Channel-size Dependent Dopant Placement in Silicon Nanowires

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***Abstract*—Sensitivity of Phosphorus dopant placement to the channel size of highly doped silicon nanowires is studied using a 10-band $sp^3d^5s^*$ tight-binding approach coupled to self-consistent simulations. Extending the simulation scope to realistically sized nanowires, we observed that uniform doping does not necessarily reduce the channel energy compared to surface-oriented doping when the diameter of a nanowire cross-section is smaller than 20nm, whilst uniform doping lowers the energy, making the channel more stable at larger cross-sections. This size-dependency, firmly connected to the recent experiment, is understood well in detail by investigating channel electrostatics.**

I. Introduction

Placing dopants in semiconductor nanocrystals causes remarkable fluctuation in electrical and material properties. It therefore has the potential as a key control factor for device engineering [1], [2], [3], [4], invoking the strong needs for understanding a pattern or a rule of thumb in dopant placement that can serve as a guideline for potential device design. A recent experimental work performed by Xie *et al.* [2], studied phosphorus (P) dopant placement in free-standing circular silicon (Si) nanowires, where, by measuring the shift of a threshold voltage, it presented an experimental message that dopant placement is not likely to be uniform and tends to be surface-oriented when the diameter of a channel cross-section is smaller than ∼20nm. While the result itself is interesting enough to attract experimentalists who are keen in building devices using doped nanowires, the relation between channel size and dopant placement is not yet fully understood in a theory perspective.

Dopants in nanowires interplay with strong quantum confinement such that details needs to be understood using a fully quantum-mechanical approach rather than classical bulk physics. Using an atomistic tight-binding approach coupled to Schröedinger-Poisson self-consistent simulations that has been validated by previous studies of highly P δ-doped Si devices [4], [5], [6], [7], we extend the simulation scope to realistically sized nanowires that are fundamentally hard to be calculated using first-principle theories such as Density Functional Theory [8], with which only surface- and interface-related dopant placement have been studied so far due to a size limitation [9], [10]. This study presents a solid understanding of the dependency of dopant placements on the channel size, establishing a strong connection to the experimental work [2].

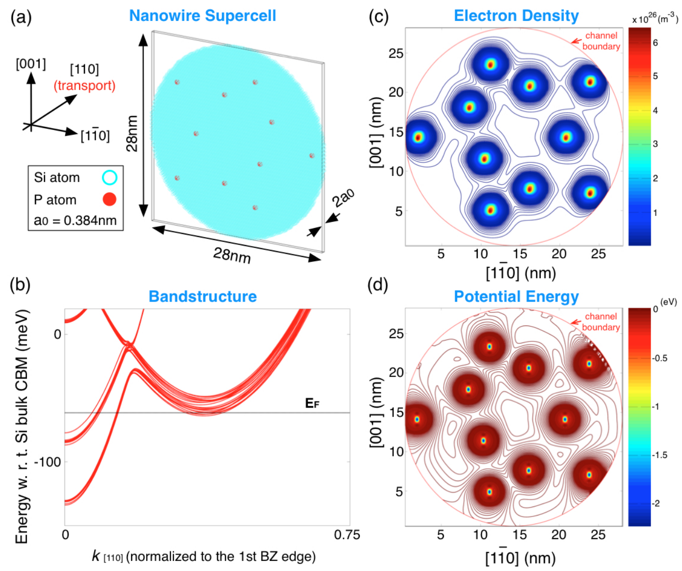

Fig. 1. **Geometry and electronic structures of P-doped Si nanowire.** (a) A 28nm, free-standing circular [110] nanowire supercell that is assumed to be periodic along the transport direction. (b) Bandstructure in equilibrium. Ionized donors pull down conduction sub-bands below Si bulk conduction band minimum. (c) Spatial distribution of electron density and (d) potential energy projected onto the channel cross-section indicates electrons are strongly confined near to donor sites.

II. Modeling Approach

[110] transport-oriented P-doped Si nanowires are represented with supercells that are assumed to be periodic along the transport direction as shown in Fig. 1(a). Structures of nanowire supercells are represented atomistically using a 10-band $sp^3d^5s^*$ tight-binding approach with no considerations of spin-orbit couplings [11]. The tight-binding Schrödinger equation is solved together with a 3D Poisson equation to obtain equilibrium channel electrostatics self-consistently [4], [7], where the potential energy is corrected by Local Density Approximation to consider carrier interactions in dense doping systems [12]. Despite being assumed to be periodic along the transport direction, nanowire supercells are still too large to be handled by Density Functional Theory, such that they have 8,672-23,618 atoms depending on the size of the channel cross-section directly comparable to the experiment [2].

We note the methodology described here has been validated well via various previous modeling works, which have success-

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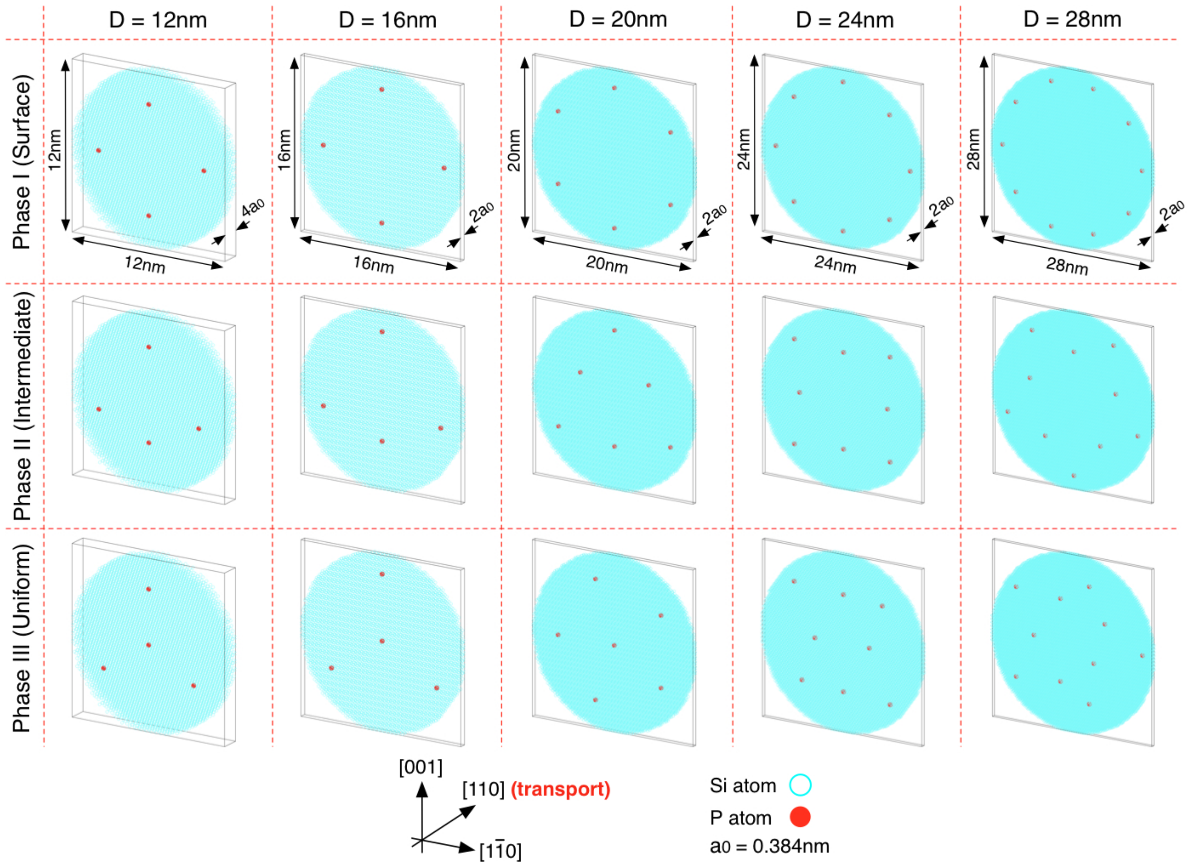

Fig. 2. **Simulated nanowire supercells.** A total of 15 [110] nanowire supercells are simulated to understand the sensitivity of dopant placements to the channel size. For each of five sizes of the channel cross-section, three different phases of dopant placements are considered - Phase I where dopants are surface-oriented, Phase II where some donors start to move to the inner side of the channel, and Phase III where donor-distribution is quite uniform. All the nanowire supercells are assumed to be doped with an average density of $\sim 2\times10^{19}\text{cm}^{-3}$.

fully explained donor physics such as electronic properties of P δ-layers in Si bulk [7], Ohmic conduction of atomic-scale P-doped channels buried in Si bulk [4], [6], electron transport in single-atom transistors [5], and binding-energy spectra of Coulomb-confined Si double quantum dot [13].

III. Results and Discussion

A. Electronic structure of P-doped Si nanowire

A supercell of the P-doped free-standing [110] Si nanowire is shown in Fig. 1(a), where the channel has a 28nm cross-section and is densely doped with an average doping density of $\sim 2\times10^{19}\text{cm}^{-3}$. Positive P-ions in the nanowire channel create attractive Coulombic force such that electrons are bound to each donor site. Although the channel remains charge-neutral in equilibrium, the P-ion (point charge) cannot be perfectly screened by electrons (cloud charge), such that a sharp confinement potential barrier is formed near each donor site. Consequently, each donor can be interpreted as a *localized quantum dot*.

When the channel is densely doped, however, these donor quantum dots start to couple one another even in equilibrium, creating paths for electron transport. Incompletely screened positive P-ions pull down these paths (*donor bands*) below undoped bulk Si conduction band minimum (CBM) as shown in Fig. 1(b). The charge and potential profile shown in Figure 1(c) and 1(d), respectively, represent the strong confinement created by P-atoms. A set of occupied donor bands (Fig. 1(b)) have finite effective masses such that they serve as paths for electron conduction, indicating the delocalization of P-donor quantum dots in densely doped nanowires.

B. Dopant placement and channel size

To carefully explore the channel-size dependency of dopant placement, we simulated a total of 15 supercell-configurations that are illustrated in Fig. 2. For each of five different sizes of a nanowire channel cross-section (diameter = 12, 16, 20, 24 and 28nm), three different dopant placements are considered - the initial stage where dopant placement is surface-oriented (Phase I), the intermediate stage where some donors start to move to inner sides of the channel (Phase II), and the final stage where donors are placed quite uniformly as they are in Si bulk (Phase III). All the supercells are assumed to be [110] transport-oriented with an average doping density of $\sim 2\times10^{19}\text{cm}^{-3}$.

Fig. 3(a) shows channel dispersions for three different doping configurations in a 12nm/28nm nanowire, where zero energy refers Si bulk CBM. Despite of the same average doping density, an interesting feature is observed from 28nm channels such that the energy of occupied sub-bands generally reduces as dopants are distributed more uniformly (Phase I

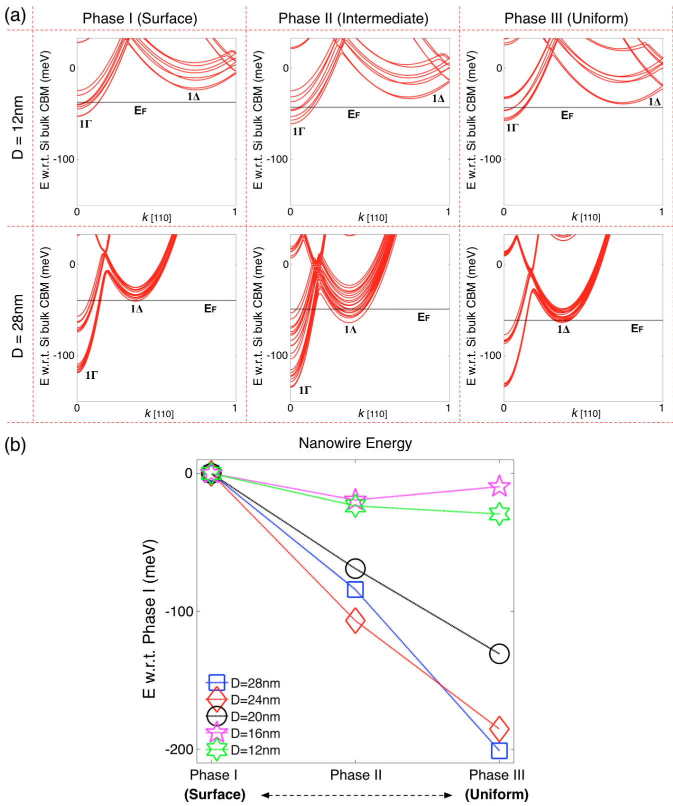

Fig. 3. **Bandstructure and channel energy of P-doped Si nanowires.** (a) Nanowire bandstructure for a channel diameter of 12nm and 28nm. As doping becomes more uniform (Phase I $\rightarrow$ Phase III), the channel of a larger cross-section shows a clear reduction of the Fermi-energy while the shift is negligible in the channel of smaller cross-sections. (b) For large cross-sections (diameters $\geq$ 20nm), the channel energy reduces as dopant distribution is more uniform. For smaller cross-sections, however, this does not necessarily happen, indicating surface donors may not be likely to diffuse into the channel.

$\rightarrow$ Phase III), which does not necessarily happen in 12nm channels. Fig. 3(b) shows the channel energies that are evaluated by Fermi-Dirac integral of channel dispersions for all the supercells (illustrated in Fig. 2). For channel cross-sections $\geq$ 20nm, the channel energy reduces as dopants are distributed more uniformly. For smaller cross-sections, however, this is not true, indicating that surface donors are not likely to diffuse into the channel. Our result here presents a strong connection to the experimental conclusion given in Ref. [2], which claimed that, for nanowires smaller than 22nm, P-dopants are likely to remain near the channel surface during the process of nanowire synthesis [2].

To understand why this pattern happens, we performed the another set of simulations changing the position of a single P-atom in a 20nm nanowire as shown in Fig. 4(a). From Fig. 4(b), we see that the channel energy increases as the dopant placement becomes closer to the surface, and the increasing becomes sharp when donors are placed within $\sim$4nm near the surface. This can be understood by exploring charge and potential energy profile shown in Fig. 4(c). If the P-atom is placed near the surface, the donor ion becomes harder to be fully screened along the direction towards the surface because there is no enough space for electrons to be piled. To maintain the charge-neutrality, the channel cannot but fill electrons in directions where there is enough room into which electrons can be piled. The spread of electrons towards the inside of the channel, therefore becomes broader and larger as the donor is placed more closely to the surface, entirely raising the channel potential energy.

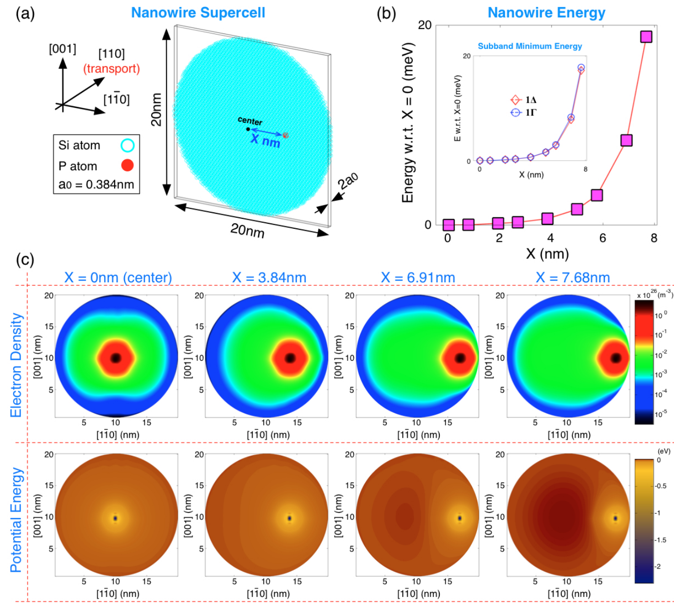

Fig. 4. **Sensitivity of channel electrostatics to dopant placement and its effect on channel energy.** (a) To study how a single dopant placement changes the channel energy, we performed simulations by changing the position of a single P-donor in a 20nm circular channel. (b) Channel energy plotted as a function of dopant position. We observe that the channel energy increases as the donor is placed closer to the channel surface. (c) Electron density and potential energy profile plotted as a function of dopant position. When a P-atom is placed near the channel surface, the donor ion cannot be fully screened due to a lack of space. To meet the charge-neutrality, electrons cannot but spread towards directions where there is enough space, raising the potential energy.

IV. Conclusions

The channel-size dependency of P-dopant placement in free-standing circular Si nanowires is understood well using a 10-band $sp^3d^5s^*$ atomistic tight-binding approach, where the charge and potential energy profiles are self-consistently determined by Schrödinger-Poisson simulations. Assuming a doping constant of $\sim 2\times10^{19}$, we study realistically sized Si nanowires that are fundamentally hard to be simulated using first principle theories. For nanowires of a channel cross-section $\geq$ 20nm, we observe more uniform doping reduces the channel energy while the pattern doesn't happen in smaller cross-sections, indicating donors are not likely to diffuse into the channel during the process of nanowire synthesis.

The reason of this pattern is investigated by simulating charge-neutral 20nm Si nanowires changing the placement of a single P-atom inside the channel. As the P-atom moves closer to the channel surface, it becomes harder to be fully screened along the direction towards the surface by electrons due to the lack of space. Consequently, electrons spread more towards the inside of the channel to maintain the charge-neutrality, increasing the overall channel potential energy. This work, combined with the strong connection to the recent experimental work [2], presents a comprehensive theoretical framework for understanding highly doped nanowires.

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REFERENCES

[1] T. Shinada, S. Okamoto, T. Kobayashi, and I. Ohdomari, "Enhancing semiconductor device performance using ordered dopant arrays," *Nature*, vol. 437, pp. 1128–1131, 2005.

[2] P. Xie, Y. Hu, J. Huang, and C. M. Lieber, "Diameter-dependent dopant location in silicon and germanium nanowires," *Proc. Natl. Acad. Sci.*, vol. 106, no. 36, pp. 15 254–15 258, 2009.

[3] J. Han, T.-L. Chan, and J. R. Chelikowsky, "Quantum confinement, core level shifts, and dopant segregation in p-doped si<110> nanowires," *Phys. Rev. B*, vol. 82, p. 153413, 2010.

[4] H. Ryu, S. Lee, B. Weber, S. Mahapatra, L. C. L. Hollenberg, M. Y. Simmons, and G. Klimeck, "Atomistic modeling of metallic nanowires in silicon," *Nanoscale*, vol. 5, pp. 8666–8674, 2013.

[5] M. Füchsle, J. A. Miwa, S. Mahapatra, H. Ryu, S. Lee, O. Warschkow, L. C. L. Hollenberg, G. Klimeck, and M. Y. Simmons, "A single-atom transistor," *Nat. Nanotechonol.*, vol. 7, pp. 242–246, 2012.

[6] B. Weber, S. Mahapatra, H. Ryu, S. Lee, A. Fuhrer, T. C. G. Reusch, D. L. Thompson, W. C. T. Lee, G. Klimeck, L. C. L. Hollenberg, and M. Y. Simmons, "Ohms law survives to the atomic scale," *Science*, vol. 335, pp. 64–67, 2012.

[7] S. Lee, H. Ryu, H. Campbell, L. C. L. Hollenberg, M. Y. Simmons, and G. Klimeck, "Electronic structure of realistically extended atomistically resolved disordered si:p δ-doped layers," *Phys. Rev. B*, vol. 84, p. 205309, 2011.

[8] M.-F. Ng, M. B. Sullivan, S. W. Tong, and P. Wu, "First-principles study of silicon nanowire approaching the bulk limit," *Nano Lett.*, vol. 11, no. 11, pp. 4794–4799, 2011.

[9] S. Kim, J.-S. Park, and K. J. Chang, "Stability and segregation of b and p dopants in si/sio2 coreshell nanowires," *Nano Lett.*, vol. 12, no. 10, pp. 5068–5073, 2012.

[10] M.-V. Fernandez-Serra, C. Adessi, and X. Blase, "Conductance, surface traps, and passivation in doped silicon nanowires," *Nano Lett.*, vol. 6, no. 12, pp. 2674–2678, 2006.

[11] G. Klimeck, S. S. Ahmed, H. Bae, N. K. R. Rahman, S. Clark, B. Haley, S. Lee, M. Naumov, H. Ryu, F. Saied, M. Prada, M. Korkusinski, , and T. B. Boykin, "Atomistic simulation of realistically sized nanodevices using nemo 3-d: Part i - models and benchmarks," *IEEE Trans. Elec. Dev.*, vol. 54, no. 9, pp. 2079–2089, 2007.

[12] E. Gawlinski, T. Dzurak, and R. A. Tahir-Kheli, "Direct and exchange-correlation carrier interaction effects in a resonant tunnel diode," *J. Appl. Phys.*, vol. 72, pp. 3562–3569, 1992.

[13] B. Weber, Y. H. M. Tan, S. Mahapatra, T. F. Watson, H. Ryu, R. Rahman, L. C. L. Hollenberg, G. Klimeck, and M. Y. Simmons, "Spin blockade and exchange in coulomb-confined silicon double quantum dots," *Nature Nanotechnol.*, vol. Advanced online publication, 2014.