Theoretical analysis on the effect of coupling between dopants and leads in Si nanodiodes for band-to-band tunneling enhancement

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Band-to-band tunneling (BTBT) [1] in silicon is a promising alternative mechanism for sub-thermal swing devices, such as tunnel field-effect transistors (TFETs). Si is an indirect-bandgap material, so this mechanism is hindered by the need for phonon assistance to conserve momentum in tunneling between bands. It can be expected, however, that the presence of dopant-induced states in the depletion region can relax this condition. As device dimensions are reduced [2], discrete dopants at front edges of the depletion region can become critical in providing pathways for BTBT transport in Si nanodiodes [3].

Here, we address key factors by simulations, combining first-principles (*ab initio*) and semi-empirical (transport) simulations to o btain current-voltage (IV) characteristics under specific conditions. Focus is on donor-acceptor (DA) pairs in different configurations between highly-doped p^+/n^+ leads.

This study considers Si nanowires oriented along <100> crystalline direction (transport direction, Z), with an atomistic structure controlled and geometrically optimized using Quantum ATK simulation [4]. **Fig. 1(a)** shows a simplified device structure with central region length of 5.43 nm, and electrostatically-doped leads of length 1.08 nm each. Electrostatic doping method consists of jellium-like uniform distribution of extra charges in Si leads, corresponding to high dopant concentrations, $N_D=N_A=2\times10^{20}$ cm^{-3}. This method is used to simply shift the Fermi levels on each lead as if dopants would be introduced in the Si matrix, without actually having such dopants incorporated in these leads. The effective zone between lead extensions that can be conceptually treated as a "depletion region" remains to have a length of 3.26 nm. Dopants are introduced in this central region (Boron (B) on left and Phosphorous (P) on right), and the entire structure is passivated by hydrogen (H) and optimized.

IV characteristics are simulated at room temperature (T=300 K). **Fig. 1(b)** shows a comparison between results obtained without dopants and with a donor-acceptor (D-A) pair, with inter-dopant distance, $d_{D\text{-}A}$=5.43 Å and 16.29 Å. First, all characteristics exhibit tunnel-diode behavior. However, it should be noted that phonon scattering is not included in these simulations. Second, it can be seen that the presence of a D-A pair induces an overall current enhancement by even an order of magnitude. This result suggests the positive effect of such front-side dopants on the current enhancement.

It will be argued that there are several key factors in further tuning this contribution, mainly dopant-lead coupling and alignment of dopant-induced energy states. **Fig. 1(c)** shows the LDOS spectra simulated without and with dopants. The presence of D-A pair makes the tunnel barrier narrower, in particular when dopants are nearer to leads. It is found that BTBT current increases with increasing the overlap of wavefunctions, as the dopant is shifted closer to its respective lead, even if the distance between donor and acceptor is also increased simultaneously.

These results can provide guidelines for tuning BTBT current enhancement in Si nanodevices.

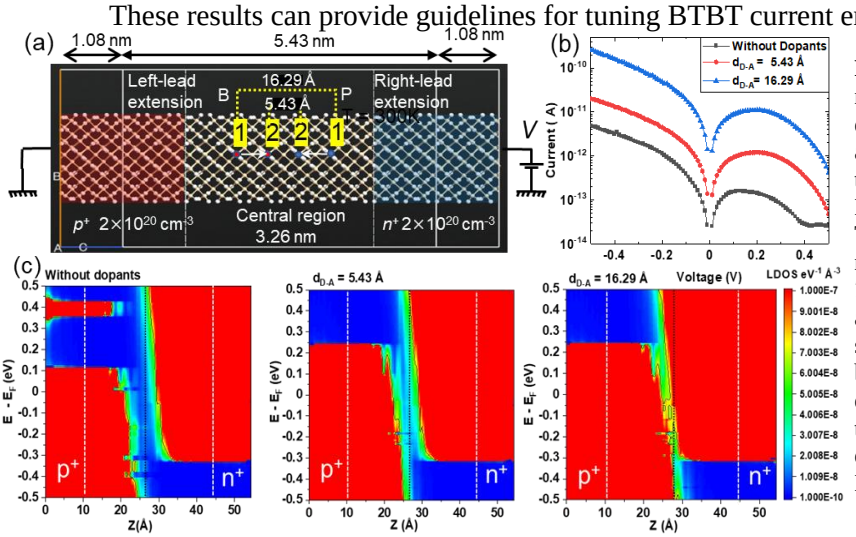

Fig. 1. (a) Atomistic view of a (100)-nanowire p^+-n^+ diode, with discrete dopants, one P-donor and one B-acceptor, substitutionally introduced in the central region (distances in each DA pair are indicated in the figure). The cross-section is on the order of ~1 nm. **(b)** *IV* characteristics simulated at *T*=300 K for a device shown in (a) with a D-A pair at different positions, symmetrical relative to center (labeled by indexes from 1 to 2). **(c)** Local density of states (LDOS) spectra for two cases at V=0 V: without discrete dopants and with a D-A dopant pair. LDOS range is valid for all graphs.

References [1] L. Esaki and Y. Miyahara, Solid State Electron. **1**, 13 (1960). [2] H. Schmid et al., Nano Lett. **12**, 699 (2012). [3] M. Tabe et al., Appl. Phys. Lett. **108**, 093502 (2016). [4] S. Smidstrup et al., J. Phys.: Condens. Matter **32**, 015901 (2020).
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