Tight-binding Simulations of Channel Modulation in a Single Atom Transistor

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Introduction

There has been remarkable progress in the use of a scanning tunneling microscope to pattern various highly phosphorus δ-doped Si (Si:P) devices [1], [2], [3]. The physical realization of a single atom transistor [3], is especially a quite remarkable achievement since it represents the ultimate limit of device downscaling. In this work, we not only perform the first tight-binding study of the gate-bias dependent shift of the electron ground state (1s(A)) in the single-atom channel, but also demonstrate strong connections between the modeling and the experiment confirming the demonstrated device is indeed a single atom transistor.

Modeling Approach

Based on the gate-bias dependent channel potential profiles that are obtained via the Thomas-Fermi approach [4], the energy-level quantizations formed by a single phosphorous atom in Si bulk are calculated with a 3-D Nanoelectronics MOdeling Tool for Petascale simulations (NEMO 3-D PETA), where the channel electronic structure is described with a $sp^3d^5s^*$ tight-binding model [5], [6]. Fig. 1(a) illustrates the simulation domain, where we only considered the gate modulation of the channel assuming the source and drain are grounded.

Result and Discussion

The equilibrium potential profile is shown in Fig. 1(b), where the 2-D surface plot on the doping plane as well as the 1-D plots along various line-cuts are presented. The phosphorous ions in highly δ-doped (1/4ML) nanowires that act as leads, pull down the conduction subbands into Si band gap creating a potential barrier over the low doped ($\sim 10^{15}/cm^3$) P-type Si channel. Strong electron confinement is created by a phosphorous atom in the channel.

Gate-bias dependent channel potential profiles are shown in Fig. 2 with energetic positions of 1s(A) state and Fermi-level. Higher gate bias reduces the channel barrier height and the energy level of 1s(A) state such that 1s(A) state meets the Fermi-level filling the first electron into the channel at the gate bias of 0.45V. Further increase of gate bias shifts up the channel potential and the 1s(A) state due to electron screening of the channel phosphorous ion. At the gate bias of 0.72V, the 1s(A) state again hits the Fermi-level filling the second electron. Fermi-level doesn't change since we assumed a zero source-drain bias for all the simulations.

The pattern of the channel modulation is summarized well in Fig. 3, which provides three strong connections to the experimental result reported in Ref. [3]. First, we obtain the energy needed to fill the first electron into the channel as 46.3 meV that is on top of the measured value. Second, the two gate-biasing points that fill a new electron into the channel, happen at Vg = 0.45 and 0.72V, where the experiment locates these *vertex points* at Vg = 0.45 (almost same) and 0.8V (10% inaccuracy). The third connection can be found from the slope of lines - the gate controllability over the 1s(A) state that is obtained as 0.15 where the experiment shows 0.12.

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Conclusion

Channel modulation in the physically realized single atom transistor (Ref. [3]) is simulated with a tight-binding approach. Results are discussed focusing on connections to the experiment that are strong enough to confirm that the device contains exactly a single phosphorous atom in the channel.

References

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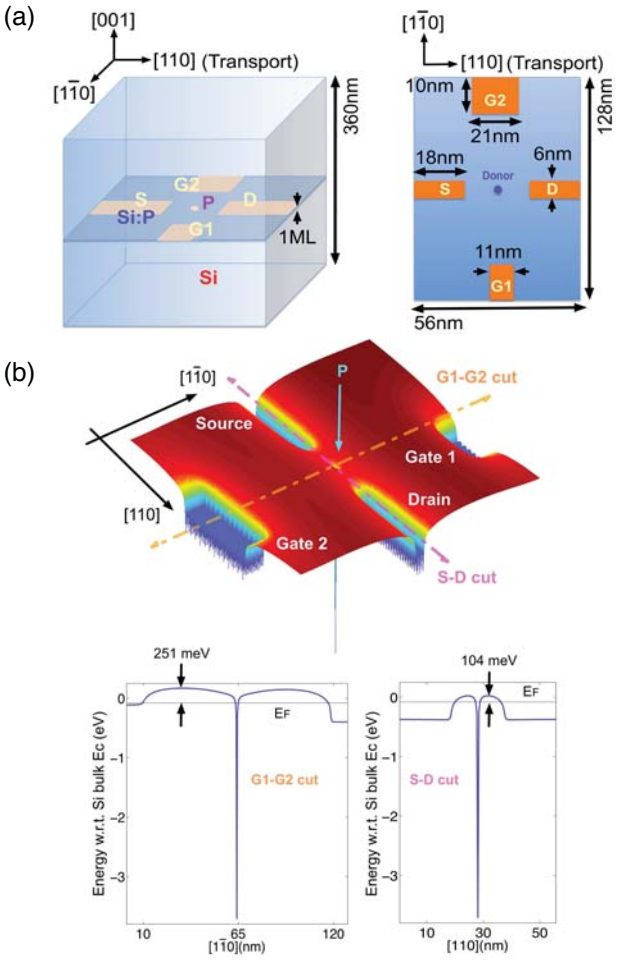

Fig. 1. (a) Simulation domain: (Left) a 3-D View (Right) a 2-D View onto the doping plane. (b) Potential profile at equilibrium on the doping plane. Densely δ-doped Si:P nanowires form leads and a single phosphorous atom creates a strong electron confinement in the channel. A zero energy references to the conduction band minimum of intrinsic Si bulk.

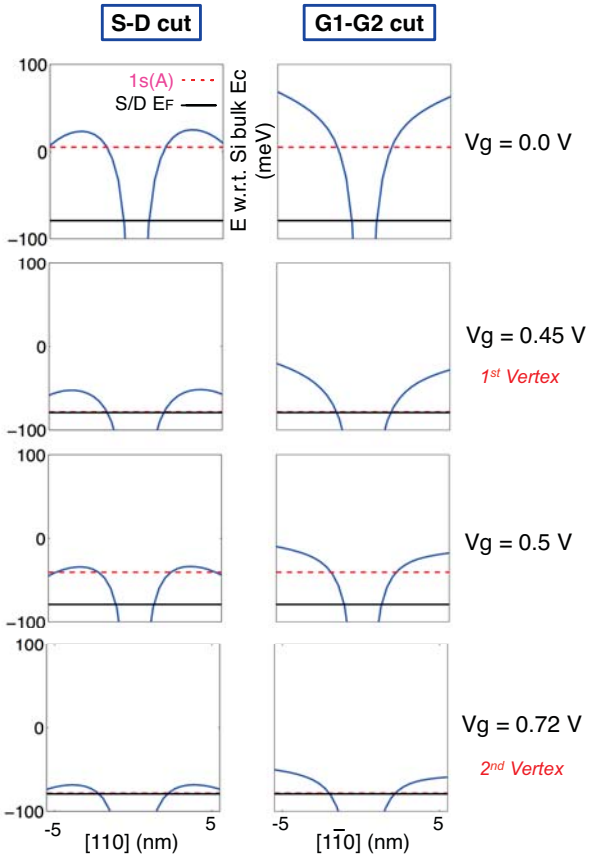

Fig. 2. Bias-dependent channel potential profile and 1s(A) state: The energetic level of electron ground state decreases with increasing gate bias such that source-drain Fermi-level meets the 1s(A) state at Vg=0.45V filling one electron in the channel. At larger gate bias, the 1s(A) state shifts up due to the electron screening over the channel phosphorous ion and decreases again filling the second electron at Vg=0.72V.

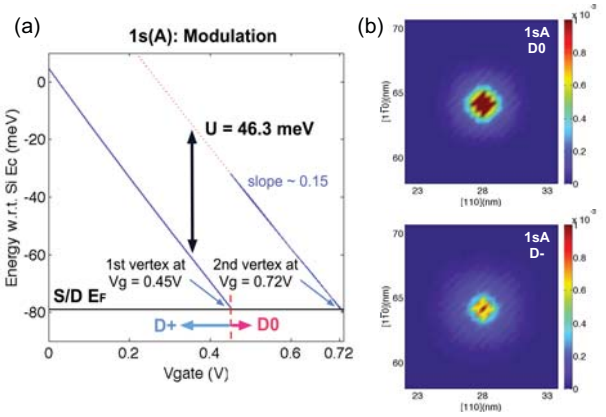

Fig. 3. (a) Gate modulation of 1s(A) state. Charging energy, lever-arm of gate bias, and the position of two vertex points (@Vg=0.45, 0.72V) demonstrate strong connections to experiment (Ref. [3]). (b) Electron wave functions at two vertex points showing a strong confinement even at the second vertex.