Strain Controlled Electronic and Transport Properties of Si-C Atomic Wire

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Abstract. An ab-initio Density functional calculations and Non-equilibrium approach have been used to study the effect of positive strain on the equilibrium geometry, electronic structure and transmission function of Si-C bi atomic wire. In the absence of strain, Si-C bi-atomic wire is found to be semi conducting. The equilibrium electronic structure of these nanowires is shown to change drastically on applying strain. The Si-C bi-atomic wire has wide zigzag (WZ) structure GM and has a direct band gap of 0.7eV and remains direct on applying small strain up to ε ~ 3.1%. At the strain value of ε ~ 3.1% the band gap widen up to 1.77eV, and becomes indirect on further increasing the strain values. We observed that at the lower bias the conductance does depend on the strain applied on the wire. From density of states we have found that the strain value of ε ~3.1% offers maximum band gap value up to the ~1.55eV bias applied. At equilibrium state the transmission through Si bands is observed slightly more, and indicates the holes tunneling through device. Application of strain provides channels for electrons tunneling.

INTRODUCTION

The scale of microelectronic devices is shrinking continuously [1], leading to increased interest on the nature of electron transport through essentially one-dimensional (1D) nanometre-scale channels such as atomic wires [2]. After the realization of carbon atomic wire, non-metals wires have gained lot of attention [3] for their application as connector within molecular electronics devices [4]. Experimentalist found that a single-walled carbon nanotube provides an ideal enclosure for the creation of such 1D wire [5]. Theoretical studies of atomic wires made of group IV, III–V, and II–VI elements suggest that linear chain of C, Si, S, Ge, SiGe, GaAs, InSb, InP, AlSb and CdTe are stable and good conductors [6]. We chose to study the effect of strain on the electronic and transmission properties of 1D bi-atomic wire of Si-C within density functional theory (DFT) formulation.

COMPUTATIONAL DETAILS

All calculations performed are based on the density functional theory [7] and A Non-equilibrium Green-Function Approach incorporated in SIESTA and TRANSIESTA codes [8, 9] within the Perdew-Burke-Ernzerhof [10] (PBE) functional. Troullier-Martins [11] ab-initio pseudo potentials has been used to describe the interaction of valence electrons with atomic cores. The charge density and potentials are calculated on a real-space grid with mesh cut-off energy of 400Ry for all systems. We sample the one-dimensional brillouin zone of the nanowires by 81 k-points for the entire lattice constants considered. Periodic boundary conditions have been used in x-direction and separate the nanowires by 15 Å in y and z directions to prevent it from interacting with its periodic image. The residual forces acting upon the atoms for globally optimized structure are no more than ~0.001eV/ Å. For transport calculation, the wire has been extended as 6x1 unit cells in the periodic direction.

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Table 1: Summary of calculated structural parameters and electronic band gap of Si-C wire at different values of strain. Here **b** is the bond length**,** $\boldsymbol{\alpha}$ is the bond angle, $\boldsymbol{E_b}$ is the binding energy, $\boldsymbol{a}$ is the lattice constant **Ɓ** is the band gap and $\boldsymbol{C}$ is the stiffness

Systems	Strain	b(Å)	α (deg)	E_b(eV)	a (Å)	Ɓ(eV)	$\boldsymbol{C(meV}$/Å)
Si-C	zero	1.695	147	-4.56	3.25	0.71 X-X	1.72
	1.5%	1.690	155	-4.56	3.30	1.01 X-X	
	3.3%	1.675	180	-4.54	3.35	1.70 X-X	
	7.1%	1.750	180	-4.28	3.50	0.97 Γ-X	
	13.8%	1.850	180	-3.53	3.70	zero	

RESULT AND DISCUSSION

Geometric Structure

Each unit cell has two atoms in y-z plane and periodic in x-direction only. We can identify each structure by the pairs of values(a, α), where a is lattice constant (LC) and α is a bond angle (BA) running from 56° to 180° angle. The geometry of atomic wire has been globally optimized for all values of BA to determine its optimum structure. Contours in the figure 1(A) represent the equipotential surface, where the global geometry is marked as a yellow mark that comes out to be wide zigzag (WZ) like geometry. On applying strain, the geometric transition comes through the change of BA and bond length (BL). For each value of strain the optimum structure by the pair of values$(\boldsymbol{a}, \boldsymbol{\alpha})$, has also been calculated and marked as a blue dot in the figure 1(A). The dotted black line, shown in figure 1(A) represents the BL with its value inline. Table I summarizes our results for BL, BA, binding energy, LC and band gap at different values of strain.

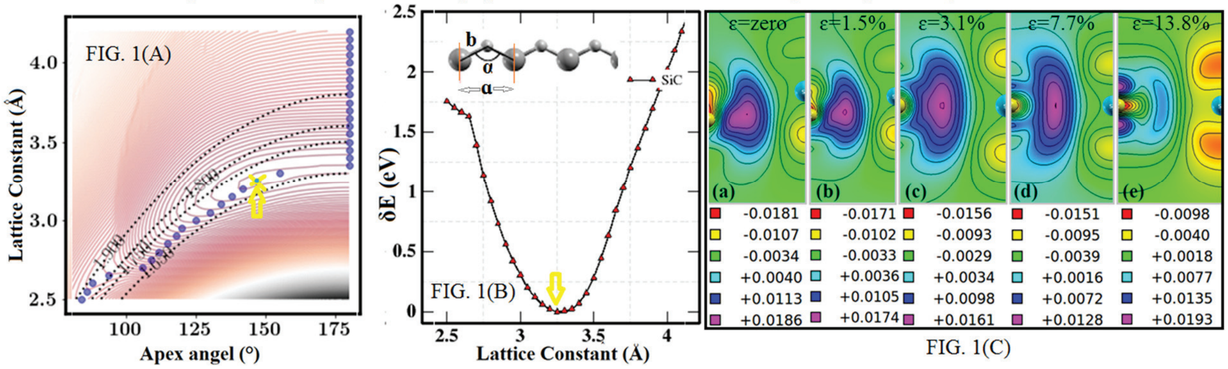

Figure 1: In fig. 1(A) each contour line represents an equipotential surface of the energy values per unit cell of Si-C atomic wires as a function of the LC $\boldsymbol{a}$ and the BA $\boldsymbol{\alpha}$. Optimized geometry at each LC is shown by the blue dots. The GM that comes naturally in transition path has been shown with yellow mark. Black dotted line denotes the BL with the values inline in **Å** unit. In fig. 1(B) the relative energy per two atom w.r.t. GM as a function of lattice parameters is plotted. Each geometry has been identified by the pairs of value$(\boldsymbol{a}, \boldsymbol{\alpha})$, where $\boldsymbol{a}$ is the LC; $\boldsymbol{\alpha}$ is the BA and $\boldsymbol{b}$ is the BL as shown in the inset. Figure 1(c): Contours plots of $\boldsymbol{\delta\rho(r\,)}$, in figure 1C(a), 1C(b), 1C(c), 1C(d) and 1C(e) are drawn for strain value **ε**~zero, 1.5%, 3.1%, 7.7.% and 13.8% respectively.

The bi-atomic wire of Si-C is found to have WZ equilibrium structure at the pair of value $(\boldsymbol{a}, \boldsymbol{\alpha})$ = (**3.25, 147**). Since, the global minimum (GM) among pairs of values$(\boldsymbol{a}, \boldsymbol{\alpha})$, is the equilibrium state with minimum energy, the change in the LC (a) is taken as applied strain, and can be defined as $\varepsilon = (\boldsymbol{a'} - \boldsymbol{a})/\boldsymbol{a}$, where $\boldsymbol{a'}$ and $\boldsymbol{a}$ are the strained LC and global LC respectively. The line stiffness **C** is calculated by fitting the strained energy **Es** i.e. the **δE** versus strain (**ε**) curve as shown in figure 1B with formula $\boldsymbol{E_S} = \boldsymbol{C_0}\varepsilon + \mathrm{C}\varepsilon^2$. By increasing strain value Si-C wire gets straightened (BA=180 degree) easily at low value of strain **ε**~3%. This suggests that the BA distortion is much easier in the Si-C wire than BL alternation. The binding energy of Si-C is **-4.*56****eV/atom***, which is smaller in magnitude than binding energy **-6.*9****eV/atom*** for C-C linear wire which we calculated for reference after optimizing its geometric structure.

Electronic Properties

Application of the strain changed the charge density and the ionic character on atoms sites. The difference in the charge density contour plots of the Si-C chains at different strain value are shown in figure 1(C), depicting the character of the bond. The difference in the valance pseudo charge density to atomic valance pseudo charge density $\boldsymbol{\rho_{atom}(r)}$ is calculated by the formula $\boldsymbol{\delta\rho(r) = \rho(r) - \rho_{atom}(r)}$. Positive values on the scale shows the amount of accumulation and negative values shows the amount of depletion in charge density. Accumulation of charge density on Carbon atom contributes more to the electronic density of states of the valance band and depletion of the charge density on Silicon atom contributes to the conduction band. In addition to the covalent character of the bonds in linear configuration as shown in figure 1C(c), 1C(d) and 1C(e), the amount of ionic character is reflected by the accumulation of bond charge near the carbon atom. In the equilibrium state as shown in figure 1C(a), there is accumulation of charges on carbon atom and depletion of charges on silicon . On increasing the strain from zero to **ε**~7.7% the charge density of bond in between the Si and C atom became delocalized at **ε**~13.8%. In contrast, silicon atom that becomes more dispersed in the region and also more cationic. This suggested that the electron affinity of atom is not the only player and the geometrical structure has the decisive effect on the ionic character of the atoms.

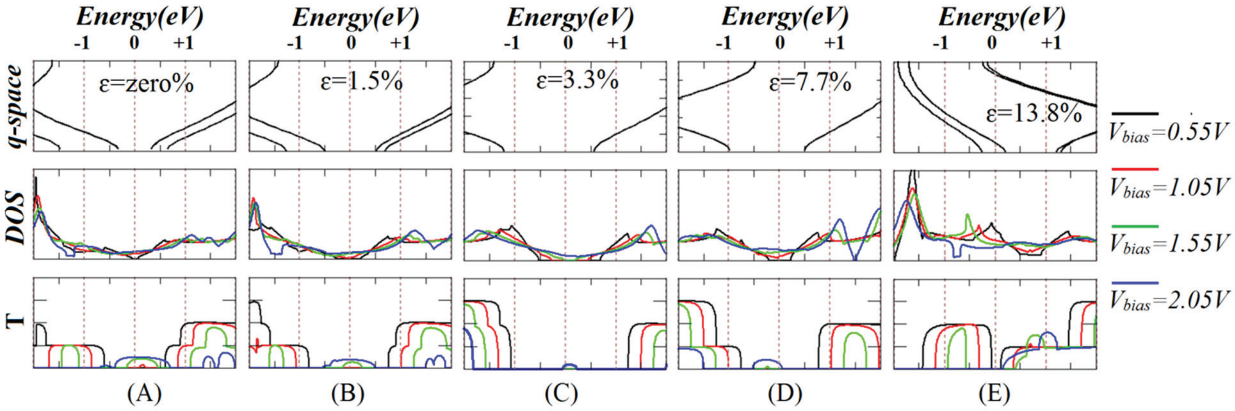

Figure 2: Top row shows the band structure with the band gap value of 0.7eV, 1.1eV, 1.7eV, 0.8eV and zero, for ε~zero**,** 1.5%, 3.1%, 7.7% and 13.8% respectively. Middle row and last row show the density of states (DOS) and the transmission between the electrodes (T) for the device, respectively at V_{bias}= 0.55V (black), 1.05V (red), 1.55V (green) and 2.05V (blue).

Unlike carbon chain, where only the $\boldsymbol{\pi}$ band crosses the Fermi level at the centre of the Brillion zone at $\mathbf{k = \pi/2d}$ [12], which leads to the Peierls distortion [13] of the chain, different situation is observed for the Si-C chains: We found that no band crosses the Fermi level, which prevents the Peierls distortion of these chains. We calculated the electronic band structure (top row of fig 2), DOS (middle row of fig 2) and transmission spectra (last row of fig 2) at different bias voltage for Si-C wires at equilibrium and strained geometry as shown in figure 2. It is quite interesting to find that the Si-C bi-atomic wire at ε~zero has a direct band gap of 0.7eV as shown in figure 2(A). On stretching the linear chain further, $\boldsymbol{\sigma_1}$* (i.e. $3s - 2p_x$) bands at Γ shift downward to Fermi energy and the $\boldsymbol{\pi}$ (i.e. $3p_z - 2p_z$) bands at X shift upward to Fermi energy level at X, as evident from band structure plot (top row) for **ε**~ 1.5%, 3.3% and 7.7% of figure 4(B), 4(C) and 4(D), respectively. Eventually, the band gap became indirect at Γ-X at the strain **ε**~7.7%. The indirect band gap decreased on increasing the magnitude of strain and system became conductor at the strain value of **ε**~13.8% by pushing the $3s - 2p_x$ band into Fermi level at Γ and also by the raising of $3p_z - 2p_z$ above Fermi level at X as evident in figure 2(E).

Transmission Spectra

In order to investigate the mechanical and electronic coupling with the charge carrier transmission we have performed the NEGF calculation for Si-C atomic wires. Summary of the calculated band gaps from DOS of device region for different bias voltage at different strain values are given in table 2. From the DOS for **ε**~zero (black), the band gap for lower value of bias voltage 0.55eV is showing the band gap 0.1eV as in figure 2(A), increases on strain ε~1.5% and 3.1% to 0.5eV and 1.2eV respectively evident from figure 2(B) and 2(C). On increasing strain further, the band gap decreases to 1.3eV and to zero for **ε**~7.7% and 13.8%. Only, for bias voltage of value 1.05eV and

1.55eV, the wire with **ε**~3.1% shows the band gap of ~0.75eV and ~0.2eV, respectively. For bias voltage of 2.05eV and 2.55eV band gap diminished for all type of wires. It is interesting to note that the transmission spectra for strained Si-C of the order of **ε**~3.1%, continue to show the plateaus like features for the higher bias voltage of 1.55eV, in contrast to rest. At, bias voltage of 1.55eV and above, the suppressed transmission, at the vicinity of Fermi level has been observed. At equilibrium state the silicon bands contributes to transmission slightly more, and indicates the holes tunnelling through device. Application of strain provides channels for electrons tunnelling.

Table 2: Summary of calculated the calculated band gap (marked with *) in eV unit from DOS of device region for different bias voltage at different strain value.

Strain	**V_{bias} (V)**			
	0.55	**1.05**	**1.55**	**2.05**
zero	0.1*	zero*	zero*	zero*
1.5%	0.5*	zero*	zero*	zero*
3.3%	1.2*	0.75*	0.2*	zero*
7.1%	0.45*	zero*	zero*	zero*
13.8%	zero*	zero*	zero*	zero*

CONCLUSIONS

The Si-C bi-atomic wire has been investigated within DFT and NEGF frame work. Our total energy calculation reveals that the Si-C structure has WZ geometry. The effect of strain on the wires suggests an increase in band gap that remains direct band up to a strain of ~3.1%. The Si-C stiffness value of the order of ~1.7meV/Å and have maximum bonding energy after carbon mono atomic wire. The charge gets accumulated near the carbon atom in the region in between the Si and C atoms. One can also conclude that the atomic sites are more ionic at GM. From, NEGF calculation we can conclude that the application of strain on the 1D Si-C wire, one can control the conductance in the bias voltage range of ~1.55eV. Also the strained Si-C wire in the range of the order of for **ε**~3% behaves as a mechanical switch for bias voltage up to the order of ~1.55eV.

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