Quantum Mechanical Simulations of Nano-Structures and Nano-Devices

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Abstract-We have investigated the quantum mechanical effects in quantum dots and nano size silicon MOSFETs using empirical pseudopotential Hamiltonian model and linear combination of bulk band (LCBB) method. Unlike the traditional effective mass approximation and kp method, our approach uses a full zone expansion to represent the electronic state. This method provides a very fast yet accurate way to simulate million atom nano structures and nano devices even on a single processor personal computer.

I. INTRODUCTION

Traditional standard approaches to simulate the nano-structures are the effective-mass envelope-function approximation (EMA) and its multiband kp generalization, where the wave function of the nano-structures is expanded in terms of zone-center (k=0) Bloch bands of the underlying periodic solid. In the past 10 years, these two methods were also used to simulate the nanometer MOSFETs incorporated with transport models such as Non-Equilibrium Green's Function (NEGF). However, as pointed by [1], these methods fail to describe the whole band structure of the constituent materials, inter-valley coupling, as well as the atomistic features and strain effects in the nano-structures and devices, which could be important to the real physical properties. One failure example has been shown by Esseni and Palestri et al. [2], that the kp method can significantly misrepresent the electron density of states (DOS) for a silicon inversion layer, and the indirect band gap nature of bulk silicon presents real challenges for this model.

On the contrary, the LCBB method [1][2][3] is an successful alternative for the theoretical simulation of nano-structures and nano-devices. By expanding the wave function in terms of full-zone Bloch states of the constituent bulk solids, LCBB represents the multi-band and multi-valley effects as well as the atomistic nature of the nano-structures and nano-devices in a very efficient way. And the calculation error is well controlled in bellow 10 meV.

II. LCBB METHOD

LCBB method is based on empirical pseudo- potential Hamiltonian model (EPM), where 4-5 EPM parameters are fitted to reproduce the bulk experimental measurements of the band structure. The fitted EPM is then used to calculate the heterostructures of constituent materials. In LCBB framework [1], the single-particle Hamiltonian is constructed as a sum of the kinetic term, a superposition of peudopotentials for different atoms, a confinement energy term which represents barriers for buffer layers of the system, and the external potential term that can be calculated from Poisson Equation. Then the single particle electronic wave function is expanded as a linear combination of full-zone bulk Bloch states. All relevant k points are included in the expansion. Detailed description of the LCBB method can be found in Ref.[1].

III. SIMULATION RESULTS

A. *Quantum Dots*

Using LCBB method, we have investigated the ground exciton energy pressure coefficients (PC) of self-assembled InAs/GaAs quantum dots by calculating 21 systems with different quantum dot shape, size, and alloying profile [4]. Consistent with the experiment, we find the PC is in the range of 60-110 meV/GPa, much smaller than the bulk InAs and GaAs PCs. The calculated PCs as a function of QD zero-pressure exciton energy is plotted in Fig. 1 with the experimental measurements. We believe that it is necessary to consider the penetration of the electron state into the GaAs barrier in order to understand the PC reductions and their large variations.

We have also studied the electronic structure of colloidal quantum dot [5], by comparing the conduction band state results from different calculation methods. We found that a colloidal quantum dot can be considered as a heterostructure system composed of the inside semiconductor material and the outside vacuum.

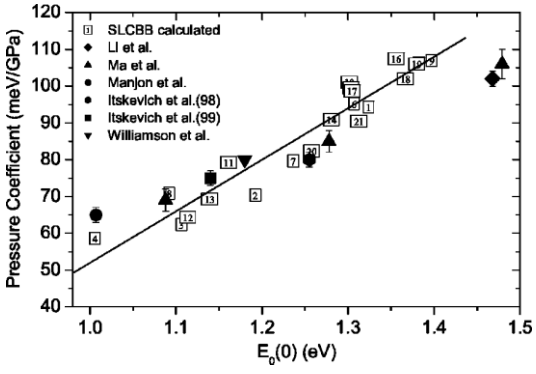

Fig. 1. The PL pressure coefficient vs PL energy

B. *Nanometer Silicon MOSFETs*

The ultimate downscaling of the MOSFET size today requires an accurate yet fast way to simulate the device

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performance before fabrication. For this motivation, we investigated the possibility of extending LCBB for device simulation [6][7][8][9][10], and we found that the same task required thousands of processors using the most widely used TB-NEGF approach can be done on a personal computer with single processor using our LCBB method without losing much accuracy. Using this quantum mechanical simulation approach based on LCBB, we have investigated the quantum mechanical effects in 25 nm MOSFET [6], including the random dopant fluctuations [8] and multi-valley coupling [7]. Based on LCBB, we have also proposed an approximated top of the barrier splitting (TBS) method to mimic the scattering states from the stationary states calculations [10].

In our simulations, we found quantum mechanical effects change the device physics in many aspects. In the simulation of 25 nm bulk MOSFET [6], we found the saturated quantum mechanical capacitance at high gate voltage is about 20% less than the classical capacitance. This is due to the fact that QM charge density is farther away from SiO2/Si interface, which is a consequence of quantum confinement effects. And the subthreshold slop is around 124 mV/dec., much larger than the theoretical limit of 60 mV/dec. This is due to the short channel effects including source to drain tunneling. In the simulation of random dopant induced fluctuation [8], we found that quantum mechanical effects increase the threshold fluctuation while decrease the threshold lowering, which is different from the results of density gradient calculations. We believe that the threshold lowering is because of the local charge density caused by the discrete dopant configuration which can be smoothed out by the quantum confinement effects, so that the quantum simulation gives a decreasing effects on threshold voltage lowering. In our investigation of multi-valley coupling [7], we found that there is very little coupling among different energy valleys and the contributions from non-X valleys are negligible. So the actual calculation can be reduced to just X valley calculation which can be further decoupled to three X valleys because the coupling among these three valleys are also negligible.

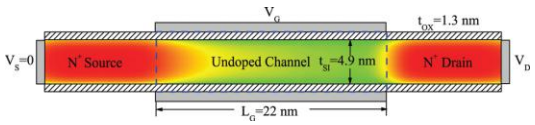

Fig.2. 22 nm DG UTB Silicon MOSFET

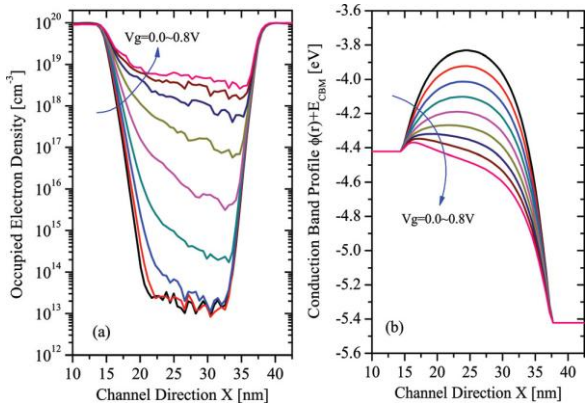

Fig.3. occupied charge density and conduction band profile along channel direction

In our method development for efficient simulation of nano-devices, we proposed a top of the barrier splitting (TBS) method to extract scattering states information from stationary states calculations using periodic boundary condition [10]. This method first calculates the electronic eigen states in a buffered periodic system. Then each calculated eigen state is decomposed into two parts, one is supposed from source side and another part is supposed from drain side. This decomposition is based on the physical insight of ballistic and tunneling transport and assumes the local density of states on top of the barrier is equally from source and drain. Then the source part is occupied by source side Fermi level while the drain part is occupied by drain side Fermi level to get the total occupied charge density and form the self-consistent calculation with Poisson Equation. We applied this approach to 22 nm double-gate (DG) ultra-thin body (UTB) silicon MOSFET (Fig.2). Fig.3 plots the occupied charge density and conduction band profile along channel direction. To verify our 3D LCBB-TBS model, we compared the simulated transfer characteristics with the tight-binding (TB) NEGF approach and found the results are very close, although the later does require hundreds to thousand processors to do the simulation. The simulated transfer characteristics is shown in Fig.4. The threshold voltages calculated from LCBB-TBS and TB-NEGF are 460 mV and 450 mV. The ON currents are 3265 uA/um and 3740 uA/um respectively. And the subthreshold slops calculated from both models are the same as 63 mV/dec.

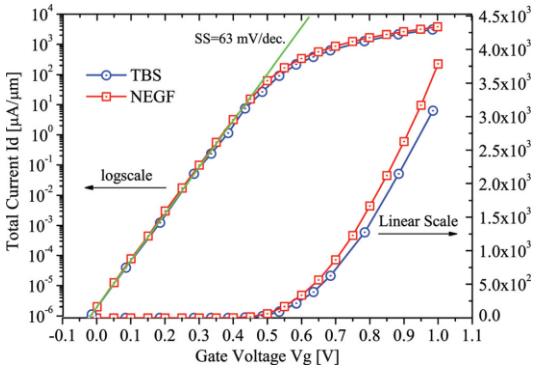

Fig.3. Simulated transfer characteristics comparing with TB NEGF method.

IV. ACKNOWLEDGMENT

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