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Linear Combination of Bulk Bands-Method and Atomistic Tight-Binding Description of Strained Silicon and Germanium Layers

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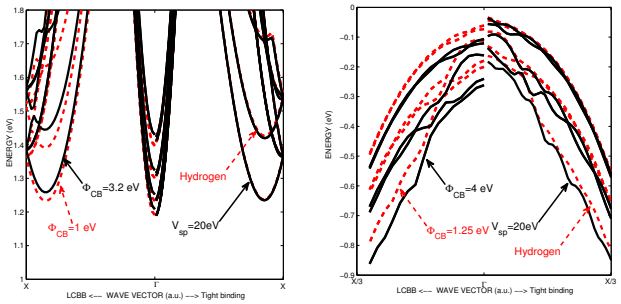
1. Introduction

During the last decade, silicon band structure engineering by means of channel rotation, mechanical strain and quantum confinement has been a very efficient way to improve Si and Ge-based MOSFETs. With a view of calculating the transport properties in such systems, the electron community has developed a large variety of computational full band methods, among which the Linear Combination of Bulk Bands-method (LCBB) [1,2] and the atomistic Tight Binding (TB) method [3,4] are now widely used.

A recent comparison between LCBB and TB simulations in strained Si 2D systems has put forth that the latter method can suffer from inaccurate parameters and fails to describe the modification of the band-structure with strain as well as the warping of the conduction band (CB) in Γ [2]. In this paper, we have revisited these conclusions using a different first-principle based TB parameterization [5] and providing a direct comparing between methods in various confined and strained Si and Ge layers.

2. Bulk Silicon and Germanium

The band-structure parameters for the empirical pseudo potential method used in the LCBB and the sp3d5s* model can be found in [5,6]. These parameters have been optimized in order to closely match first-principle simulations of relaxed but also strained Si and Ge.

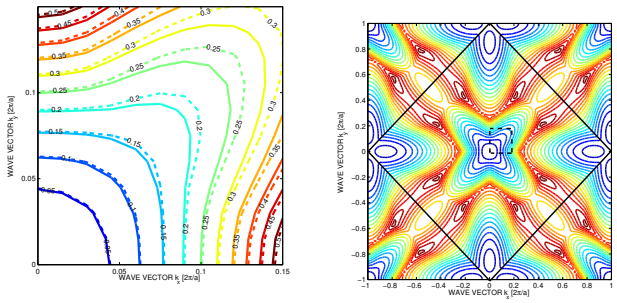


(a) Conduction bands (b) Valence bands

Figure 1: Dispersion relation along the Γ-X direction in a 5 nm silicon well calculated with a tight binding model with hybridized orbitals and with Hydrogen passived surfaces. Comparison with LCBB model using various barrier potential heights. For each plot, the tight binding results span on the right part, and the LCBB ones on the left.

3. Two-Dimensional Sub-Band Structure

We first consider the case of carrier confinement in the channel of FD-SOI Si-based MOSFEFs. In such devices, the semiconductor channel is embedded in SiO_2, which forms a [0 0 1]-oriented quantum well. Accurate simulations require in principle an accurate description of both the semiconducting channel and the surrounding oxide layers. Within the framework of the LCBB the confinement in the semiconductor layer can be obtained using an additional positive (negative) potential for the CBs (and the VBs) at the Si/SiO_2 interfaces. There is no simple way to do so with a tight binding model. For that reason, in the tight binding community it is a common practice to simulate MOSFETs devices [3,4] without the SiO_2 regions and to use a 'standard' surface state amorphization technique such as raising the energy of a hybridized orbital [7] or connecting the surface atoms to monovalent atoms [8]. However, with these two techniques different results can be found, as depicted in Figure 1 in case of a 5nm Si well. These results can be compared to the LCBB ones simulated with realistic Si/SiO_2 band offsets (ϕ_{BC}=3.2 eV for electrons and ϕ_{BV}=4eV for holes), but also with lower band offsets. As can be seen, the VBs sub-band structure is relatively different, but surprisingly, the CBs match relatively well.



(a) Zoom of the lowest energy sub-band in the near Γ-region. The equi-energy contour plots from the bottom of the sub-band are spaced by 50 meV.

(b) Lowest energy sub-band as a function of in-plane vectors. The limits of the 2D Brillouin zone are shown with solid lines. Dashed lines show the zoomed region in (a).

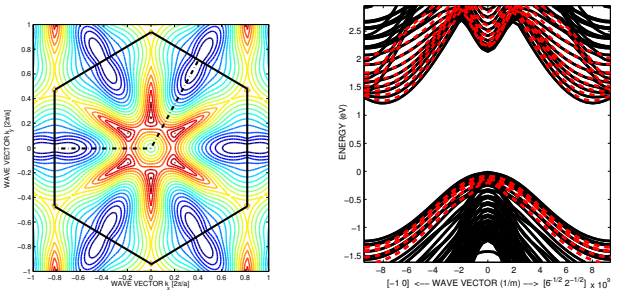
Figure2: Sub-band structure as a function of in-plane wave vectors components for a 2.26 nm germanium quantum well 'embedded' in SiO2. Dashed lines: LCBB and Solid lines: tight-binding.

Moreover, and in contrast with the results shown in [2], the warping of the CBs in Γ is well aligned between the two models as shown in Figure 2. Figure 3 shows that the relatively good matching holds for the [111]-quantization direction.

4. Wave Functions penetration in the Oxide region

Including the oxide regions in a tight binding simulation is still in progress. Since oxide is an amorphous material the exact nature of which is not know, several research groups have proposed to introduced a

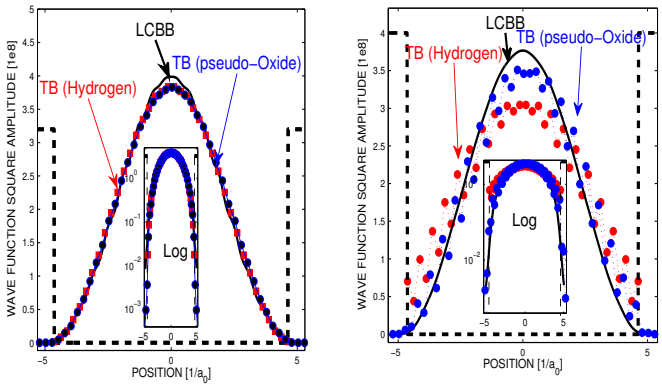
pseudo-Zinc-blende oxide material, acting as a virtual buffer all around the semiconductor regions [9]. Such pseudo-oxide is an efficient and versatile way to capture the main features of the Si/SiO_2 interface (finite band offsets, change of the effective mass, and penetration of the waves in the oxide). Figure 4 shows the wave function square modulus for electrons and holes at $\mathbf{k}_\perp = \mathbf{0}$. The carriers are not perfectly confined into the well and their wave functions penetrate into the oxide region (in contrast with the TB model when the dangling bounds are passived with Hydrogen).



(a) Electron lowest energy sub-band as a function of in-plane vectors. The limits of the 2D Brillouin zone are shown with solid lines. Doted dashed lines indicate the high symmetry directions along which the sub-band structure is shown in (b).

(b) Electron and holes sub-band structure along high symmetry directions in reciprocal space.

Figure3: Sub-band structure for a 5 nm silicon quantum well oriented along the [111]-direction. Dashed lines: LCBB and solid lines: TB.



Lowest quasi-degenerate conduction band states.

Highest valence band states

Figure 4: Si layer of size 5 nm embedded in Oxide; Lines: LCBB, Symbols: TB (with and without a pseudo-oxide buffer).

5. Si/sGe/Si Heterostructure

During the last decades, Si/sGe/Si epitaxial heterostructures have received a continuous attention due to the challenges in the fabrication of efficient light emitting devices exploiting the silicon-based integrated circuit technology. Besides its great technological interest, such structure is also a good candidate to bench models. The boundary conditions used in both methods are comparable: the strained germanium layer is embedded in a silicon buffer exhibiting a similar crystallographic structure. However, with the LCBB method presented in [1,2] the Block functions in both material are identical. This is not the case with the tight binding model in which either silicon or germanium parameters are used depending on the atom position in the heterostructure. In addition, results obtained with the full zone **k.p** method of [10] (using position dependent parameters [11]) are compared to the previous ones. Figure 5 shows the VBs dispersion relation for a 2nm strained Ge layer embedded in a large (L=50nm) relaxed Si buffer. The states confined in the buffer are clearly visible and form a quasi-continuum in energy. Some differences between the LCBB method and the two others can be observed, which highlight the limitation of the single material approximation in such a slightly confined system (ϕ_{BV}=0.54eV for holes).

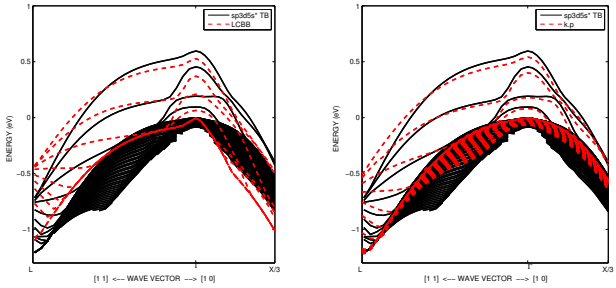


Figure 5: Sub-band structure in a Si/sGe/Si heterostructure. Solid lines: TB, Dashed lines: LCBB calculation (left) and k.p (right).

6. Conclusions

A comparison between the atomistic TB and the LCBB model is provided for particular structures featuring strain and confinement. The impact of the boundary conditions is also highlighted. In particular, we briefly discussed the treatment of oxide boundaries with a TB model using a pseudo oxide buffer. The issue of band mixing at interfaces will be addressed during the conference.

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