

Diameter Dependency of Characteristics of Ultrathin Si Nanowires

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Abstract. In the present paper, we have presented electronic and transport properties of silicon nanowire (SiNW) using density functional theory. Electronic and transport properties are computed for a different diameter of zigzag structure. These nanowires show metallic nature at a nano-scale. With increasing in diameter SiNWs are becoming more metallic. Out of 1R, 2R and 3R zigzag SiNWs, 1R zigzag serves a potential applicant as a electronic and thermal conducting material.

INTRODUCTION

Nanotechnology and semiconductor devices are the most researched topics of the decade. In nanotechnology widely researched topics are nanowires and nanotubes which it opens a large scope of research in research community [1, 2]. More and more study of one dimensional semiconductor have been reported because of their unique electronic and structural properties [3], such as thermal and chemical stabilities, excellent mechanical strength and good heat transfer [4, 5]. Si nanowire (SiNWs) has importance in several technological fields like a nano electronics, detectors and biochemical sensors [6-8]. But there is no systematic research done on ultrathin SiNWs; Si nanowire and nanotubes are most capable building blocks for nano technology [9, 10].

For NWs, diameter of NWs plays a vital role in the characteristic. In this study, we had done study the effect of diameters depended structural, electronic and transport properties in SiNWs with zigzag arrangement. Firstly we give the computational detail for this study, followed by the section of result and discussion in which we will discuss the stability and different characteristic and which will be followed by conclusion.

METHODOLOGY

Simulations of the paper are done with the Quantum Espresso [11] based on density functional theory (DFT). To represent electron ionic core relation we used norm-conserving pseudo potential. To get the correct ground state structure of the system we used the Rappe Rabe Kaxiras Joannopoulos method, Perdew Burke Ernzerhof (PBE) exchange and correlation of the generalized gradient approximation (GGA). The Brillouin zone integration is done with the gamma centered Monkhorst Pack $1 \times 1 \times 29$ k-point mesh and cutoff energy for plane wave basis set of 1088 eV were considered to get the electronic properties convergence. All the considered SiNWs are elongated to z-directions. For avoiding interaction in x and y direction, vacuum of 12 Å is applied. Schematic diagram and charge density contour were taken with the help of XCRYSDEN [12]. Electronic Transport properties were computed using BoltzTraP code [13]

RESULTS AND DISCUSSIONS

Computed values of binding energy E_b , lattice constant, nearest neighbor distance N_D , diameter of wire D and conduction channel for considered SiNWs states are presented in Table 1. Distance between two neighboring atoms is liable for the deviation in binding energy. As per previous reported work the bond length between Si-Si atoms varies between 2.34 Å to 2.86 Å which is in good agreement with our work [14]. The binding energy for every atom of considered structure computed with subsequent equation,

$$E_b = \left(\frac{E_{system} - nE_{atom}}{n} \right) \quad (1)$$

Here, E_b is the binding energy, E_{system} and E_{atom} are the energy of the considered structure and individual isolated atom, and n is the number of atoms in considered structure. It is defined in such a way that positive binding energy per atom is consideration that system is stable than isolated atom. Schematic structure and variation in binding energy with lattice constant of computed 1R, 2R and 3R SiNWs are shown in Fig. 1, and STM images for SiNWs are shown in Fig. 2.

Table 1. Binding energy (E_b), Lattice constant (LC), Nearest neighbor distance (N_D), Diameter of wire (D) and conduction channel (G) of considered SiNWs

System	E_b (eV)	LC (Å)	N_D (Å)	D (Å)	G (G_0)
1R	4.14	2.49	2.49	-	2
2R	4.53	2.49	2.49	2.45	2
3R	3.59	3.33	2.40	3.43 & 5.05	5

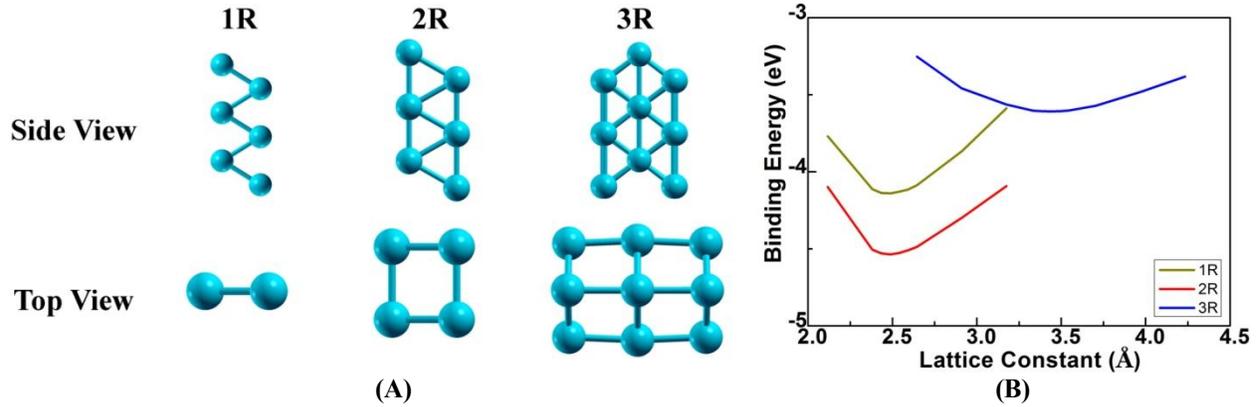


FIGURE 1. (A) Schematic structure of considered zigzag 1R, 2R and 3R SiNWs (B) Variation in binding energy with lattice constant of 1R, 2R and 3R SiNWs

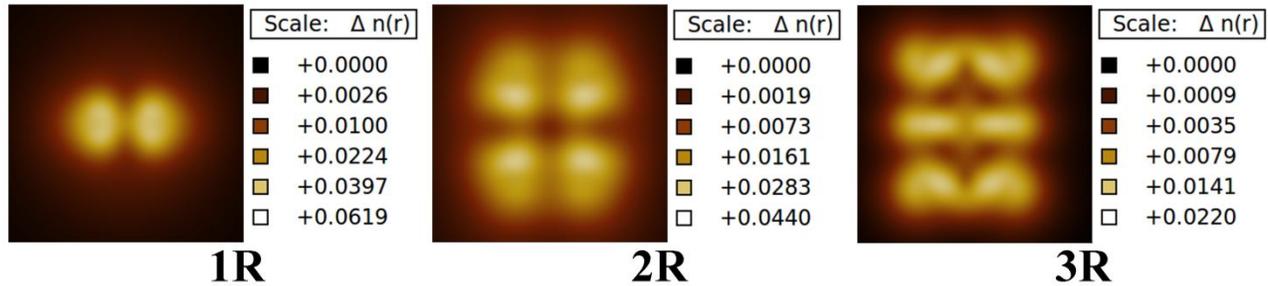


FIGURE 2. STM image of of 1R, 2R and 3R SiNWs

In 1R SiNWs, there is single zigzag chain of Si and optimized lattice constant and binding energy is 2.49 Å and 4.14 eV. In 2R SiNWs, there are two zigzag chains with the separation of 2.49 Å which has lattice constant of 2.49

\AA and binding energy of 4.53 eV. In 3R SiNWs, as shown in Fig. 1, there are nine atoms distributed in two planes which are normal to the nanowire axes. In 3R structure lattice constant and binding energy of system is 3.33 \AA and 3.59 eV. Binding energy of considered structure is in good agreement with Si crystal which is 4.63 eV [15], but lattice constant is less than the Si crystal which is 5.43 \AA [15]. Similar kind of behavior was reported for Au nanowire by Jariwala et al [16].

Electronic Properties

Electronic density of states and band structure for computed SiNWs systems with optimized lattice constant have been computed and shown in Fig. 3. It is undoubtedly seems that 1R, 2R and 3R SiNWs are metallic in nature which is in agreement with previous work for SiNWs reported by Jariwala et al [14]. Among the considered NWs 3R SiNWs having a highest number of conduction channel, which is states in Table 1.

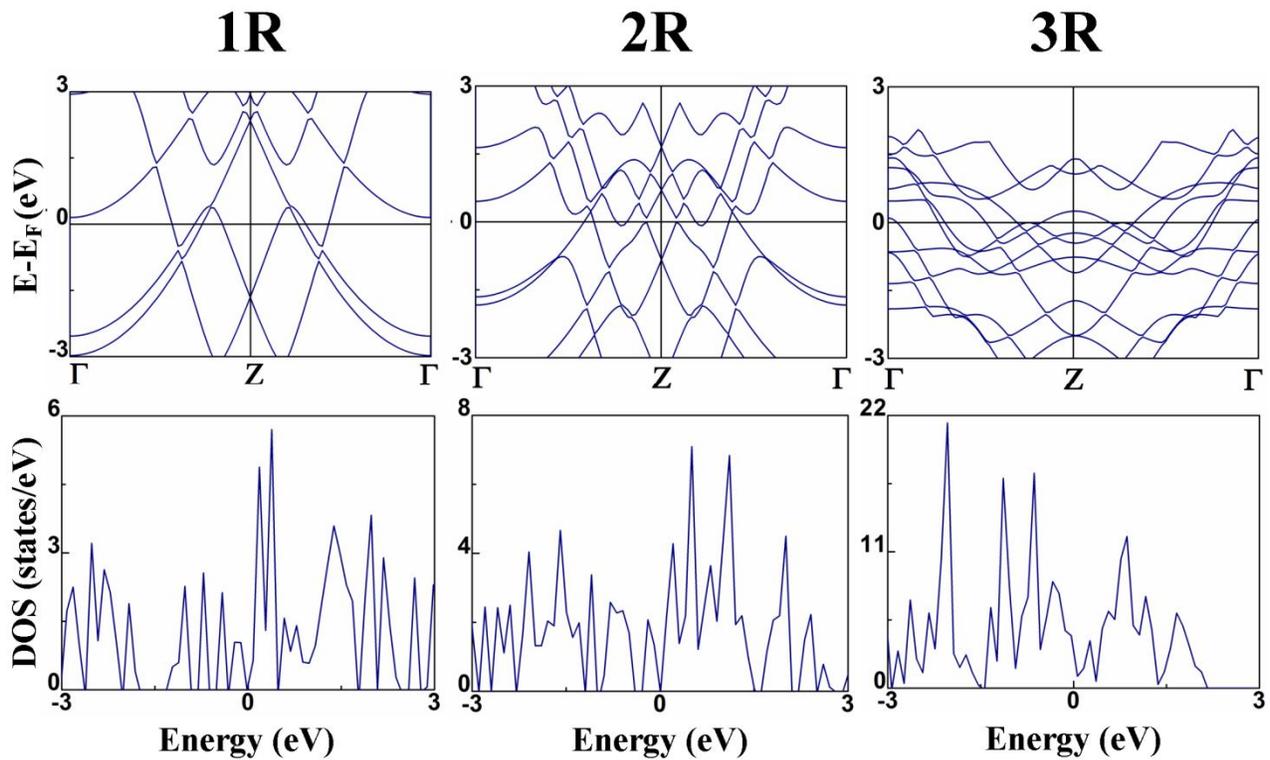


FIGURE 3. Density of States (DOS) and electronic band structure of 1R, 2R and 3R SiNWs

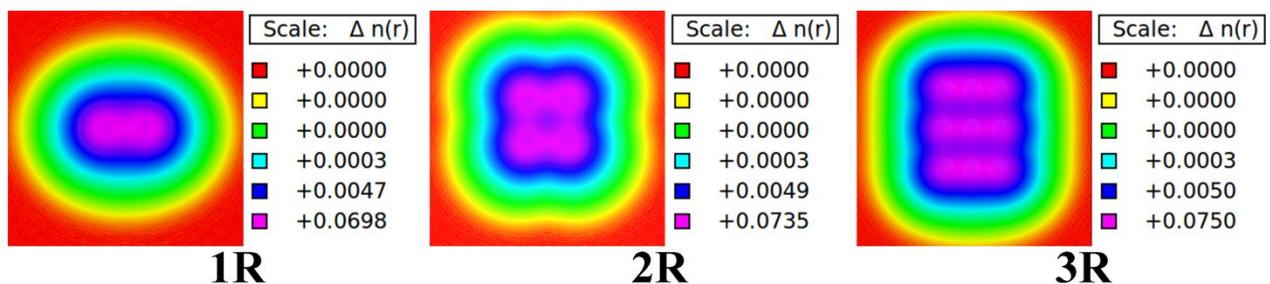


FIGURE 4. shows a charge density contour of SiNWs with (001) plane of SiNWs. All the charge contour shows metallic behavior of 1R, 2R and 3R SiNWs.

Transport Property

Transport characteristic of considered SiNWs have computed by BoltzTraP code which is governed by Boltzmann theory. Fig. 5 shows the variation in electronic conductivity and thermal conductivity of SiNWs for temperature ranging from 50 K to 800 K. For 1R and 2R SiNWs, electronic conductivity is decreased with increasing in temperature and in 3R SiNW electronic thermal conductivity is increasing with increasing in temperature. While for thermal conductivity all SiNWs increases with the increment in temperature.

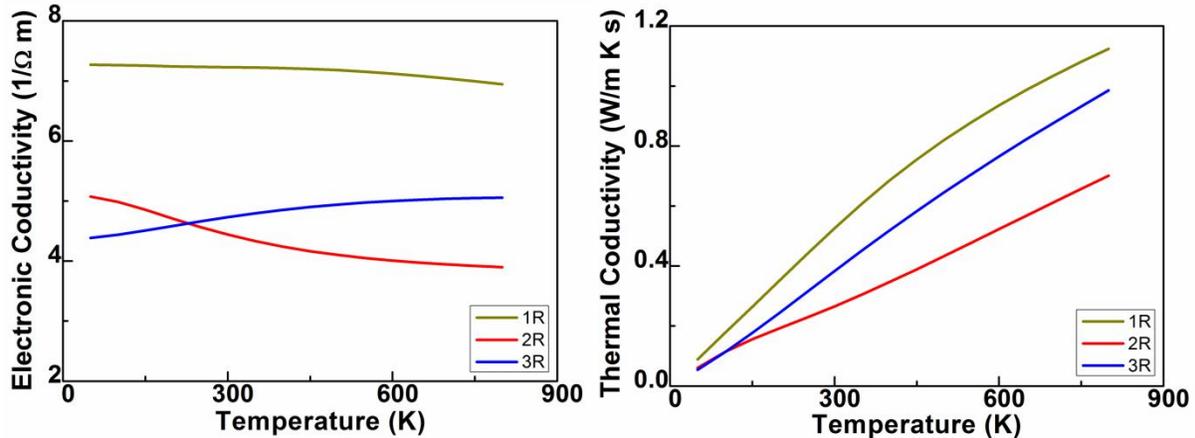


Figure 5. Variation in Electronic and Thermal conductivity with temperature for 1R, 2R and 3R SiNWs.

CONCLUSIONS

We have systematically computed the SiNWs with different diameter using density functional theory. Here we conclude that with increasing in diameter of SiNWs it becomes more metallic. The DOS and electronic band structure of all the SiNWs shows delocalized bonding. Si as a bulk shows a semiconductor behavior but in a 1D configuration it shows metallic nature. This SiNW have potential applicant for the electronic and thermal conducting material.

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