A self-consistent calculation of band structure in silicon nanowires using a Tight-Binding model

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***Abstract*—The properties of silicon nanowire (SNW), resulting from the band structure calculation using a four-orbital *sp*^{3} tight-binding method, are discussed in this paper. A number of intrinsic properties including band gap, density of states and parabolic effective masses have been derived from the computed electronic structure for different SNW widths. A self-consistent solver of coupled 3D Poisson-Schrödinger equations using the tight-binding model has been developed to analyze the effect of gate bias on the SNW band structure at room temperature. The spatial distribution of carriers in the nanowire is calculated and the impact of gate bias on subbands is discussed. Finally, effective mass model is compared to tight-binding model to assess the validity of this approximation in narrow SNW.**

Band structure; silicon nanowire; self-consistent solution; tight-binding

I. INTRODUCTION

With the downscaling of bulk MOS transistors and the issues encountered to keep on improving their performance, new architectures are becoming of great interest. Conventional transistors begin to evolve towards 3D nonplanar devices at nanometer scale. Among these new architectures, nanowire transistors are promising devices. Indeed, it is predicted that narrow nanowires with a surrounding gate will lead to superior electrostatic control of the conductivity in the field effect transistor channel. Recently, the fabrication of silicon nanowire (SNW) transistors with nanometer diameter has been demonstrated by various experimental groups [1-3].

Nevertheless, as the dimensions of future devices approach the atomic scale, simulation appears to be essential for a better understanding of electronic transport in these devices. In particular, the band structure calculation is a crucial step to obtain the electronic material properties, which are necessary for transport simulation. In order to describe the SNW electronic structure and transport properties, several methods can be used: *ab initio* methods [4][5], kp method [6], pseudo-potential method [7] and tight-binding method [8]. In this paper, we chose to use a tight-binding (TB) model [9], which is a semi-empirical method based on a set of parameters fitted to accurately reproduce the electronic structure obtained by *ab initio* calculations or experiments. This method has the advantage of dealing with larger systems and being faster than *ab initio* methods, while keeping a good description of electronic structure.

In Sec. II, the TB model used for describing SNW band structure is detailed. Then, electronic structure is computed and intrinsic properties are calculated for different widths of SNW with a square cross-section. In Sec. III, the effect of gate bias on the band structure is discussed thanks to a self-consistent Poisson-Schrödinger solver. Finally, in Sec. IV, the validity of the effective mass approximation is studied and corrections are proposed to obtain a better agreement with TB model for wire (W) width down to 2 nm.

II. BAND STRUCTURE CALCULATION

A. The tight-binding model

The TB model used is a *sp*^{3} third nearest neighbors three centers model optimized to accurately reproduce the effective mass values of bulk silicon [8] [10]. The tight-binding fitting parameters for Si, employed in this work, have been taken from [10]. In order to calculate the electronic structure, an infinite silicon nanowire with a square cross-section and oriented along [001] is considered. The unit cell is carved out of the bulk silicon by keeping all atoms inside a parallelepiped. At the surface, dangling bonds are saturated with hydrogen atoms in order to avoid energy states in the band gap. This approach does not take into account surface reconstruction effects but succeeds in describing the quantum confinement [10].

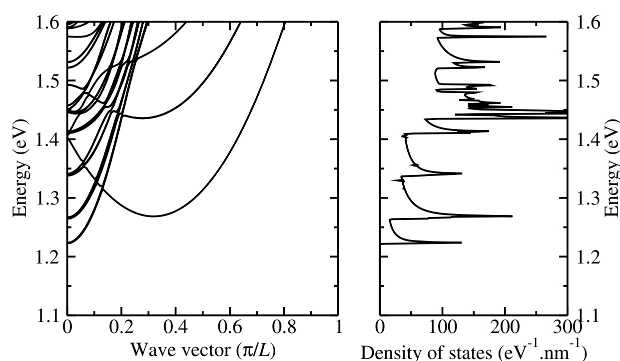

Figure 1. Conduction band structure and density of states of a [001]-oriented Si nanowire of 5 nm in width.

Because of 2D quantum confinement in SNW, the reciprocal space is restricted to 1D and the first Brillouin zone extends over [-π/*L*;π/*L*], where *L* is the length of the unit cell. For a [001]-oriented Si nanowire, *L* is equal to the lattice parameter (a_0 = 0.543 nm). In bulk Si, conduction bands have six minima, which belong to six valleys named Δ valleys. These six minima are localized at 0.83 from the Γ point along the *X* direction. In SNW, the position of conduction band minima is different and depends on the nanowire orientation. Indeed, the six Δ valleys of bulk Si are projected on the nanowire axis. For a [001]-oriented Si nanowire, the six Δ valleys split into two groups: one group of four valleys ($[100]$, $[\bar{1}00]$, $[010]$ and $[0\bar{1}0]$) is projected at $k = 0$ and the other group ($[001]$, $[00\bar{1}]$) is projected at $|k| \sim 0.33\pi/L$. In the considered range of SNW widths (2 nm ≤ W ≤ 20 nm), the minimum of the conduction bands occurs at $k = 0$, therefore SNW is a direct band gap material contrary to bulk Si. Furthermore, as the nanowire width decreases, the subband minima of the second group (at $|k| \sim 0.33\pi/L$) progressively shift towards $k = 0$. The density of states can be computed from the band structure. It is composed of Van Hove peaks corresponding to energy subbands. Fig. 1 shows the conduction band structure and density of states of a [001]-oriented Si nanowire of 5 nm in width.

It should be noted that the electronic band structure significantly evolves according to the nanowire width. Consequently, intrinsic properties like band gap and effective mass evolve as well. The variations of the energy gap ε_g and of the effective mass values as a function of the nanowire width are plotted in fig. 2 and 3, respectively. The effect of quantum confinement on the band gap is clearly shown with a dramatic increase of ε_g as the width is reduced below 5 nm. The effective mass values are extracted at the energy minima of the two groups of valleys previously described thanks to,

$$m_n^* = \hbar^2 \left[\frac{d^2E(n,k)}{dk^2} \right]^{-1}, \quad (1)$$

where *n* is the subband index. The effective mass calculated for the first subband at $k = 0$ corresponds to the transverse mass of the bulk Si ($m_t^* = 0.19\ m_0$), while the effective mass calculated for the first subband at $|k| \sim 0.33\pi/L$ corresponds to the longitudinal mass of bulk Si ($m_l^* = 0.916\ m_0$). It is observed that for large cross sections of nanowire, the bulk mass values are recovered. More generally, nanowire electronic properties tend towards those of the bulk, when the nanowire width increases.

B. Self-consistent calculation of band structure

In order to investigate the role played by the gate bias V_g on the band structure, we have coupled the TB Schrödinger equation to a 3D Poisson solver. The SNW is now surrounded by two dielectric materials (1 nm of interfacial SiO_2 layer and 3 nm of HfO_2) and a mid-gap metal gate. The dielectric materials are treated as a continuum medium through dielectric constants equal to 3.9 for SiO_2 and 19 for HfO_2. SNW are assumed to be undoped, so that the Fermi energy ε_F is located at the middle of the band gap at $V_g = 0$ V.

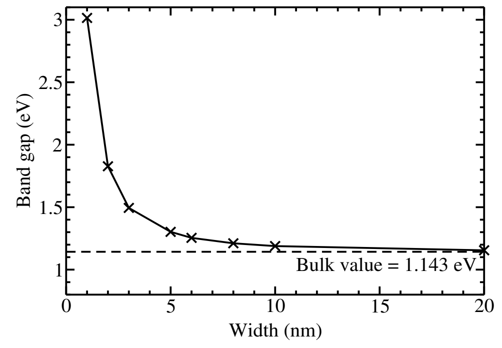

Figure 2. Evolution of band gap as a function of the width for a [001]-oriented Si nanowire.

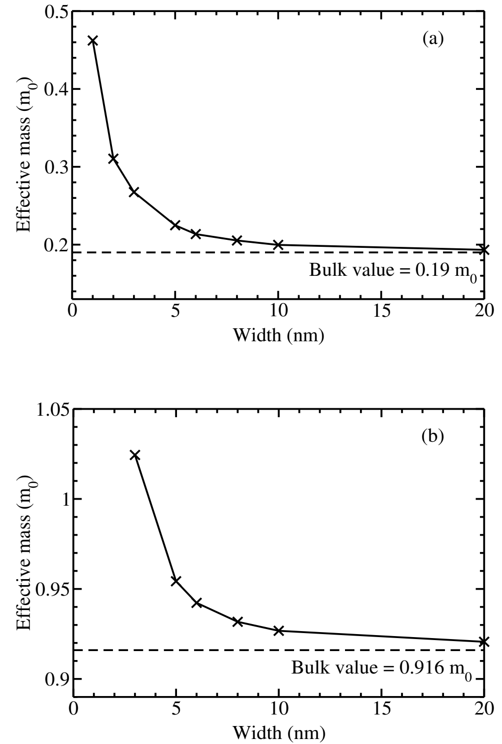

Figure 3. Evolution of electron effective mass values of the first subband at $k = 0$ (a) and at $|k| \sim 0.33\pi/L$ (b) as a function of the width for a [001]-oriented Si nanowire. m_0 is the electron mass.

For each gate bias, Schrödinger's and Poisson's equations are self-consistently solved at room temperature in order to obtain the electron density and the potential inside the nanowire. Fig. 4 shows the cartographies of electron density for 2 nm and 5 nm-wide nanowires. In the narrower nanowires, the electrons are localized at the centre while they are closer to Si/SiO_2 interface in the larger nanowires. The effect of gate bias on band structure is shown in fig. 5 and 6. The band structure is plotted at $V_g = 0$ V and $V_g = 1.5$ V for [001]-oriented Si nanowires of 2 nm and 5 nm in width, respectively. We observed that the bias has little impact on the dispersion relation *E(n,k)* inducing a very slight modification of masses as

a function of the gate bias. When V_g varies from 0 V up to 1.5 V, the effective mass of the first subband at $k = 0$ increases of 0.5% (respectively 2.7%) for a 2 nm-wide (respectively 5 nm-wide) SNW. The modification of effective mass at $|k| \sim 0.33\pi/L$ is still negligible (0.1%) for a 5 nm-wide SNW. While the effective masses extracted from the curvature of the energy subbands are not much sensitive to the gate bias, the quantum confinement varies significantly with V_g. This alters the energy levels. The band structure is not simply shifted by a constant, but the energy difference between two subbands is modified when the gate bias is ranged from 0 V up to 1.5 V. As illustrated in fig. 6, the variation of the relative position of two subbands is more important for large nanowires.

III. Comparison with the Effective Mass Approach

In this section, tight-binding model and effective mass approximation are compared. For both models, the same geometry and dimensions are considered and dielectric parameters are identical. The comparison between both models focuses on the electron density and the potential inside the nanowire.

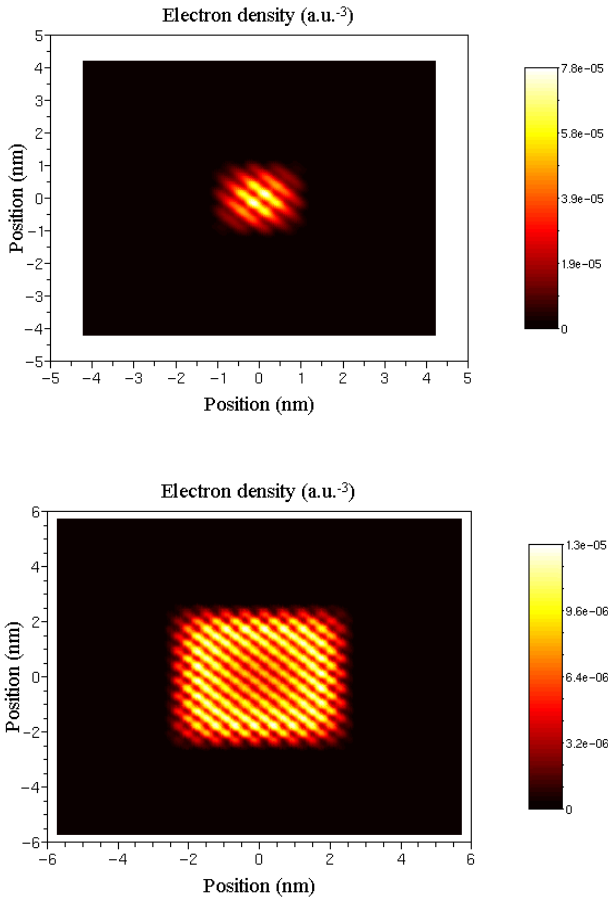

Figure 4. Electron density in a section of [001]-oriented Si nanowires of 2 nm in width (top) and of 5 nm in width (bottom) at $Vg = 1.5$ V.

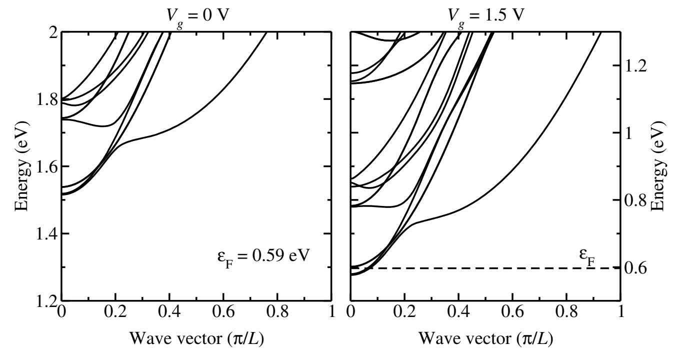

Figure 5. Band structure of a [001]-oriented Si nanowire of 2 nm in width at two gate biases $V_g = 0$ V (left) and $V_g = 1.5$ V (right).

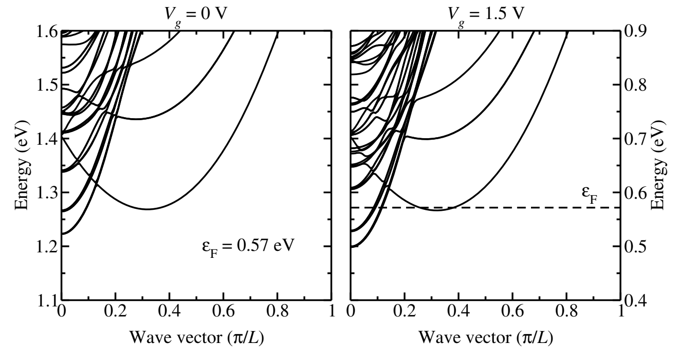

Figure 6. Band structure of a [001]-oriented Si nanowire of 5 nm in width at two gate biases $V_g = 0$ V (left) and $V_g = 1.5$ V (right).

First, the calculations with effective mass model are done without correction: the effective mass values for each valley correspond to the bulk values ($m_l^* = 0.916\, m_0$ and $m_t^* = 0.19\, m_0$) and the nonparabolicity coefficient α is set to 0 eV^{-1}. The number of electrons n_e in the unit cell derived from atomistic and effective mass model is plotted in fig. 7 for a large range of gate voltages. Without correction in the effective mass model, n_e for both models matches for large nanowires ($W \geq 5$ nm) but not for narrow nanowires ($W < 5$nm). As illustrated in fig. 7, the threshold voltage shift between both series of results increases when the nanowire width decreases. Consequently, for narrow nanowires ($W < 5$ nm), the corrections to the effective mass model are necessary to obtain a better agreement with the tight-binding model.

In order to reduce the threshold voltage shift, the bulk effective masses are replaced by those resulting from the band structure calculation using tight-binding model (cf. fig. 3). These corrections lead to a clear improvement. Indeed, the threshold voltage shift is strongly reduced even for narrow nanowires (cf. fig. 8). This improvement is explained by the fact that with corrections the energy levels computed with effective mass approximation are closer to those computed with tight-binding model.

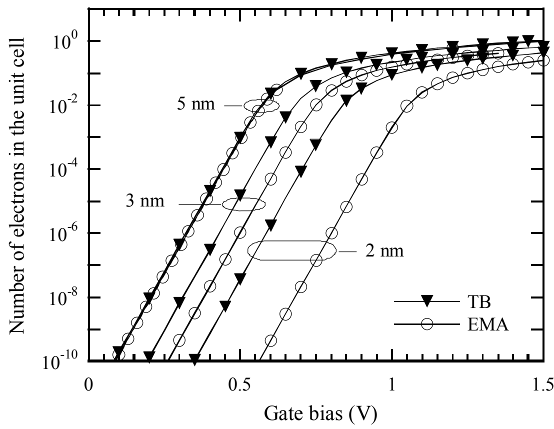

Figure 7. Comparison of the number of electrons in the unit cell between tight-binding model (TB) and effective mass approximation (EMA) without corrections

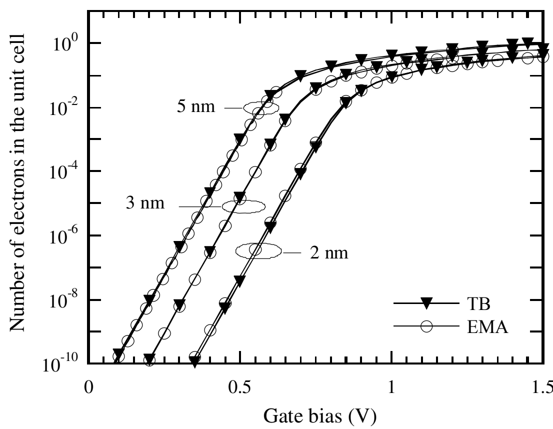

Figure 8. Comparison of the number of electrons in the unit cell between tight-binding model (TB) and effective mass approximation (EMA) with corrections.

IV. CONCLUSION

By comparison with the bulk silicon, silicon nanowire has a direct band gap. Intrinsic properties evolve according to the nanowire width. Indeed, the energy gap and the effective mass values increase with the reduction of width. Thanks to self-consistent simulations, the effect of gate bias on the band structure of a nanowire has been highlighted. The gate bias does not modify the subband shape of the band structure, but alters the energy difference between two subbands. Finally, the comparison between effective mass and tight-binding models made appear that corrections to the effective masses are required to maintain a good agreement with the tight-binding model for nanowire width lower than 5 nm.

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