The 19th International Conference on Global Research and Education (Inter-Academia 2021)

Theoretical study of the impact of a donor-acceptor pair on tunneling current in Si nanodiodes

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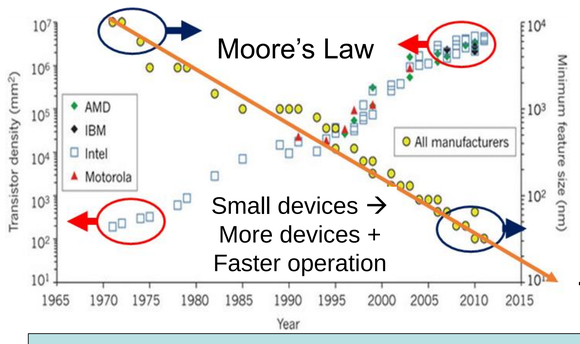
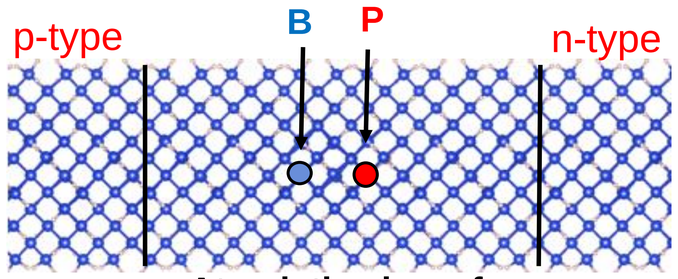
Dopant individuality and its role in *p-n* and p^+-n^+ junctions

I. Ferain *et al*., Nature 479, 310 (2011)

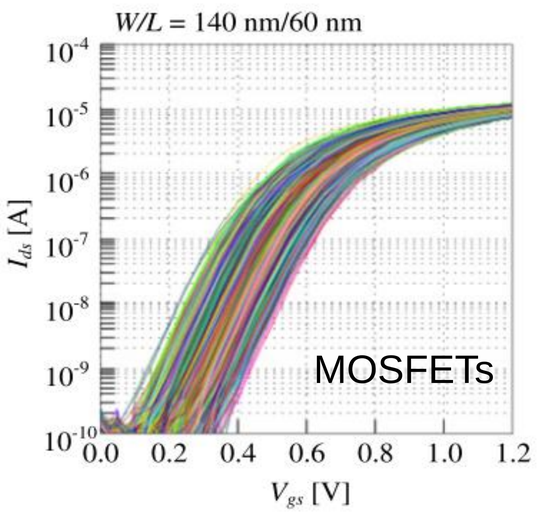


< 10 nm

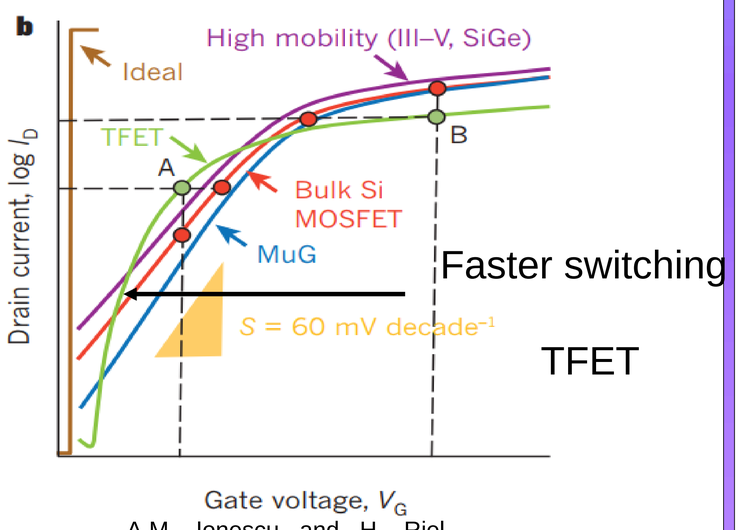


Atomistic view of nanoscale *p-n* junctions

Conventional dopants (Phosphorus and Boron) can mediate transport in even in an "atomic"-level diode



T. Tsunomura, A. Nishida, and T. Hiramoto, Jpn. J. Appl. Phys. **49**, 054101 (2010).



A.M. Ionescu and H. Riel, Nature **479**, 329 (2011).

<u>Purpose</u>: to study the impact of conventional dopant-atoms on BTBT in nanoscale Si Esaki diodes

Simulation Methodology : QuantumATK

First-principles simulation flow

Electronic states

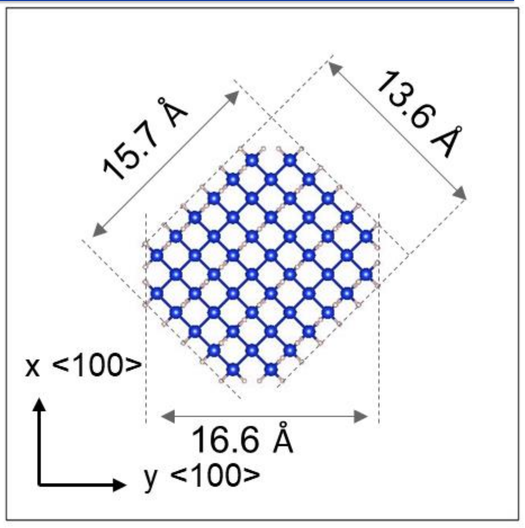
1. Density Functional Theory (real space)
2. LCAO basis function
3. Pseudopotential
4. Structural optimization (important)

***D*: Nonequilibrium Density Matrix**

***H*: Hamiltonian**

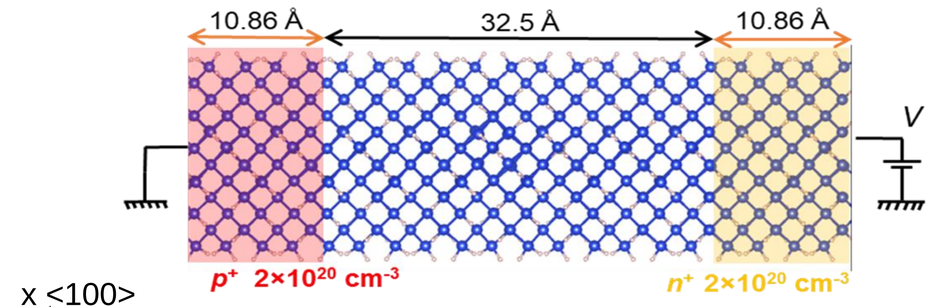
Quantum transport

1. Modelling contact electrodes using *ab-initio* self-energy
2. Non-equilibrium carrier distribution based on Non-Equilibrium Green Function (NEGF)
3. Transmission spectrum & tunneling current



❑ Dopants are inserted substitutionally in a Si nanowire

❑Geometry optimization is carried out after H-passivation and doping

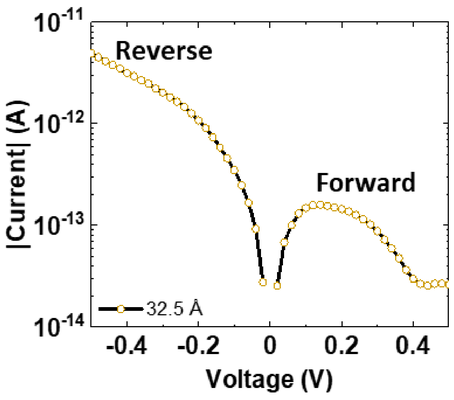


❑ *E*lectrostatically doped leads

❑ Non-Equilibrium Green's Function (NEGF)

✓ I-V Characteristics & LDOS (local density of states) are calculated

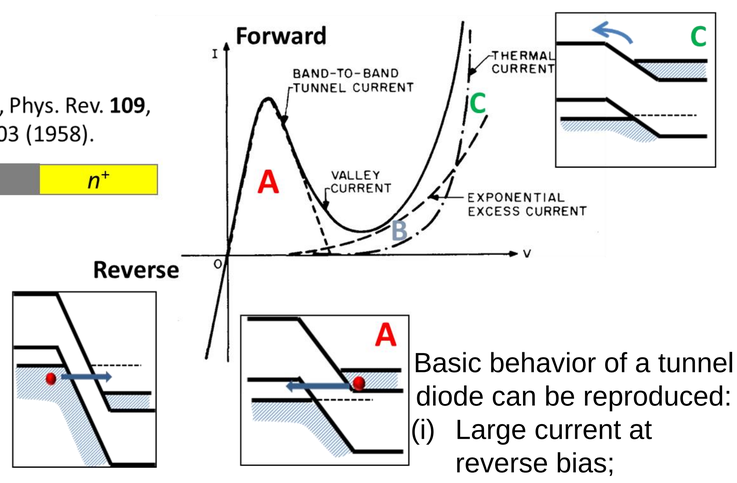
Device Structure: Tunnel Diode with (undoped) central region



- No phonon contribution
- No excess current
- Quantum size effect

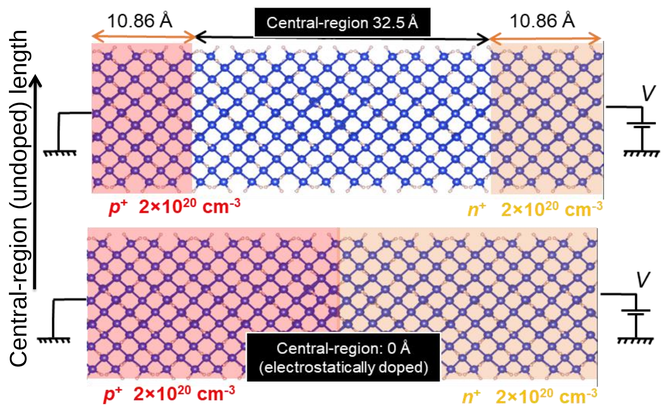
L. Esaki, Phys. Rev. **109**, 603 (1958).

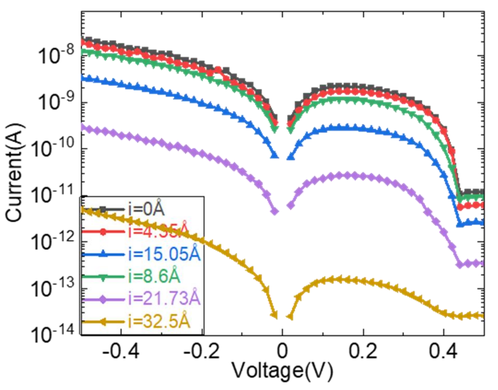
p^+ n^+



Basic behavior of a tunnel diode can be reproduced:
(i) Large current at reverse bias;
(ii) NDC at forward bias.

Effect of central-region length: tunnel rate modulation



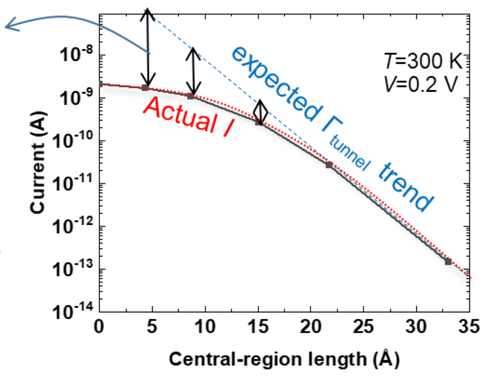


Large central region

Δ*I* = deviation of the actual current from the "ideal" expected trend of tunnel rate (exponential)

⇩

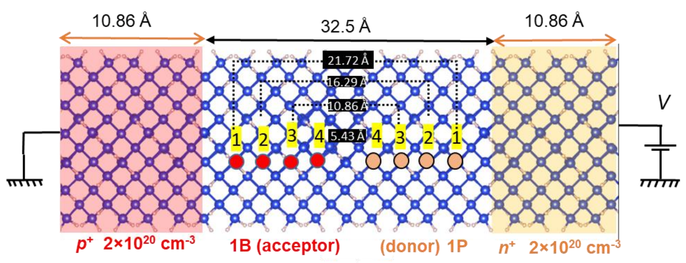
Formation of a natural "**depletion layer**" as p^+ and n^+ regions approach each other

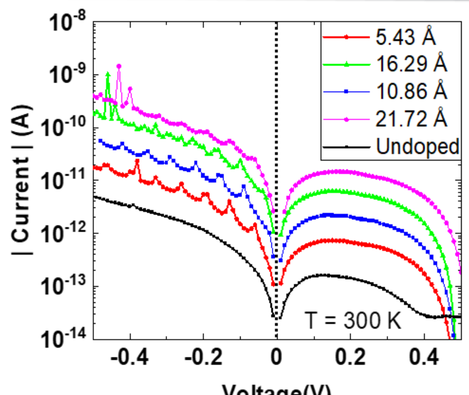


Systematic decrease of $L_{central}$ ↓ Systematic increasea of Γ_{tunnel} ↑

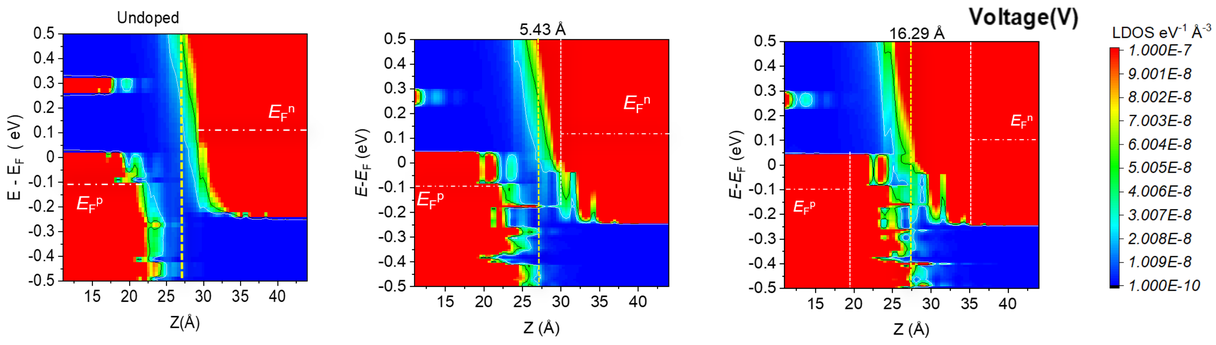
Central region: consumed by (electrostatic) doping

Effect of donor-acceptor (DA) pair in the central region





- 1P-1B cases give all higher currents than undoped case
  - Two orders increase in the current levels occurs with changing the configuration of D-A pairs (1P-1B).



Local Density of States (LDOS) interpretation for V_{bias}=0.2 V

➢D-A pair makes the tunnel barrier narrower, depending on the configuration of the donor-acceptor pair

Conclusions

❑ **Transport via highly-doped Si Nanodiodes**

✓Basic tunnel-diode features are mostly reproduced

❖ "electrostatic doping" = an approximation of actual doping
→ effect of the central-region length has been studied

❑ **Discrete doping with donor-acceptor pair in central region**

✓Tunnel-diode features are maintained, but current level depends on D-A pair configuration

❑ **Electric field and Energy states**

✓Electric field induced effect → modifications of the band edges

✓Energy alignment is also important (may lead to strong enhancement for particular configurations)

- **new properties of (highly codoped) Si**
- **new functionalities for BTBT devices**