Full-band Study of Ultra-thin Si:P Nanowires

Hoon Ryu[1], Sunhee Lee[2], Bent Weber[3], Suddhasatta Mahapatra[3], Michelle Y. Simmons[3],
Matthias Yui-Hong Tan, L. C. L. Holleberg[4], and Gerhard Klimeck[2]

[1] Supercomputing Center, Korea Institute of Science and Technology Information,
Daejeon 305-806, Republico f Korea
[2] Network for Computational Nanotechnology, Purdue University, West Lafayette, IN 47907, USA.
[3] Centre for Quantum Computation and Communication Technology, School of Physics,
University of New South Wales, Sydney, NSW 2052, Australia.
[4] Centre for Quantum Computation and Communication Technology, School of Physics,
University of Melbourne, Parkville, VIC 3010, Australia.
[1] e-mail: elec1020@gmail.com

INTRODUCTION

With a recent progress in scanning tunneling microscope (STM) technology which can control dopant placements within a single atomic layer, experimentalists proposed various prototypes of highly phosphorous δ-doped Si (Si:P) devices [1-3], motivating modeling works in a theoretical perspective. Previous studies modeled equilibrium electronic properties of Si:P devices [4-6]. They are, however, limited to the analysis of 2-D planar doping device [4-5], or by assuming 1-D uniform doping in nanowire (NW) channels [6].

With the tight-binding (TB) model, we present a detailed modeling study of ultra-thin Si:P NWs which represent the limit of channel-downscaling. We confirm the experimentally observed metallic property of Si:P NWs by looking into equilibrium dispersions, and demonstrate a connection to the recent experiment [7]. This work should be highlighted as the first modeling study of Si:P NWs based on the atomistic full-band approach.

METHODOLOGY

Assuming long channels, NWs are represented with a periodic boundary condition along a [110] transport direction (Fig. 1(a)) and the 10-band sp3d5s* TB model validated via modeling works with the 3-D Nanoelectronics Modeling Tool [8]. The charge-potential self-consistency is obtained by solving a 3-D Schrödinger-Poisson (SP) equation. The potential is corrected with Local Density Approximation (LDA) to consider carrier interactions in highly doped devices [9] (Fig. 1(b)). For all the channels, a doping level of 1/4 monolayer (ML, 1 P atom per every 4 Si atom) is assumed.

RESULT AND DISCUSSION

Equilibrium Bandstructures: The equilibrium dispersion of a [110]-transport, 1/4ML doped and 2 Dimer Row (DR) wide (~1.7nm) Si:P NW is shown in Fig. 2, where 0.0eV references to the conduction band minimum of Si bulk. A few sub-bands are pulled down into the bulk band gap by phosphorus ions creating donor bands. A metallic property of Si:P NW is supported by a large density of electron states near the Fer-mi energy.

Experimental Samples: Recently, Weber et al., have experimentally demonstrated that the ohmic conduction is still observed even in ultra-thin Si:P NW up to 2DR width (Fig. 3). A total of 4 NW samples are measured to show that the Si:P NWs shows a quite constant resistivity regardless of the channel width (Table I) [7].

Connection to Experiment: By calculating the number of sub-bands (modes) crossed by the Fermi-energy at equilibrium, we approximated NW resistances in the ballistic regime for the 4 NW samples shown in Table I, and corrected ballistic resistances with a mean-free path ranging from 3.0 to 8.5nm for the scattering-involved transport [10], where 8.5nm is the mean-free path of 1/4ML doped Si:P 2-D δ-layer [11], and we assumed a shorter mean free path in NW channels due to the 2-D confinement of Si layers. As Fig. 4 indicates, modeling results exhibit quantitatively excellent agreement with the experiment.

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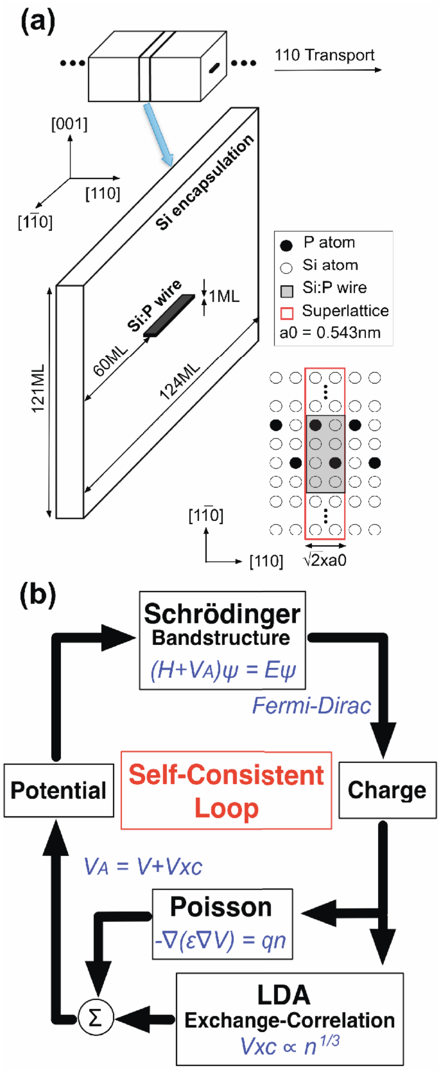

Fig. 1. (a) Geometry of 1/4ML doped 1.7nm wide Si:P NW and atomic distribution in the channel (b) Flow chart LDA-corrected SP self-consistent simulations.

Sample	W_{ch}(nm)	L_{ch}(nm)	R_{ch}(kΩ)
S1	4.6 (~6DR)	47	5.2
S2	2.3 (~3DR)	54	10.1
S3	2.3	20	17.1
S4	1.7 (~2DR)	106	82.3

Table I. Width (W_{ch}), length (L_{ch}) and measured resistance (R_{ch}) of four sample Si:P NWs (taken from Ref. [7]).

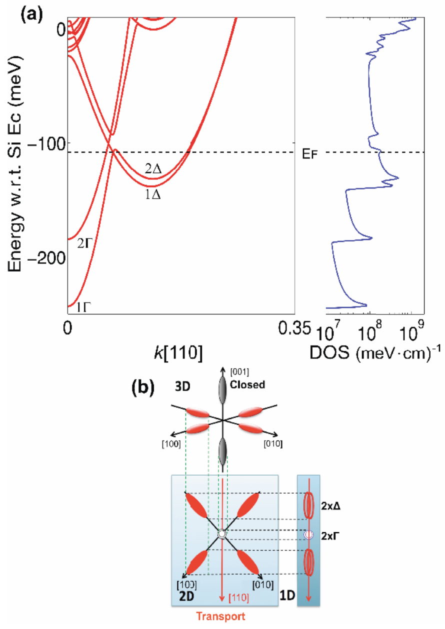

Fig. 2. (a) Equilibrium dispersion of the [110]-oriented, 2DR wide, and 1/4ML doped Si:P NW. Donor bands are observed below Si bulk conduction band minimum (0eV). Density of state profiles show the target NW is metallic. (b) Projection of 6 ellipsoids in Si bulk conduction band along the [110] direction, explaining why two Γ/Δ valleys are observed in the 1-D NW bandsturcture.

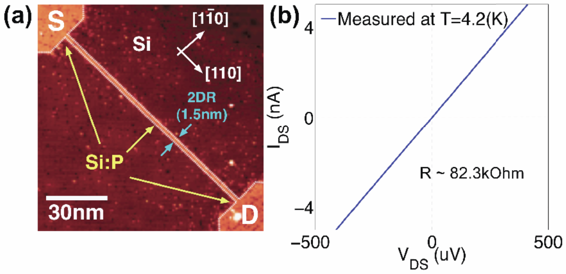

Fig. 3. (a) STM image, and (b) measured ohmic conduction property of the Si:P NW Sample 4 (See Table I).

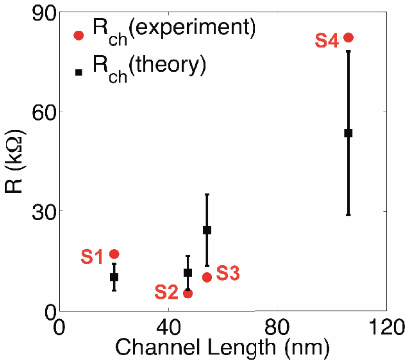

Fig. 4. Measured and calculated channel resistances of four Si:P NW samples at equilibrium.