

A Study on Electronic Structure of Silicon Nanowires with Diverse Diameters and Orientations for High Performance FET

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1 Introduction

From the scaling limit issues in a planar MOSFET, 3D MOSFETs including a fin FET have been focused for future LSI devices, owing to its ability to reduce the off current (I_{off}), which eventually reduces the power consumption. These 3D MOSFETs also provide larger on current (I_{on}) by adjusting the threshold voltage (V_{th}). However, the total current required for driving the circuit would be limited due to its narrower cross section. This concern is also applied to a nanowire FET which is the ultimate 3D MOSFET. One way to improve the I_{on} at small cross section is to achieve one dimensional transport [1]. In order to investigate the properties of the nanowire FET, we analyzed the electronic structure of silicon nanowires (SiNWs), which are used as a channel for the nanowire FET.

2 Method

The electronic structure of SiNWs was calculated by the first principles calculations with local density functional approximation (LDA) [2, 3] using ultrasoft pseudo-potential proposed by Vanderbilt [4]. All the calculations are done by Tokyo Ab-initio Program Package (TAPP) [5]. We analyzed the dependence of cross section diameter on the band structure of SiNWs having [001], [011] and [111] orientation with a circle cross section. The dangling bond of peripheric atom was passivated by hydrogen atom. SiNWs with [001] orientation having Si atoms bonding of three hydrogen atoms were not adopted. The diameter indicates twice distance between center and Si atom which is the farthest from center. In our parameters for first principle calculation, periodic-boundary conditions were employed in xy plane with a supercell which is large enough to eliminate the interaction between neighboring wires. Neighboring wires are separated by 0.7 nm. Brillouin zone integral was done by two sample k points. The energy cutoff set to 12.25 Ry.

From these calculation, the diameter dependence on band gap, electron and effective masses (m_e^*), hole effective mass (m_h^*) and the number of subbands were estimated. The obtained band gaps are shifted by 0.6 eV, which is required to reproduce the bulk silicon band gap value.

3 Result and Discussion

Band structures of SiNWs are shown in Fig. 1. When diameters are about 1 nm, SiNWs with each orientation

have a direct band gap at gamma point, which are in contrast to bulk Si. SiNW with [111] orientation and diameter of 1.93 nm has indirect band gap.

Fig. 2 indicates band gaps dependence on diameter for SiNWs with each orientation. The band gap of SiNWs becomes wide as diameter decreases and band gaps over 2 eV is obtained with small diameter SiNWs. SiNWs with each orientation have direct band gap in small diameter. However, SiNWs with [111] orientation and diameter above 1.93 nm have indirect band gap.

Fig. 3 indicates m_e^* and m_h^* dependence on diameter for SiNWs with each orientation. The m_e^* of SiNW with [001] orientation becomes heavy as the diameter increases. The m_e^* of SiNW with [011] orientation becomes heavy as the diameter increases. Moreover, the m_e^* moves towards the bulk m_e^* of 0.19 m_0 , which correspond in first Brillouin zone of SiNWs with [001] and [011] orientation, when the diameter of SiNWs increases for SiNWs with [001] and [011] orientation. The m_h^* of SiNW with [111] orientation becomes light as the diameter increases. The m_h^* of SiNW with [011] orientation have almost constant value, despite of diameter's variation. Both electron and hole effective mass of SiNW with [011] orientation have smaller values than effective mass of SiNWs with other orientation. From the viewpoint of only effective mass, SiNW with [011] orientation may have high mobility.

When one dimensional ballistic conduction is achieved, the conductivity of SiNW FET is basically determined by the number of subbands near conduction band minimum (CBM) in n-channel FET and valence band maximum (VBM) in p-channel FET. Here, the numbers of subbands within 50 meV from CBM and VBM are plotted in Fig. 4. The number of subbands within 50 meV from CBM and VBM increase, as the diameter of SiNW increases. About SiNWs with diameter of not over 2.5 nm, SiNWs with [001] orientation have larger number of subbands within 50 meV from both CBM and VBM than value of other orientation SiNWs. Therefore, SiNWs with larger diameter and with [001] orientation can achieve higher conductivity from the viewpoint of the number of quantum channels near each edge.

However, as the density of subbands increase, the spacing of each band becomes narrow, which will allow inter subband scattering, eventually reduces the conductivity. Here, we propose a model that there exists a trade off between the number of subbands and conductivity,

lowering due to subband scattering. An optimum diameter exists for the SiNW with each orientation (Fig. 5).

4 Conclusions

In conclusion, the tendency of band gap, m_e^* , m_h^* and the number of subbands for different diameters in SiNWs has been calculated. A trade-off model for I_{on} is proposed for SiNW FET.

Acknowledgement

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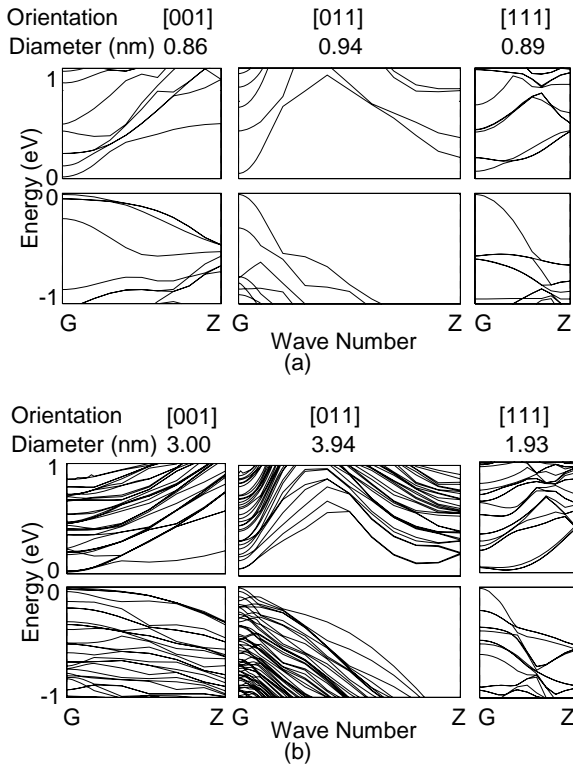


Fig. 1 (a) The band structure of SiNWs with small diameter. (b) The band structure of SiNWs with larger diameter. The upper (lower) pictures indicate band structure near CBM (VBM). The longitudinal axis indicates relative value. The transverse axis each orientation is coupled with same scale.

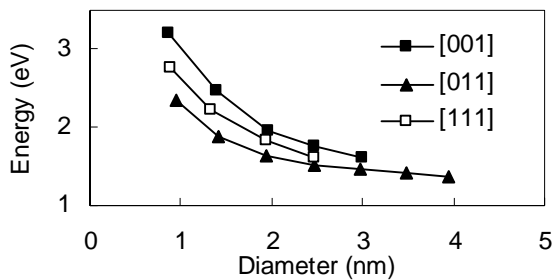


Fig. 2 Band gap dependence on diameter about SiNWs having

[001], [011] and [111] orientation. Solid square, solid triangle and empty squares indicate [001], [011] and [111] orientation. A large band gap is obtained with small diameter. When diameters increase, band gaps of each SiNW become lower.

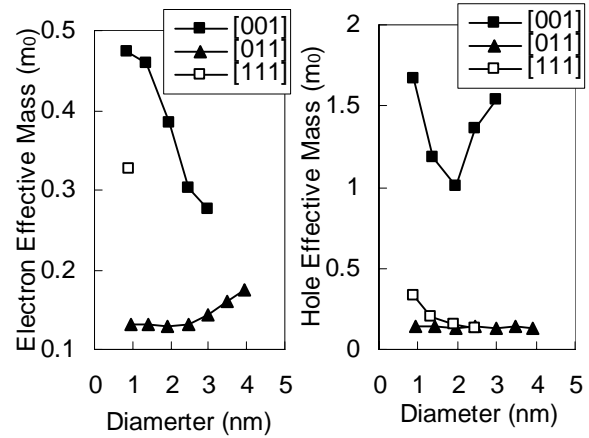


Fig. 3 Calculated electron (left) and hole (right) effective mass in the unit of free electron mass, m_0 , plotted as a function of diameter. m_e^* of SiNWs having [001] orientation moves towards the bulk m_e^* , $0.2 m_0$, when diameter increases.

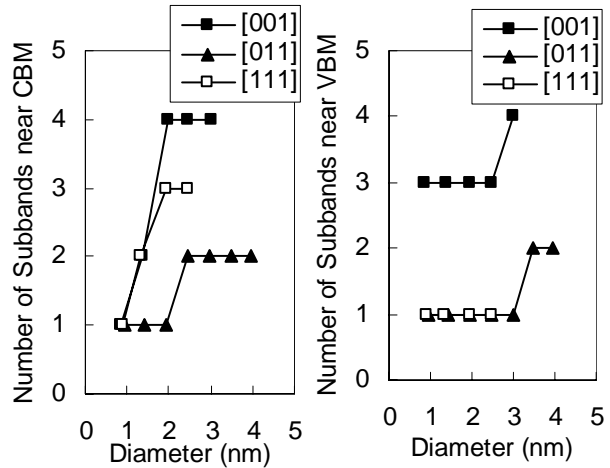


Fig. 4 The number of subbands within 50 meV from the CBM (left) and VBM (right) versus diameter.

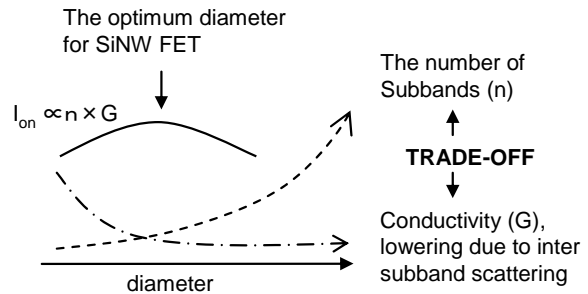


Fig. 5 The trade off model between the number of subbands (n) and the conductivity (G) with inter subband scattering.