Extended Abstracts of the 2004 International Conference on Solid State Devices and Materials, Tokyo, 2004, pp. 726-727

A-9-1 (Invited)

Nanoscale Device Simulation at the Scaling Limit and Beyond

Anisur Rahman[1], Gerhard Klimeck[1] , Nizami Vagidov[2], Timothy B. Boykin[3], Mark Lundstrom[1]

[1]School of ECE, Network for Computational Nanotechnology Purdue University, West Lafayette, IN 47907, USA
[2]Department of EE, State University of New York, Buffalo, NY 14260
[3]Department of Elec. and Comp. Engineering, University of Alabama, Huntsville, AL 35899
E-mail: rahmana@purdue.edu

1. Introduction

Metal Oxide Semiconductor Field Effect Transistors (MOSFETs) have been aggressively scaled over past three decades and according to the ITRS 2001 roadmap projection the 2016 devices are going to have channel lengths of 10nm. To ensure electrostatic control, new device geometries need to be explored such as thin semiconductor-on-insulator (SOI). For improved transport properties Ge channel devices are also considered. The design studies of such devices have revealed that in order to curb short channel effects, their body thickness should not exceed 2-3 nm [1, 2]. For such extreme thin body the underlying atomistic texture makes the use of ubiquitous effective mass (EM) approach questionable and an atomistic treatment of the device becomes essential. Here the semi-empirical tight-binding (TB) theory is applied to semiconductor thin films on (001) wafers and the subband structure as well as the effect of valley interaction are investigated.

2. Approach

The explored semiconductor thin film on (001) wafers is schematically presented in fig. 1. The crystal structure for cubic semiconductors, e.g. Si, Ge, is FCC lattice with two atoms associated with each lattice point—the lattice atom at the lattice site and the basis atom at a quarter of body diagonal away shown by black and white circles. The thin film is made by alternatively stacking these two types of atomic layers.

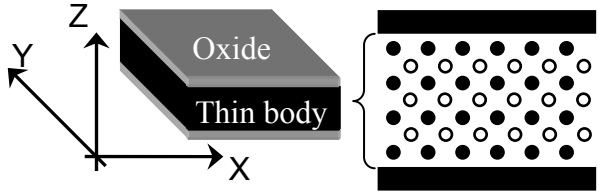

Fig. 1 The thin film on (001) wafers modeled in this work. The film is composed by alternately repeating two types of atomic layers, lattice atoms (black) and basis atoms (white).

The $sp^3d^5s^*$ tight-binding model used here has been described elsewhere [3]. Spin-orbit coupling is used in all simulations and each atomic layer contributed a 20x20 block to the block tri-diagonal thin-film Hamiltonian. This model enables the exploration of body thickness of both even and odd numbers of atomic layers. At the top and the bottom interface of the film, zero wavefunction boundary condition is applied. The dangling bonds at these surfaces are pacified according to the BC II technique described in [4]. The subbands are the stationary states, formed in this quantum well due to energy quantization along the thickness direction (Z axis). A typical TB ground state wavefunction for silicon subband is presented in fig. 2 where the atomistic nature is visible.

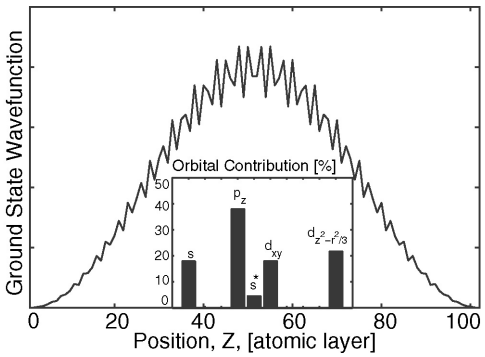

Fig. 2 Typical TB wavefunction in Si (001) films. The sum of squared orbital contribution is plotted. Inset: The individual orbital contribution. Only the orbitals shown contribute to wavefunction.

3. Results

Inside the first Brillouin zone, the Si conduction band (CB) has six ellipsoidal X valleys along Δ and Ge has eight half L valley ellipsoids along Λ. When quantum confinement is present along the [001] direction, the traveling states from these valleys combine to form subbands. In the EM formalism, each of these valleys is modeled separately, and any interaction between valleys is ignored. The difference of mass along confinement direction results in two subband ladders in Si—two-fold degenerate unprimed ladder and four-fold degenerate primed ladder. In ultra-thin Si body, the primed ladder is higher in energy—thereby not crucial for transport properties; therefore, this work will focus on the unprimed ladder and will refer to those as "the subbands". Similarly, in Ge only the fourfold degenerate L valley subbands will be considered.

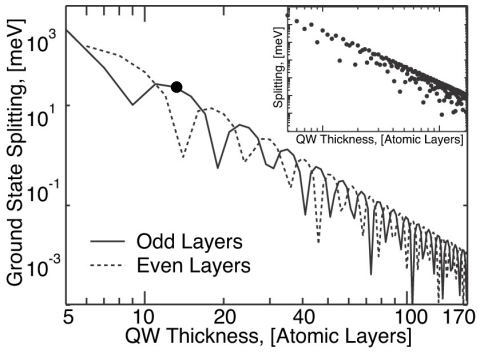

Fig. 3 The splitting vs. quantum well thickness in silicon using TB. The odd and even number of atomic layers show similar splitting profile. This is not obvious from the inset plot where the odd and even layers are not distinguished from each other.

The coupling between bulk conduction band valleys becomes important as the film thickness decreases. The interaction between valleys causes the two-fold degenerate subbands in silicon to split in energy [5], and the splitting vs. body thickness is plotted in fig. 3. It can be seen that for extremely thin body, e.g. 5 atomic layers, the splitting approaches hundreds of meV. Silicon film of such thickness has already been reported in [6]. Such splitting reduces the band edge effective mass, alters the scattering process for electrons and can result in completely different carrier transport properties for the end of ITRS roadmap devices. Our TB simulation also shows that similar interaction is present in germanium thin films and the corresponding splitting of germanium L valley subbands is plotted in fig. 4.

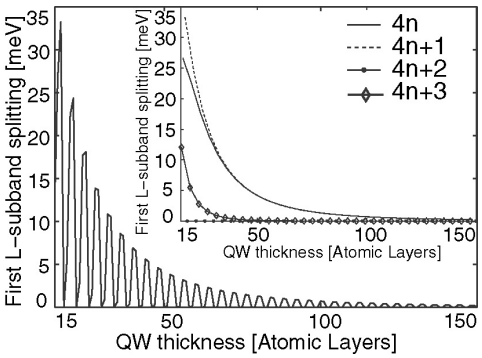

Fig. 4 The L valley subband splitting in Ge thin film shows interesting characteristics. Four different groups can be identified according to body thickness in atomic layer, $4n+i$, where n is an integer and i = 0, 1, 2 or 3 (inset). Interestingly, for i = 2 the splitting becomes practically zero.

The origin of subband splitting in Si is explained in fig. 5, which is also true for Ge L valleys [5]. Here the dispersion $E(0,0,k_z)$ has two minima at $k_z=\pm k_m$, near the respective centers of the two vertical ellipsoids, so that there are four traveling states $\pm k_1^{(n)}$, $\pm k_2^{(n)}$, at each energy E_n. When confining barriers are added, only a linear combination of all four states can satisfy the boundary conditions; for symmetric barriers the orbital coefficients of the lowest two states are sums of cosines or sums of sines, characterized by $k_1^{(n)} \approx k_m + \pi/t$ and $k_2^{(n)} \approx k_m - \pi/t$. At large t ($k_m >> \pi/t$) the lowest two states have nearly equal energies and k, while at small t the splitting becomes large as shown in fig. 3. In fact, as $t \approx \pi / k_m$ the four states in fig. 5 are nearly equally spaced along the k-axis.

In fig. 6, the two-dimensional density-of-states (2D DOS) for a 13 atomic layer (2nm) Si (001) film is shown and is compared with the EM calculation. The dashed line is for TB simulation and the associated bandstructure is shown in the inset. The lowest subband is X type and in the 2D Brillouin zone the projection of the Δ-line along [001] is at the Γ point, therefore, we observe the lowest subband at this point in the inset figure. At the band edge, the TB results shows subband splitting effects (~25meV). Due to removal of two-fold subband degeneracy, the TB DOS is 50% of what calculated from EM approach. Both the higher unprimed subbands and the primed subband ladder, formed by other four X valleys and modeled by transverse mass m_t, suffers from non-parabolicity and the first TB primed band edge (starting at about 1.52 eV) doesn't agree well with EM calculation. Fortunately, such higher subbands seldom play role in transport in ultra-thin body MOSFETs and are usually ignored.

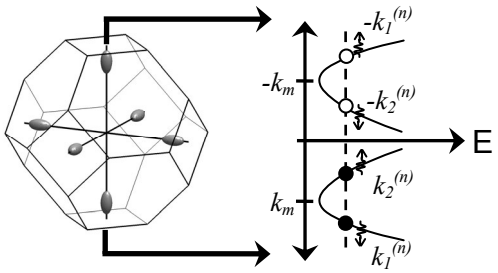

Fig. 5 The origin of subband splitting. The bulk Brillouin zone is shown left and the E-k along Δ at $k_x=k_y=0$ is shown on right. The black and white circles represent four traveling states around the two band minima which combine to form two subbands. At small body thickness these states move higher in energy and the interaction between them becomes stronger. This interaction is the origin of subband splitting [5].

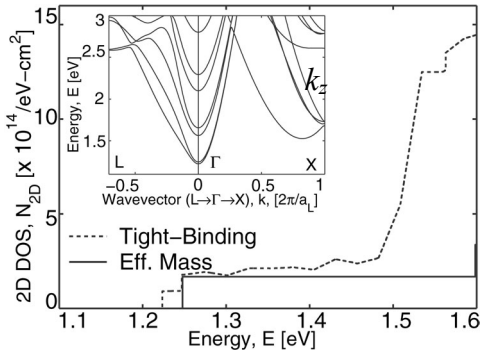

Fig. 6 DOS vs. E plot for 13 atomic layers (~2nm) silicon (001) film—tight-binding (dash) and effective mass (solid). The TB shows a DOS turn on that is split into two even steps that are due to valley splitting. The EM model can only predict the accumulative DOS. The step width corresponds to about 1 kT and will have impact of the transport properties. The first subband edges from two approaches agree well. The primed subbands suffer from non-parabolicity. The inset figure shows the E-k of conduction subbands from TB calculation.

4. Conclusion

Atomistic modeling of thin Si and Ge films is performed in this work. The $sp^3d^5s^*$-SO tight-binding simulation reveals interesting features in the ultra-thin-body MOSFETs, which otherwise is not captured by the traditional effective mass approach. Valley interaction causes subband degeneracy removed, which may have crucial effect on the transport properties of the end of the roadmap CMOS devices and beyond.

Reference:

[1] Hasan *et al,* SSE, Vol. 48, No. 6, pp. 867-875, June 2004.
[2] Rahman *et al.*, IEDM Technical Digest. Dec. 2003.
[3] Boykin *et al*, PRB, Vol. 69, No. 11, 115201, 2004.
[4] Lee *et al*, PRB, Vol. 69, No. 4, 045316, 2004.
[5] Boykin *et al*, APL, Vol. 84, No.1, 115, 2004.
[6] Uchida *et al.*, IEDM Tech. Digest. Dec. 2003.

Acknowledgements

This research has been done under the SRC contract no. 1042 and NSF contract no. EEC-0228390.