A Tight-binding Study of Channel Modulation in Atomic-scale Si:P Nanowires

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Abstract—It has been well understood that ultrathin, highly P δ-doped Si (Si:P) nanowires are metallic at charge-neutrality (Ref. [5]). This work extends the scope of tight-binding modeling beyond charge-neutrality to examine the channel modulation of a 1.5nm wide, 1/4 monolayer(ML)-doped Si:P nanowire and its effect on the channel conductance. Subband-anticrossing plays a key role in the channel modulation, creating a local minimum in the ballistic conductance as the channel is occupied with more electrons. While the channel modulation causes a fluctuation in the conductance, nanowires still remain metallic boding well for their utility as potential interconnects.

I. INTRODUCTION

Remarkable progress in scanning tunneling microscope (STM) lithography have realized various atomic-precision STM-patterned highly P δ-doped Si (Si:P) device architectures with a major effort underway to develop a Si-based quantum computer [1], [2], [3], [4]. In particular, the observation of Ohmic conduction in 4-atom wide ($\sim$1.5nm), single mono-layer (ML) thick highly P δ-doped Si (Si:P) nanowires [2], bodes well for the utility of charge-neutral Si:P nanowires as ultrathin interconnects for atomic-scale devices, and has been theoretically confirmed by our previous modeling work [5].

If perfectly metallic, nanowires should exhibit a consistent conduction behavior regardless how many electrons fill the channels. Since Si:P nanowires are made of semiconducting materials. An interesting area of research is to study the channel modulation of Si:P nanowires, especially to see how the metallic property changes if the channel is subjected to a varying number of electrons. Using an atomistic tight-binding approach, this work extends the scope of Si:P nanowire modeling beyond charge-neutrality to understand the channel modulation and its effect on the channel's metallic property.

II. MODELING APPROACH

4-atom wide ($\sim$1.5nm), single atomic ML thick [110] Si:P nanowires are assumed to have long channels, and are thus described by a supercell with a periodic boundary condition along the transport direction (Fig. 1(a)). Bandstructures, charge densities and potential profiles are calculated with a 3-D Nanoelectronics MOdeling Tool for PETAscale simulations (NEMO 3-D PETA), where channel electronic structures are
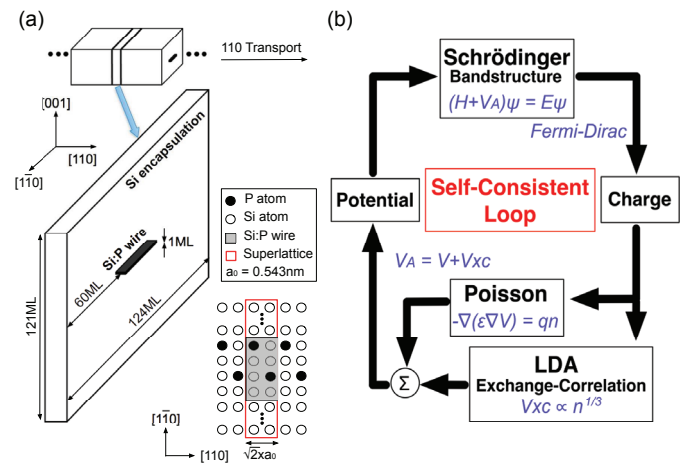

Fig. 1. (a) Supercell of a 1/4ML-doped, 1.5nm wide and single ML thick [110] Si:P nanowire. Atomic placement in the central P-doped channel region is also shown. (b) Flow-chart describing the LDA-corrected Schrödinger-Poisson self-consistent loop for electronic structure calculations.

described with a 10-band nearest neighbor $sp^3d^5s^*$ tight-binding model [5], [6], [7]. The charge-potential is calculated self-consistently by solving a 3-D Schrdinger-Poisson equation, where the mean-field based electrostatics are corrected in the Local Density Approximation (LDA) to consider carrier interactions in highly doped devices (Fig. 1(b)). [8] All the channels are assumed to have an areal doping density of 1/4ML ($\sim$2$\times$10$^{14}cm^{-2}$, corresponding to one P atom per every four Si atoms). All the simulations have been performed at a low temperature of 4.2K.

III. RESULTS AND DISCUSSION

A. At charge-neutrality

The electronic structure of the [110] transport-oriented, 1/4ML doping, 1.5nm wide Si:P nanowire is calculated, where a total of two electrons are filled in the supercell (Fig. 1(a)) to place the Fermi-level into charge-neutrality. Fig. 2 shows the bandstructure dispersion, density of states and the spatial distribution of the electron density across the channel cross-section. Fig. 3 illustrates the electrostatic potential profile along various line-cuts. As the positive donor ions pull down the Si
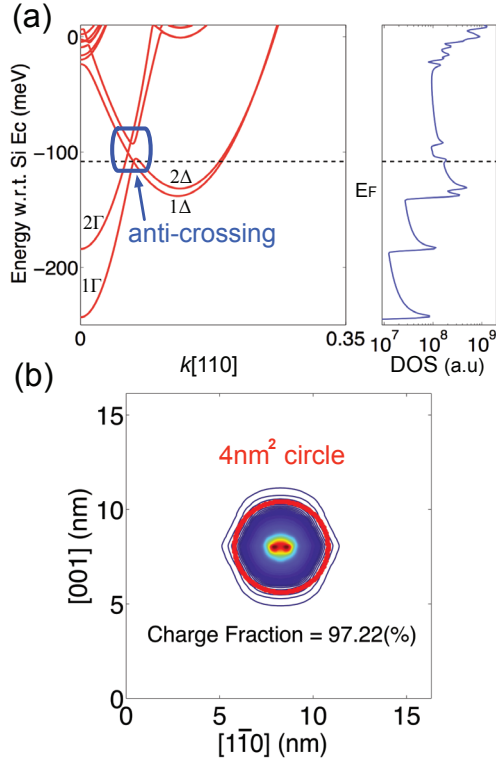
Fig. 2. (a) Nanowire bandstructure with a density of state (DOS) profile in equilibrium. The bandstructure and DOS confirm the electron conduction via donor bands, and that the channel is metallic. The dispersion shows an anti-crossing (highlighted) of $\sim$15meV (a small energy-gap that disconnects 1Δ and 2Γ sub-band). (b) Spatial distribution of the electron density on a channel cross-section. 97% of total electrons exist within a 4nm^2 circle showing the conduction path is indeed in a nanometer-scale.
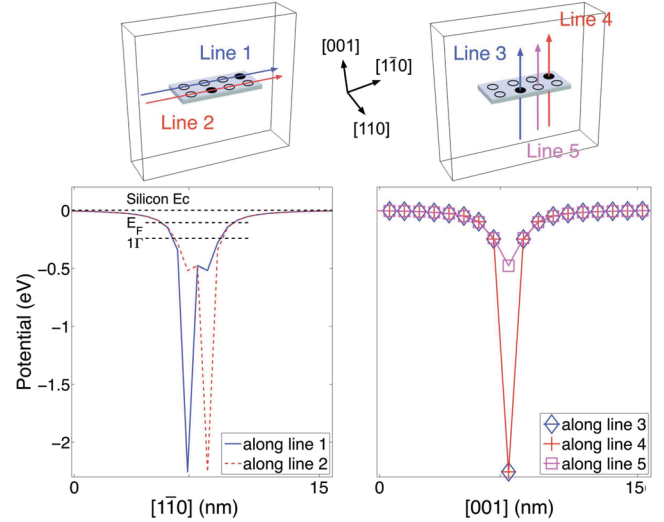

Fig. 3. Electrostatic potential profile as a function of position along transport-perpendicular directions. The potential at impurity sites is symmetric and decays rapidly in the space along the direction vertical to the channel. Along the lateral direction (line 1, 2), the potential shows significant variation but second-nearest neighbor impurities influence the intermediate Si sites significantly to create a wider quantum well compared to the vertical direction (line 3-5).

conduction bands, a couple of sub-bands, which we call as *donor bands* are observed below the Si bulk conduction band minimum (CBM) that is referenced at a zero energy. The high density of states (DOS) near the Fermi-level indicates that the channel is metallic (Fig. 2(a)). The donor bandstructure shows a *band-anticrossing* that is placed between the 1Δ and 2Γ subband, with a remarkable energy gap of $\sim$15meV. This band-anticrossing, which is known to be observed in alloy materials [9], turns out to affect the channel modulation, as will be discussed in detail in the next subsection.

The spatial distribution of the electron density and the electrostatic potential (Fig. 2(b) and Fig. 3) show that the channel electrons are strongly confined to the lithographically defined channel. At charge-neutrality, we observe 97% of electrons are placed within a 4nm^2 circle centered to the P-doping region, which represents that the conducting path (the electrostatic channel size) is still in a nanometer-scale.

B. Channel modulation: Beyond charge-neutrality

While Si:P nanowires have densely doped channels, they are still semiconducting materials such that the channel could be modulated when the number of channel electrons changes. To understand how the electrostatic potential, electron densities, dispersions and channel conductances change, we extend the scope of simulations beyond charge-neutrality where we changed the number of electrons filled in the nanowire from

2.0 (charge-neutral) to 2.8 with a step of 0.05 (a total of 17 cases are calculated).

Fig. 4 illustrates the dispersion, electron density and potential profile of a 1.5nm wide, 1/4ML [110] transport-oriented Si:P nanowire for the four selected cases (2.0, 2.2, 2.5 and 2.7 electron-filling) 3-D electron density profiles are projected to the transport-perpendicular ((110)) plane. Potential profiles are cut along the four lines (1,2,3,5) shown in Fig. 3. Dispersion and potential profiles are represented with respect to the Fermi-level that is fixed due to the DC-grounded source and drain lead. As addressed in Fig. 2(b), 97(%) of total electrons are placed near the P-doping region indicating a strong channel channel confinement at charge-neutrality. As the channel electron increases, however, electrons spread and are penetrated into the Si layer. Electrons screen donor ions more strongly such that the channel confinements become weaker as the potential profiles in Fig. 3 also indicates. While the channel is lithographically defined to be 4-atom wide and 1-atom thick, the electron density profiles on the channel cross-section claim that the channel can serve as a ultrathin metallic nanowire only within a certain range of electron-filling. If the channel is filled with too many electrons, i.e. the case of 2.7 electrons in Fig. 4, $\sim$12% of the electrons come from occupied bulk conduction subbands rather than donor bands, and conducting electrons are not thus confined to the narrow P-doping region any more.

Fig. 5 describes the pattern of channel conductances that are calculated in the ballistic regime. It is commonly known that the channel conductance of typical n-type field effect transistors is proportional with increasing number of channel electrons [10]. For ultrathin Si:P nanowires, however, a clear local minimum in they conductance is observed with increasing channel electrons, although the finite curvatures of donor subbands near the Fermi-level indicates that the channel is not quite localized (and still metallic). Rather than a channel-
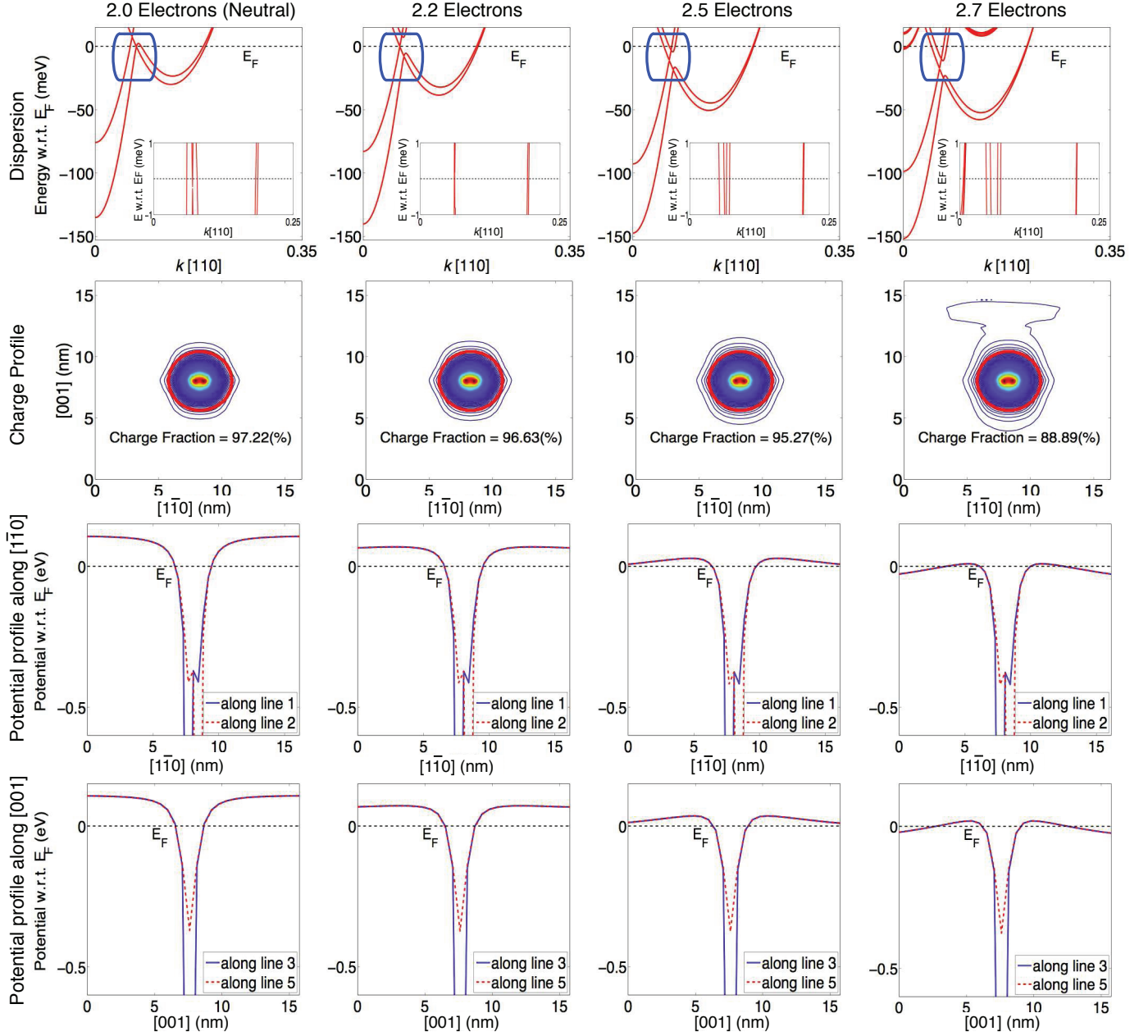
Fig. 4.   Illustration of charging effects on the nanowire properties. Dispersion and potential profiles with different electron-filling are represented with respect to the Fermi-level that is assumed to be fixed by in-plane source-drain Si:P contacts. Band-anticrossings are highlighted in the dispersion profiles to focus on their effects on the nanowire transport, and dispersions zoomed-in within $\pm 3k_B T$ from the Fermi-level are provided in the inset. 3-D potential profiles are cut with four lines depicted in Fig. 2(c). Charge profiles projected to the transport-perpendicular plane are shown with the effective channel region. Fractions of electrons in the effective channel region are also indicated in the inset.

localization, a subband anti-crossing serves as a reason for this local minimum of the channel conductances as dispersion profiles in Fig. 4 indicate. At charge-neutrality (2.0 electrons), a total of six subbands are observed in the Fermi-tail such that the channel conductance becomes $6(2e^2/h)$. With 2.2 electrons, the Fermi-level is placed in the anticrossing gap so the channel conductance reduces to $4(2e^2/h)$. As the channel is populated with more electrons, the conductance increases again as the Fermi-level crosses more subbands.

A ~30% reduction in the channel conductance (observed in the local minimum) may weaken the metallic conduction in utlrathin Si:P nanowires. In spite of the degradation, however, the channel conductance of STM-patterned Si:P nanowire is still extremely small when compared to the conventional P-doped Si nanowires that have a radius of a few nanometers [11]. When the channel has more than 2.6 electrons, conductance again increases sharply but the conduction path is not in a nanometer-scale any more since the channel electrons comes from the Si bulk conduction subbands.
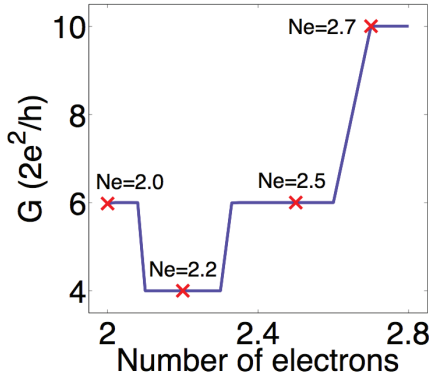
Fig. 5. Ballistic channel conductance that are calculated as a function of a number of channel electrons. The four cases (2.0 (charge-neutral), 2.2, 2.5 and 2.7 electrons) shown in Fig. 4 are also marked. A local minimum in the conductance is observed due to the band-anticrossing. The (30%) reduction in conductance however is not large enough to undermine the metallic conduction of thin channels when compared to Ref. [11]. When the change has more than 2.6 electrons, conductance increases sharply but the conduction path is not in a nanometer-scale any more.

IV. CONCLUSIONS

Channel modulation in ultra-thin Si:P nanowires has been studied with a $sp^3d^5s^*$ tight-binding approach coupled to a LDA-corrected Schrdinger-Poisson equation. Various patterns of channel conductances and electron profiles are simulated to understand how the metallic property of nanowires changes with channel electron-filling. A local minimum in the ballistic channel conductance is observed with increasing channel electron-filling due to a subband anti-crossing. Fluctuations in the channel conductance, however, are not strong enough to undermine the metallic conduction via ultrathin channels, boding well for the utility of Si:P nanowires as interconnects.

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