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Tight-Binding Calculations of Ge-Nanowire Bandstructures

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INTRODUCTION

Recent development of CMOS industry has demonstrated the possibility to fabricate ultimate semiconductor nanowire MOSFET [1]. Since this device represents a promising candidate due to its better electrostatic control, it then becomes relevant to develop modeling tools based on atomistic and quantum methods capable to calculate nanowire bandstructures [2,3]. In this work, we study Ge nanowires using a tight-binding approach. We consider a sp^3 model which includes the third-neighbor-interactions as well as the spin-orbit coupling. The present model was developed by Niquet *et al.* [4] and gave very good agreement with the $sp^3d^5s^*$ [5] tight-binding approach and ab initio LDA calculations.

RESULTS AND DISCUSSION

We investigate germanium nanowire bandstructures. The [100] orientation is first adopted as the wire axis and the square cross-section (size D) is confined with four {100} faces (Fig. 1). The wire surfaces are saturated by hydrogen atoms in order to removes the dangling bonds. We consider the standard sp^3 tight-binding scheme using a supercell periodically repeated along the nanowire axis and setting 4 orbitals (one *s* and three *p*) on each Ge atom. In the sp^3 model, each orbital interacts with the third neighbors whereas its $sp^3d^5s^*$ counterpart, which has more orbitals per atom, only includes the nearest neighbor interactions. As a result, the number of orbitals and the number of neighbor-interactions compensate each other, and these two tight-binding models finally provide very close physical features. Figure 3 shows the energy bandstructures of the Ge nanowires previously described. For large cross-sections (D>4 nm), the minimum of the conduction band is determined by four degenerated half-bands at the limits of the Brillouin zone ($k_x \pm \pi/a$, where a is lattice constant of the Ge) and represents the eight projected L-valleys of the bulk. When quantum confinement becomes stronger (D<3 nm) the L-valleys are lifted, showing that the effective mass approximation (EMA) is no longer valid. Figure 4 compares the energy bandgap for Ge and Si [2] nanowires (with the same surface configuration) as a function of the diameter D. For the two materials, the bangbap increases by reducing the cross-section as predicted by the EMA. Although the silicon bandgap is the largest, the increase of the Ge bandgap is more pronounced as expected from the transverse effective mass difference [6]. At the ultimate scaling, Ge nanowires have then a bandgap very close to the one of Si. We can note that such effect should have a beneficial impact on the leakage current of Ge nanowire-transistors. Figure 5 shows the hole effective mass of the valence band versus the diameter calculated from the E-k_x dispersion relations. Strong transverse confinement (*i.e.* diameters smaller than 4 nm) induces a significant variation of the hole effective mass from $-0.20\times m_0$ to $-0.46\times m_0$.

Different wire orientations and confinement directions have also been studied. As a conclusion, we found that the physical properties of Ge (bandgap, effective masses) are more dependent to the quantum confinement than in Si and should have an important impact in the transport of ultimate Ge-nanowire MOSFETs.

ACKNOWLEDGEMENT

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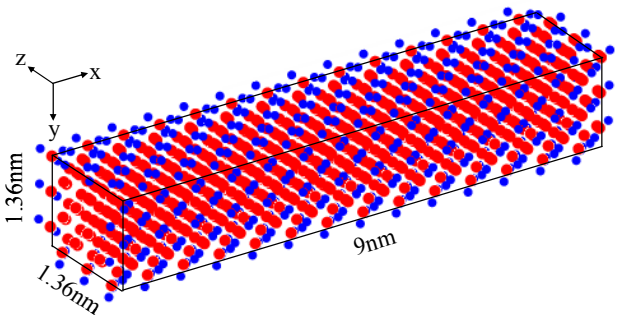

Fig. 1. Atomistic view of a Ge square nanowire [1.36nm × 1.36nm × 9nm] playing the role of the conduction channel in the active region of the transistor. Germanium atoms are in red and the dangling bonds are saturated by hydrogen atoms (in blue).

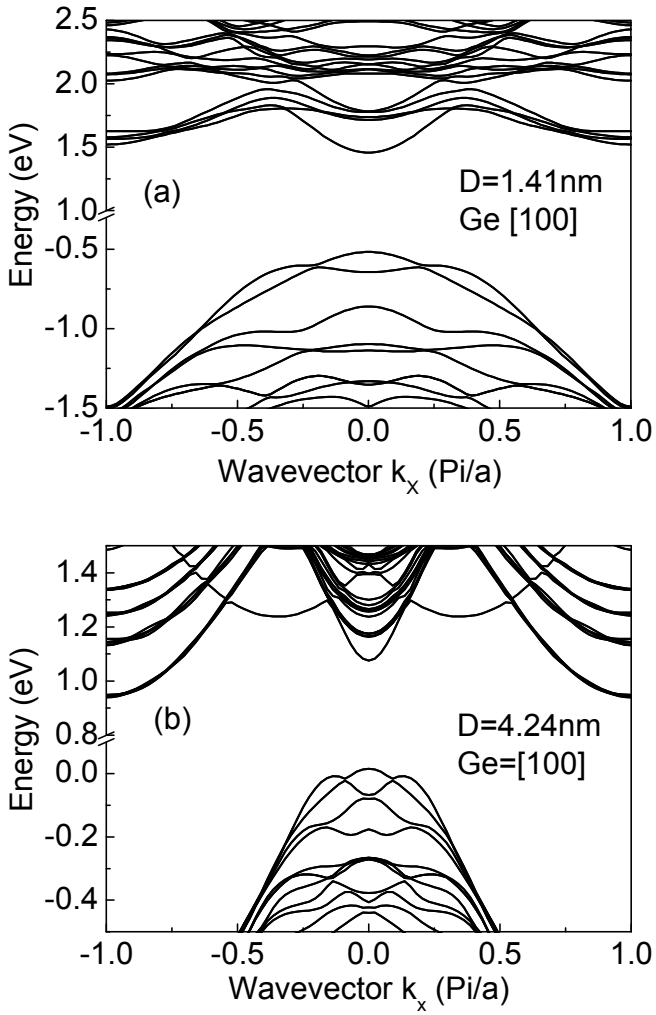

Fig. 2. Energy bandstructures of [100]-oriented Ge nanowires with two diameters: a) 1.41 nm and b) 4.24 nm. The transverse surfaces are {100} faces with dangling bonds pacified by hydrogen. The lattice constant a=0.5658 nm and k_x is the wavevector along the nanowire axis.

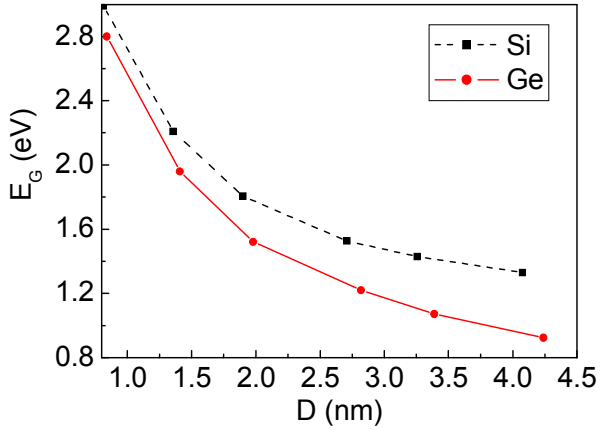

Fig. 3. Bandgap versus the diameter D of Ge and Si [2] nanowires with axis oriented along the [100] direction. The same surface configuration (orientation and boundary conditions) is considered for the both materials.

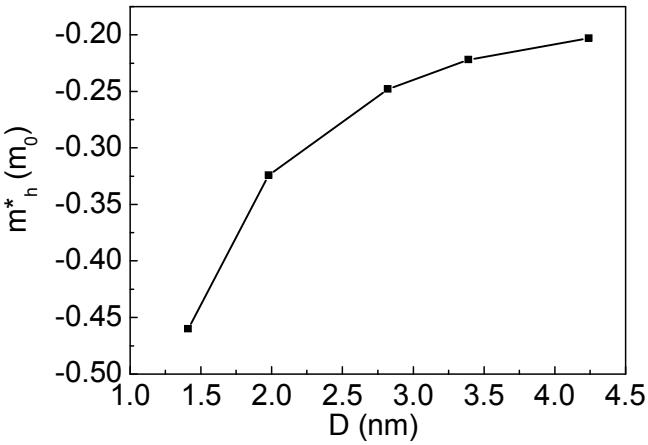

Fig. 4. Hole effective mass m^*_h at the Γ point in the valence band versus the wire diameter D for a [100]-oriented Ge nanowire. m_0 is the free electron mass.

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