Contact Block Reduction (CBR) for Ballistic Transport with Atomistic Basis Sets

nanoHUB online simulation and more — an NCN project

Objective:

- Evaluate Retarded Green's Function (G^R) for open systems in an atomic basis set with reduced computational cost.

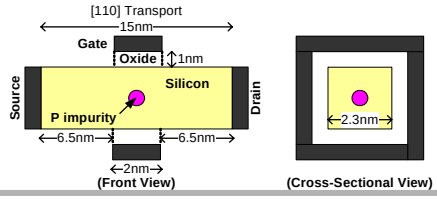
Approach:

- Use ***Contact Block Reduction*** (CBR) with atomistic tight binding (TB) band model.
- Identify ***basis-dependent efficiency criteria.***

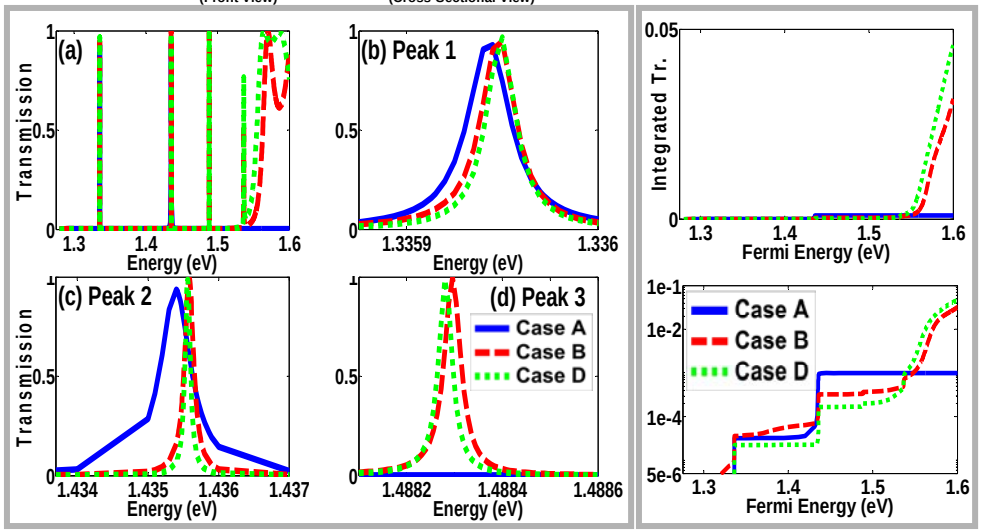
Result:

- The numerical efficiency of CBR is hard to be achieved unless **BM has cubic-grid bases**.
- CBR is still efficient with TB for ***the RTD-like device***, where a few strongly confined states dominate transport in a narrow energy range.
- ***k·p* can be the optimal solution** to attack following problems at one time:
  - Modeling of ***the hole-transport*** through wires with acceptable accuracy.
  - Modeling of ***multi-contact effect* (>2).**
  - Evaluation of G^R with good efficiency.

[TB]

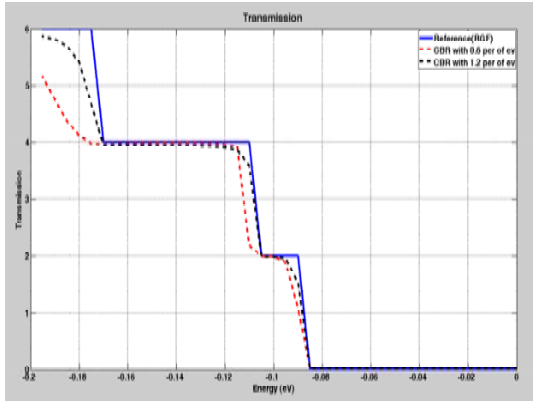


Method	Number of used ev's	Subdivision of boundary block	Time for sim. (s)
A: CBR	3(0.013%)	Use	658
B: CBR	10(0.044%)	Use	647
C: CBR	10(0.044%)	Don't Use	3341
D: RGF	----	----	7737



[*k·p*]

Hole transmission in Si wire of 2n square cross-section at equilibrium



[1] D. Mamaluy *et al*, J. of Appl Phys 93:4628 (2003)
[2] H. Ryu and G. Klimeck, Proceedings of ICSICT 2008

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