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Effect of Al atom Doping on Band Gap of Rectangular Cross Section Si nanowire

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Abstract
In this work band gap of hydrogen-passivated, free-standing silicon nanowires, oriented along [111] direction with rectangular cross section was studied. Further the effect of doping of Al atom on band structure is also analyzed by using GGA approximation. it is found that the band gap of H-SiNW dramatically reduced upon doping and nanowire start behaving as bulk silicon.
Keywords:DFT, GGA, nanowire

Introduction:

In the last few years quantum wires, or nanowires are studied both experimentally and theoretically .Semiconductor nanowires exhibit a variety of unique material properties, including mechanical flexibility, size-dependent optical and electronic properties, and solution process ability. In particular, silicon nanowires (SiNWs) have been studied both theoretically and experimentally and they have attracted much attention due to their applications in various field, like nanosensors [1,2], solar cells [3,4], Field effect transistor [1,5], and energy conversion devices [6,7], to use nanowire for these applications, it is necessary to control the electronic properties of nanowires (NWs), which depends on the diameter of nanowire, crystallographic orientation [8] ,doping element, doping concentration ,cross sectional geometry and optimized structure of the nanowires [9]. Band structure of SiNWs can be modified by changing cross sectional area, cross sectional geometry, orientation, surface morphology, dangling bond passivation, and by doping of impurity atom[10,11]. Reduced dimensionality systems are characterized by a large surface-to-bulk ratio and offer the possibility of doping through the external adsorption of molecules [12] rather than the incorporation of substitution impurities [13]. Álvaro Miranda [14] has studied NH_3 molecular doping of silicon nanowires grown along the [112], [110], [001], and [111] orientations. most of the nanowire are of free-standing type; typical dimensions are tens of nanometers in lateral size and microns in length, although nanowires as small as 3 nm in diameter have been reported [15] .Not only cubic but wurtzite structure nanowires have been synthesized. They can be assumed to have low defect concentrations and close to bulk structure, few research studies have carried out on strained nanowires[16], a number of studies have already been made to study polarized photoluminescence[17,18] and Raman scattering experimentally [19] . Riccardo Rurali et al.[20] has studied Nanowires with diameters below 10 , where quantum effects become important and the properties diverge significantly from those of bulk silicon. They have studied the structural properties of silicon nanowires, emphasizing the close connection between the growth orientation, cross section, and bounding facets. Many unique properties of these systems are at the same time defying challenges and opportunities for technological advances. Structures and energetic of H-SiNWs were reported by using DFT tight binding method[21] .By passivating the SiNWs surface with H and some halogens including Br, Cl, and I, the electronic structure of wires with diameter ranging from 0.6 to 3 nm has been studied using ab initio DFT calculations[32]. Impurity doped SiNWs have also attracted attention since the dopant atoms provide excess carriers required in device applications, such as diodes and transistors. Doping of H-SiNW by Mn, B and P impurities and its effect on the electronic structure and band gap have been investigated by calculations based on DFT by Fernandez-Serra et al[22]. Furthermore, growing research interest has been devoted to the functionalization of SiNW surface with various species to study the chemical and biological sensitivities of silicon nanowires. Few ab initio calculations now reported for InP nanowires[23] though only for the band gap and not for the whole band structure. In this article we extend our earlier study in which we have studied the effect of doping on band gap of silicon nanowire of triangular cross section along [1 1 1] direction by implementing density functional theory using GGA, in this research paper effect of doping on band gap of silicon nanowire of rectangular cross section along [1 1 1] direction is analyzed by implementing density functional theory using GGA

Table-1
Band Gap of SiNWs Along [1 1 1] Direction

Si	**H**	Al	Lattice parameters(A	Cell Angles	**Cross sectional area (nm^2)**	**Band Gap(eV)**
32	30	0	a = 30.454426 b = 30.499196 c = 9.621926	alpha = 90.000000 beta = 89.836100 gamma= 89.999999	.388	2.380
32	28	2	a= 27.037097 b= 30.991761 c=9.552908	alpha=90.000000 beta= 89.750330 gamma=90.00000	.388	1.621

SiNW with rectangular cross section was chosen and the electronic band structure of these SiNWs was studied by using DFT calculation. Silicon nanowire as a prototype was taken which has N=44 Si atoms in its primitive unit cell, and grown along [1 1 1] direction. we import the crystal structure of bulk Si and Create a [111] surface then Specify the surface [111] and the number of layers . the surface is converted to crystal structure by building a vacuum layer of 4.0A^o thickness. we Find out the periodic lattice length along Z direction, which is 9.406 angstrom. All the the redundant atoms along Z direction are deleted. the structure according to the periodic lattice length is Rebuild then a supercell in the X-Y plane is build. the redundant atoms in the X-Y plane is deleted. After Rebuilting the cell shape the nearest atom length between neighbor cells is checked. If the length is less than 10 angstrom, that time the cell size is changed so that the distance between nearest neighbor cells should be greater than 10 angstrom. Now, the final structure of Si nanowire with rectangular cross section along [111] direction is shown in Fig.1(a). The cross sectional View of silicon nanowire along [111] direction is shown in Fig.1(a), Yellow spheres stand for silicon atoms and white spheres for hydrogen. Hydrogen passivation is used to eliminate the defect states within the band gap so that the band structure of the chain should briefly feature the characteristics of silicon. for eliminating the inter-layer interaction a vacuum layer of thickness 4 Å is built between two neighboring chains . Upon relaxation, the structure of the ideal bare nanowire get reconstructed . Furthermore, to allow possible reconstructions involving two unit cells, structure optimization of an ideal nanowire is performed. In the later optimization, the energy per Si atom and the atomic structure did not change from the single cell optimization. Table 1 lists the studied cases with the atomic numbers within them, the area of the cross section and band gap. The lattice constants along the chain axis were optimized, involving variations within 3.5%.We have performed first-principles plane wave calculations[24,25] within DFT [26] using ultrasoft pseudopotentials.[27,28] The exchange correlation potential has been approximated by generalized gradient approximation GGA using Perdew Burke Ernzerhof exchange correlation functional[29] both for spin-polarized and spin unpolarized cases. For partial occupancies, we use the Methfessel-Paxton smearing method[30] The adopted smearing width is 0.1 eV for the atomic relaxation and 0.05 for the accurate band structure analysis and density of states calculations.Here total energy / atom convergence tolerance is 0.1000E-05 eV. All structures have been treated within a super cell geometry using the periodic boundary conditions. The lattice constants of the tetragonal super cell in the x-y plane are taken as asc=23.10918, bsc=22.661879 Å and csc=9.616978 Å along the z axis For the double unit cell calculations, the lattice constant is taken as csc=2co to prevent the interactions between the nearest neighbor impurity atoms located in adjacent cells. In the self consistent potential and total energy calculations, the Brillouin zone of SiNW is sampled in the **k** space within the Monkhorst-Pack scheme[31] by 1x1x40 mesh points as determined by the convergence tests and k-point separation of 0.02 1/A is taken for a geometrical optimization. A plane wave basis set with kinetic energy 230 eV has been used. All atomic positions and lattice parameters are optimized by using the BFGS where total energy and atomic forces are minimized. The convergence or energy is chosen as 10^{-4} eV between two ionic steps, and the maximum force allowed on each atom is 0.3000E-01eV/A. The band structure and density of state for rectangular cross sectional Si nanowire along [1 1 1] direction are displayed in Fig.1(b) and Fig.1(c) respectively. Note that for a SiNW passivation with H and subsequent optimization, most of the peak positions coincide with those of the ideal SiNW.

Effect of Doping of Al atoms on band gap:
Until now we have discussed hydrogen passivated SiNWs. However, impurity and dopant may be adsorbed on the SiNW surface in the practical usage. The adsorbents could take effect on the electronic structures and thus other related properties. The doping of single B or P atom in [110] SiNWs has been studied in Ref [22],where

the authors found that impurity favors the surface position and doping reduces the density of carriers. It means that the doping influences the electrical properties of the [110] SiNW remarkably. But it is unknown whether a similar conclusion could be drawn with [111] SiNWs. Therefore we studied a single Al atom adsorbed on the surface of SiNW oriented along [111] direction. Starting with the hydrogen terminated SiNWs, we replaced the Si atoms with Al atoms as shown in Fig. 2(a) and then optimized the structure by using generalized geometry approximation. Optimized structure of Al doped silicon nanowire along [1 11] direction is shown in Fig.3, from the optimized structures, we found that the adsorbed structure kept almost the original feature of the SiNW without impurity. The Si-Al bond length was about 2.5 Å and there was a distortion around the Al atom locally as shown in Fig.3.Surprisingly, Al doping causes energy levels to shift closer to the conduction band. The location of impurity states in the band gap occurs in a reverse order as compared to the n-type (N, P, As) and p-type (Al, Ga) dopants in bulk Si crystal. We found that the band gap surprisingly decrease to 1.621 eV by replacing two hydrogen atoms by two Al atoms at the edges as shown in Fig.2(b). Due to the reduced adatom-adatom interaction, dispersion less impurity bands are obtained. Electronic band structures of hydrogen passivated and doped Si nanowire were different from that of the bare wire since a defective state emerged in the middle of the band gap, and some bands appeared at the bottom of the conduction band. The band decomposed charge density analysis indicates that these levels originate from doping elements. H-SiNW semiconductor can be modified as a p type through substitution of Al . In view of the above results, one can contemplate that metallic, n and p-type zones or any sequence and size of them can be generated according to a desired device functionality.

FORMATION ENERGY:

We studied the relative stability of structures as a function of the wire size by calculating the formation energies of the nanowires. Formation energy is defined as the total energy difference between the reactants and the products. it is the (total energy of Si nanowire without H + total energy of the H atoms in the H2 form or other) - total energy of Si wire with H.

In calculations we have taken a supercell of 1x1x40 relative to the primitive cell, containing 32 ions. The Formation energy on hydrogen termination silicon nanowire and Al doped Silicon nanowire were calculated to be 0.369 eV and 0.371 eV respectively, indicating only a very minor change in formation energy take place due to doping of Al atoms.

Conclusion

Our results show that doping of Al atoms could reduce the band gap of silicon nanowire and at that time silicon nanowire will start behaving as bulk silicon. Some of the parameters that characterize the electronic band structures are listed in TABLE-1 It has been found that the band gap of the SiNWs decreases as the doping concentration increases. it is found that doping of Al atoms does not affect the geometry of silicon nanowire along [1 1 1] direction very much which is clear from Fig.2(a) and Fig.3.The optimized structure of hydrogen passivated silicon nanowire is nearly similar to the optimized structure of silicon nanowire which is doped with Al atoms. from this study it is clear that the doping of Al atom does not affect the geometry of nanowire but it could reduce the band gap of silicon nanowire upto great extent.

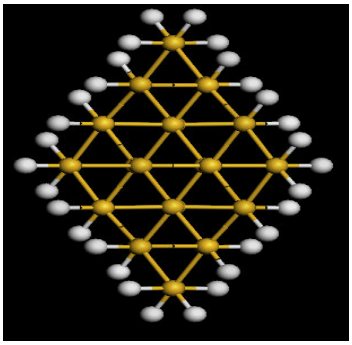

Fig.1(a)

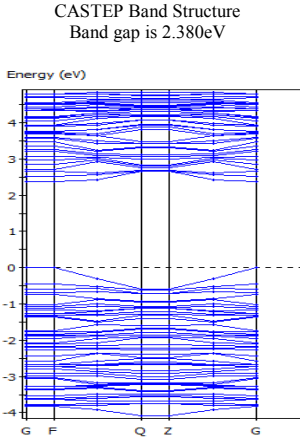

Fig.1(b)

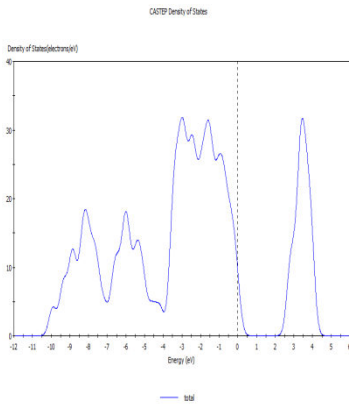

Fig.1(c)

Figure 1. in Fig.1(a) shows the rectangular cross sectional nanowire along [111] direction. Yellow sphere represents the silicon atom and white spheres represent hydrogen atoms In Fig.1(b) energy band structure of Si nanowire along [111] direction is presented. Fig.1(c) represent the density of states

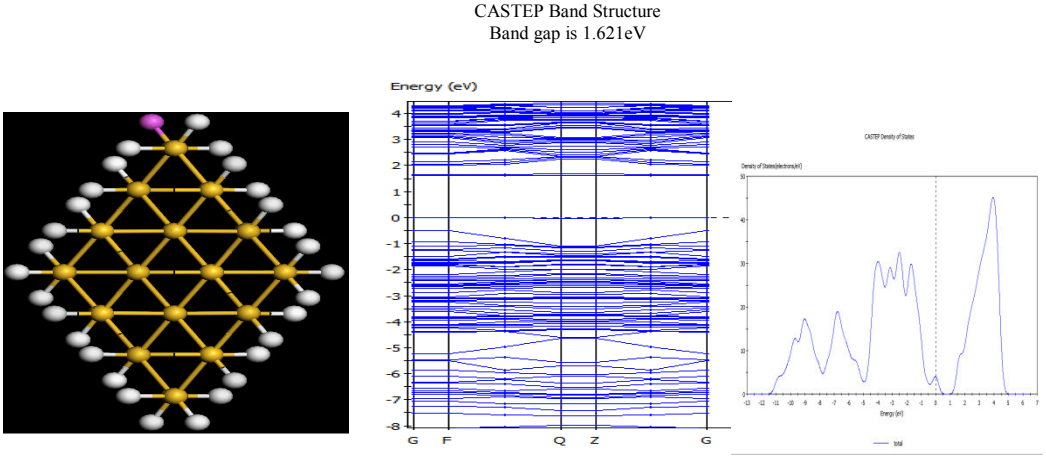

Fig.2(a) **Fig.2(b)** **Fig.2(c)**

Figure 2. in Fig.2(a) Al replaced the core Si atoms Yellow sphere represents the silicon atom and white spheres represent hydrogen atoms and violet sphere represents the Al atoms. In Fig.2(b) energy band structure of Al doped Si nanowire along [111] direction is presented. The energy band structure at the bottom indicates a p-type behavior.Fig.2(c) represent the density of states

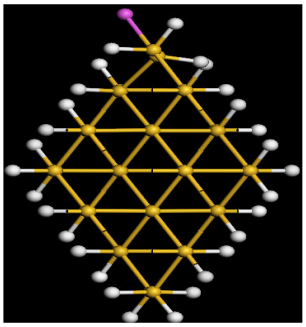

Figure 3.*Optimezed geometry of doped silicon nanowire.*

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