

Equilibrium Bandstructure of a Phosphorus δ -doped Layer in Silicon using a Tight-binding Approach

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Abstract—Emerging STM technology opens the possibility of creating ultra-high doped silicon devices. For the theoretical analysis of Si:P QW devices, an atomistic tight-binding approach with self-consistent potential calculation is used. Fermi-level, 1Γ , 2Γ and 1Δ bands are of the same order with previous studies. Impurity bands can be simply explained by the band projection of silicon bulk bandstructure. The potential profile, in comparison with the single impurity potential, indicates that ionized donors are not only coupled to each other but also the impurity ions are screened by the electron charge. To demonstrate the advantage of atomistic simulation, the equilibrium bandstructures of δ -layers with different doping density and dopant configuration are computed. Increased number of dopants causes down-shift of valleys and the disordered configuration of donor atoms breaks the symmetry of 2D bands. This approach allows us to study more realistically extended and disordered devices in the future.

I. INTRODUCTION

Importance of Si:P technology: There has been rapid progress using scanning tunneling microscope (STM) patterning of donors in silicon, and experimentalists can control dopant placements with atomic scale precision to build a variety of planar δ doped devices, such as quantum dots and wires [1] [2] [3]. The 2D δ -layers serve as conducting leads to such devices, motivating the need for theoretical analysis of phosphorus δ doped layer (Si:P δ -layer) at equilibrium and investigate notable properties of doping dependency.

Previous works: Several theoretical studies analyzed the electronic properties of dense Quantum Wells (QW). Qian *et al.* used planar Wannier orbitals based on the empirical pseudopotential method (PP) assuming the parabolicity of sub-bands [4]. Cartoixa *et al.* calculated temperature and doping dependence of the equilibrium Fermi level in the Si:P δ layer structure based on atomistic sp^3s^* tight-binding (TB) with anti-bonding orbital model [5]. However, sp^3s^* is known to represent the X points in the conduction band badly [6], and it is unclear whether the number of basis is enough since additional basis is needed to appropriately describe L and X valleys in the bandstructure [7]. Most recently, Carter *et al.* calculated bandstructures of the Si:P δ layer in different configurations using Density Functional Theory (DFT) approach [8]. However, the computational burden of DFT calculation

prevents them from simulating realistically extended device structures.

Atomistic modeling and NEMO 3-D: The effects of the silicon bandstructure and potential profile due to ionized donors have been quantitatively explored with our empirical TB model for single donors [9] [11]. The Nanoelectronic Modeling Tool (NEMO 3-D) [10] can simulate atomistic structure of realistic size and to include non-parabolicity of bulk materials automatically by using empirical $sp^3d^5s^*$ TB model. NEMO 3-D was successful in many problems that simplified EMA failed to tackle [10], one of which was to predict the spectrum of single phosphorus impurity in Si FinFET [11]. Here, we explore the validity of NEMO 3-D based calculation for Si:P δ -doped system to ultimately model realistically extended and disordered systems.

This paper is organized as follows. In Section II, the simulation approach and device is introduced. Section III is divided into two parts; in part A, the atomistic TB approach is benchmarked with previous studies and a couple of examples - doping density and donor configuration - that exhibit unique capabilities of atomistic simulation is demonstrated in part B. Section IV summarizes and concludes the paper.

II. METHODOLOGY

Self-consistent calculation: The major simulation scheme used in this work is to obtain the potential profile and bandstructure using the charge density based on a self-consistent calculation. This has been implemented to run in parallel on super computers, and this self-consistent loop was initially applied to observe the temperature dependence of electronic properties of Si:P QW [12] [13].

The Density of States (DOS) and Local DOS are computed over the 2D k space. Subject to the charge neutrality condition in equilibrium, where the total electron number equals the number of positively ionized donors, the Fermi level of the system and electron charge profile are determined self-consistently with the potential profile. Exchange and correlation effects are taken into account within the Local Density Approximation (LDA) [14]. Typical calculations require 128 cores for about 30 hours. A graphical representation of this self-consistent scheme is depicted in Fig. 1.

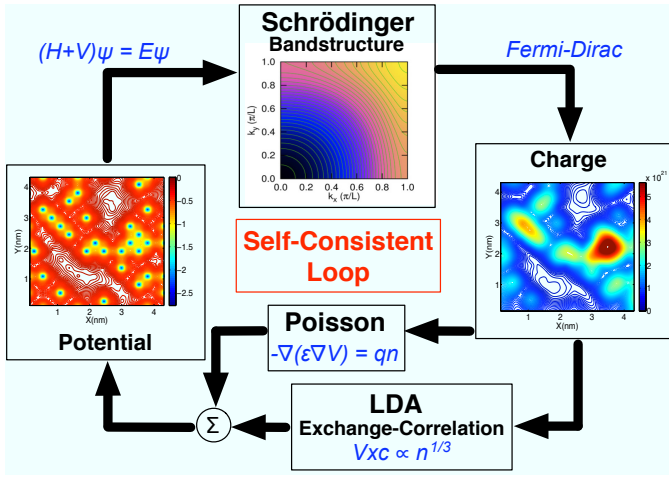


Fig. 1. Self-consistent bandstructure calculation scheme used in this simulation. An atomistic $sp^3d^5s^*$ TB Hamiltonian is used for charge integration. Potential profile is computed from FDM Poisson solution. LDA correction is included for exchange-correlation effects.

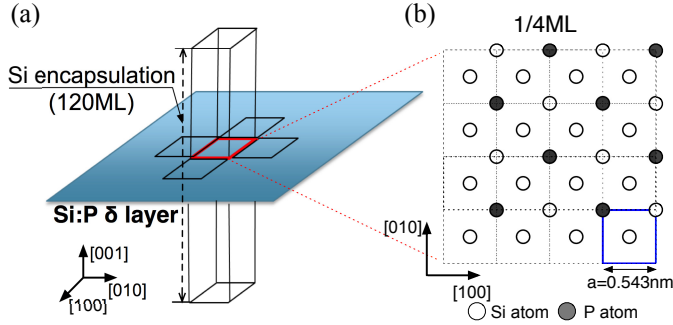


Fig. 2. (a) Simulation structure of Si:P δ -layer encapsulated by silicon. (b) Cross-sectional view of Si:P δ -layer with 1/4ML doping (corresponds to $1.7 \times 10^{14} \text{ cm}^{-2}$). The superlattice is large enough to simulate various doping configurations.

Simulation structure: The physical structure used in this work is depicted in 2(a). Periodic boundary conditions are applied to the in-plane directions of the Si:P δ layer. The silicon encapsulation layer is assumed to be intrinsic and should be thick enough (120ML at $<4\text{K}$) to prevent the impurity states from moving due to the confinement wall. Increasing the cap layer from The size of the 2D periodic super cell used in this simulation is set to $4a \times 4a$, $a = 0.543\text{nm}$, which is large enough to account for various doping density. The ordered placement of dopant atoms with 1/4ML doping constant is shown in Fig. 2(b). For the Hamiltonian, the $sp^3d^5s^*$ TB basis without spin-orbit coupling is used. We assumed 4K as the electron temperature throughout the paper.

III. SIMULATION RESULTS AND DISCUSSION

A. Validation of Si:P δ -layer equilibrium properties

Bandstructure: Table I provides a comparison with previous methods and shows that the atomistic TB approach predicts the reasonable band minima and Fermi level with respect to the other methods. Fig. 3(a) shows the equilibrium bandstructure

TABLE I
COMPARISON DATA FOR THE FERMİ ENERGY, 1Γ , 2Γ AND 1Δ OF Si:P QW BANDSTRUCTURE (REFERENCE: SILICON $E_C=0.0\text{eV}$)

Energy(meV)	$sp^3d^5s^*$	PP [4]	sp^3 [5]	DFT [8]
E_F	-110	-111	~ -110	-110
1Γ	-394	-410	N/A	-540
2Γ	-369	-400	N/A	-420
1Δ	-242	-270	N/A	-210

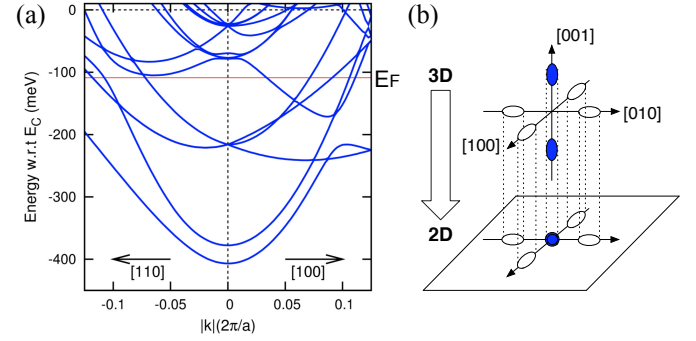


Fig. 3. (a) Bandstructure of a δ -layer of 1/4ML at 4K plotted with respect to *silicon bulk band minima*. The impurity band is shown below the silicon conduction band minimum. Zone folding is observed due to the two-fold redundancy of the supercell, hence the 1Δ valley resides at $k_x = 0.07(2\pi/a)$. (b) The 2D band projections of silicon bulk bandstructure. Two valleys are projected to the gamma point, changing the valley landscape from 6Δ to $2\Gamma+4\Delta$.

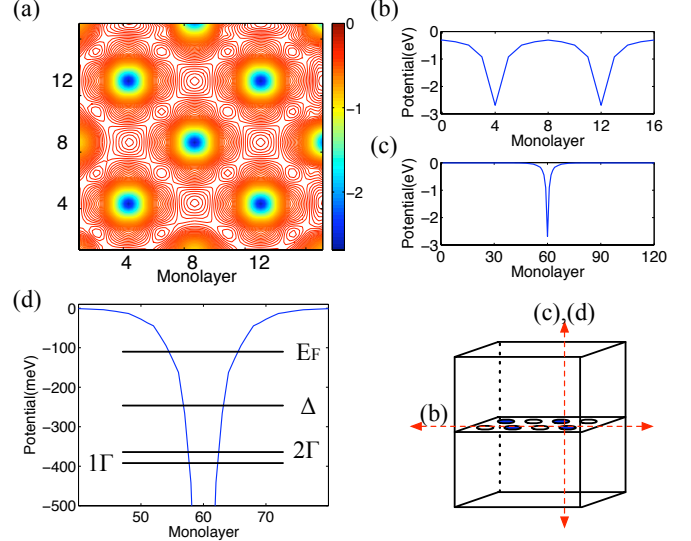


Fig. 4. Equilibrium potential profile of the 1/4ML δ -layer at 4K (a) in the δ -layer plane, (b) along one of the in-plane monolayer, (c) along the confinement direction and (d) zoom-in plot of (c) with corresponding Fermi level, 1Γ , 2Γ and 1Δ positions. Note x is in *monolayers*; in $[100]$ oriented structure, the distance between the monolayers is $a/4 = 0.1358(\text{nm})$.

of the Si:P δ -layer plotted with respect to the *silicon bulk band minima*. It turns out that the LDA treatment results in 30meV downshift of bands [13]. Due to the potential from the ionized donors, bands are pulled down below the bulk

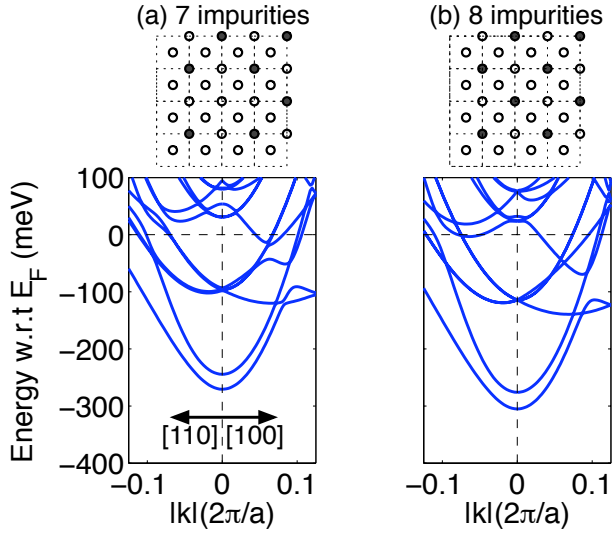


Fig. 5. Bandstructures of δ -layers with different number of impurities plotted with respect to the Fermi level: (a) 7 impurities, (b) 8 impurities (default). The doping configuration for (a) is chosen such that the impurities are regularly positioned throughout the domain.

silicon conduction band minima. Unlike EMA, TB can not only observe atomistic effects, such as, dopant configurations and including randomness but also automatically take into account the six-fold degeneracy of silicon bandstructure and the coupling between the valleys. Since the supercell is repeated, zone folding is observed, where the position of the 1Δ band appears around $0.07(2\pi/a)$. As shown in Fig. 3(b), two out-of-plane valleys are projected to $k_x - k_y$ plane to form 1Γ and 2Γ bands, while remaining four in-plane valleys stay along $\langle 100 \rangle$ as in bulk. The confinement mass is larger in gamma-projected valleys ($m_l = 0.91m_0$) than remaining in-plane valleys ($m_t = 0.19m_0$), resulting in lower quantization energy ($\propto m^{*-1}$) of gamma-projected valleys. However, the Γ projected bands interact with each other creating a sizeable valley splitting (VS). Since the quantum well is very thin, the valley splitting can reach tens of meV [16] [17]. An analytical model for VS in V-shaped QWs has previously been developed [17].

Potential profile: Fig. 4 shows various potential cut of the simulated device. Fig. 4(a) and (b) shows perfect periodicity of the potential profile in such $1/4\text{ML}$, regular patterned 2D layer. In contrast to the single impurity potential [15], charge screening and electrostatic coupling between impurities significantly alter the in-plane potential landscape. The effect of charge screening in such Si:P δ doped devices is further described in [13]. The strong electrostatic confinement of this δ -layer is shown in Fig. 4(c). In conjunction with Fig. 3, where the valley splitting of 25(meV) is observed, the confinement from donor potential provides strong confinement of impurity states below silicon conduction band minima. The position of Fermi level and valley minimum points plotted with respect to the confinement potential are indicated in Fig. 4(d) and this plot represents similar pattern with previous studies [4] [8].

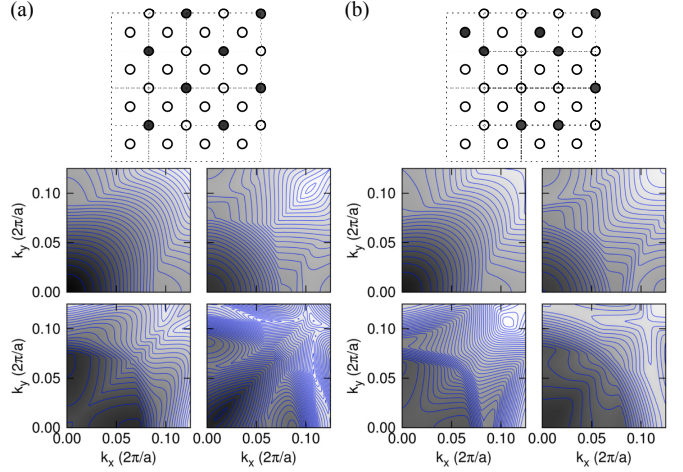


Fig. 6. 2D contour plot of first four subbands of $1/4\text{ML}$ δ -layer with (a) ordered configuration and (b) disordered configuration. Compared to the perfect case (a), disordered configuration breaks the periodicity within the supercell and it results in the symmetry breaking of bandstructure.

B. Atomistic effects

Motivation: From the bandstructure studies, the Si:P δ -layer turns out to be *semi-metallic*; it conducts since there always exist states available around Fermi level. However, it is not expected to behave as perfect metal because of the non-uniform distribution of density of states and it will exhibit unconventional conductance pattern. This information can be crucial when it is coupled to wires and quantum dots in cryogenic environment. Therefore, it is worthwhile to investigate the bandstructure of δ -layer with variety of doping densities and dopant configurations in atomistic treatment with the self-consistent method described in previous section. In this section, a couple of examples are demonstrated before exploring realistic and extended devices.

Doping density: To examine the doping density dependence of the δ -layer bandstructure, different numbers of impurities can easily be placed in the simulation domain by substituting silicon atoms to donor atoms. Fig. 5 depicts an example with different doping density. It is clearly shown that as more impurities are in the domain, more subbands are included below the Fermi level to satisfy charge neutrality.

Dopant configuration: Using the atomistic tight-binding simulation, it is also possible to introduce different donor configuration in the simulation domain simply by putting impurities on available sites at random. Fig. 6(b) shows an example of disordered donor configuration in the δ -layer. A notable observation from the bandstructure comparison in Fig. 6 is that in the disordered cell, the subbands are not in perfect symmetry. Similar effect is observed in random alloys in III-V or SiGe systems, where atom placement and/or strain play a significant role to the modification of states [10] [18] [20]. In Si:P δ -layers, the electrostatic potential from donors introduces disorder in the Hamiltonian and it breaks the symmetry of the bandstructure.

IV. CONCLUSION

For the theoretical analysis of Si:P QW devices, an atomistic TB simulation with self-consistent calculation is used. Results are in good agreement with previous studies and the band projection and coupling can be reasonably explained for small cells. The potential profile, in comparison with the single impurity potential, indicates that ionized donors are not only coupled to each other but also impurity ions are screened by electron charge. Next, we investigated the effect of doping density of the δ -layer. We expect a linear down-shift of subbands as the doping increases, which may be used to predict correct density of state distribution and electrical characteristics in real δ doped devices. Atomistic disorder effects can be captured automatically and it breaks the symmetry of impurity bands. With this new methodology, we are now ready to explore realistically disordered systems which may contain tens of thousands to millions of atoms [10].

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