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Study of structural and electronic properties of metallic nanowires: Bi, Na, Cu, Pb

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Abstract. The properties of electrons become more striking when progressing from the three-dimensional to lower dimensions; thus there is a need to investigate and recognize the properties of metallic structures at the nanoscale. Devices made from nanowires have several advantages over those made by photolithography. A variety of approaches have been devised to organize nanowires via self-assembly, thus eliminating the need for the expansive lithographic techniques normally required to produce devices of the size of typical nanowires. In the present work, an ab-initio self-consistent density functional method in the local density approximation is employed to study structural and electronic properties of some metallic nanowires such as Bismuth (Bi₅), Sodium (Na₅), Copper (Cu₅), Lead (Pb₅) where n=5. We explored the lowest energy structure and investigate the various physical properties of Bi₅, Na₅, Cu₅, Pb₅ (n=5) nanowires. Calculations of lattice parameter, bond length, bond angle, binding energy (BE), internal energy, pressure, band structure and the density of states (DOS) have been carried out in a large energy interval for different isomeric forms like linear chain, zigzag, equilateral triangle, dumbbell, pyramidal, pentagonal, tetrahedral etc. and thereby analyzing the size effects on nanowires.

1. Introduction
The most fundamental properties of materials get changed at the nanoscale with respect to any other scale, the behaviour of a material like its physical, chemical, biological, electrical, magnetic properties is modified when compared to the bulk. Generally, there are two distinct approaches for creating small objects, one by top-down as lithography, etching and deposition techniques and microelectronic devices and other by a bottom-up approach which aims to start with the smallest possible building material- atom, to create a desired product, and this was very well proven by two IBM researchers by creating STM (Scanning tunnelling microscope), to place every atom at the right place. Nanotechnology promises putting essentially every atom in the right place, making almost any structure consistent with the laws of physics and chemistry. The present work is focused on nanowires. Nanowires are playing an integral part in the design and construction of both electronic and optoelectronic nanodevices [1]. Many analyses have been performed in various materials, for example Cu, Si, Ag, Pb, Ni, Al etc. nanowires [2-7] and successful fabrication has been achieved [8]. The increased surface area, very high density of electronic states and joint density of states near the energies of their van Hove singularities, enhanced exciton binding energy, diameter-dependent bandgap, and increased surface scattering for electrons and phonons are just some of the ways in which nanowires differ from their corresponding bulk materials.

2. Methodology
Although a lot of work has been done, the study of metallic nanowire is still at an early stage; hence an extensive investigation is yet to be done. We analyzed the structural and electronic properties of some isomeric structure of metallic nanowires (Bi, Na, Cu, Pb) using computational methods. We have investigated various geometries for different metallic nanowires and then predict the most stable geometry for those particular metallic nanowires in terms of their physical properties. For our computational work ABINIT code [9] has been used to determine the total energy of an assembly of nuclei and electrons placed in a repeated cell according to Density Function
Theory. The computation can be done using plane waves and norm-conserving pseudopotentials. In this code, self-consistent calculations will generate the DFT ground-state, with associated energy and density. Afterwards, a non-consistent self calculation might generate Eigen energies at a large number of k-points, for band structures. The electronic density of states can be computed either within the tetrahedron method, or using a smearing technique. There are many advantages of ABINIT code, such as the computation is done using plane waves and pseudopotentials, admits various types of pseudopotentials, the total energy computation is done according to the DFT and LDA, metallic as well as insulating systems can be treated, cell may be orthogonal or non-orthogonal and the code can provide an automatic analysis of bond lengths and angles, and the atomic coordinates.

3. Results and Discussion

3.1 Bi₈ (N=1-5) nanowires: Bismuth is really an interesting material to investigate on the nanoscale because bulk Bismuth has very small effective mass carriers, highly anisotropic carrier pockets and a very long mean free path. Thus, these bulk properties lead to a quantum nature that can be observed in nanowires of relatively large diameter. In fact, Bismuth in bulk form is a semimetal and therefore it is not a good thermoelectric material. However, with the introduction of quantum confinement it can be given small diameter nanowire.

Theoretically, Schmidt and Springborg [10] studied a one dimensional chain of metal atoms including Bi chains but considering only three structures. Lin et al [11] studied the transport properties of Bi nanowires arrays by employing a semi classical transport model. However, our current knowledge of the structural and electronic properties of various technologically important metallic nanowires is still quite limited. We are also not aware of any ab-initio theoretical work on the structural and electronic properties of Bi nanowires in various isomeric forms, since the study of metallic nanowires is at early stage. Extensive investigation of semi-metallic Bi nanowires is required. Figure 1 represents the obtained results for Bi nanowires. It has been observed that the equilateral triangle shape is more stable for the Bi nanowire metallic character. The maximum DOS is seen for a three atom triangular wire. A summary of the results is presented in Table 1.

Figure 1 Bismuth nanowire (a) 3-atom triangle (b) Band structure (c) Density of states

Figure 2 Sodium nanowire (a) 5-atom tetrahedral shape (b) Band structure (c) Density of states
In order to understand the size effect and stability of alkali metals for quantum quantization we have chosen sodium nanowires for our analysis. Although a great deal of work has been done for transition metallic nanowires, so far as alkali metals are concerned more research is needed. Yannouleas et al [12] studied the energetics, forces and quantized conductance in jellium-modelled metallic nanowires theoretically. The effect of atomic and electronic structure on mechanical properties of a piece of sodium nanowire was studied with a total energy method based on the Density Functional Theory by Hakkinen and Manninen [13]. Kobayashi et al [14] employed first-principles method to study the electron transport through monatomic Al and Na wires. The stability of sodium nanowires was studied by Yanson et al [15] by modelling them as infinite uniform jellium cylinders. Tsukamoto and Hirose [16] studied the electron-transport properties of Na nanowires under applied bias voltages, by using first principles calculations. They predict that a voltage drop locally occurs on the negatively biased end of the nanowire. Sen et al [17] studied the atomic and electronic structure of pentagonal nanowires of some alkali, simple transition, noble and inert gas atoms. Qi et al [18] analyzed the size effect on the cohesive energy and the lattice parameter of nanoparticle. They revealed that the cohesive energy and the lattice parameter of nanoparticles depend on its size i.e. both of them are size dependent.
3.3 Cuₙ (N=1-5) nanowires: Sen et al [17] have used first principles calculations to study two pentagonal Cu nanowires along the direction and concluded that these wires should be stable and metallic. The energetics of nanowire of several materials including Cu is studied by quenched molecular dynamics by Tommei et al [20] with the aim of comparing wires i.e. fcc and pentagonal which are expected to be among the most favourable ones for wires of intermediate thickness. They revealed that the best pentagonal wires are always those including marks truncations, but the fcc wires are more favourable than the pentagonal ones in any size range. Figure 3 represents the obtained results for Cu nanowires. The highest binding energy is seen in four atom dumbbell shape and hence more stable. Therefore, the maximum DOS is seen for a five atom pyramidal wire followed by four atom dumbbell shape wire

3.4 Pbₙ (N=1-5) nanowires: Lead is unique among all metals. Pure lead has little strength and is very soft, because its inter-atomic bonding forces are weak and its melting point is very low. Its resistance to corrosion in aggressive environments is well known. In fact, a very reactive metal, therefore it is commonly used in corrosive environments. The understanding of the conductive properties of extremely small metallic structure is of utmost importance for the potential use in nano electronic devices and as interconnects. Theoretically, Sen et al [17] performed a first principles study of lead nanowires only in various pentagonal structures and concluded that staggered pentagons have a stable structure. Figure 4 represents the obtained results for Pb nanowires using our ABINIT code. Pb nanowires show more stability in an equilateral triangle shape; thus the maximum DOS is seen for three atom triangular wires. The DOS of three atom triangular wires reveals that the electron are highly delocalized near the Fermi level in comparison to other structures. All the band structure calculations show that large number of channels is available for the electronic conduction hence ballistic conductance is possible.

4. Conclusion
The results of our calculations for various nanowires giving the observed shape and number of atoms are summarized in Table 1. As we found that an equilateral triangle shape is more stable for Bi nanowire metallic character, the maximum DOS is seen for a three atom triangular wire. For Na nanowires, a five atom tetrahedral wire is the most stable; the maximum DOS is seen for a five atom tetrahedral wire. In the case of Cu nanowires, the highest binding energy is seen in a four atom dumbbell shape and is hence the most stable. Therefore, the maximum DOS is seen for a five atom pyramidal wire followed by a four atom dumbbell shaped wire. Whereas Pb nanowires show more stability in the equilateral triangle shape; thus the maximum DOS is seen for a three atom triangular wire. The DOS of three atom triangular wires reveals that the electrons are highly delocalized near the Fermi level in comparison to other structures. All the band structure calculations show that a large number of channels are available for electronic conduction hence ballistic conductance is possible.

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