International Journal of Science and Research (IJSR)
ISSN (Online): 2319-7064
Impact Factor (2012): 3.358

Structural, Electronic and Optical Properties of Doped Titanium Nanowire

Florina Regius[1], Gnaneshwar.P.V [2], Arjun Senthil[b], Moon Paul [c], Varun Nair[d]

[1]Advance Materials Research Lab, Indian Institute of Information Technology and Management, Gwalior, Madhya Pradesh, India

[1, 2, 3, 4, 5]SRM University, Department of Physics and Nanotechnology, Katankulathur, Kancheepuram Dt, Tamil Nadu-603203, India.

Abstract: ***Electronic optical and structural properties of Titanium Nanowire (TiNW) when doped with Al and P atoms are obtained from simulation studies have been reviewed. The band gap, density of states, optical spectrum and Structural property of Titanium Nanowire has been compared when this nanowire is doped with phosphorus and aluminium atoms. We observed that decrease in band gap increases the metallic property of silicon. Total energy is maximum then the structure is least stable. So we can say that total energy is inversely proportional to stability. In density of states, we clearly see the decline in DOS/eV with the increase of doping Al and P atoms. In this paper, we have discussed all the electronic and structural properties.***

Keywords: Band structure, Band gap, Density of States, TiNW

1. Introduction

The nanowire, a structure that has an amazing length-to-width ratio. Nanowires can be incredibly thin -- it's possible to create a nanowire with the diameter of just one nanometre, though engineers and scientists tend to work with nanowires that are between 30 and 60 nanometres wide. Scientists hope that we will soon be able to use nanowires to create the smallest transistors yet, though there are some pretty tough obstacles in the way. Nanowires possess unique electrical, electronic, thermo electrical, optical, magnetic and chemical properties, which are different from that of their parent counterpart. Titanium NW are the answers for ongoing obstacles in electronic field. These Ti NW are the one-dimensional structures. Their electronic conduction can be controlled by doping. Ti NW can be used from field effect transistor to Biosensors.[4,5] The photoluminescence in Ti NW and nanoparticle have been observed [7,8] which is an experimental evidence of the quantum confinement.[6] Titanium-wire research started in the mid 1990s, when advances in microelectronics triggered a renewed interest in silicon—now nanowire—research. [1] Last, we will turn our attention to the electrical properties of Titanium nanowires and discuss the different doping methods. Then, three effects essential for the conductivity of a Titanium nanowire are treated. [9]Experimentally it has been observed that the band Gap can be tuned by choosing different growth directions and diameters of wire. [10] The electronic structure of Ti NW being critically depends on the size, orientation, passivation and doping level of Nano structure. These are the diameter dependence of the dopant ionization efficiency, the influence of surface traps on the charge-carrier density, also causing diameter dependence, and the charge-carrier mobility in titanium nanowires. [1]Many techniques, including both top-down and bottom-up approaches, have been developed and applied for the synthesis of Nanowires. Vapour–Liquid–Solid (VLS) Mechanism, Chemical Vapour Deposition (CVD), Evaporation of SiO, Molecular Beam Epitaxy (MBE), Laser Ablation and Electroless metal deposition and dissolution (EMD) [2]. These days Ti NW are used for enhanced thermo electric performance [3]. Titanium nanowire can be uniformly made at low temperature using Vapour-Liquid-Solid growth.

2. Computational Method

We have performed the calculation using the ab-intio psuedopotential method which is based on the density functional theory and analyse the electronic properties of Titanium Nanowire (alpha). We have used atomistix toolkit (ATK)[11] for computation, a further development of TranSIESTA-C[13,14] which, in turn, is based on the technology, models and algorithms developed in the academic code TranSIESTA and,in part, McDCal [12], employing localized basis sets as developed in SIESTA[15]. The computation has been made in self-consistent manner using steepest descent geometric optimization with Pulay Algorithm for iteration mixing. A mesh cut-off of 70 Hartre has been used throughout the study. The Brillion-zone (BZ) integration is performs with a Monkhorst-Pack scheme using 1*1*11 k points. The cut-off energy and the number of k points are varied to test the convergence and are found to converge within the force tolerance of 0.05eV/A for the reported value. The exchange correlation functional described within the extended huckel and with generalised gradient approximation revised-PBE (rev-PBE) as proposed by Zhang and Yang [16] are used for the computation of total energies of Titanium Nanowire and its doping with aluminium and phosphorous atoms. The total energy for Titanium Nanowire extended huckel potential is -2426.37 eV. The extended huckel potential is quite good for the computation of total energy.[17]The nanowires are placed in the super cell along the wire length in z-direction while the super cell lengths in the x and y direction are chosen big enough to avoid interaction between nanowire and its periodic image.[18] For better understanding of fundamental physics associated with different structures, the binding energies of Titanium nanowire have also been analysed and to understand the nature of material, localization and delocalization of states near the Fermi level, we have analysed the electronic band structure and density of states for all the doping configuration of Titanium Nanowire.

3. Results

3.1 Structural Properties

The atomic configurations of the Titanium Nanowire are presented in the Fig 1. It may be cautioned that these figures are schematic and separations between atoms are not to scale. As these figures depicts the structures quite clearly and hence have not been discussed separately in the text. The stability energetic in the various nanostructures of titanium has been performed under the extended huckel with the revised PBE type exchange correlation functional. We observe that Titanium Nanowire has the lowest energy is visible at -3426.37 eV which shows it is the most stable structure and when it is doped with one aluminium atom the total energy is -3375.27 eV which is less lower than earlier which shows it is next stable structure. In this way total energy increases with the increase of doping of Aluminium atoms in Titanium Nanowire. Now after doping with phosphorus atoms, the total energy has a great variation. -3468.46 eV is the lowest energy found when Titanium Nanowire is doped with the four phosphorus atoms. This shows it is highly stable structure. -3510.69 eV is the next lower energy found when Titanium Nanowire is doped with the three phosphorous atoms. It is also highly stable but lesser then earlier. Here, we observe that with increase in doping of atoms, total energy decreases and stability increases. Now for detail of structural stability, the formation energy and binding energy are calculated. [19]

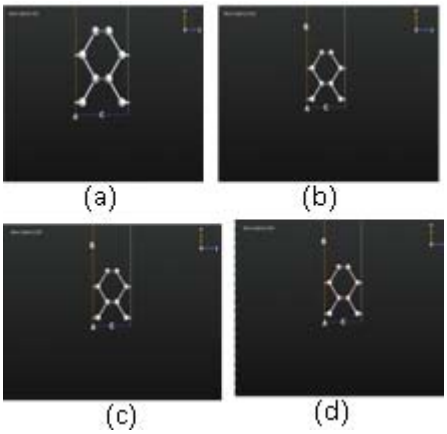
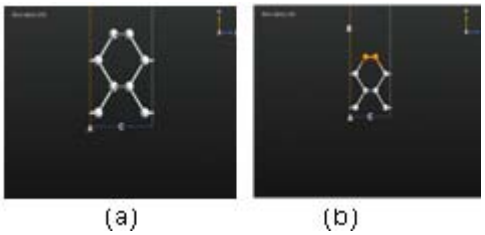


Figure 2: The atomic Configurations of Titanium Nanowires (a) TiNW without doping, (b) TiNW doped with 2 Al atom, (c) TiNW doped with 4 Al atoms, (d) TiNW doped with 6 Al atoms



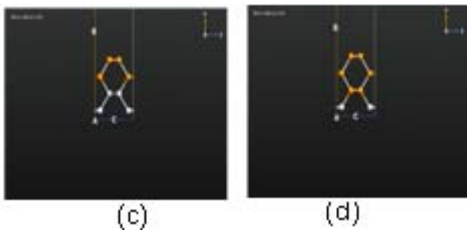
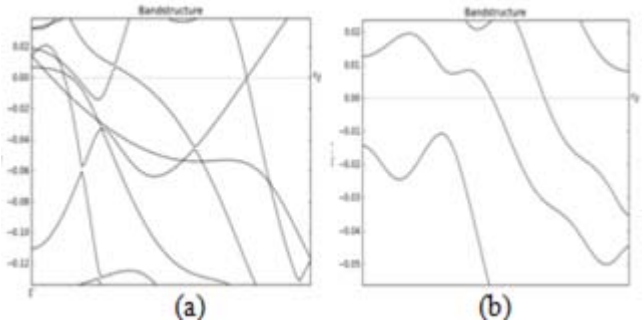


Figure 3: The atomic Configurations of Titanium Nanowires (a) TiNw without doping, (b) TiNw doped with 2P atom, (c) TiNw doped with 2 P atoms, (d) TiNw doped with 3 P atoms and

3.2 Band Structure Analysis

By observing the below graphs, we can clearly say that when titanium is not doped with any atoms still it shows metallic nature. That's why the Fermi level is crossed by many lines. The last curve above the Fermi level is at 0.01 and the last curve below the Fermi level is -1.0. There is no band gap which shows it is metal.When titanium is doped by two aluminium atoms, then metallic nature increases. The curve which is above the Fermi level at 0.03 and the curve which is below the Fermi level is -0.013. Now titanium is doped by four aluminium atom, then metallic nature increases. The curve which is above the Fermi level at 0.05 and the curve which is below the Fermi level is -0.013. As usual there is no band gap, still there crossing of lines in Fermi level. This clearly shows the doping nature.Finally. Titanium is doped by six aluminium atoms, then metallic nature increases. The curve which is above the Fermi level at 0.01 and the curve which is below the Fermi level is -0.012 . This depicts the increase in metallic property. But when titanium is doped by two phosphorous atoms, then metallic nature increases. The curve which is above the Fermi level at 0.03 and the curve which is below the Fermi level is -0.013. When titanium is doped by four phosphorous atoms, then metallic nature increases. The curve which is above the Fermi level at 0.05 and the curve which is below the fermi level is -0.013. As usual there is no band gap, still there crossing of lines in Fermi level. This clearly shows the doping nature.Hereby titanium is doped by six phosphorous atoms, then metallic nature increases. The curve which is above the Fermi level at 0.01 and the curve which is below the fermi level is -0.012 . This graph clearly has lot of dense lines crossing each other which shows it has maximum metallic nature



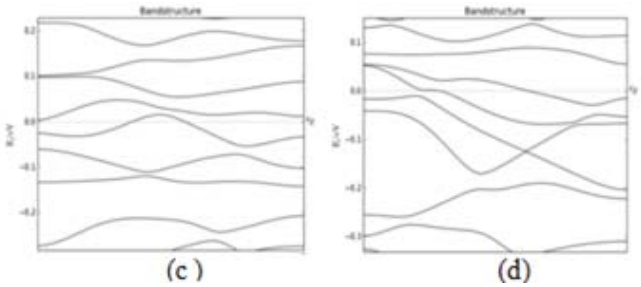


Figure 4: The Bandstructures of Titanium Nanowires (a) tiNW without doping, (b) tiNW doped with 2 Al atom, (c) tiNW doped with 4 Al atoms, (d) tiNW doped with 6 Al atoms

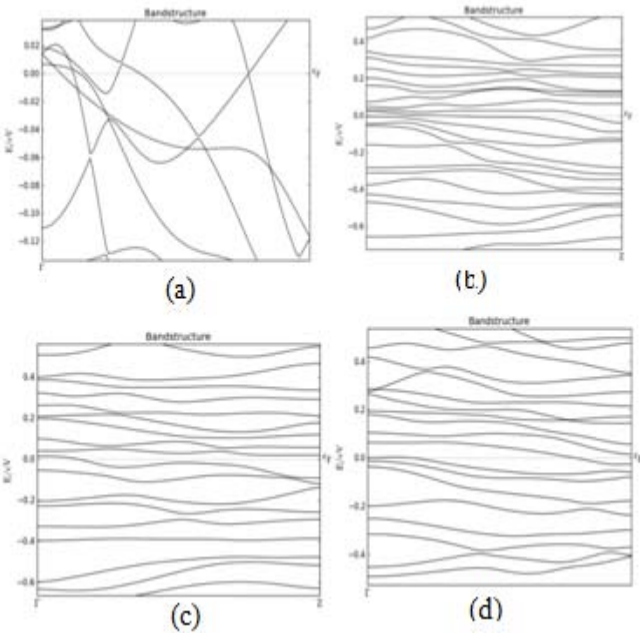


Figure 5: The Bandstructures of Si nanowires (a) tiNW without doping, (b) tiNW doped with 2 P atom, (c) tiNW doped with 4 P atoms, (d) tiNW doped with 6 P atoms

3.3 Density of States

By increasing the doping, we see doping become closer and denser which shows metallic property is increasing. And obviously Fermi level is decreased. By clearly noticing, it shows states are decreasing on Fermi level because of shifting.It decreased from 45 -30 level on doping Phosphorous atoms.Even the other peaks are showing the decline.We can c see the decrease in the height and width of the peak on creasing the doping atoms.There is decrease in density of states from 50-35 level in case of aluminum atoms.The peaks on the right side is decreasing from 30-22 level in case of Al atoms but in case of Phosphorous atoms it is decreasing from 28 -18 level.But the peaks on the left side are decreasing from 28-17 level in case of Al atoms doping and in case of P atoms doping,the peaks are decreasing from 22-18 level.From the above comparison,we can see the graph which depicts the doping of 6 Al atoms which shows denser graph and on the other hand the graph of 6 P doping shows highest denser graph Which depicts it is highly metallic. It clearly shows phosphorous increases more metallic nature in comparison to aluminum

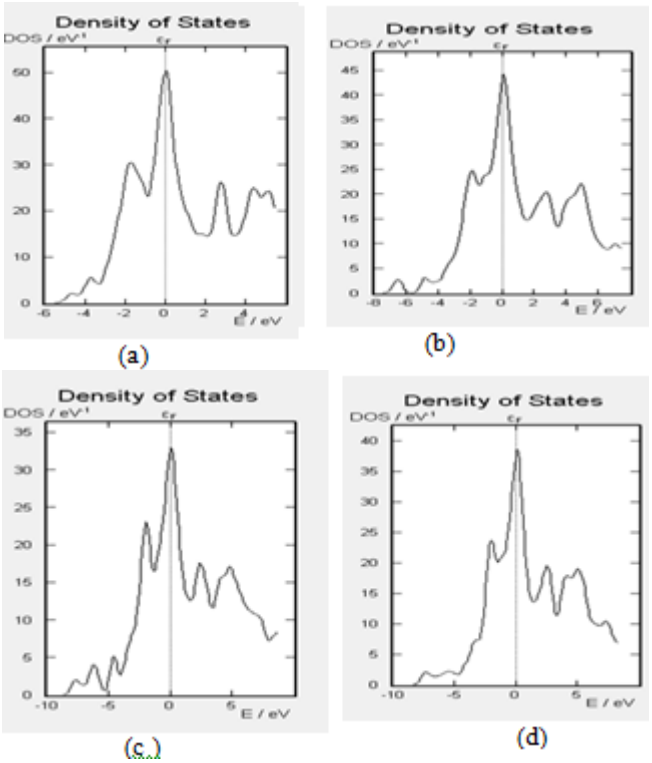


Figure 6: The Density of States of Titanium Nanowires (a) TiNw without doping, (b) TiNw doped with 2 Al atom, (c) TiNw doped with 4 Al atoms, (d) TiNw doped with 6 Al atoms

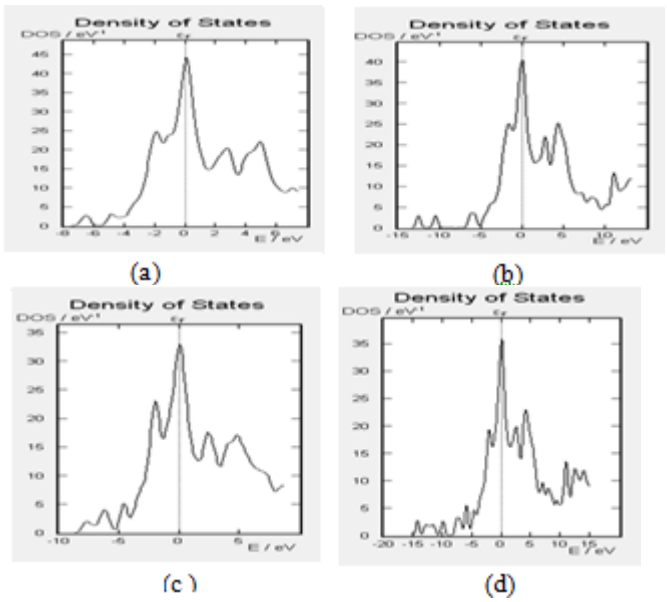


Figure 7: The Density of structures of Titanium Nanowires (a) TiNw without doping, (b) TiNw doped with 2 P atom, (c) TiNw doped with 4 P atoms, (d) TiNw doped with 6 P atoms

3.4 Optical Spectrum

- We must see the onset in this graph which tells about the electronic transition.Band offfsets can be known by Brus model We see that EF -0 which represents the gap opening And region around them denotes density of states for holes as well as electrons Moreover we can't make use of linear plot As it can bo done by log scales.The peaks play their own role but some are small and some high It signifies multirelaxation among them.that means no direct

transition for Germanium nor for Gas Here, we see so many multirealxation peaks mingle Which signifies deep or shallow level defect The real part usually give absorption energy and imaginary part gives the information on loss or extinction coefficient The multicolour lines refer 3D info on one scan axis which is to be confirmed for the uniformity as well as monodisperse that is not true always

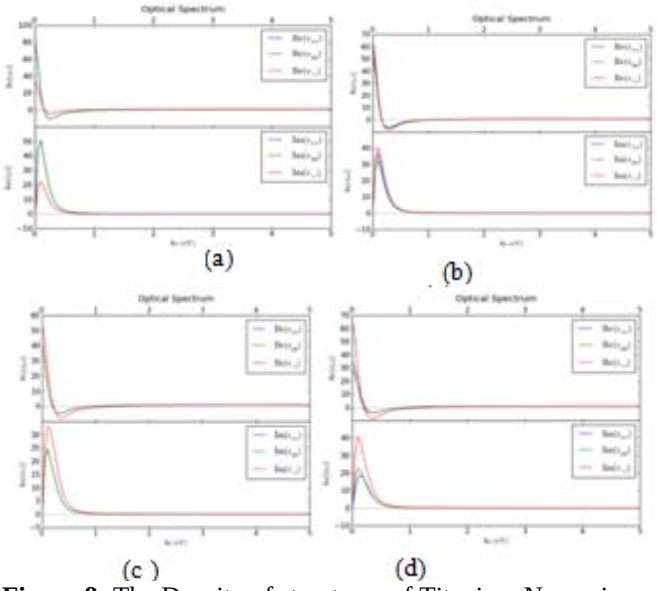


Figure 8: The Density of structures of Titanium Nanowires (a) TiNW without doping, (b) TiNW doped with 2 Al atom, (c) TiNW doped with 4 al atoms, (d) TiNW doped with 6al at atoms

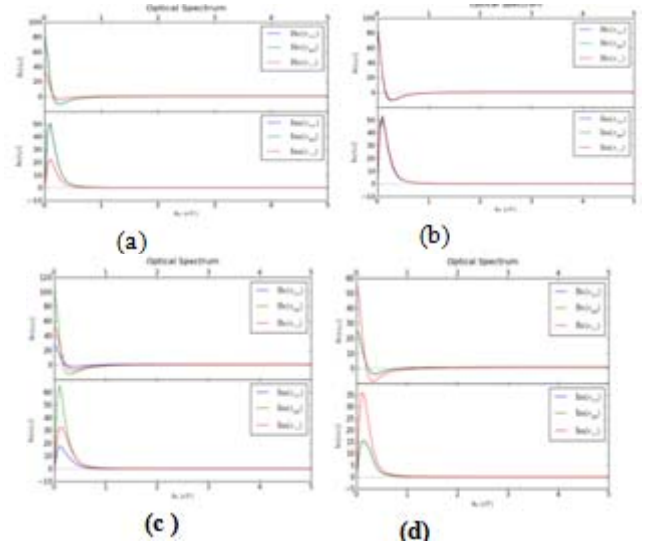


Figure 9: The Density of structures of Titanium Nanowires (a) tiNW without doping, (b) tiNW doped with 2 P atom, (c) tiNW doped with 4 P atoms, (d) tiNW doped with 6 P atoms

4. Conclusions

After analysing the structural, optical properties and electronics properties Titanium nanowire, we can conclude that in case of structural property, if total energy is maximum then the structure is least stable. So we can say that total energy is inversely proportional to stability. With the increase of doping Al and P atoms, total energy is increasing. In density of states, we clearly see the decline in DOS/eV with the increase of doping Al and P atoms. But the graph was getting denser and crowded with conduction lines as the metallic property is increasing. Finally, in Band structure, we observe that band gap gets hidden because of crowded conduction lines while doping it with Al and P atoms which depicts the increase of metallic nature as earlier in case of ti NW, there was small band gap available depicting semiconductor property.

5. Acknowledgement

Authors greatly acknowledge the support from ABP-IIITM Gwalior for providing the infrastructure support in doing the research work.

References

[1] Volker Schmidt,* Joerg V. Wittemann, Stephan Senz, and Ulrich Go¨sele, Adv. Mater. 2009, 21, 2681–2702
[2] Mehedhi Hasan1, Md Fazlul Huq2* and Zahid Hasan Mahmood, © 2013 Hasan et al.;licensee Springer
[3] Kui-Qing Peng[a], Xin Wang[a], Li Li[a], Ya Hu[a], Shuit-Tong Lee, 10.1016/j.nantod.2012.12.009
[4] F.Patolsky and C.M.Lieber, Mater. Today 8,20 (2005)
[5] A.M.Morales and C.M.Lieber,Science 279,208 (1998)
[6] Bozhi Tian[1,3], Xiaolin Zheng[1,3], Thomas J. Kempa[1], Ying Fang[1], Nanfang Yu[2], Guihua Yu[1], Jinlin Huang[1] & Charles M. Lieber, *Nature* 449, 885-889 (18 October 2007
[7] Z.G.Bai,D.P.Yu,J.J.Wang,Y.H.Zou,W.Qian,J.S.Fu,S.Q. Feng,J.Xu and L.P. You, Mater.Sci.Eng.,B 72, 117 (2000)
[8] D.B.Geohegan,A.A.Puretzky, G.Dushcher and S.J. Pennycook, Appl. Phys Lett.73.438
[9] M. Hofheinz, X.Jehi, M. Sanquer, G.Molas, M.Vinet and S.Deleonibus,Eur.Phys.J.B 54, 299 (2006)
[10] D.D.D.Ma,C.S.Lee, F.C.K.Au, S.Y. Tong and S.T.Lee, Science 299, 1874 (2003)
[11] http://www.atomistix.com
[12] Jeremy Taylor, Hong Guo and Jian Wang,Phys.Rev.B 63,245407 (2001)
[13] Mads Brandbyge, Jose-Luis Mozos, Pablo Ordejon, Jeremy Taylor and Kurt Stokbro, Phys.Rev. B 65, 165401 (2002)
[14] Kurt Stokbro, Jeremy Taylor, Mads Brandbyge and Pablo Ordejon, Annals N.Y.Acad.Sci.1006,212 (2003)
[15] Jose M. Soler, Emilio Artacho, Julian D.Gale, Alberto Garcia, Javier Junquera, Pablo Ordejon and Daniel Sanchez Portal,J.Phys.Cond.Mat.14,2745 (2002)
[16] B. Hammer, L.B. Hansen and J.K. Norskov, "Improved adsorption energetics within density Functional theory using revised Perdew-Burke-
[17] Anurag Shrivastav, Neha Tyagi and R.K.Singh, JCTN, Vol.8.1-6,2011
[18] Anurag Shrivastav, Neha Tyagi and R.K.Singh, Materials Chemistry and Physics 127 (2011)489-494
[19] Anurag Srivastava,[1] Mohammad Irfan Khan,[1,2] Neha Tyagi,[1] and Purnima Swaroop Khare' Volume 2014 (2014), Article ID 984591