Modeling Transport in Phosphorus δ-Doped Silicon Tunnel Junctions

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There is growing interest in electrical devices based on phosphorus-doped Silicon (Si:P) δ layers, which can be fabricated with atomic precision using scanning tunneling microscope (STM) lithography. A STM is used to make lithographic patterns by selectively removing hydrogen from a hydrogen-passivated Si surface. Phosphene gas is then introduced and adsorbs where the hydrogen has been removed. The result is precise, planar structures made from a high density ($\approx 1.7 \times 10^{14} cm^{-2}$) of P donors. While great strides have been made in fabricating nanoelectronics from Si:P δ layers, the electronic structure (Figs. 1, 2) of the Si:P δ layers deviates significantly from that of silicon at normal levels of doping, and theoretical studies have produced inconsistent predictions (Table 1). This makes it difficult to accurately model devices made from Si:P δ layers.

In this work, we flip the problem around and use experimental transport measurements from nanoscale tunnel junctions to study the electronic structure of Si:P δ layers. We model tunnel junctions both with (Fig. 2) and without (Fig. 4) a gate to modulate the potential in the junction. We show that the transport properties of tunnel junctions depend strongly enough on the electronic structure that measurements could provide insight into the electronic structure (Fig. 3). We also model the effect of in-plane (patterned phosphorus, Figs. 4, 5) and surface (metal-dielectric) gates, since such gates will be necessary for more advanced devices. We compare our model to experimental results and find good agreement.

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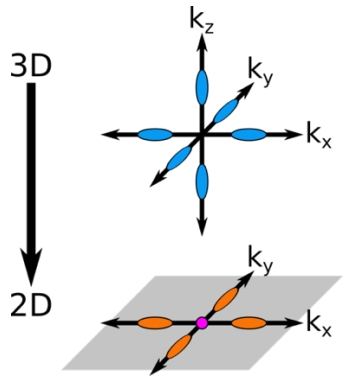

Fig.1: Basic band structure in a δ-layer. The charged δ-layer confines the electrons to a 2D plane. The six valleys in bulk Si (top) are effectively projected into 2D (bottom) — forming two types of bands: The two bulk Si bands along $\pm k_z$ are transformed into two Γ bands centered at $\vec{k} = 0$ (magenta), and the remaining four bands become known as Δ bands (orange).

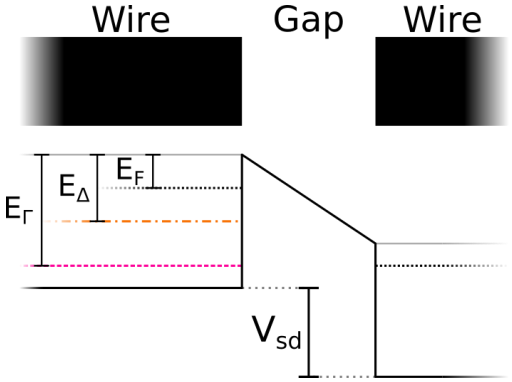

Fig.2: Top: top view of a δ-layer tunnel junction. Bottom: cross section of potential barrier along the wire axis. The barrier is trapezoidal due to a source-drain bias V_{sd} across the junction. The Γ and Δ bands and quasi-Fermi level E_F are shown as dashed curves. The grey curve is the bulk Si conduction-band minimum.

Model	E_{Γ_1}	E_{Γ_2}	E_Δ	E_F
DFT (1D) [1]	296	288	165	72
DFT (3D) [2]	369	269	68	23
TB (3D) [3]	401	375	249	115
DFT (1D) [4]	419	394	250	99
TB (3D) [5]	427	421	287	142

Table 1: Predicted band energy minima (see Fig. 1) and Fermi level E_F for quarter-layer doped δ-layer sheets — computed with density functional theory (DFT) and tight binding (TB). Values are measured in meV below the conduction-band minimum.

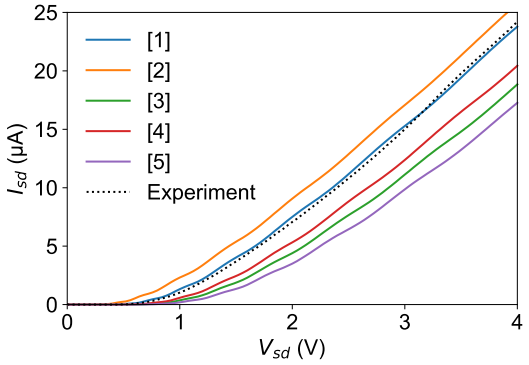

Fig. 3: Predicted total current through a tunnel junction formed from a 35-nm-wide wire with a 15-nm-wide gap for all parameters in Table 1 (references for parameters in legend) as well as experimental data (dotted). For this calculation, a 78 kΩ resistance is placed in series with the tunnel junction to better replicate experimental conditions.

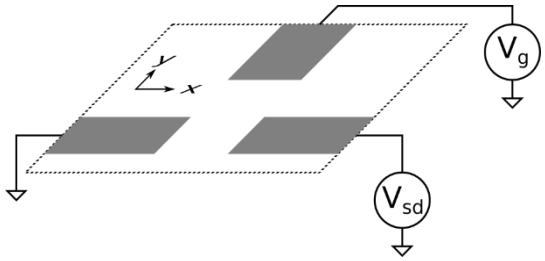

Fig. 4: A more complicated geometry includes an in-plane gate in addition to the tunnel junction. This requires an electrostatics simulation and a 2D treatment of tunneling through the barrier.

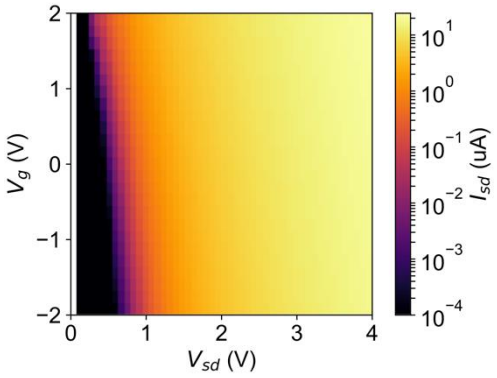

Fig.5: Current through a 35-nm-wide wire with a 15-nm-wide gap with the addition of an in-plane gate (Fig. 4).