Nanowire transport and edge passivation

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ABSTRACT

The influence of edge passivation on quantum transport simulations of a silicon nanowire is revisited. Thanks to a combination of non-equilibrium Green's functions and state-of-the-art band structure calculations we extract I(V) characteristics of a p-doped and n-doped nanowire MOSFET (NWFET). A self-energy of passivation is parametrized, allowing us to gauge the impact of various edge chemistry on electrical characteristics.

INTRODUCTION

Non-equilibrium Green's functions (NEGF) allow us to perform a quantum transport simulation of an NWFET made of two leads and an active region, where carriers move according to a custom band structure (BS) [1].

One of the most efficient ways to describe the BS of a material is the Slater-Koster (SK) tight-binding (TB) model. The set of SK-TB parameters is usually based on accurate experimental measurements and can be extended to state-of-the-art density functional theory (DFT) data, including results of hybrid functionals [2].

We focus here on an NWFET structure made of pure Si [100] along the transport direction, with 3x3 nm^2 square cross-section. The two contacts are highly-doped Si with an intrinsic channel surrounded by SiO_2, see Fig. 1. NEGF calculations are performed using a recursive Green's function with low-rank approximation [3] and an sp3d5s* TB-basis. The transferability of the basis for correct description of the NW BS can be affected by the scheme employed to passivate the silicon dangling bonds. They are located around the nanowire, and to avoid too high complexity the Si /SiO_2 interface is usually not described explicitly.

MODEL

The BS obtained in DFT of the Si NW passivated with hydrogen are shown in Fig. 2 and Fig. 3. Thanks to a self-energy technique [4] a fit to the DFT results is performed both for the valence and conduction bands. Note that this technique can be extended to a more complex Si / SiO_2 interface as shown Fig.4 obtained thanks to ab initio molecular dynamics [5] with the resulting band structure Fig. 5.

Taking into account the self-energy effect of passivation, the NEGF results for an n-doped and p-doped NWFET are shown Fig. 6 and Fig. 7 respectively. The passivation effect shows a decrease of the electronic current at high gate voltage and more pronounced for a p-NWFET.

CONCLUSION

Essentially the edges passivation of a nanowire can be included implicitly thanks to a custom self-energy. I(V) characteristics are influenced by the corresponding set of parameters, and conversely one can seek a good set of parameters as a function of passivation chemistry engineering.

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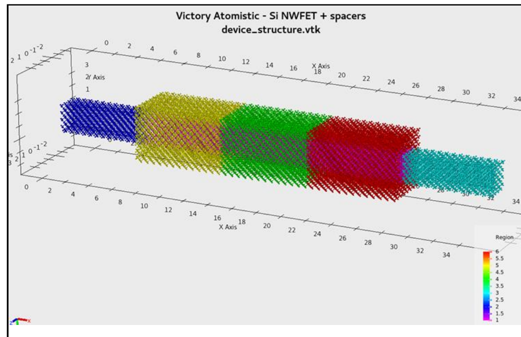

Fig. **1**. MOSFET structure of a silicon nanowire oriented [100] with a square cross-section of 3x3 nm^2.

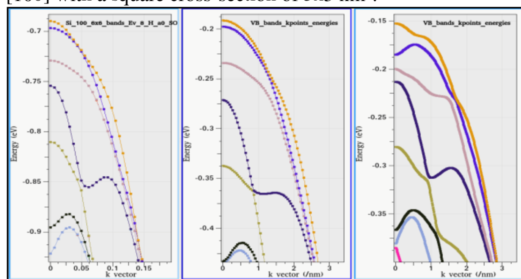

Fig. 2. Valence band structures of a slice of Si NW [100] obtained in DFT (left) and Tight-Binding (middle and right) with two different passivation schemes (fitted vs original).

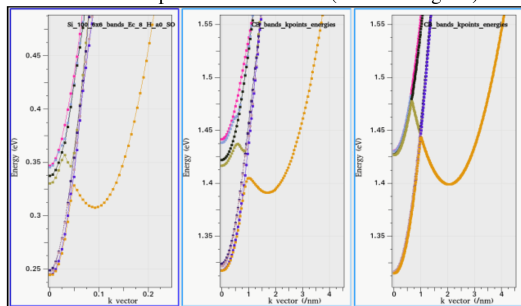

Fig. 3. Same as Fig. 2 for the valence band structures of a slice of Si NW [100] DFT (left), TB (middle and right).

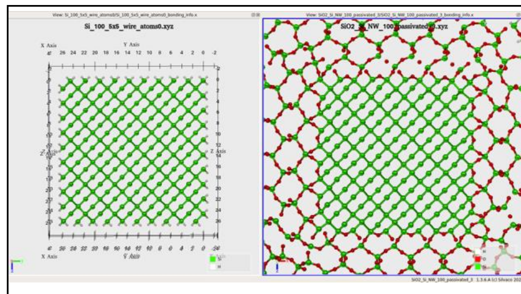

Fig. 4. Si NW [100] passivation of the dangling bonds with hydrogen atoms (left), with cristobalite SiO_2 (right).

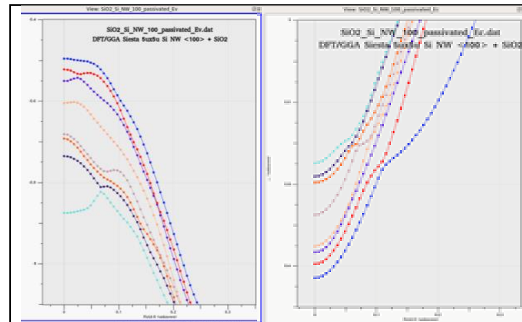

Fig. 5. Valence and conduction band structures of a slice of Si NW [100] (left and right respectively) with SiO_2 passivation obtained in DFT.

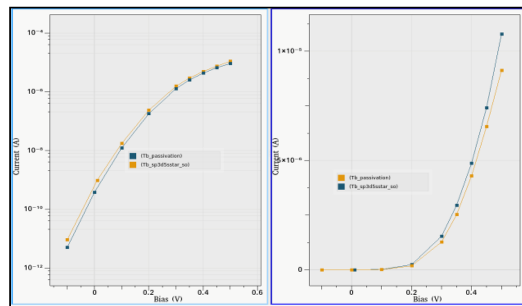

Fig. 6. I(V) curves of Si NW n- MOSFET with two different passivation schemes, one conventional with H- termination, and one that mimics the passivation obtained in DFT.

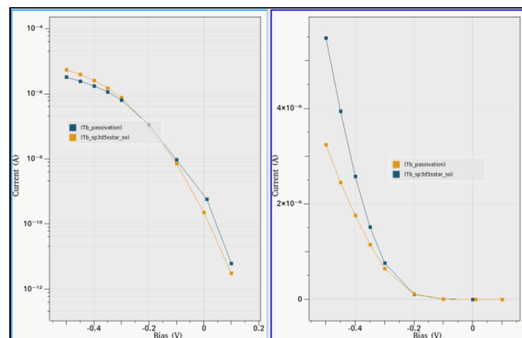

Fig. 7. I(V) curves of Si NW p- MOSFET with two different passivation schemes, one conventional with H- termination, one that mimics the passivation obtained in DFT.