Density functional tight binding modeling in the context of ultra-thin SOI MOSFETs

S. Markov[*], C. Y. Yam[*], B. Aradi[+], G. Penazzi[+], A. Pecchia[^], T. Frauenheim[+] and G. H. Chen[*]
[*]Department of Chemistry, The University of Hong Kong, Hong Kong
[+]BCCMS, University of Bremen, Bremen, Germany, [^]University of Rome "Tor Vergata", Rome, Italy
e-mail: figaro@hku.hk

We investigate the applicability of density functional tight binding (DFTB) theory [1][2], coupled to non-equilibrium Green functions (NEGF), for atomistic simulations of ultra-scaled electron devices, using the DFTB+ code [3][4]. In the context of ultra-thin silicon-on-insulator (SOI) transistors we adopt atomic models that include not only the Si channel, but also the interfacial SiO_2, and look at the change of electronic, dielectric and transport properties as Si film thickness is reduced from 10 nm to less than 1 nm. We build on our previous reports [5][6], and draw a systematic comparison against a corresponding model that employs H-passivation of the channel, and against known experiment.

DFTB derives as an approximation of density functional theory (DFT). It is computationally more efficient since part of its Hamiltonian is pre-computed in tight-binding terms over extended neighbors, employing non-orthogonal basis. This makes DFTB readily applicable to larger structures even with disorder, e.g. as found in SiO_2. An additional part in the DFTB Hamiltonian approximates effects of second-order charge fluctuations, which allows DFTB to capture more accurately not only permanent charge transfer due to bond asymmetry, but also induced polarization due to applied electric field, and hence to model dielectric response.

DFTB relies however on 1 to 3 parameters (typically) per chemical element. We recently reported good parameterization for Si and O that yields accurate band-structure for bulk Si, as shown in Fig 1. Although the band-structure of bulk oxide is not as accurately reproduced, the error is still around 20%, and a large-gap insulator results, as seen in Fig 1. Fig. 2 shows a fragment of an atomic model of an Al–amorphous-SiO_2–Si structure, and the corresponding density of states as a color-map. From the on-atom projected DOS we extract the profile of the conduction and valence band-edges across the MOS junction, superposed on the color-map. Notable is the gradual initial opening of the gap on the Si side, and the penetration of states in the insulator from both the metal and the semiconductor. We attribute the somewhat inaccurate band-offsets between SiO_2 and Si to the weakly expressed CB minimum of SiO_2 at Γ. This should have relatively small influence on the confinement effects in the channel, because of the abrupt change in gap after 0.7 nm from the interface. Indeed, Fig. 3 shows very good agreement between experimental [7], and calculated dependence of Si band-gap and CB/VB-edge shifts on Si film thickness. This is in contrast to the simulations with H-passivated Si channel, which overestimates the effects ~2 times. Similar comparison is drawn in Fig. 4 for the dependence of Si permittivity on Si thickness, calculated as described in [8]; experimental data is from [10]. The microscopic permittivity profile across 0.8 nm SOI structure is shown in the inset of Fig. 4, and the interface transition agrees with more accurate studies [9].

Beyond the electronic structure and dielectric properties, we compare I_DV_G characteristics of junctionless-SOI transistor with 3 nm gate length and 0.8 nm Si body thickness, calculated in DFTB+NEGF (ballistic limit) and the measured from a similar device [11] in Fig 5. Model compares well with experiment in the sub-threshold regime, after small work-function adjustment. There is significant difference however, between the models with H- and SiO_2-passivated Si channel, as seen in Fig. 6.

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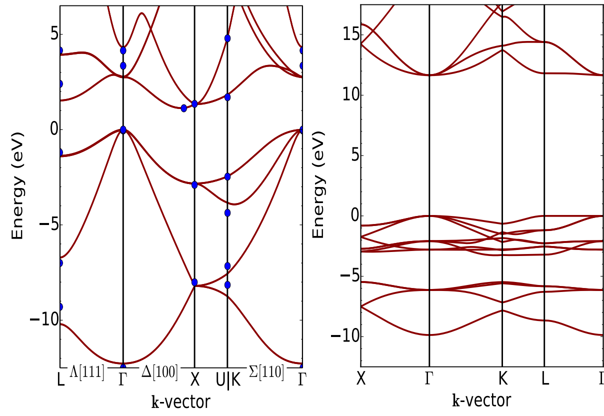

Fig.1. Band-structure of bulk Si (left) and β-cristobalite SiO_2 (right) show very good agreement for Si, and a large gap for SiO_2 at the same time, with the same DFTB parameters for Si.

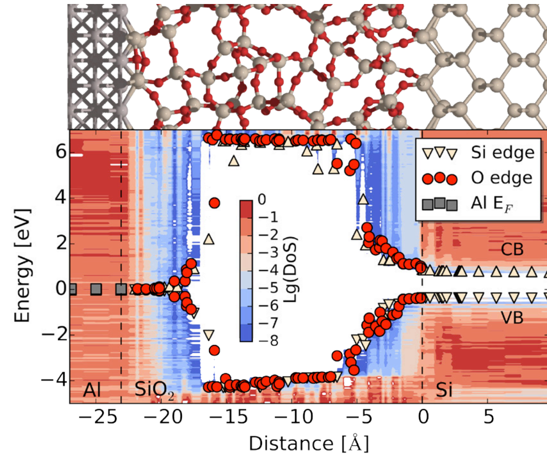

Fig. 2. Density of states, and conduction and valence band profiles across Al–SiO_2–Si structure, calculated in DFTB, show penetration of states in SiO_2 from both Al and Si.

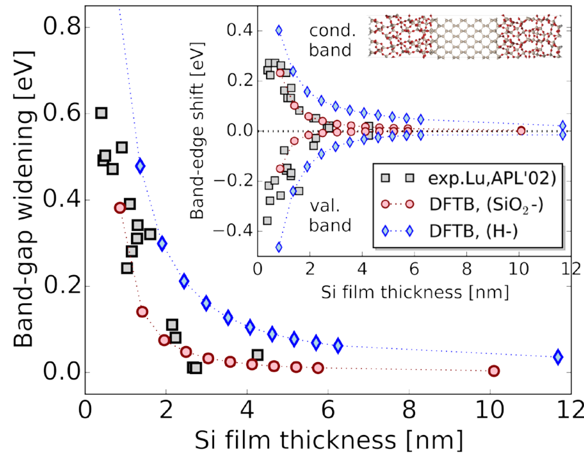

Fig. 3. Band-gap widening and edge-shift of the conduction and valence bands of ultra-thin Si vs. Si thickness, for SiO_2- and H-passivation. Band-edge shifts lead to appreciable change in gate work-function difference, with thinning Si.

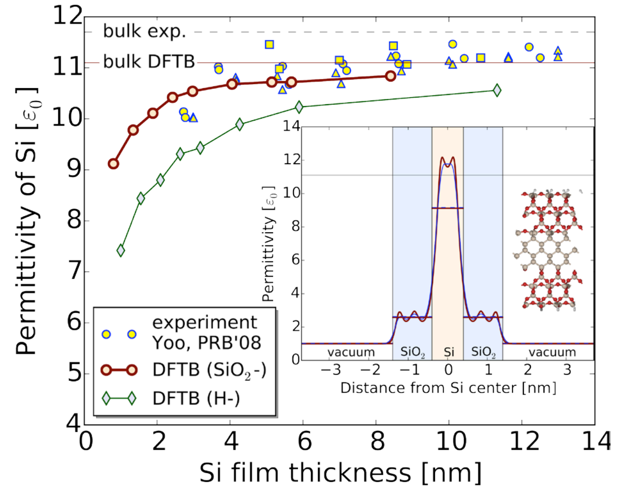

Fig. 4. Permittivity of Si versus Si film thickness for SiO_2- or H-passivated channel. Inset: microscopic permittivity profile for SiO_2 passivated, 0.8 nm Si film and the atomic model.

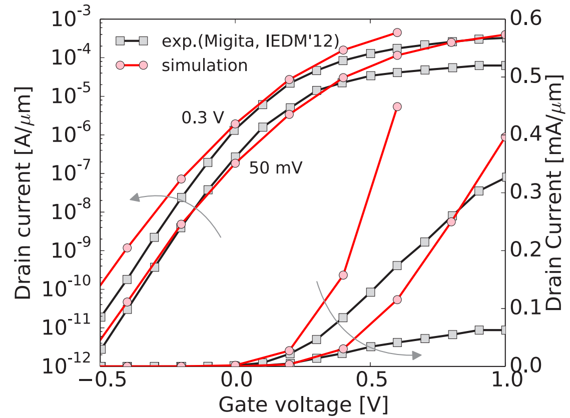

Fig. 5. Transfer characteristics of a junctionless SOI MOSFET with 3 nm gate length and 0.8 nm Si channel compare well in the subthreshold regime against experiment with the given critical dimensions

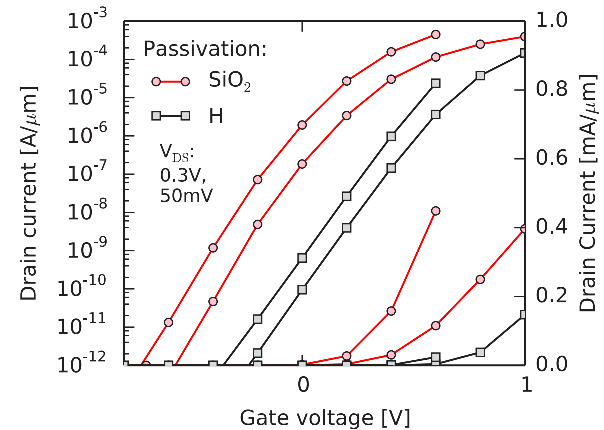

Fig. 6. Transfer characteristics of ETSOI transistors modeled with H- and SiO_2-passivation show large difference due to the differences in the electronic and dielectric properties.