to an external bias. D denotes the active device region. S_L (S_R) represents the interface between D and L(R).

$$T(E,V) = \mathrm{Tr}[\Gamma_L(E)G^r(E,V)\Gamma_R(E)G^a(E,V)] \quad (9)$$

where $\Gamma(E)$ is the coupling at energy E between the device and the leads. The approach discussed in this subsection follows ref. 7, which implemented NEGF approach for the DFTB method. Recently, DFTB method for quantum transport in time domain has also been developed.[16]

2.3 Coupled electromagnetics semiconductor method

The electromagnetic environment and wave propagation in a given device are governed by the Maxwell's equations or its subset. To model electromagnetic wave interacting with physical structures, the EM solvers exploit the fundamental Maxwell's equation to describe the EM field in the media.[8] The Maxwell's equation is give by,

$$\nabla \cdot \vec{E} = \frac{\rho}{\varepsilon}$$

$$\nabla \cdot \vec{B} = 0$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\nabla \times \vec{B} = \mu_0 \vec{J} + \mu_0 \varepsilon \frac{\partial \vec{E}}{\partial t} \quad (10)$$

where $\vec{E}$, $\vec{B}$, ρ and $\vec{J}$ denote the electric field, magnetic field, charge density and current density, respectively. μ_0 and ε are permeability and permittivity of the medium, respectively. In our simulations, the contribution from magnetic field is neglected and thus only the Gauss' law for electricity is solved.

Depending on the media under consideration, the current density $\vec{J}$ relates to electric field and carrier density in different ways.[11,12] For metal or conductor, the current density is determined by the Ohm's Law,

$$\vec{J} = \sigma \vec{E} \quad (11)$$

together with the current continuity equation,

$$\nabla \cdot \vec{J} + \frac{\partial \rho}{\partial t} = 0 \quad (12)$$

In a dielectric, there are no free charges and therefore, no current continuity equations need to be solved in the dielectric materials. The Maxwell's equation is coupled with the drift-diffusion equation to calculate the current and charge distribution in semiconductor materials. The current densities of electron (n) and hole (p) are split into the drift and diffusion terms,[9]

$$\vec{J}_x = q\mu_x x\vec{E} + kT\mu_x \nabla x,\ x \in \{n,p\} \quad (13)$$

and satisfy the current continuity equation,

$$\nabla \cdot \vec{J}_x \mp q\frac{\partial x}{\partial t} = \pm U(x),\ x \in \{n,p\} \quad (14)$$

where U is the generation/recombination of charge carriers and μ_x is the carrier mobility. And the charge density is given by,

$$\rho = q(p - n + N_D - N_A) \quad (15)$$

where N_D and N_A are the donor and acceptor concentrations due to the doping, respectively.

2.4 Multiscale QM/EM method

The methods described in the preceding subsections are combined to study transport phenomena in nanoscale electronic devices. The QM/EM method combines the strengths of both QM (accuracy) and EM (efficiency) methods. As shown in Fig. 2, the system of interest is partitioned into an active scattering region which is described quantum mechanically and the rest includes interconnects and semiconductor matrices where a classical description is sufficiently accurate. In our approach, the QM region is simulated using the combined DFTB + NEGF method described in Sections 2.1 and 2.2, while the outer EM region is simulated using the semi-classical drift-diffusion model described in Section 2.3. Similar to the QM/MM method, the two models communicate through the interface between the two regions. In the QM/EM method, the system is discretized into regular Cartesian grids. The boundary conditions for Poisson equation are applied on the boundary of the outer EM region. Specifically, Dirichlet boundary condition is applied to the metal region while Neumann boundary condition is applied to remaining part of the boundary. Poisson equation coupled with drift-diffustion equation is solved first on the whole system to obtain the potential on every grid points. The grids in the QM region is then divided into finer grids and inherit the potential of their parent grids. In DFTB + NEGF calculations, the Fock and density matrices are obtained self-consistently by solving eqn (4)–(7) and eqn (5) (Poisson equation) is solved on the finer set of grids with potential at the QM/EM interface acting as the boundary condition. The current flowing through the interface is computed using eqn (8). In addition to the boundary conditions on the outer EM region, the obtained current is used as a boundary condition at the QM/EM interface for the next EM calculation. The current is computed again for the new values of the electric potential as boundary condition. The whole process is iterated until the convergence of current and potential at the interface is reached.

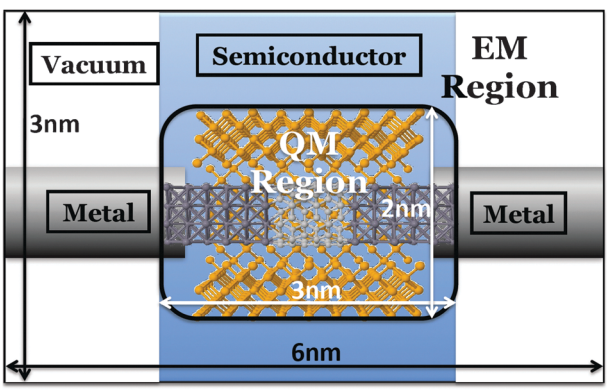

Fig. 2 Schematic diagram to illustrate the multiscale QM/EM approach. Region enclosed in the central box is simulated by quantum mechanical transport model with full atomistic details while the outer EM region is simulated using the coupled EM semiconductor method.

3 Results and discussions

The method described above has been applied to a carbon nanotube (CNT) based electronic device[17] embedded in a silicon block. Fig. 3 shows the atomistic details of the electronic device included in the QM region which is simulated using the combined DFTB + NEGF method. The electrodes are given by aluminum (Al) nanowires of finite cross sections oriented in (100) direction. Both ends of the CNT are connected to the Al electrodes with a preset separation of 1.5 Å. We include explicitly in the simulation box 48 Al atoms of the left electrode and 48 Al atoms of the right electrode along with 60 C atoms of the CNT. The electronic device is then embedded in a silicon block with a dimension of 3 × 2 × 2 nm. The dynamic response of the CNT molecular device had been studied elsewhere.[18] The surroundings are included in the EM region with a dimension of 6 × 3 × 3 nm which is solved by the coupled EM semiconductor method. The QM region is surrounded by silicon with a dielectric constant of 11.9[19] and connected to two Al nanowire of length 1.5 nm with conductivity equal to 3.3 S/m.[19] The remaining is vacuum space (see Fig. 1).

Fig. 4 depicts the *I–V* curves of the system in linear response regime. For comparison, we perform a full QM simulation for the same system containing more than 1200 atoms using DFTB + NEGF method. The covered bias voltage ranges from 0 to 5 mV. It is shown that the *I–V* curve simulated by QM/EM method reproduces precisely that of the full QM simulation which justifies our multiscale QM/EM approach. Despite its accuracy, QM/EM method provides a more efficient way for electronics simulations. We report also the CPU time for the simulations presented. The calculations were carried out on a single core of an Intel Xeon E5620@2.40 GHz multicore processor. For the full QM simulations, one self-consistent iteration in DFTB + NEGF method took roughly 77 CPU minutes while in the QM/EM simulations, one self-consistent iteration took 15 CPU minutes and the EM solver took about 10 CPU minutes. QM/EM method is overall much more efficient, moreover, the EM region of the system can easily be scaled up with minor computational efforts. This provides an efficient means for electronic device simulations in nanoscale.

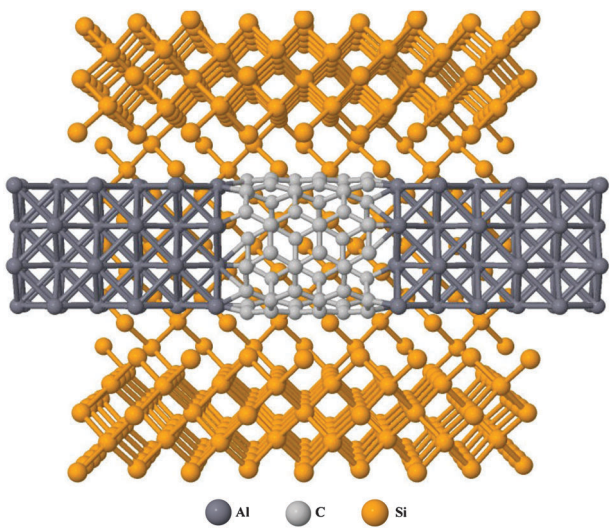

Fig. 3 Atomistic details of the electronic device in QM region where electron scattering process takes place. The electronic device contains a (5,5) carbon nanotube connected to aluminum leads.

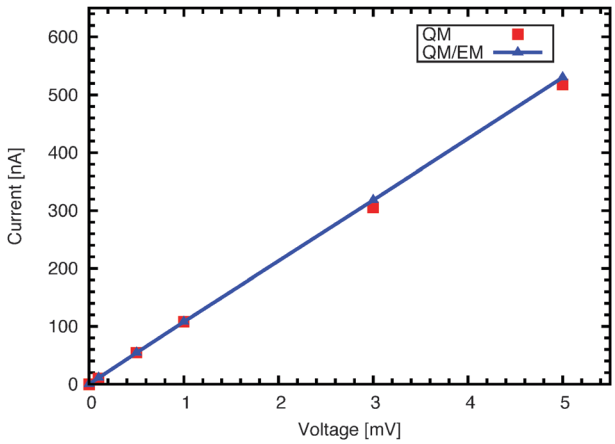

Fig. 4 Comparison of the full QM and QM/EM simulations of *I–V* curves of a CNT based molecular device.

EDA tools are routinely used to design new electronic integrated circuits and devices. Individual electronic devices are simulated and characterized by the compact models. The QM/EM method allows a multiscale approach to the simulation of electronic devices. Individual electronic components in the integrated circuit under different operating conditions can be simulated and the resulting *I–V* curves can be utilized to construct the compact models, and the outputs of the compact model are coupled to circuit simulators (for instance, SPICE[20,21]) to simulate the electric signal propagation through the integrated circuit. The QM/EM method thus provides an efficient alternative for the construction of compact models in current EDA tools. Moreover, this multiscale QM/EM approach applies not only to the field of electronics, but also to areas like photonics. Whereas the current work presents electronic device simulations in steady state, the QM/EM method can be easily generalized for frequency domain and time domain simulations.[22–24] This makes possible the real time simulations of electromagnetic wave propagation in various electronic and photonic devices.

4 Summary

To summarize, we have shown a multiscale QM/EM approach for electronic device simulation. The method includes both macroscopic drift-diffusion current model and quantum tunneling model which are solved together in a self-consistent fashion. Through application to a CNT based molecular device, the method is shown to be both efficient and accurate.

Acknowledgements

We thank the Hong Kong University Grant Council (AoE/P-04/08), Hong Kong Research Grant Council (HKU700909P, HKUST9/CRF/08, HKU700808P and HKU701307P) and The University of Hong Kong (UDF on Fast Algorithm,

Seed Funding Programme for Basic Research 2010-11159085 and 201010159001) for the support.

References

1 L. Lavagno, G. Martin and L. Scheffer, *Electronic Design Automation for Integrated Circuits Handbook*, CRC Press, 1st edn, 2006.
2 M. Auf der Maur, M. Povolotskyi, F. Sacconi, A. Pecchia and A. Di Carlo, *J. Comput. Electron.*, 2007, **7**, 398–402.
3 L. P. Kadanoff and G. Baym, *Quantum statistical mechanics: Green's function methods in equilibrium and nonequilibrium problems*, Addison-Wesley, 1989.
4 A. Warshel and M. Levitt, *J. Mol. Biol.*, 1976, **103**, 227–249.
5 D. Porezag, T. Frauenheim, T. Köhler, G. Seifert and R. Kaschner, *Phys. Rev. B: Condens. Matter*, 1995, **51**, 12947–12957.
6 M. Elstner, D. Porezag, G. Jungnickel, J. Elsner, M. Haugk, T. Frauenheim, S. Suhai and G. Seifert, *Phys. Rev. B: Condens. Matter*, 1998, **58**, 7260–7268.
7 A. Pecchia, G. Penazzi, L. Salvucci and A. di Carlo, *New J. Phys.*, 2008, **10**, 065022.
8 D. J. Griggiths, *Introduction to Electrodynamics*, Addison Wesley, 3rd edn, 1999.
9 D. Vasileska, S. M. Goodnick and G. Klimeck, *Computational Electronics*, Morgan and Claypool, 1st edn, 2006.
10 W. C. Chew, M. S. Tong and B. Hu, *Integral Equations Methods for Electromagnetic and Elastic Waves*, Morgan and Claypool, 1st edn, 2007.
11 P. Meuris, W. Schoenmaker and W. Magnus, *IEEE Trans. Comput.-Aided Des. Integr. Circuits Syst.*, 2001, **20**, 753–762.
12 W. Schoenmaker and P. Meuris, *IEEE Trans. Comput.-Aided Des. Integr. Circuits Syst.*, 2002, **21**, 534–543.
13 G. H. Chen and S. Mukamel, *J. Chem. Phys.*, 1995, **103**, 9355–9362.
14 R. Landauer, *IBM J. Res. Dev.*, 1957, **1**, 233.
15 M. Büttiker, *Phys. Rev. Lett.*, 1986, **57**, 1761–1764.
16 (*a*) Y. Wang, C. Y. Yam, G. H. Chen, T. Frauenheim and T. A. Niehaus, arXiv:1101.5929v1, 2011; (*b*) X. Zheng, F. Wang, C. Y. Yam, Y. Mo and G. Chen, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 2007, **75**, 195127; (*c*) X. Zheng, G. Chen, Y. Mo, S. Koo, H. Tian, C. Yam and Y. Yan, *J. Chem. Phys.*, 2010, **133**, 114101.
17 X. Zheng, G. H. Chen, Z. B. Li, S. Z. Deng and N. S. Xu, *Phys. Rev. Lett.*, 2004, **92**, 106803.
18 C. Y. Yam, Y. Mo, F. Wang, X. Li, G. H. Chen, X. Zheng, Y. Matsuda, J. Tahir-Kheli and A. G. William III, *Nanotechnology*, 2008, **19**, 495203.
19 W. M. Haynes, *CRC Handbook of Chemistry and Physics*, CRC Press, 91st edn, 2010.
20 L. W. Nagel and D. O. Pederson, *SPICE (Simulation Program with Integrated Circuit Emphasis)*, University of California, Berkeley Memorandum No. ERL-M382, 1973.
21 L. W. Nagel, *SPICE2: A Computer Program to Simulate Semiconductor Circuits*, University of California, Berkeley Memorandum No. ERL-M520, 1975.
22 (*a*) L. Y. Meng, C. Y. Yam, G. H. Chen, Q. Chen and N. Wong, *to be submitted*, 2011; (*b*) C. Y. Yam, S. Yokojima and G. H. Chen, *Phys. Rev. B: Condens.Matter*, 2003, **68**, 153105; (*c*) W. Z. Liang, S. Yokojima, D. H. Zhou and G. H. Chen, *J. Phys. Rev. A*, 2000, **104**, 2445–2453.
23 M. Sukharev and M. Galperin, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 2010, **81**, 165307.
24 K. Lopata and D. Neuhauser, *J. Chem. Phys.*, 2009, **130**, 104707.