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Transport Calculation of Semiconductor Nanowires Coupled to Quantum Well Reservoirs

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INTRODUCTION

Semiconductor nanowires represent an attractive material system since they can be now produced with controlled material composition, physical dimensions, and electronic properties. Furthermore they can function at the same time as interconnects and as devices: with an individual nanowire, nanoscale field effect transistors (FETs) have already been realized [1].
On a simulation perspective, semiconductor nanowires are also very interesting because they exhibit electronic properties that can not be found in the usual MOSFET, like the 2D confinement of the electrons (or holes) in the channel. This implies that the widely spread effective-mass approximation can no more be used for transport calculation in devices with strong confinement, where the bandstructure plays a crucial role. In this work, therefore, an atomistic treatment of silicon nanowires is proposed with not only perfect contacts but also transitions from 1D (quantum well) to 2D (quantum wire) confined structures.

RESULTS

To account for bandstructure effects in Si nanowires, the $sp^3d^5s^*$ empirical tight-binding method is applied. Its parameters are optimized to reproduce the bulk bandstructure [2] and are assumed unchanged for nanostructures. The wire itself is constructed by translating the primitive unit cell of the semiconductor crystal, composed of two atoms. A small example with two additional quantum well reservoirs is shown in Fig. 1: the two different atoms of the primitive cell are plotted with different colors. Others than (100) growth directions can also be selected.

Any quantum transport problem requires appropriate open boundary conditions. The usual technique assumes semi-infinite reservoirs (Source and Drain) that are the prolongation of the device. In the present case this means a 2D electron confinement for the reservoirs. However, realistic devices have larger Source and Drain regions than the nanowire channel, leading to a transition from a 1D confined electron gas to a 2DEG one. This has a strong influence on the characteristics of the device, such as the transmission and the density of states, as shown in Fig. 2 and 3 but also on the computational effort.
The device is solved with an atomistic Green's function method whose boundary conditions are represented via self-energies. Their calculation can be accomplished via a recursive algorithm [3]. However 80% of the CPU time is still dedicated to that process. To improve the numerical efficiency a new algorithm was developed, based on the propagating waves in the reservoirs. It is 15-20 times faster than what is presented in Ref. [3] for this specific problem. The well established algorithm is labeled "Sancho-Rubio", the new one "injection" in Fig. 3.

CONCLUSION

A more realistic treatment of Si nanowires is presented where perfect contacts are replaced by quantum wells. A new algorithm is used to solved the resulting problem.

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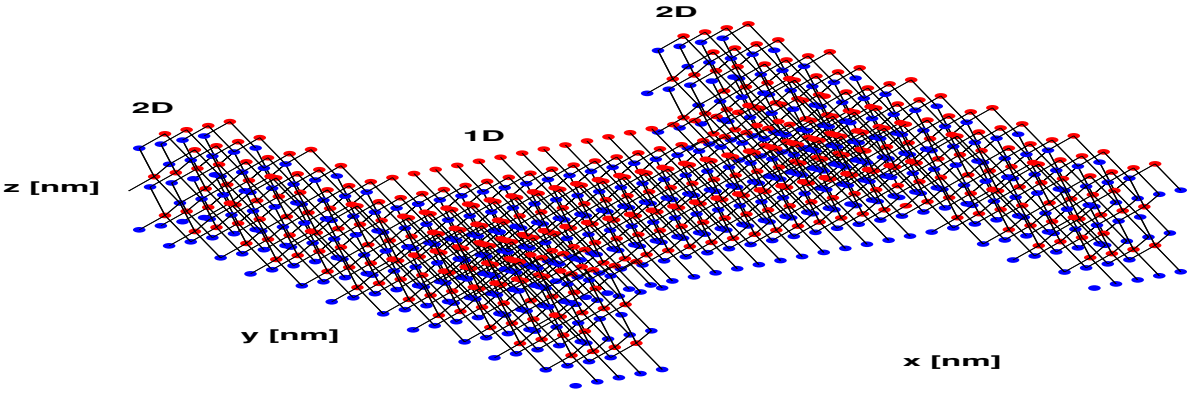

Fig. 1. Schematic view of a Si nanowire (1D electron gas) with quantum well Source and Drain (2D electron gas). Benchmark example for the wire: x=22 nm, y=1.6 nm, z=1.6 nm. Source and Drain are assumed infinite in the x and y directions.

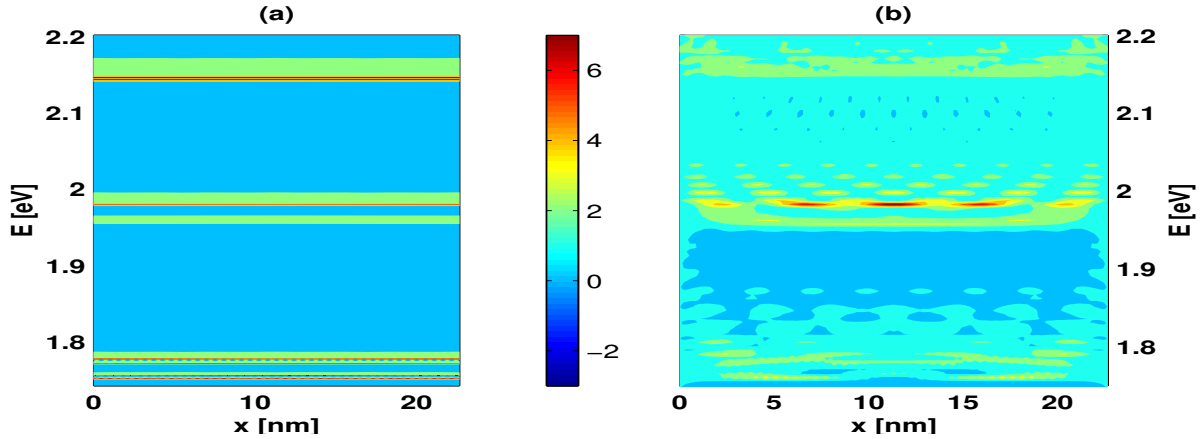

Fig. 2. Spectral density of states for the wire from Fig. 1, (a) with perfect boundary conditions (BC) where Source and Drain are the same as the Device, DOS is perfectly smooth in x and step-like in E, (b) with discontinuity in BC (2DEG-1DEG transition) inducing evident interference effects in the inhomogeneous DOS.

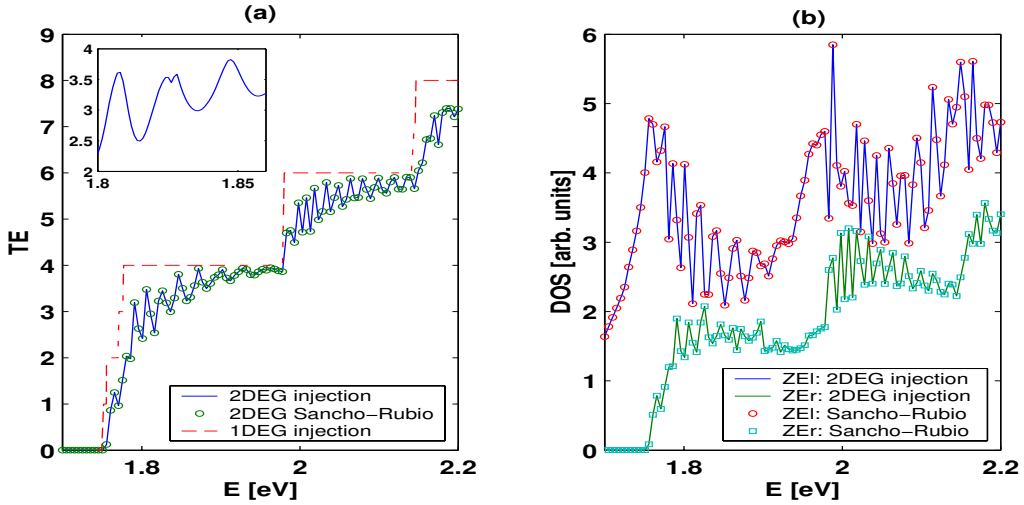

Fig. 3. (a) Transmission through the wire from Fig. 1 with quantum well (circled line + zoom) and perfect contacts (dashed line). "Injection" labels the new algorithm, "Sancho-Rubio" the usual one. (b) Density of state at x=0 nm (Source) coming from left (Source, solid line with circles) and right (Drain, solid line with squares) quantum well reservoirs.