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Quantum Transport in Ultra-scaled Phosphorous-doped Silicon Nanowires

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***Abstract* – Highly phosphorous-doped nanowires in silicon (Si:P NW) represent the ultimate nanowire scaling limit of 1 atom thickness and a few atoms width. Experimental data are compared to an atomistic full-band model. Charge-potential self-consistency is computed by solving the exchange-correlation LDA corrected Schrödinger-Poisson equation. Transport through donor bands is observed in [110] Si:P NW at low temperature. The semi-metallic conductance computed in the ballistic regime agrees well with the experiment. Sensitivity of the NW properties on doping constant and placement disorder on the channel is addressed. The modeling confirms that the nanowires are semi-metallic and transport can be gate modulated.**

I. Introduction

With a recent progress in the scanning tunneling microscope (STM) technology which can control dopant placement within a few atomic layers, experimentalists proposed various prototypes of highly doped Si:P devices [1-3] and have motivated detailed electronic structure modeling. Previous studies have calculated equilibrium properties of Si:P devices with the pseudo-potential method (PP) and the density functional theory (DFT) [4-6], but they were limited to δ-doped plane devices (PD) [4-5] or by the assumption of 1-D uniform doping [6].

Electronic properties of Si:P NW's are studied with the tight binding (TB) band model. Conductance of a [110], 1/4 mono-layer (ML) doping (1 phosphorus in every 4 Si atom) and 2 dimer-row (DR) wide Si:P NW is calculated and compared with experiments. Dependencies of the Si:P NW conductance on doping constant and dopant placement disorder on the channel are studied.

II. Methodology

Devices are described with the atomistic $sp^3d^5s^*$ TB model that has been experimentally validated by various modeling works with the Nanoelectronics Modeling Tool (NEMO 3-D) [7-9]. Charge-potential self-consistency is calculated with a parallelized 3-D Schrödinger-Poisson solver [10]. The potential is LDA-corrected to consider carrier interactions in densely-doped devices [11].

III. Result and Conclusion

Validation of methodology Fig. 1(a)-(b) shows the superlattice (SL) of δ-doped Si:P PD where a periodic boundary condition (PBC) is used to the in-plane direction of 1/4ML δ-layer. Along the [001] direction, a 120ML thick Si encapsulation is used to eliminate effects of the confinement wall. Equilibrium properties at T=1.2K agree well with previous studies as shown in Fig. 1(c) and Table I.

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Si:P NW in equilibrium The [110]-transport, 1/4ML and 2DR Si:P NW is calculated with PBC in the transport direction. SL of Si:P NW and electronic properties at T=1.2K are shown in Fig. 2 and Table II. A few Si conduction bands are pulled down into the bulk band gap by phosphorus ions creating donor bands. The PD shows a stronger semi-metallic property than the NW due to the wider doping. A band anti-crossing of 15meV gap is observed in (1Γ, 2Δ) sub-bands due to the atomic treatment of Si:P alloys [12].

Transport through donor-bands Fig. 3(a) shows a STM image of the [110]-transport, 1/4ML and 2DR Si:P NW. The ballistic source-drain conductance (dI_d/dV_d) is calculated to compare with the experimental result measured at T=1.2K. The effect of gate biasing on the NW is approximated by controlling the number of electron-filling in Si:P NW SL, which is a reasonable approach due to the weak control of the in-plane gate over the NW channel.

Fig. 3(b) shows the conductance computed with the change of electron-filling from 2.0 (neutral) to 2.6. Our TB result shows a good quantitative agreement with the measured data corrected by contact resistances. A local minimum is observed in patterns of conductance due to the band anti-crossing as illustrated in Fig. 3(c). Transport through impurity bands is confirmed by electron profiles on the NW cross-section, which indicates that carriers are strongly bound to impurity spots.

Engineering of Si:P NW properties The doping profile on δ-doped NW channels can modify NW properties. The effect of the doping constant is studied with 1/4, 1/16 and 1/64ML Si:P NW SL's. Lower doping pushes donor bands toward the Si CBM as depicted in Fig. 4. A perfect depletion of Δ-bands is observed in the 1/64ML case. The effect of dopant placement is studied with three 1/64ML Si:P NW SL's of different dopant placements on NW channels. Equilibrium bandstructures and charge profiles on channels along the transport direction are shown in Fig. 5. Donors on NW channels are localized more strongly as doping becomes less uniform (SL01→ SL03). The effective masses of donor bands become larger and conductance reduces as the Fermi level crosses fewer modes.

Conclusion Atomistic TB simulations can describe the physics of ultra-scaled Si:P NW's which gives a reasonable estimation of experimentally verified device behaviors. The strength of our approach is the ability to study disordered Si:P devices of realistic dimensions.

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TABLE I
SI:P QW BAND-STRUCTURE: COMPARISON WITH PREVIOUS STUDIES
(REFERENCED TO SI BULK CONDUCTION BAND MINIMUM)

Energy (meV)	1Γ	2Γ	1Δ	E_F
PP [3]	-410	-400	-270	-110
DFT [4]	-540	-420	-210	-111
$sp^3d^5s^*$ TB	-415	-384	-242	-110

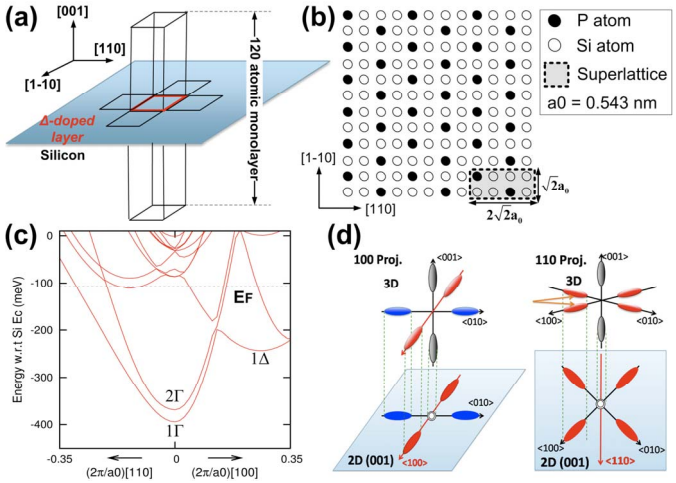

Fig. 1. (a) 3-D schematic of Si:P PD SL (b) Atomic structure of δ-doped layer (c) [110]/[100] bandstructures at T=1.2K in equilibrium (d) 2-D projections of Si bulk bandstructure.

TABLE II
SI:P NW BAND STRUCTURE IN EQUILIBRIUM
[110]-TRANSPORT, 1/4ML DOPING AND 2DR WIDTH AT T=1.2K
(REFERENCED TO SI BULK CONDUCTION BAND MINIMUM)

Energy (meV)	1Γ	2Γ	1Δ	2Δ	E_F
$sp^3d^5s^*$ TB	-242	-183	-137	-130	-106

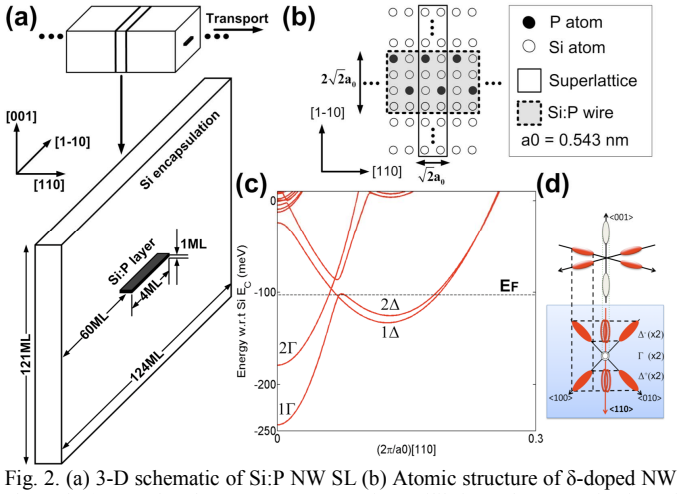

Fig. 2. (a) 3-D schematic of Si:P NW SL (b) Atomic structure of δ-doped NW channel (c) [110] bandstructure at T=1.2K in equilibrium (d) 1-D projection of Si bulk bandstructure along [110] direction.

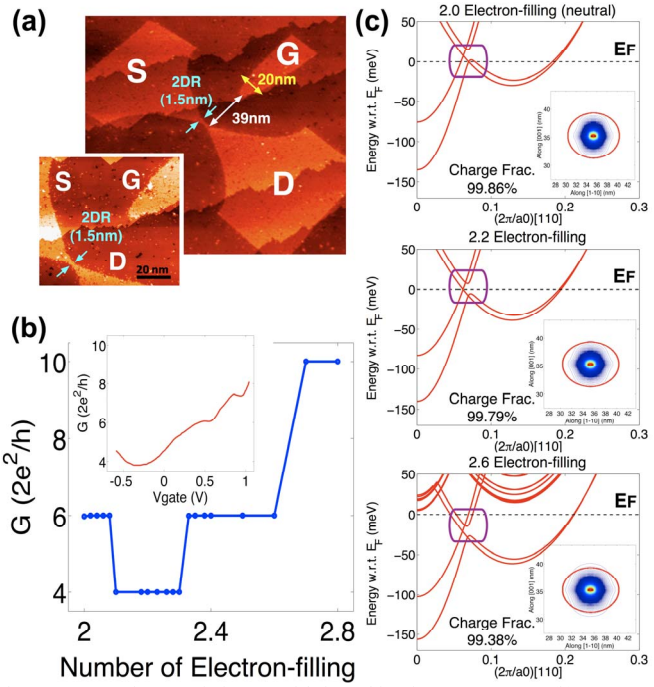

Fig. 3. (a) STM image of Si:P NW fabricated in Simmons's group (b) Computed and measured conductance (inset) at T=1.2K (c) Bandstructures with different electrons focused on the band anti-crossing (Inset: a latitudinal view of electron profiles with the fraction of charge in the arbitrarily defined central area).

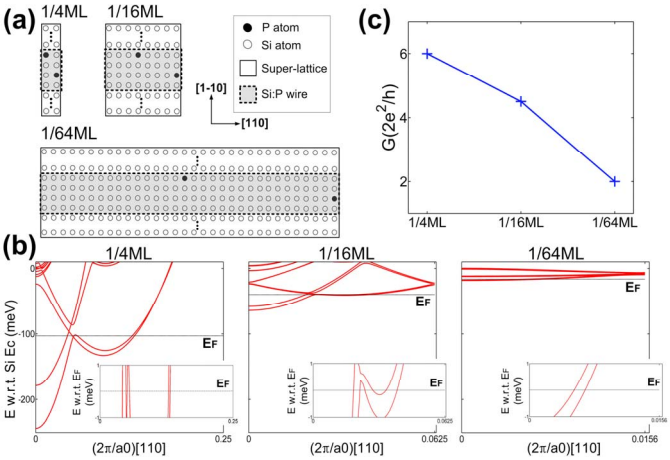

Fig. 4. (a) Atomistic structure of NW channels of the 1/4, 1/16 and 1/64ML Si:P NW SL (b) Bandstructures at T=1.2K in equilibrium (Inset: Zoomed in within ±10kT from E_F) (c) (dI_d/dV_d) with 2 electrons.

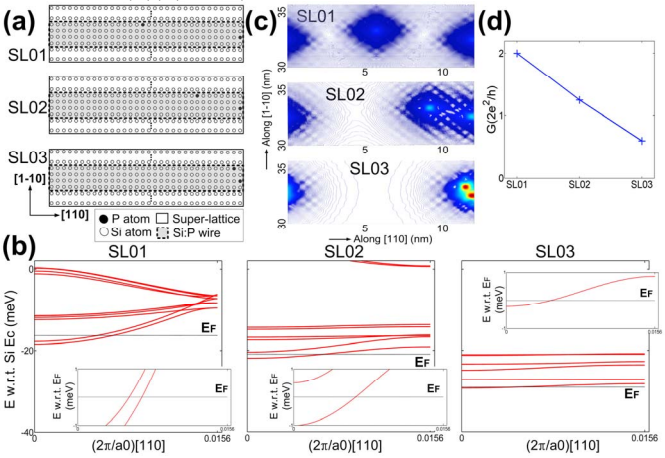

Fig. 5. (a) Atomistic structures of NW channels of the 3 1/64ML Si:P NW SL's (b) Bandstructures at T=1.2K in equilibrium (Inset: Zoomed in within ±10kT from E_F) (c) Lateral charge profile on δ-layer (d) (dI_d/dV_d) with 2 electrons.