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Band Structure of Surface Terminated Silicon Nanowire

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Silicon nanowires (SiNW) exhibit interesting physical properties that are noticeably different from those of the bulk and they are among the most competitive candidates of nanoscale building blocks. The advent of nano-technology made it possible to fabricate SiNWs with diameters of several nanometers [1-3]. Simulations have also been done to predict the feasibility of potential electronic devices applications [4-7]. However, most of the simulation works focus on [100] hydrogen-passivated SiNWs(SiNWH), while recent experiments have provided convincing evidence that the SiNWs grown by experiments were mostly along the [110] and [112] direction and covered by an oxide sheath[1].

In this paper, we present a systematic theoretical study of O-passivated SiNW(SiNWO) along [100] and [110] directions for the first time. Also, SiNWH is brought into comparison. We fix our attention on the electronic properties such as the band gap, density of state (DOS), projected DOS (PDOS), and effective masses (EM) as functions of Si core orientation and dimension. These properties are all relevant to the performance of ultra-scaled FETs built with SiNWs.

We consider [100]-oriented crystalline SiNW whose cross section has the shape of a square with four equivalent side faces corresponding to the (110) surfaces of bulk silicon. The corresponding diameter varies from 0.815nm to 5.16nm. As for the [110]-oriented SiNW, the cross section has the shape of a hexagon with two side faces of (100) and four side faces of (111). The corresponding diameter varies from 0.77nm to 3.16nm. Hydrogen or Oxygen atoms passivate all the dangling bonds at the surface of SiNW. First principle density functional theory (DFT) calculation was employed, with the interaction between the ions and electrons described by ultra-soft pseudo-potentials and the electron exchange-correlation potential treated with the generalized gradient approximation in PW91 form.

According to the calculation, SiNWH and SiNWO of both [100] and [110] direction are direct band gap semiconductors, with the valence band maximum (VBM) and conduction band minimum (CBM) at Γ point. Quantum confinement effect results in larger band gaps and distinct variation of effective mass in the transport direction. Generally speaking, the energy gap and the hole EM of SiNWO are both smaller than those of SiNWH of the same size. We will discuss below in the case of different orientation.

[100] SiNW

Fig.1 shows the effective masses of H and O passivated [100] SiNW at (a) the VBM and (b) the CBM. As the result of quantum confinement, the effective mass of band edge is increasing with the decreasing of wire thickness. The electron effective masses of [100] SiNWH and SiNWO for the thick wires correspond to the electron transverse EM of bulk Si (in our calculation, m_t of bulk Si is $0.21m_0$) which is consistent with other reports. The EM of hole for the thickest SiNWH is $1.03m_0$, which is about four times heavier than that for the [100] bulk heavy hole (also observed by TB calculation in [7]), while the hole effective mass of SiNWO is only $0.5m_0$.

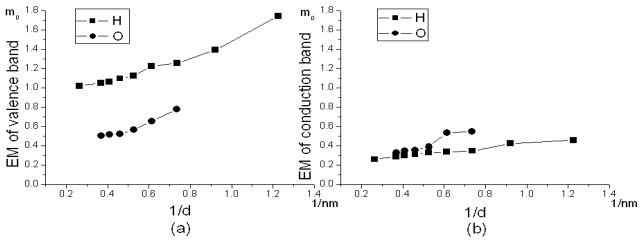

Fig.1 EM of H/O passivated [100]SiNW (a)VBM (b) CBM

This result can be explained after comparing the total DOS and PDOS distribution shown in Fig.2. The CBM in both H- and O- passivated case is mainly contributed by 3p orbit of center Si atoms in the wire. The introduction of O-termination modifies the electronic structure of VBM. The VBM is contributed by 3p orbit of surface Si atoms and 2p orbit of O atoms which is quite different from the case of SiNWH. An effect called σ-n mixing effect[8], which means orbit mixing between σ bond of valence Si 3P orbit and non-bonding lone pair states of O atom, weakens the localization of the valence electron and

decreases the EM of the hole greatly. Also, with the modification of VBM, the band gap of SiNWO is minishing.

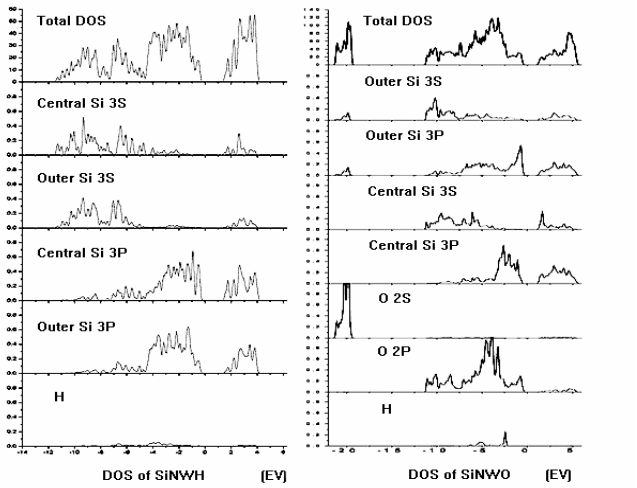

Fig.2: Total DOS and PDOS of [100] SiNWH and SiNWO. Fermi level is set to zero(eV).

[110] SiNW

Fig.3 shows the relation between effective masses and the thickness of [110] SiNW. One distinct characteristic can be observed: the calculated electron and hole EM of [110] SiNWH is much smaller than that of [100] SiNWH and bulk Si. Foremost, electron and hole EM is very close to each other, which is especially beneficial to CMOS application. Moreover, the band gap of [110] SiNWs is less than that of [100] (not shown here). According to our calculation, there is particularly about 3% strain in SiNWH and 12% strain in SiNWO along the axis for the thickest SiNW considered in this work. Such large strain is obviously overestimated since the interfacial structure is considered as ideal situation in the simulation. It has been demonstrated that the strain along [110] reduces the m_t of conduction band [9], and we got the smaller EM of electron than that of bulk m_t. The strain also eliminates the degeneracy of valence band, inducing the ascending of light hole band. Therefore, the hole EM of [110] SiNWH corresponds to that of light hole in bulk Si. Same as [100] SiNW, the introduction of O-termination modifies the electronic structure of VBM.

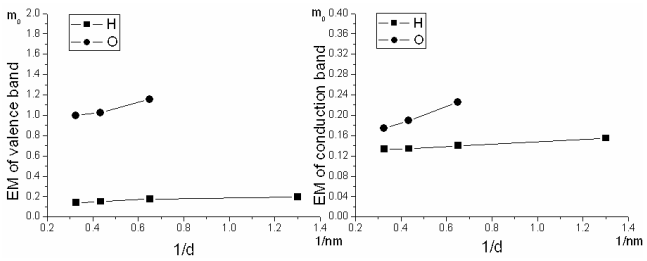

Fig.3 EM of H/O passivated [110]SiNW (a)VBM (b) CBM

From PDOS analysis in Fig.4, we also can find that the CBM in both cases are made of nearly the same composition, but there is some distinct difference in the VBM. Apart from the quantum effect, the modification of VBM is apparently the result of O-affiliation together with the intensive strain. The large strain, which may cause band warps, results in the abnormal enhancement of the hole effective masses in SiNWO.

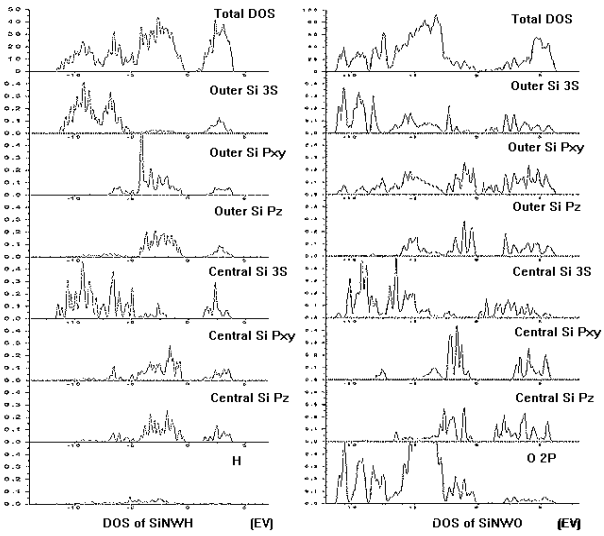

Fig.4 DOS and PDOS of [110] SiNWH and SiNWO,

Here we address our conclusion. The introduction of O-termination mainly modifies the electronic structure of VBM, resulting a smaller band gap and hole EM; there is a large strain existing in [110] SiNW which also decreasing the EM; with less band gap, as well as less EM, [110] SiNWs show some predominance over [100] counterparts; however, excessively large strain in [110] SiNWO which induces the hole EM increasing must be avoided; [100] SiNWO and [110] SiNWH are the best choices for the CMOS blocking cell according to our calculation.

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