

9-15-2008

Electronic structure and transport in silicon nano-structures with non-ideal bonding environments

Amritanshu Palaria

Purdue University - Main Campus

Gerhard Klimeck

Purdue University - Main Campus, gekco@purdue.edu

Alejandro Strachan

Purdue University - Main Campus

Follow this and additional works at: <http://docs.lib.purdue.edu/nanodocs>

Palaria, Amritanshu; Klimeck, Gerhard; and Strachan, Alejandro, "Electronic structure and transport in silicon nano-structures with non-ideal bonding environments" (2008). *Other Nanotechnology Publications*. Paper 140.
<http://docs.lib.purdue.edu/nanodocs/140>

This document has been made available through Purdue e-Pubs, a service of the Purdue University Libraries. Please contact epubs@purdue.edu for additional information.

Electronic structure and transport in silicon nano-structures with non-ideal bonding environments

*Amritanshu Palaria, Gerhard Klimeck, Alejandro Strachan,
Network for Computational Nanotechnology, Birck Nanotechnology Center,
Purdue University, West Lafayette, IN 47907*

Abstract

As semiconductor devices scale down, the role of surfaces and interfaces becomes increasingly important. This effort seeks to develop methods for analysis of nano-structures, including the effect of surfaces, which represent a broader family of non-ideal bonding environments in the material, and evaluate the effects of such environments on device behavior. The presented work focuses on surfaces in 1-D silicon nano-structures. While a lot of theory and computational methods, particularly the empirical $sp^3d^5s^*$ tight-binding (TB) and the non-equilibrium Green's function (NEGF) approach, already exist for predicting electronic structure and transport through nano-devices, the lack of knowledge of the modified Hamiltonian that includes the effect of changes in the bonding at surfaces and interfaces inhibit the use of such theory for a full and precise analysis of devices. Even worse, sometimes the actual atomic configuration might be unknown. Hence, we first present a viable technique to predict atomic configuration for structures where nothing or very little is known a priori and show novel low energy structures of silicon nano-tubes and their properties. We then present how the use of density functional theory (DFT) helps one construct the proper TB Hamiltonian including the effects of non-ideal bonds. We show that the bulk empirical parameters give an electronic structure that qualitatively matches well with DFT-LDA and GW results, but the band gap is lower than the GW corrected gap. We also present the electronic structure of small dimension silicon nano-wires and show how surfaces can play an important role in futuristic small dimension devices.

Introduction

Silicon has been the treasure of the semiconductor industry for four decades. Its major attractions have been its abundance in the Earth's crust and its readiness to form an insulating oxide. Miniaturization has driven device sizes to the nanometer scale and the conventional MOS transistors fail to be miniaturized at the same pace, now primarily due to heat dissipation and gate leakage issues. New materials like high-k dielectrics have been introduced to replace the well-developed SiO_2 . But silicon still remains among the cheapest materials to use for large-scale production of electronics. With this in mind, there continues to be a drive to design new nanoelectronic devices based on silicon.

Design of novel nanoelectronic devices is challenging because it requires one to take into account not only the device level quantum effects due to miniaturization, but also the changes in properties of the material itself, which can once again be explained by quantum mechanics. A very good example in this regard is provided by carbon, the group IV material just above silicon in the periodic table. Depending on its molecular structure, pure carbon can range from being a pure insulator (diamond) to semiconducting (some nanotubes) and metallic (some other carbon nanotubes, graphite). This shows how the atomic arrangement or the molecular structure determines the electronic structure of a material in general. Therefore, as the dimensions of the silicon devices get closer to atomic dimensions, the effect of any deviations from the ideal bonding environments observed in bulk silicon would have to be taken into consideration because these effects are expected to become proportionately large at such small device dimensions. This

motivates the need to carry out a full range analysis, right from the atomic arrangement in the material to transport characteristics of the full device, what could be termed ‘bottom up’ approach, to fully explore and understand the behavior of nanoscale devices.

Method and Results

We describe a multi-scale simulation approach to investigate the structure of 1-D nanoelectronic materials and their electronic properties. While the methodology described here is generally applicable, the focus of this work is on silicon. The procedure envisioned here consists of the following steps:

1. The structure of the nano-material, if unknown, is deduced from an integrative approach using molecular dynamics and density functional theory. We have applied this methodology to predict low energy silicon nano-tube structures.
2. The electronic structure is obtained using extended orthogonal $sp^3d^5s^*$ tight binding using empirical parameters for bulk silicon. We report here our results for Si (100) surfaces and compare them with the electronic structures obtained from density functional theory using local density approximation (LDA) and GW correction.
3. The Hamiltonian determined in step 2 is used in the standard non-equilibrium Green’s function (NEGF) approach to obtain transport characteristics of a nano-device.

Silicon nanotubes

In recent years, researchers have succeeded in producing small dimension (~ 1 nm) silicon nanotubes in the lab [1,2], but the atomic configuration of these tubes has remained an open question. To investigate the possible structures of these tubes, we combined the popular computational methods of molecular dynamics (MD) and density functional theory using the generalized gradient approximation (DFT-GGA) [3]. Using the reactive force field ReaxFF [4], which is accurate enough to describe chemistry, we carried out MD simulations of cyclic expansive and compressive loading of tubes with initial cross sections of pentagonally and hexagonally arranged atoms under various conditions. This annealing process results in fully relaxed hollow structures the most promising of which then refined using density functional theory. We obtained a number of low energy tubes with comparable energetics and disparate Young’s moduli, reported for the first time. These tubes were found to have a high atomic disorder and reduced symmetry. Their structures emphasized the major influence surface forces can have on very small 1-D structures and underscored the importance of non-ideal bonding at low dimensions.

Si (100) surface and electronic structure

DFT is well known to under-estimate band gaps. The GW correction provides realistic band gaps but is computationally expensive. An alternative to these *ab initio* electronic structure methods is provided by the empirical tight binding method, which can calculate electronic structure for several million atoms. However, the transferability of the $sp^3d^5s^*$ orthogonal TB parameters fitted for bulk Si [5,6] to non bulk-like bonds has to be investigated first if TB is to be used for strongly deformed nano-scale structures; since any change in the connectivity and bond angles would affect the Hamiltonian and hence

the TB parameters. The easiest test bed for this investigation is the reconstructed Si (100) surface, which is also of practical utility. Of the several possible reconstructions of the Si (100) surface, the symmetrical p(2X1)s and the asymmetrical p(2X1)a (figs. 1a and 1b respectively) are among the most likely [7,8].

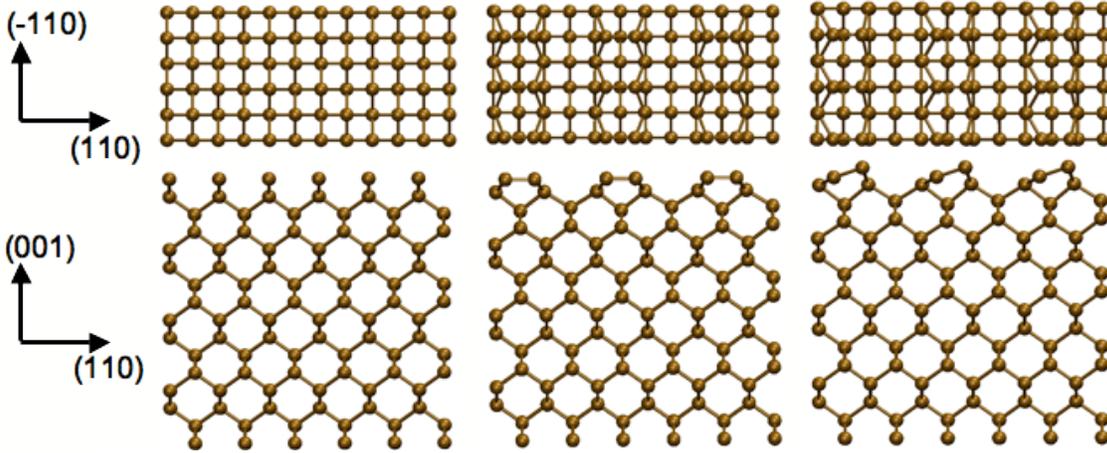


Fig 1. Silicon slab (a) ideal bulk-like (no reconstruction of free surface), (b) top surface symmetrically reconstructed p(2X1)s, and (c) top surface asymmetrically reconstructed p(2X1)a.

In fig. 2, we show the electronic structure we obtain with the use of silicon bulk-fitted $sp^3d^5s^*$ TB parameters for the slabs shown in figure 1 with p(2X1)s and p(2X1)a reconstructions respectively on the top surface. The bottom surface of both slabs is bond

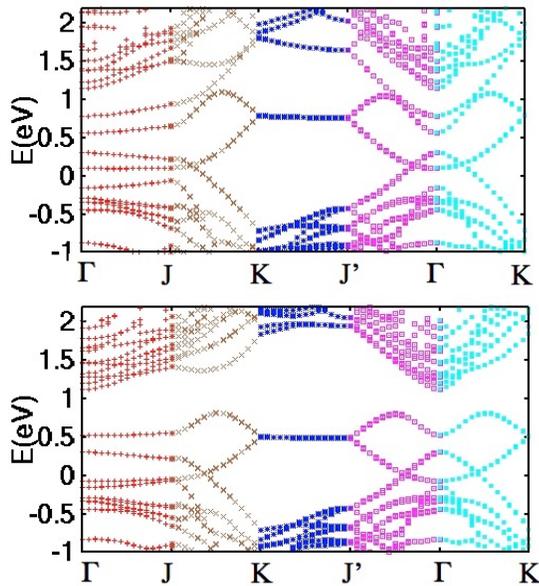


Fig 2. Electronic structure for the reconstructed Si(100) surface slabs obtained from bulk Si $sp^3d^5s^*$ parameters for orthogonal TB. The top band diagram is for p(2X1)s and the bottom one for p(2X1)a reconstruction.

passivated according to the procedure outlined in [9], such that the states due to that surface get pushed away from the gap into the bulk state region. We find that orthogonal TB with bulk parameters reproduces the well-known result that the p(2X1)s surface is metallic. For the p(2X1)a surface, we obtain a band gap of 0.304 eV from the bulk TB parameters while the GW band gap is 0.65 eV [10]. The TB band gap is still better than the LDA band gap of 0.25 eV. We also note that in both the p(2X1)s and p(2X1)a cases, the bands qualitatively match well with the LDA and GW results [8]. This tells us that the bulk TB parameters need a modification for the surface atoms quite like the GW correction for DFT, which increases the separation between the valence and conduction bands.

The presence of surface states on open surfaces will affect transport characteristics of 1-D nano structures by providing extra “stepping stones” for electrons in the band gap. For instance, in

figure 3, we consider a (110) silicon wire with the top surface asymmetrically reconstructed (100) (fig. 3a) and compare its tight-binding-based electronic structure (fig. 3b) to that of a similar wire with no reconstructions on any surface (fig. 3c). For both wires, all non-reconstructed surfaces were passivated [9]. The two dispersions look relatively similar in the valence and the conduction band, except for one additional branch in the valence band of fig. 3b. A folded band with a relatively heavy mass is showing up with a peak at $k=0.55$. Additional simulations are under way to examine the nature of this additional dispersion branch and to possibly relate it to surface states as seen in fig. 2.

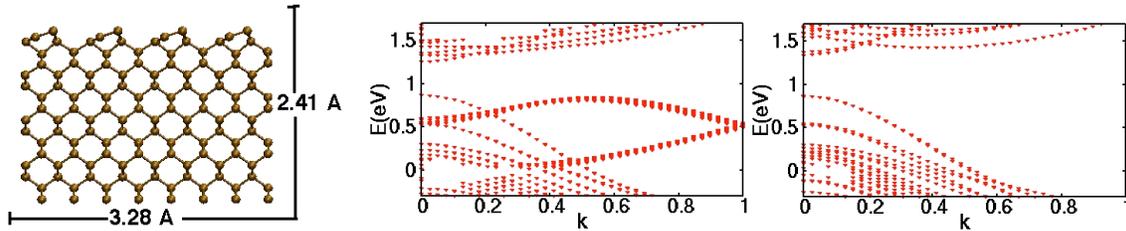


Fig 3. (a) The Si (110) wire with top (100) surface reconstructed. (b) Band diagram for the wire in (a) obtained using bulk TB parameters. (c) Band diagram for a similar ideal wire (no reconstructed surface).

Conclusions

Combined use of MD and DFT is an effective means of obtaining novel nanostructures and predicting their bond environments. For electronic structure, empirical tight binding can be used on these geometries. Even though the bulk TB parameters give good qualitative band structures, they need to be modified for the surface atoms to enable them produce realistic band gaps.

Acknowledgements

Financial support by SRC, FCRP MSD, Purdue CRI, and Purdue NCN cost-share, as well as the use of nanoHUB.org computational resources are gratefully acknowledged.

References

- [1] B. Marsen and K. Sattler, *Phys. Rev. B* **60**, 11593 (1999)
- [2] M. De Crescenzi et al., *Appl. Phys. Lett.* **86**, 231901 (2005)
- [3] A. Palaria, G. Klimeck and A. Strachan, submitted for peer review (2008)
- [4] M.J. Buehler, A.C.T. van Duin and W.A. Goddard, *Phys. Rev. Lett.* **96**, 095505 (2006)
- [5] G. Klimeck et al., *Superlattices and Microstructures* **27**, 77 (2000)
- [6] T.B. Boykin et al., *Phys. Rev. B* **66**, 125207 (2002)
- [7] R.A. Wolkow, *Phys. Rev. Lett.* **68**, 2636 (1992)
- [8] A. Ramstad, G. Brocks and P.J. Kelly, *Phys. Rev. B* **51**, 14504 (1995)
- [9] S. Lee et al., *Phys. Rev. B* **69**, 045316 (2004)
- [10] M. Rohlfiing, P. Kruger and J. Pollman, *Phys. Rev. B* **52**, 1905 (1995)