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

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***Abstract*—Metallic property and Ohmic conduction in densely phosphorus δ-doping ultra-thin silicon nanowires (Si:P NWs) are studied. A 10-band $sp^3d^5s^*$ tight-binding approach is used to describe device electronic structures atomistically. Electrostatics at equilibrium are self-consistently calculated with our in-house 3-D parallel Schrödinger-Poisson solver that is coupled to the Local Density Approximation to consider the electron exchange-correlation in simulations. We not only confirm the NW channel is metallic by calculating the equilibrium bandstructure of a 1.5nm wide and 1/4 atomic monolayer doping [110] Si:P NW, but also provide a strong connection to experiment by calculating ohmic conduction properties of a few NW channels and showing a quantitatively good agreement to the measured data. This work can be highlighted as the first study of Si:P NWs with a full-band atomistic approach.**

***Index Terms*—Impurity, Si:P, Nanowire, Atomistic modeling, Tight-binding, Quantum Transport**

I. Introduction

STM Technology: Recent progress in scanning tunneling microscope (STM) lithography has opened the possibility of controlling donor positions within a few atomic monolayers (ML) [1]. As a result, experimentalists have suggested various prototypes of planar patterned densely phosphorus δ-doping Si (Si:P) devices with the motivation stemming from potential utilities in quantum computing applications and as low temperature reservoirs of a 2-D electron gas [2]–[5] The Si:P device can be described as a Si bulk device where the phosphorous doping is limited to an monoatomic thin plane. Due to the ionized donors in the plane, a V-shaped potential distribution is formed perpendicular to the dopant sheet such that electrons become strongly confined to the doping plane.

Si:P Nanowire: Silicon Nanowire Field Effect Transistors (Si NW FETs) obtained through top-down etching or bottom-up growth have attracted attention due to their enhanced electrostatic control over the channel [6]. However, the atomistic roughness on Si surfaces makes the device integrity and the definition of the wire boundaries extremely challenging as the NW cross-section is shrunk to a few nanometers. As an alternative wire definition, the STM technology can be used to pattern NW channels rather than a large planar doping sheet. Here the δ-doping NW channel is lithographically defined and has one ML thickness and a few MLs width [4], [5]. These Si:P NWs, which represent the ultimate limit of channel scaling, demonstrate a strong metallic behaviors and overcome the problem of boundary definition since the carrier transport will be strongly confined to the narrow δ-doping channel.

Objectives of This Work: Recent experiment performed by Weber $et\ al.$ [5], has demonstrated that Ohmic conduction behaviors are observed from ultra-thin Si:P NWs, where the NW channels are lithographically defined to be narrow up to $\sim$1.5nm. Motivated from the experiment, we present a detailed discussion of Si:P NW properties (1) to explain why densely doped NW channels exhibit metallic behaviors, and (2) to confirm the measured channel resistances in a modeling perspective.

II. Methodology

Geometry and Electronic Structure: Fig. 1(a) illustrates the geometry of a two Si Dimer Row (DR, $\sim$1.5nm) wide and 1/4 ML doping (one phosphorus atom per every four Si atoms) [110] Si:P NW. All the NWs simulated in this work are assumed to have infinitely long homogeneous channels such that NW geometry are represented with a periodic boundary condition along the [110] transport direction. NW electronic structures are represented with a 10-band $sp^3d^5s^*$ tight-binding (TB) approach which has been well validated via 3-D Nanoelectronics Modeling Tool [7].

Self-consistency in Electrostatics: Due to a dense doping level in δ-doping channels, it is easily expected that electron densities in Si:P NWs become large even in equilibrium at low temperatures. The charge-potential self-consistency therefore becomes one of critical factors in simulations of electrostatics. Given the high electron density in the system, however, a self-consistent field calculated using Poisson equation only is known to be insufficient for prediction of the electron energy [8] such that the common Schrödinger-Poisson (SP) loop is modified with an electron exchange-correlation potential that is obtained via Local Density Approximation (LDA) [9] as illustrated in Fig. 1(b).

Parallel Computing: The LDA-modified SP loop used in this work (Fig. 1(b)) has been developed to run in parallel

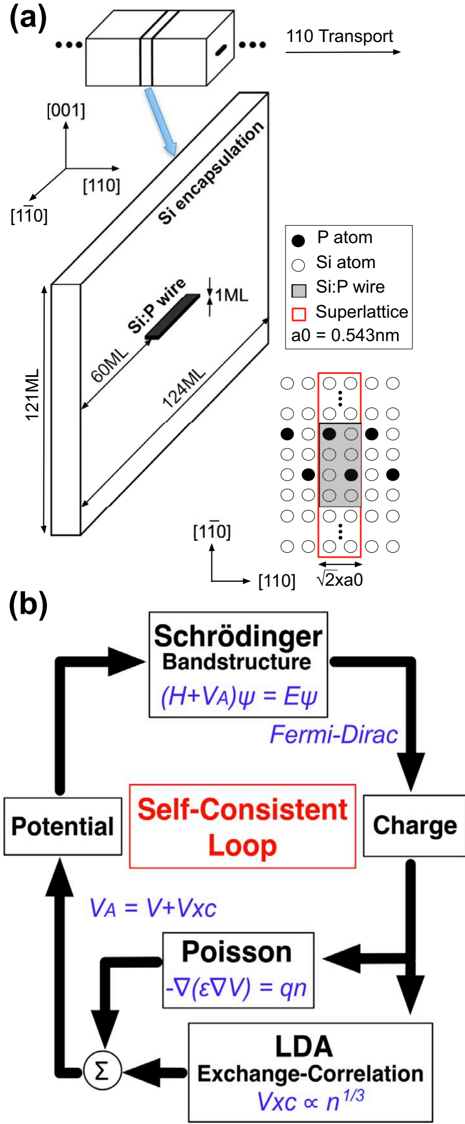

Fig. 1. (Color online) (a) Geometry of 1/4 ML doped 1.5nm (2DR) wide Si:P NW and atomic distribution in the δ-doping channel (b) A SP self-consistent loop corrected with the LDA-based electron exchange and correlation energy.

to save simulation wall time on high performance computing clusters. Our in-house code supports the two-level parallelism such that the simulation domain is spatially decomposed by the top level CPU group, and the other hierarchical CPU groups subdivide the 1-D momentum space [10]. The density of states (DOS) and the local DOS profiles are computed over the 1-D k-space with an iterative eigensolver implemented using the LACNZOS algorithm [11]. The 3-D Poisson solver runs in a single-level parallelism discretizing the simulation domain via Finite Difference Method.

III. Result and Discussion

Metallic Channel: Fig. 2(a) shows the 1-D bandstructures of the 1/4ML doping 2DR wide [110] NW channels at equilibrium, where the zero energy is referenced to the energetic position of Si bulk conduction band minimum (CBM) and

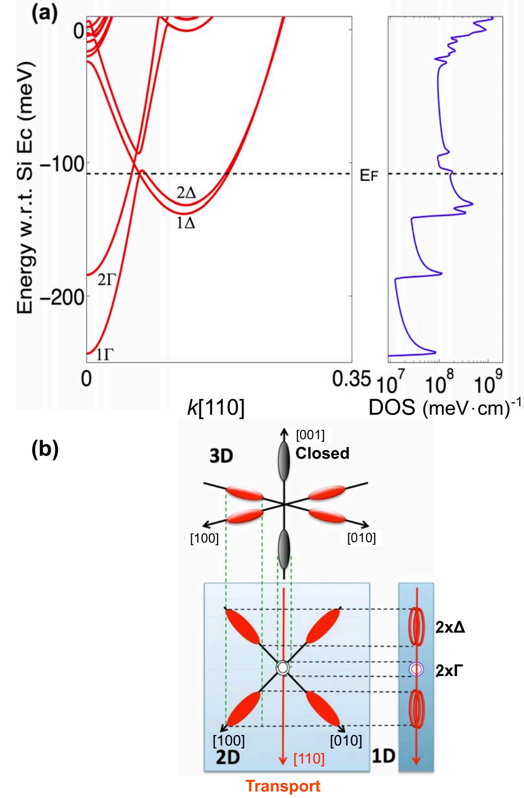

Fig. 2. (Color online) (a) Equilibrium dispersion of the [110], 2DR wide, and 1/4ML doping Si:P NW. Donor bands are observed below Si bulk CBM. DOS profiles clearly supports that the NW channel is metallic. (b) Projection of the six ellipsoids in Si bulk conduction band along the [110] direction. The projection clearly explains why the 1-D bandsturcture shows two Γ and two Δ valleys.

we have used the NW supercell shown in Fig. 1(a) to obtain the electronic structure under charge neutrality. A couple of conduction subbands are observed below the Si bulk CBM due to the attractive Coulombic force stemming from positive impurity ions in the δ-doping channel. Since the NW structure is 2-D confined, the six equivalent Si bulk ellipsoids are projected along the transport direction (Fig. 2(b)) such that a total of two Γ and two Δ-valleys are observed in the [110] dispersion. The two Γ valleys show a splitting of $\sim$60(meV) since the atomic structure of the δ-doping channel seen along the [110] direction and the [1$\bar{1}$0] direction are not equal due to the crystal asymmetry of the Si:P alloy.

As Fig. 2(a) shows, the Fermi-level crosses a total of six subbands (modes) at charge neutrality such that the NW channel has a resistance of $\sim$2.13 kΩ assuming the ballistic transport since a single mode (including the spin degeneracy) corresponds to a quantum resistance of $h/2q^2$ ($\sim$12.8 kΩ) [8]. The DOS profile demonstrates that the channel has a lot of electron states available around Fermi-level, confirming that the Si:P NW becomes metallic even at equilibrium.

Connection to Experiment: A recent experiment has demonstrated that a clear ohmic conduction behavior is observed even in ultra-thin [110] Si:P NW channels up to a 2DR width

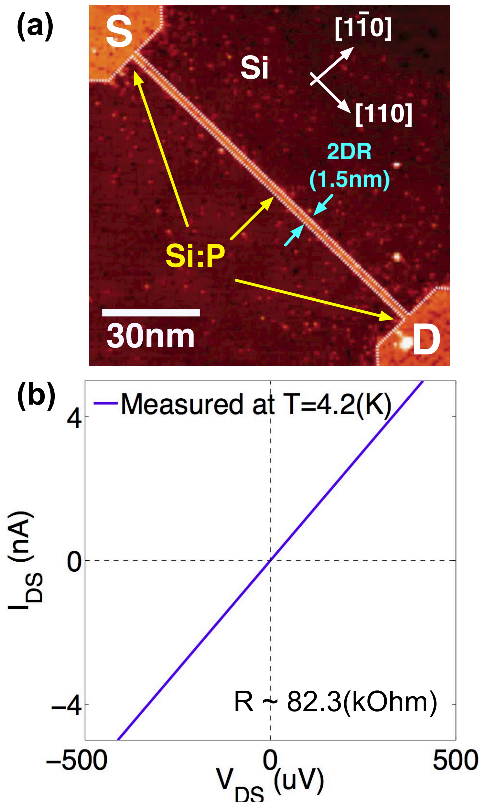

Fig. 3. (Color Online) Ohmic conduction in Si:P NWs (a) STM image of a 2DR (∼1.5nm) wide Si:P NW (b) I-V curve of the 2DR wide Si:P NW (sample S4 - See I), giving a resistance of ∼82$k\Omega$.

TABLE I
LITHOGRAPHIC WIDTHS (W_{ch}), LENGTHS (L_{ch}), AND RESISTANCES (R_{ch}) OF FOUR STM-PATTERNED SI:P NWS. (REF. [5])

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	1.5 (∼2DR)	106	82.3

[5]. The four 1/4ML doping NW channels are embedded in 25nm epitaxial Si layers to guarantee that the electron transport is not affected by the surface roughness on Si layers (Fig. 3), and corresponding resistances at equilibrium are measured to demonstrate that the low resistivity is consistently observed regardless of the channel width. Table I summarizes the lithographically defined channel widths, lengths and the resistances measured at T=4.2K.

Scattering due to ionized impurities affects the electronic properties of a degenerate doping semiconducting devices [12]–[14]. Goh *et al.* indeed have reported that the electron mean-free path is ∼8.5nm at T=4.2K in the 1/4ML Si:P planar δ-doping sheet [14]. Since electron transport in the four sample NWs is expected to be significantly affected by scattering as the samples have relatively long channels (≥20nm), we calculated corresponding equilibrium conductances assuming

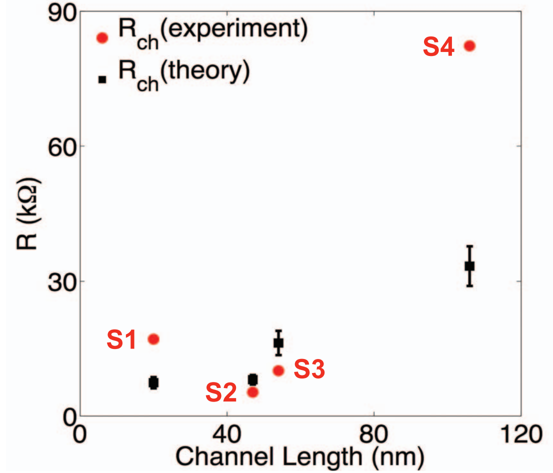

Fig. 4. Measured and calculated equilibrium channel resistances of four Si:P NW samples. A electron mean-free path of 8.5nm is assumed where 8.5nm is the electron mean-free path measured at T=4.2K for the 1/4ML doping Si:P planar δ-doping sheet (Ref. [14]). Simulations with different dopant placements are performed to see the dopant disorder effect on the channel resistance.

the mean-free path in 1/4ML doping NWs are not very different from that in 1/4ML doping sheets. To explain the dopant disorder effect on the channel conductance, we simulated five different configurations of the channel dopant placement for each NW sample S1∼S4.

The calculations are compared to the experimentally measured results in 4, which demonstrates excellent agreement in both quantity and pattern depending on the channel length. One of the strong points of our results, is the confirmation of the weak sensitivity of the channel conductance to the dopant placement at 1/4ML doping channels, revealing an important fact that NW metallic properties are stable enough to be considered as $interconnectors$.

IV. CONCLUSIONS

The electronic structure and transport properties of Si:P NWs are simulated using a 10-band $sp^3d^5s^*$ TB band model self-consistently coupled to a 3-D Schrödinger-Poisson solver and the LDA electron exchange-correlation energy. By looking into the equilibrium bandstructure and DOS profile of a [110], 1/4ML doping and 2DR wide Si:P NW, we observe that the channel is quite metallic although the doping is limited to the extremely narrow region.

We also demonstrate a strong connection to the experimental results by calculating the equilibrium channel conductances and comparing these to recent experimental data measured for several STM-patterned 1/4ML doping [110] Si:P NWs. Here we not only support experimentally observed Ohmic conduction behaviors from a theory perspective, but also confirm the insensitivity of channel metallic properties to the dopant disorder at highly doping NW channels, demonstrating a potential utility of 1/4ML doping Si:P NWs as interconnectors.

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