

Short Communication

Physical Study of Nano Ribbon and Tetragonal Bundled and Isolated Nano Tube SiC (7,0)

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Abstract

Physical study of nano ribbon, tetragonal bundled and isolated nano tube SiC (7,0) are part of our project in knowing new nano material such a silicon carbide. These studies have been performed by density function theory. Effect of ribboning, tubulating and tetragonal bundling on the physical properties such as stability, structural constants, optical physics, chemical parameters and magnetization have been investigated by PWSCF software. These factors are very important tools for materials engineering in nano science and technology. There is an inter-tube interaction at bundled structure that changes its physical properties.

Keyword: *Physical property, Density function theory, SiC nanotube, Ribbon, Semiconductor, Density of state, PWSCF, Simulation.*

1. INTRODUCTION

Low-dimensional materials refer to a new class of material with reduced dimensionality with one or more physical dimension(s) constrained to the nanometer scale. Two-dimensional (2D) nanosheets, one-dimensional (1D) nanotubes, and zero-dimensional (0D) fullerenes represent typical examples of such materials. When compared to three-dimensional (3D) bulk substances, low-dimensional structures are anticipated to exhibit new properties due to quantum confinement and/or surface and interfacial effects. Therefore in recent years, materials scientists have drawn particular attention to these nano systems to make sense of their unusual physical

and chemical properties that can promote novel applications in engineering [1].

Nano science is the study, understanding and control of phenomena and manipulation of material at the nano scale, so nano science is the world of atoms, molecules, macromolecules, quantum dots, and macromolecular assemblies. Nanotechnology describes many diverse technologies and tools, which do not always appear to have much in common. Therefore, it is better to talk about nanotechnologies, in the plural. In 1985, scientists discovered new material by founding strange results in mass spectra of evaporated carbon samples. Therefore, fullerenes were discovered and their

stability in the gas phase was proven. CNTs have been discovered in 1991 after discovering fullerene [2]. CNTs have attracted a lot of interest due to their unique properties and have many applications in industry [3,4]. CNTs are a layer of graphene sheet which is rolled up as a tubular form. Chiral vector defines the structure of a CNT with a pair of integers (n,m)[5,6]. Nowadays, many types of semiconductors such as SiGe[7], BN[8], GaN[9] and SiC[10] have been fabricated. A CNT is cylindrical, the ends of some CNTs are open; the others are closed with full fullerene caps. Bulk silicon carbide has different structural form such as cubic form or hexagonal form. These polytypes are semiconductors with the zinc blend (3C) or the wurtzite (2H). polytypes. For high temperature, high power and high frequency devices, these materials are suitable. Nowadays silicon carbide nano tubes (SiCNTs) are synthesized [11]. SiCNT were also synthesized by the reaction of CNTs and SiO at different temperatures. Depending on chirality vector, CNTs are either metallic or semiconductor but SiCNTs are always semiconductor. The zigzag tubes are a direct band gap but the armchair tubes are an indirect band gap. A Si-C bond is more stable than that of Si-Si or S-C. The kind of chemical bond of CNT and SiCNT is different. Owing to electronegativity the carbon atom respect to the silicon atom, SiCNT has polar property. Therefore, SiCNTs may exhibit some unusual physical properties respected to CNT. Such an example, zigzag SiCNT may be piezoelectric that can show second order nonlinear optical response. SiCNT are not only in single wall form but also are in multi wall form with a common axis. SiCNT same as CNT has the strong

aromaticity that can absorb other elements or materials even for tradition metal. CNTs can also be bundled to tetragonal or hexagonal form. Graphene is a planar layer of sp^2 bonded carbon atoms in honeycomb arrangement.

Here, with ab initio density functional theory, physical study of nano ribbon and tetragonal bundled and isolated nano tube SiC (7,0) was investigated. The results consist mainly of physical properties such as structural, optical and electrical properties.

2. COMPUTATIONAL METHOD

Ab initio calculation for silicon carbide low dimensional was performed using Quantum SPRESSO Software [12]. This software is based on density functional theory (DFT) with the pseudo potentials. We applied Xcrysden program for the visualization of molecular and/or crystalline structures from the specified input data and for the visualization of properties [13]. A super cell $1 \times 1 \times 1$ is selected for all samples which have 28 atoms. The atomic potential of silicon and carbon are the ultra-soft pseudo potentials. The number of the valence electrons of the outer shell for the C and S atoms in the pseudo potentials is 4 and 4, respectively with configurations C: $2s^2, 2p^2$ and Si: $3s^2$ and $3p^2$ that treated as valance state electrons. For main calculations, the primary calculation is necessary. For example, total energy of unit cell versus k point and plane wave cut off energy must be optimized. Total energy of unit cell versus its volume must also be optimized for stability of system. The k-space integration in a uniform mesh ($1 \times 1 \times 12$) and ($1 \times 12 \times 12$) was performed for one and two dimensional super cell by Monkhorst-Pack grids. Although, atoms Si and C are not a magnetic atom, the spin polarization is applied to it for studying the magnetic property. SiCNT (7,0) are constructed by rolling up a graphitic hexagonal SiC sheet.

The atomic positions and then lattice constants were fully relaxed. The type of ionic dynamics selected at this paper is BFGS quasi-newton algorithm, based on the trust radius procedure for structural relaxation. Convergence threshold for self-consistency that estimated energy error was selected less than 10^{-7} Rydberg. The convergence criterion is satisfied when the total energy changes less than etot_conv_thr (energy total Convergence threshold) between two consecutive scf steps. Note that etot_conv_thr is extensive, like the total energy. Default amount is less than 10^{-4} Ry. convergence threshold on forces (a.u) for ionic minimization is satisfied when all components of all forces are smaller than forc_conv_thr (force Convergence threshold). Default amount is less than 10^{-3} Ry/au

3. RESULTS AND DISCUSSION

3.1. Structural Property

3.1.1. Unit Cell

The most important parameter for calculation is the suitable selection of atomic position and crystalline structure. Figure 1 illustrates the atomic position and the crystalline structure for a) ribbon, b) isolated single wall NT (ISWNT) (7,0) and c) the bundled structure. Figure 1d and 1e show unit cell in real space and reciprocal space. Bigger atom is silicon and small atom is carbon. This figure shows the atomic position and the crystalline structure after relaxing. At calculation of relaxing, force and pressure were optimized to the minimum amount.

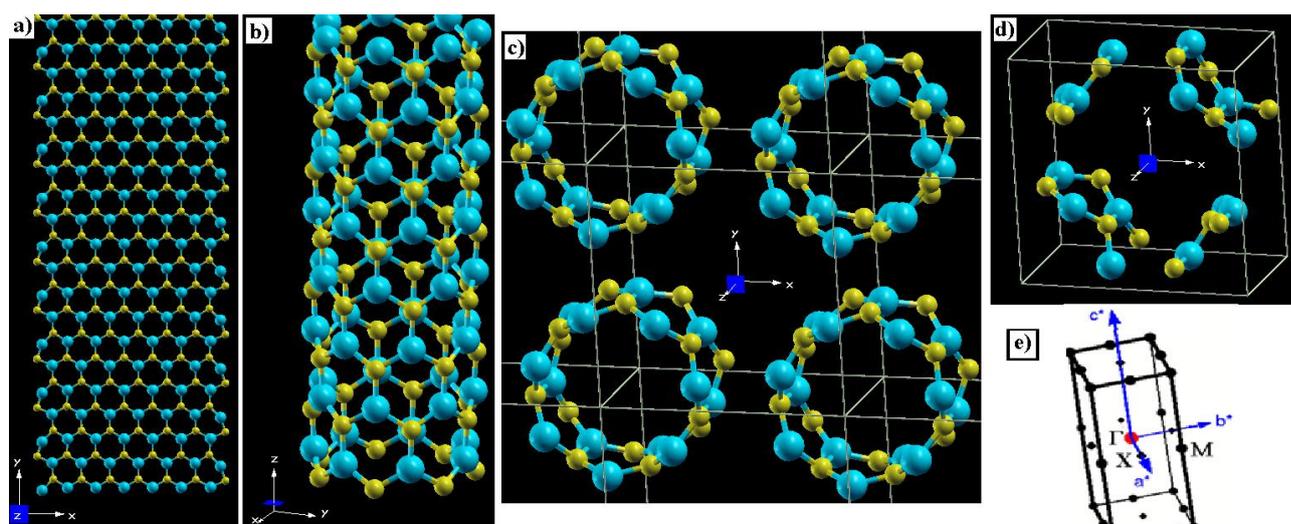


Figure 1. The atomic position and the crystalline structure after relaxing for a) ribbon b) isolated single wall NT (7,0) c) the bundled structure d) unit cell in real space e) unit cell in reciprocal space

3.1.2. Lattice Constants

For determining lattice parameter, total energy of unit cell respect to volume must be minimized. Figure 2 depicts the changes of energy (energy – minimum energy of stability) versus to the changes of volume (volume – volume related to minimum energy of stability). Ribbon (7,0) is a tape part of SiC sheet. The diagram of stability

for ribbon at figure 2 shows that nano ribbon is stable in real space. Width before and after relaxing is 21.47 \AA and 20.96 \AA , respectively. Owing to the atomic pull of inner atoms from atoms of sheet's edge, the width of nano ribbon is decreased. At the lengthwise direction, lattice constant is 5.293 \AA and the transversal pull certainly affects on that and increases it. Single Wall

SiCNT (7,0) are formed by rolling up a graphitic hexagonal SiC sheet. Figure 2 shows the probability of its stability. Calculations show lattice parameter 5.313Å at the tube axis and SW-SiCNT represents one dimensional system. When SW-SiCNT comes to the neighbor of one another, an inter-tube interaction is created. This force makes a new style of crystalline structure which is named the bundle structure. Here, the bundle structure changes the geometric and electronic

properties SW-SiCNT. The crystalline structure is also tetragonal or hexagonal form. We investigation each of two states but here is only reported the tetragonal bundle structure. Figure 2 foresees a lattice parameter 10.16Å at the transverse. The axial lattice constant 5.324Å is bigger than that of ISW-SiCNT. This value refers to force due to inter-tube interaction. Then if ribbon is tubulated and tube is bundled, the axial lattice constant will increase such as others [14-16].

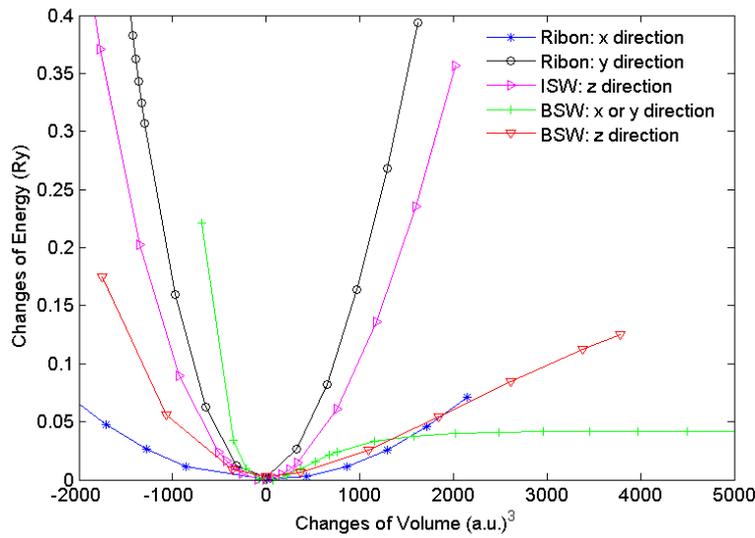


Figure 2. Energy versus volume for computing lattice constant. Representation of stability of samples.

3.1.3. Symmetry

Physics is the study of symmetry. Symmetry in physics has been generalized to mean invariance. If there is high symmetry in unit cell, the volume of calculations will be less and system will be more stability. The symmetry with stability has direct line relation. By increasing the material's symmetry, its stability increases too. Base on table 1, stability of ISW is more than BSW.

3.1.4. Buckling

It is thought that Si and C atoms are placed on the perimeter of one circle at ISW-SiCNT, but it was not true. Because of the electronegative difference and the radius difference of atoms Si and C, these are place in the perimeter of two different circles. The difference between the radii of these circles is defined buckling ($\beta = |r_C - r_{Si}|$). The calculated buckling at table 1 shows that buckling of BSW is less than that of ISW due to the inter-tube interaction that tubes were pulled from

four sides at the tetragonal bundled structure.

3.1.4. Hardness of Materials

The Hardness of samples were calculated by the bulk modulus or some indispensable energy for changing the form of a material. The bulk modulus was obtained by fitting data of the energy versus the volume with Murnaghan's state equation [17]. Table 1 shows the calculated bulk modulus (kbar) of samples. As it can be seen, the

transverse hardness of nano ribbon (801 kbar) is less than the longitudinal hardness (861 kbar). For ISW-SiCNT, there is only the axial hardness (677 kbar). At BSW-SiCNT, there is not only the axial hardness (4222 kbar) which is nota bene but also the transverse hardness (120 kbar) because of the inter-tube interaction. Then, being bundled to the tetragonal form increases the hardness of nano tubes.

Table 1. Structural properties of materials.

Physical properties		Ribbon	ISW-NT	BSW-NT
Number of atoms at unit cell		28	28	28
Lattice constant (Å)	x=a	40	25	10.16
	y=b	5.293	25	10.16
	z=c	12	5.313	5.324
Young's modulus (kbar)	a	801	-	120
	b	861	-	120
	c	-	677	4222
Symmetry	number	2	4	4
	Point group	C _{2v} (m)	C _{2v} (mm2)	C _{2v} (mm2)
Tubular diameter D(Å)		-	6.9202	6.9286
Translational vector		b	c	a+b+c
Radial buckling β (Å)		-	0.11	0.1

3.2. Optical Properties

3.2.1. Bandgap

The band gap study is a suitable way for knowing a material that is metal or semiconductor. The calculated band structure of nano materials along the higher symmetric direction Z, gamma, X and M in the Brillouin zone are given in figure 2 accompany with total density of state. Being zero at density of state prerequisites for existing band gap. The Fermi's level is zero. It is seen that nano ribbon has an indirect band gap 1.593 eV from gamma to X point. The first effect of being tubulated of nano ribbon is reduction of bandgap from 1.593 to 1.16 eV. The second effect is the band gap change from indirect to direct. And finally the third effect is degeneracy increase. When ISW-SiCNT is bundled to the tetrahedral form,

several phenomena happen such as material properties transition to the metal state and reduction of band structure degeneracy. For determination of the locality of Fermi's energy at band gap, $E_F - E_{VBM}$ and $E_{CBM} - E_F$ have been calculated. E_{VBM} (E_{CBM}) is maximum and minimum of valance and conduction energy, respectively. It can be seen that Fermi's energy is near to the conduction band and this vicinity is increases for ribbon such as others [11-13].

3.2.2. Partial Density of State (PDOS)

Figure 3 shows partial density of state of nano ribbon, ISW-SiCNT and BSW-SiCNT. The charges of energy are between -15 eV and 3 eV and PDOS change is also from zero to 1.5 states on electron volt.

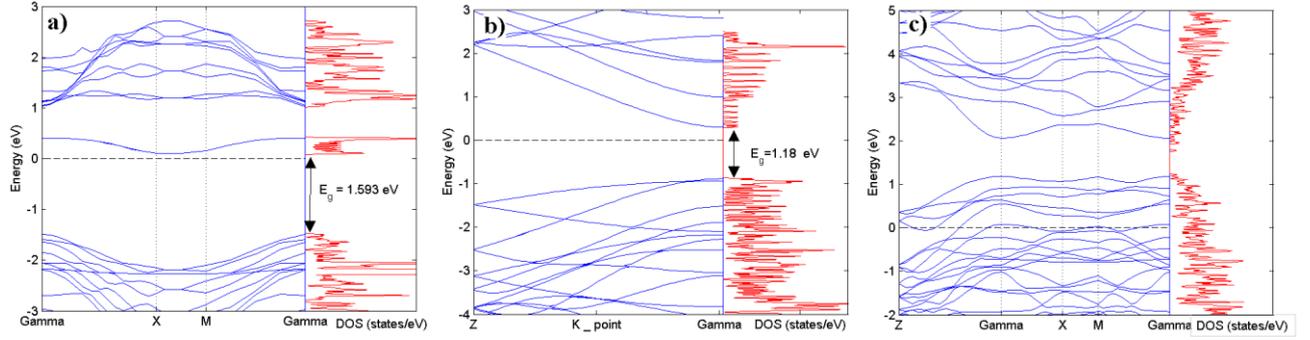


Figure 3. Band structure and density of state: a) nano ribbon b) ISW-SiCNT c) BSW-SiCNT.

Table 2. Optical properties of materials.

Physical properties		Ribbon	ISW-NT	BSW-NT
Energy band gap (eV)		1.593	1.18	-
		$\Gamma \rightarrow X$	$\Gamma \rightarrow \Gamma$	-
		indirect	direct	-
$E_F - E_{VBM}$ (eV)		1.492	0.884	-
$E_{CBM} - E_F$ (eV)		0.101	0.297	-
Effective mass m/m_o	C.B	1.1959	0.2677	-
	V.B	0.4784	0.4207	-
V (cm/s)	C.B	6.9018×10^6	3.8633×10^6	-
	V.B	4.6012×10^6	3.0907×10^6	-

The partial density of state of materials shows the role of each atomic orbital at band structure. At nano ribbon, all atomic orbital have an important role at creating the conduction band but for valance band, the role of orbital p of atoms C and Si is

higher. For ISW-SiCNT, the roll of orbital p of atom Si (C) at conduction (valance) band is more. At BSW-SiCNT, the Fermi's energy level has been formed compound from orbital p of atom C and Si.

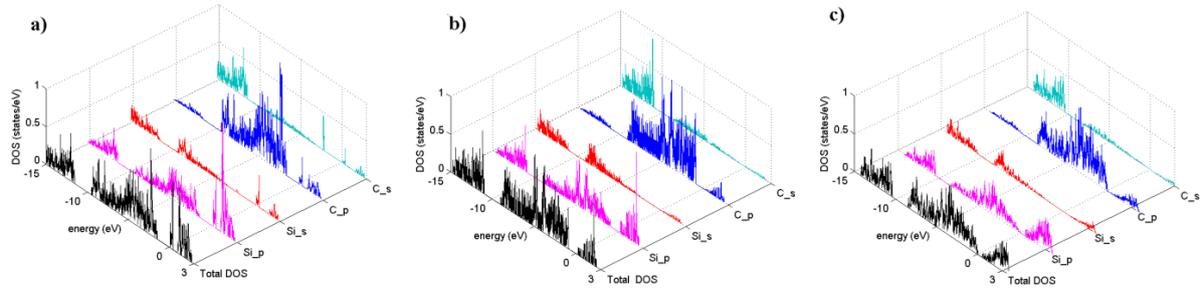


Figure 4. Partial density of states: a) nano ribbon b) ISW-SiCNT c) BSW-SiCNT.

3.2.3. Velocity

The mean velocity of an electron (hole) in a definite Bloch level was calculated for a semiconductor. Table 2 shows the result. This velocity describes the motion of Bloch electrons (holes) between collisions at x (gamma) point and gamma (z) point for ribbon and ISW-SiCNT, respectively. As seen, being tubulated causes to decrease the velocity at between collisions, both for

electron in the conduction band and for hole in valance band.

3.2.4. Effective mass

The mass tensor plays an important role in determining the dynamics of electron (located in minimum conduction band) and hole (located in maximum valance band). The effective mass was calculated by using the band structure. Table 2 illustrates the

effective mass nano ribbon and ISW-SiCNT. As seen, being tubulated decreases the effective mass.

3.4. Chemical Property

3.4.1 Cohesive Energy

The cohesive energy of a crystal is defined as the energy that must be given to it for separating its component into neutral free atoms or the difference between the average energy of the atoms of a solid and that of the free atoms.

For each structure, formula of computing of cohesive energy is $E_c = E_{total} - \sum_i n_i E_i^{free}$

. Cohesive energy, total energy of a crystalline structure, energy of formation a free atom and number of atoms have been shown by E_c , E_{total} , E_i^{free} and n_i , respectively.

Table 3 shows the cohesive energy of the samples. By decreasing the cohesive energy, its stability increases. Base on the cohesive energy of BSW-SiCNT, its stability enhancement can be concluded.

3.4.2. Bond Length

The bond length or bond distance is the average distance between nuclei of two bonded atoms in a molecule. Table 3 illustrates the bond length before and after relaxation. Picking out a ribbon from sheet SiC causes that atoms sit closer together and the bond length is decreased. When ribbon is rolled up, inner pressure increases the place of atoms and consequently the bond length is increases. For ISW-NT, the increase of the bond length is more. As a result, being tubulated increased the bond length. The chemical bond type is polar covalent bond because the electronegativity of carbon atom (2.55) is more than silicon atom (1.9).

3.4.2. Charge Density

Charge density can refer to the charge distribution over the volume of a particle; such as a molecule, atom or ion. The

electronic configuration of the valance electrons for atom C (Si) is $2s^2 (3s^2)$ and $2p^2 (3p^2)$. When a molecular bond Si-C is formed, the distribution of the charge density is changed due to the electronegative difference of atoms Si and C. More electron affinity of carbonic rather than Si atom causes the electron cloud of Si atom attracts forward to atom C and its charge density is consequently increases. This is the reason of more charge average of atom C at table 3.

3.5. Magnetic Property

C and Si atom are nonmagnetic elements and also SiC Graphene-like sheet is a nonmagnetic material so it can be hypothesized that ribboning, tubulating and bundling can produce the magnetic property. The calculations of the spin polarizations show that these factors have not any effect on the magnetic property and are nonmagnetic materials.

4. CONCLUSION

In this paper, the physical properties such as structural, optical, chemical and magnetic property of nano ribbon, isolated single wall- silicon carbide nano tube and tetragonal bundled single wall- silicon carbide nano tube have been studied by first-principles calculation within density functional theory. We found that ribboning, tubulating and bundling can change the physical properties. These methods can be a suitable way for engineering of materials. Stability of BSW-SiCNT is more respected to other materials because of high symmetry and low energy. BSW-SiCNT is metal but nano ribbon and ISW-SiCNT are indirect and direct semiconductors. The chemical bond type Si-C of all is a polar covalent bond. Calculations show that these nano structures are nonmagnetization. Results of this research can be used to in SiC bundled such as the doping, storage and absorption phenomena.

Table 3. Chemical properties of materials.

Physical property		Ribbon	ISW-NT	BSW-NT	
Bond length (Å)	Before relaxation	1.771	1.764	1.768	
	After relaxation	1.65	1.783	1.782	
Cohesive energy (eV)		-13.024	-13.418	-13.442	
Average of charges (e)	s	C	1.1647	1.1402	1.1403
		Si	0.8378	0.8381	0.8385
	p	C	3.8748	3.9120	3.9017
		Si	2.0047	1.9979	2.0137
Total charges (e)		7.8820	7.8882	7.8942	

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