NANOMATERIALS FOR SILICON NANOTECHNOLOGY

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Abstract

Nanomaterials could play important roles in the silicon nanotechnology platform. Silicon nanotechnology is the production reality and follows famous Moore's law. There are some significant challenges must be overcome for nanomaterials to be useful in future silicon technology. As silicon scaling leads to materials challenge for fabrication, package, interconnects and lithography, new structures like molecular assembly, macromolecules and sub 100 nm structures are needed in the future. This paper discuss about nanomaterials needed for Lithography challenges and Resist challenges. Silicon devices with materials like strained silicon, poly silicon and silicides are incorporated which overcomes the challenges mentioned above. This paper also describes about the characterization, analysis, electrical and mechanical properties of the mentioned nanostructures. We also simulated nanostructures like molecular structures, Spin quantum dots, nanowiers and nanotubes using nanomaterials.

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1. Introduction

Silicon is a production reality and material for integrated circuit manufacturing and follows famous Moore's law, Nanodevices has structure dimension less than 100 nm, already 22 and 20 nm experimental data's on nano devices are available. So silicon nanotechnology is extendable till 2015. Nano materials plays very important role in silicon nanotechnology platform. By scaling the devices the dimensions of the transistor goes down and manufacturers faces many challenges from materials to fabrication of the devices.[1] So silicon scaling gives rise to materials challenges like lithography, interconnects, packing and transistors. Nanotech building blocks like sub 100 nm particles and structures, macromolecules, molecular assembly (both directed and self assembly) are going to find birth inside the silicon devices. This paper discuss about the simulation of nano structures and its electrical and mechanical properties. For lithography scaling new materials, mast, design techniques are need for lithography challenges. To overcome this, materials like silicides, strained silicon and high k dielectrics are added to the transistors to improve their performances. Silicides (metal silicides) can be added in the gate region of transistors. Strained silicon (Silicon and Germanium) can be added in the channel region to increase the conduction. High K dielectrics in the oxide region of less than 3 atomic layers thickness are used to improve dielectric characteristics. Figure 1 shows the transistors [1] with silicides, strained silicon and high k dielectric.

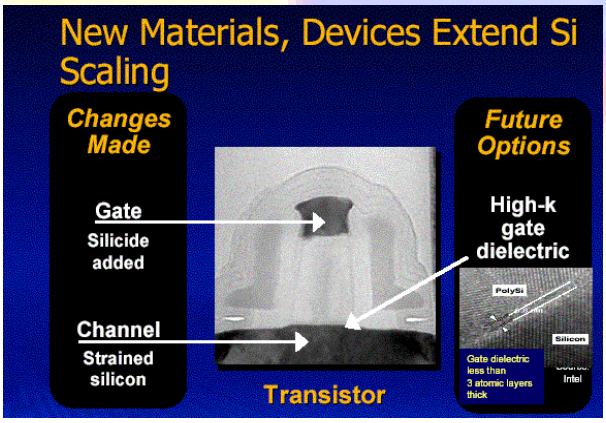

Figure 1 shows the transistor with silicides, strained silicon and high k di-electric added [1] The above mentioned materials may help silicon scaling down to 10 nm. The characterization for the materials is physics based computer vision and quantitative understanding of the materials. This paper discusses about the structural analysis and the simulation of nanostructures. Nanostructures like nanoparticles, nanowires, nanotubes, molecular assembly structures are simulated. The

characteristics of molecules sandwiched between two metals are also studied. Future nanodevices like quantum dots, quantum cellular devices are also studied. Any solid material in the form of particle with a diameter comparable to the wavelength of electron is quantum dot. Silicon nanowire has diameter smaller than 100 nm. Figure 2 a and b shows the quantum dot and slicon nanowire.

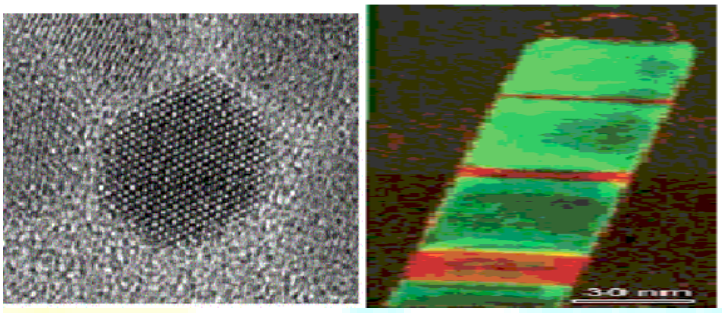

Figure 2 a and b shows the quantum dot and silicon nano wire.

The reasons for choosing nanostructure materials are due to its electronic, optical, thermal, mechanical and chemical properties. Nanowires and nanotubes are most confining electrical conductors. It is small enough and ideal from defect free. It can be designed to conduct heat substantially better than bulk materials. It has large surface to volume ratio. It has quantum confinement and tunable optical properties. [2]. Nanostructured materials has applications in biomedicine, structural re-enforcenment in composite materials, as tunable lasers and light emitting diodes, high surface area sensors and conducting channels for electronics.

2. Properties and characterization of polysilicon

In applications involving surface micromachining, thin films of silicon are needed as a Structural material. Since it is difficult to grow thin films of single crystal silicon, thin films of polysilicon are grown instead.[3]] These materials are now finding extensive use in the IC industry. The mechanical properties of polysilicon films depend greatly upon the process used in deposition. The residual stress can be controlled almost entirely by varying deposition pressure and temperature. It has also been discovered that there is a direct link between the presence of <110> oriented grains and residual stress in films. The strength of polycrystalline silicon is less well understood. Different researchers have Reported a Young's modulus ranging between 140 to 210 GPa,[4] with these values having a dependence on crystal structure and orientation. Recent

research has shown that the Young's modulus of polycrystalline films is highly dependent upon deposition conditions. The films exhibit preferential grain orientations that vary with temperature. Since an ideal film does not exhibit orientation dependence for its mechanical properties, researchers have found that depositing films at 590 oC, which is the transition point between polycrystalline and amorphous silicon, is an effective method of producing an isotropic film of polysilicon. At this temperature, the amorphous silicon will recrystalize during annealing, which produces films with a nearly uniform Young's modulus of 165 GPa. In polycrystalline materials, the fracture strength is dependent upon two factors, the grain size, d, and the fracture surface energy, gs. This stems from the fact that the size of a dislocation is usually governed by the grain size, which, by Griffith's equation, shows that the fracture strength of this material is:[5]. In polycrystalline materials, the fracture strength is dependent upon two factors, the grain size, d, and the fracture surface energy, gs. This stems from the fact that the size of a dislocation is usually governed by the grain size, which, by Griffith's equation, In several studies, the mean fracture strength of polysilicon has been found to be between 2 to 3 GPa, which is clearly less than that of single crystal silicon. Polysilicon fracture samples have been reported to have a Weibull modulus similar to that of single crystal silicon, which would indicate a similar reliability of the two materials. Table 1 shows the mechanical properties of polysilicon.

3. Properties of strained silicon and its characterization

Strained silicon is exactly what the name implies: silicon that is elastically deformed, as a rubber band is elastically deformed when it is extended. Strained silicon can be strained compressively (i.e., the atoms are being squeezed together) or tensile (i.e., the atoms are being stretched apart). The most established and proven method of straining silicon involves the deposition of a silicon-germanium (SiGe) thin film on top of a traditional silicon wafer, which then acts as an atomic template for deposition of a subsequent thin film of silicon. The thin film of silicon conforms to the atomic spacing of the underlying SiGe layer, which has a larger atomic spacing, and assumes a state of biaxial tension (*i.e.*, it is being pulled in stretched apart in two orthogonal directions). A schematic of how the crystalline structure of the strained silicon thin film is distorted is shown in Figure 3. [6] Although it is not readily apparent that the mechanical deformation of silicon would have any positive impact on the electrical properties of silicon, there are indeed benefits to straining silicon. Specifically, the distortion of the crystalline structure changes the properties of the charge carriers in silicon, allowing the carriers to move

more quickly in response to an applied voltage. These charge carriers, electrons (negative charge carriers) and holes (positive charge carriers), are said to have a higher *mobility* when silicon is strained. The higher the Ge content in the SiGe alloy, the greater the strain and the corresponding increase in the mobility of electrons and holes. AmberWave's strained silicon solution targets a Ge content between 15-20%, where the exact target specification is determined. Table 3 shows the stained silicon properties.

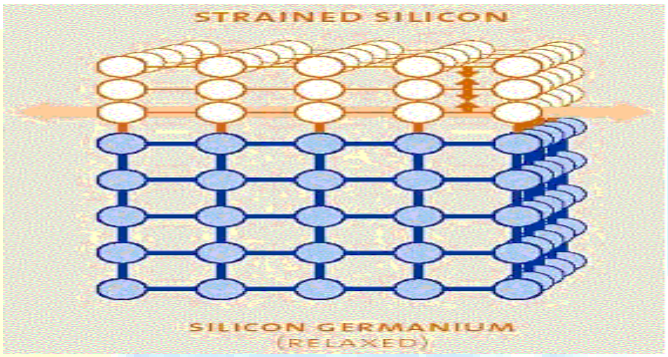

Figure 3 a silicon germanium of strained silicon crystal lattice [6]

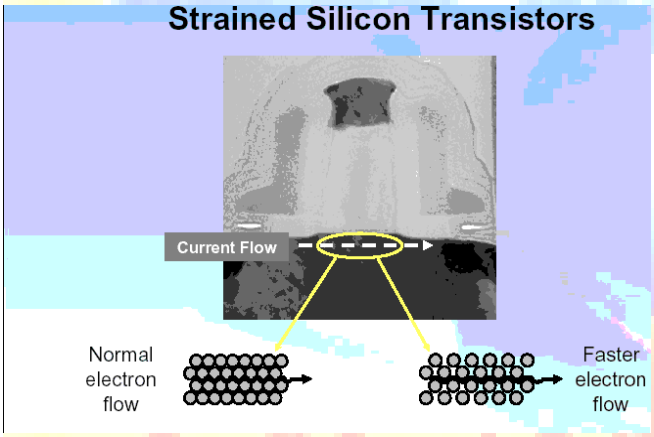

Figure 3 b faster electron flow of strained silicon transistors [1]

Figure 3 a shows the germanium on silicon to form strained layers and figure 3 b shows current flow of strained silicon transistors [1]. Figure 4 shows the formation of silicon germanium layers. Strained Silicon on silicon process flow schematic shown in figure 4. Figure 4 a shows the wafer bonding. It has five layers of si substrate, silicon germanium layer graded silicon and strained silicon. Wafer bonding is done suing UV bonding machine. Figure 4 b shows the KOH etching and removal of silicon substrate. Figure 4 c shows the final structure.

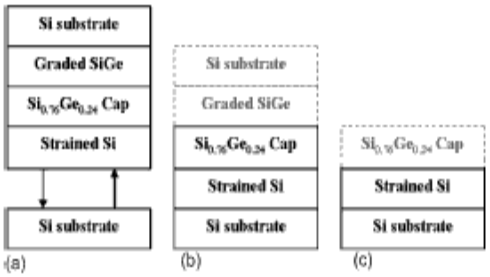

Figure 4. SSOS process flow schematic showing _a_ wafer bonding; _b_ back side removal via mechanical grinding and KOH etching; and _c_ final structure after SiGe removal. [7]

4. Properties and characterization of silicides

The use of silicides in electronic technology has been motivated by the fabrication of contact structures where both the metallurgical and electrical properties of the contacts were important. For almost all uses of silicides in today's integrated circuits, electrical and metallurgical behaviors are equally important. For example, the diffusion of boron, probably along the grain boundaries, of conductors made of CoSi2 may not be very important in itself (since it will not greatly affect the resistance of the conductors) but it may significantly affect the electrical properties of materials found at both ends. Thus, in considering the use of silicides and the role that interfaces play in that use, one is obliged to consider almost simultaneously electrical and metallurgical factors, with the primacy being given to one or the other depending on the specific application. While pure metals have good electrical conductivity, they are not suitable, for different reasons, for VLSI/ULSI applications. Metal silicides, on the other hand, are compounds formed by metals and silicon. Many of them exhibit metallic conduction behavior and have attracted much attention in the past three decades in the context of metallization applications because of their low and metal-like resistivity, high temperature stability, and high electro migration resistance. Table 2 shows the properties of silicides.

Tabel 1,2,3 shows the properties of materials that is needed for silicon industry.

5. Simulation work of nanostructures

5.1. Nanotube

As mentioned in the previous section, nanotubes and nanowires are the nanostructures made up of nano materials. Carbon nanotubes are the prominent nanotube technology in the future. Here we have simulated the carbon nanotube structure. We have used nanotube simulator for simulating and generating carbon nanotubes structure. Figure 5 a shows nanotube simulator. Figure 5 b and c shows the armchair and Zig zag nanotubes.

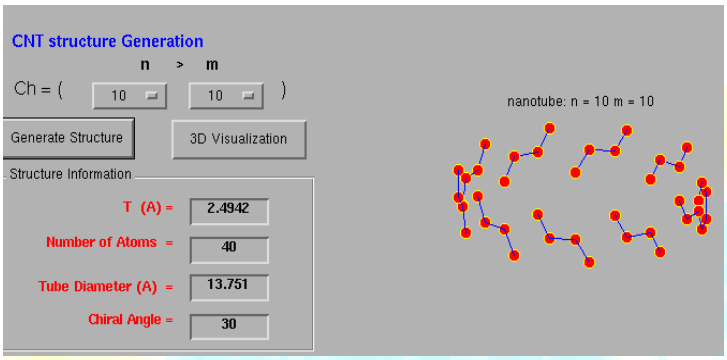

Figure 5 a Nanotube simulator.

Nanotube simulator gives tube diameter, chiral angle and band structure calculations.

For armchair type nanotube simulated values are tube diameter of 13.7, chiral angle is 30^{o} and chiral vector n=10 and m=10. Band structure gives conduction band, val;ence band and band gap with lattice point.

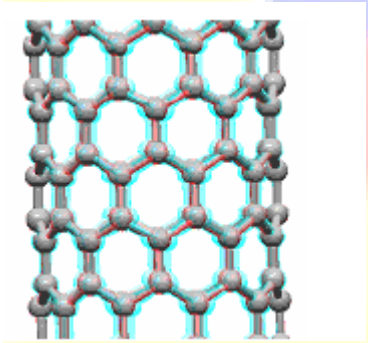

Figure 5 b shows the zigzag type Carbon nanotube.

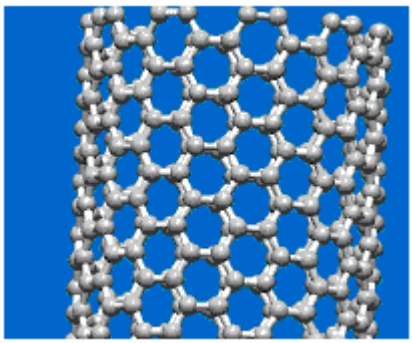

Figure 5 c shows armchair (10,0) carbon tube

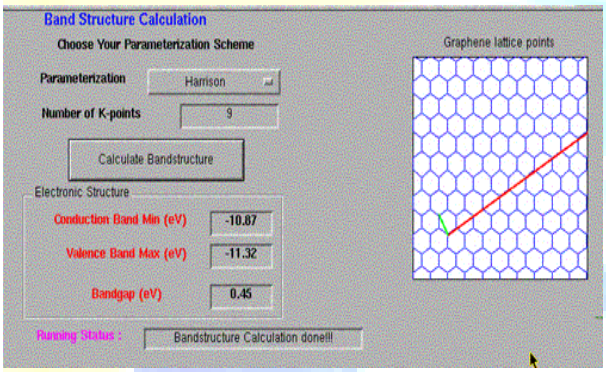

Figure 5 d shows the band structure calculation of nano tube with graphite sheet lattice points.

Figure 5 b,c shows the types of carbon nano tubewith armchair and zig zag type. Figure 5 d shows band structure calculation. The conduction band for nano tube is -10.87 eV,valence band -11.32 eV and band gap of 0.45 eV. These simulation are useful for study for future nanodevices.

5.2. Nanoparticles

The second type of structure generation is using nanoparticles. Nanoparticles are small cluster of atoms with nanoscale size in all three dimensions. Due to their large surface area and different physical properties, nanosparticles are being investigated for advanced computing. Energy storage, packaging etc. Transition metals such as Pt, Ru and Re make good catalyst materials and are being investigated as elements for nanoparticles. In this simulator we optimize the nanoparticle shape according to the surface energies of a selected particle size. In an FCC system, the nanoparticle has (100),(110) and (111) surfaces. So given nanoparticle, we find the shape and lowest total surface energy system. By selecting the different surfaces energies

induced by surface modification. Figure 6 a and b shows the nanoparticle with structure generation. The number of atoms taken for carbon is 365, radius 8 A^o The surface energies at 100 orientation is 0.386 eV, 110 is 0.388 and 111 is 0.317. Figure 6 b shows the diameter of the nanoparticle. The structure simulated gives the idea of nanoparticle made of carbon.

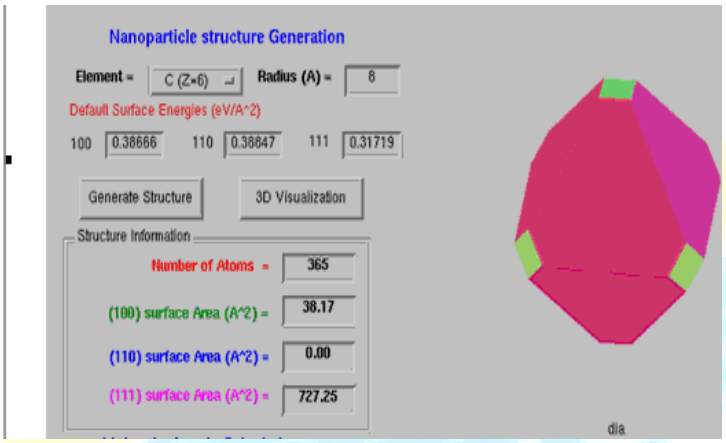

Figure 6 a shows the nanoparticle structure generation

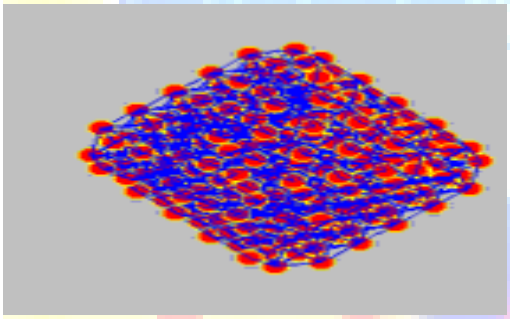

Figure 6 b shows the diameter of nanoparticle.

5.3. Nanowires

Like nanotubes semiconductor nanowires exhibit one dimensional geometries and physical properties. We used MSL simulator for simulating the structure of nanowires. Semiconductor nanowires can be thought of a cylinder cut out of bulk materials. Figure 7 a and b shows the silicon nanowire with unit cell length 5.4 A^0, 9 silicon atoms and wire diameter 7.37 A^o with growth direction 100 orientation.

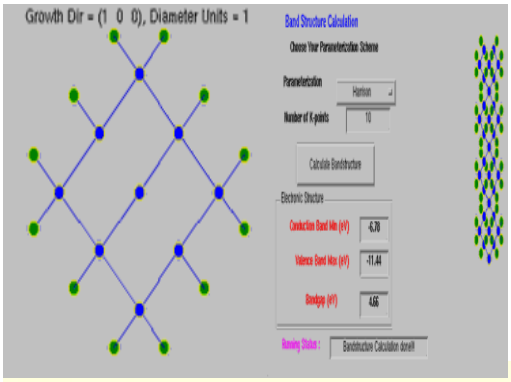

Figure 7 a and b shows the silicon nanowire structure generation and bandstructure calculation.

Figure 7 b shows the nanowire with conduction band -6.78 ev, valence band -11.49 and band gap 4.66 ev. The nanowire silicon simulation gives in depth of its usage in silicon nanotechnology.

5.4. Molecular structure conduction

Molecular assembly structures can be used as nanodevices and its usage can be understood through its electrical conduction. Figure 8 a shows the Molecule in between two metals with energy levels.

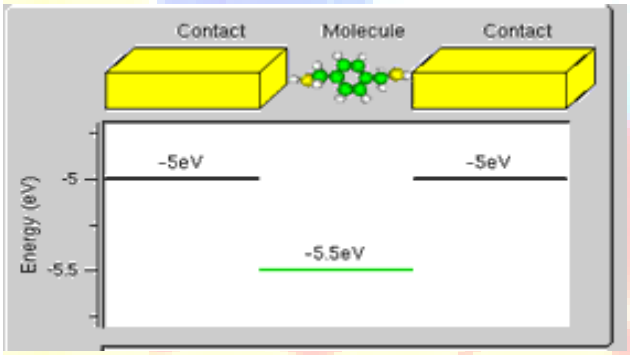

Figure 8 a molecule between two metals with energy diagram.

A virtual experimental set up is made to study the I-V characteristics and conduction characteristics of given molecule. The simulation is carried out with the following conditions. Temperature – 300^0K, single electron charging energy 1 eV, Coupling factor 0.1, Fermi level – 5eV, energy level -5.5 eV and voltage level 0 to 4 volts. Figure 8 b, c and d shows the I-V, Conductance and no of electrons per voltage characteristics are studied

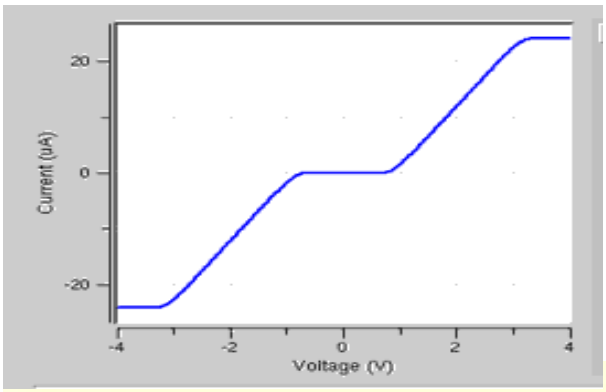

Figure 8 b I-V characteristics of Molecule

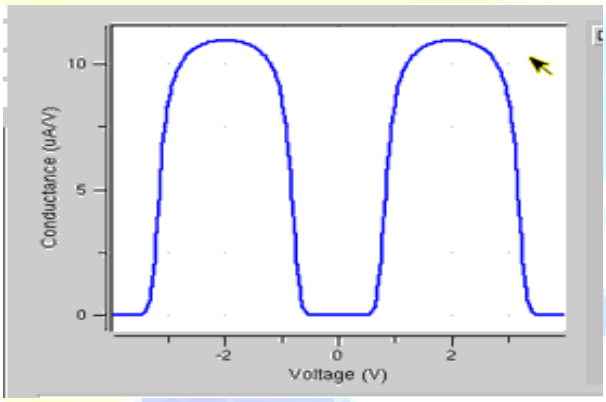

Figure 8 c-v characteristics of a molecule

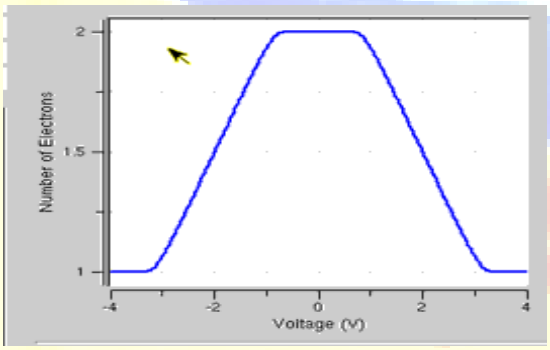

Figure 8 d shows the No of electrons per given voltage.

I-V characteristics resemble exactly as forward diode characteristics with 0.8 volts threshold voltage and saturates at the current of 24 micro amps. Conductance and voltage characteristics gives conductance value of 12 micro amps per volt at 1.8 volts, so there is sharp conduction between 1 to 3 volts. The conduction is possible for the positive and negative voltages also. Figure 8 d shows no of electrons takes place in the conduction, here two electrons take part in conduction between 0 to 1 volt above 1 volt one electron in the conduction process.

The behavior of the molecules and its electrical properties clearly gives conduction is possible as well as acts as molecular diode device.

5.5 Spin Quantum dots

We have simulated gallium arsenide quantum dots with rectangular and pyramid shape with X,Y,Z dimensions using MSL simulator. Figure 9 a shows the rectangular quantum dot with 5, 5.5 and 6 nm dimensions. Figure 9 b shows the pyramid quantum dot with 10,10.5 and 5 nm dimensions. We have simulated the energy states of a quantim dot

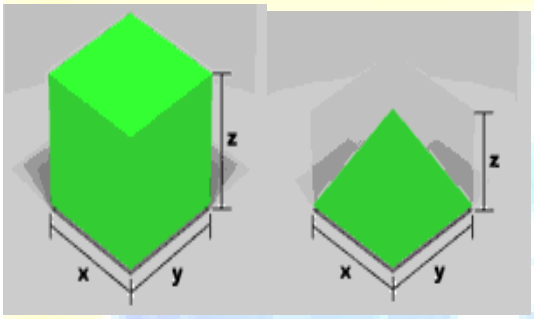

Figure 9 a and b shows the rectangular and pyramid quantum dot.

Figure 10 shows the energy states of a quantum dot with ground state of 4.087 ev and excited state of 5.65 ev with band energy of 1.57032 ev. Quantum dots are used to store one electron and by applying external force electrons come out of the dot and move to the near by dot, by this way the movement of electrons can be controlled.

6. Conclusion:

This paper discussed about the usage of silicides, polysilicon and strained silicon for the silicon nanotechnology. The mechanical and electrical properties are also studied for silicon nanotechnology. We have simulated nanotube, nanowire, nanoparticle, and molecular conduction and quantum dots. The structure and electrical properties are studied using Nanotube, MSL simulators. In conclusion, the lithography and resist challenges can be overcome by using above mentions nanostructures using nanomaterials.

7. Reference

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Table 1 Mechanical properties of polysilicon as gate element [8]

S.NO	Parameters	Values
1	Young's modulus (Gpa)	169 +/- 6
2	Poisson's Ratio	0.22 +/- 0.01
3	Tensile strength (Gpa)	1.2 + / - 0.15

Table 2 Silicides properties [9]

S.NO	SILICIDE	RESISTIVITY MICRO OHM CM	STABLE ON SILICON UP TO ^{0}C	SILCION CONSUMED PER NM	BARRIER HEIGHT (ev)
1	PtSi	28 - 35	750	1.12	0.84
2	$TiSi_2$	13 -16	900	2.27	0.58
3	$CoSi_2$	14 - 20	950	3.64	0.65
4	$NiSi_2$	40-50	650	3.63	0.66

TABLE 3 lists physical mechanical and electrical properties of Si, Ge, and SiGe

Properties	$Si_{.25}Ge_{.75}$	$Si_{.5}Ge_{.5}$	$Si_{.75}Ge_{.25}$
Atoms/cm^3	*4.415 x 10^{22}	*4.61 x 10^{22}	*4.805 x 10^{22}
Atomic weight	*61.4725	*50.345	*39.2175
Breakdown field (V/cm)	*1.5 x 10^5	*2 x 10^5	*2.5 x 10^5
Crystal Structure	Diamond	Diamond	Diamond
Density (g/cm^3)	*4.577	*3.827	*3.078
Dielectric constant	*14.975	*13.95	*12.925
Electron affinity *X*(V)	*4.0125	*4.025	*4.0375
Minimum Indirect Energy Gap (eV) at 300K	***0.804	***0.945	***1.05

Minimum Direct Energy Gap (eV)	1.6	2.5	3.1
Intrinsic carrier concentration (cm^{-3})	*1.8 x 10^{13}	*1.2 x 10^{13}	*0.6 x 10^{13}
Intrinsic Debye length (μm)	*6.51	*12.34	*18.17
Intrinsic resistivity (Ω-cm)	*.575 x 10^{5}	*1.15 x 10^{5}	*1.725 x 10^{5}
Lattice Constant (A)	***5.5960	***5.5373	***5.4825
Linear coefficient of thermal expansion, $\Delta L/L\Delta T$ ($°C^{-1}$)	*5.0 x 10^{-6}	*4.2 x 10^{-6}	*3.4 x 10^{-6}
Melting point (°C)	*1056.5	*1176	*1295.5
Minority carrier lifetime (s)	*1.375 x 10^{-3}	*1.75 x 10^{-3}	*2.125 x 10^{-3}
Mobility (drift) (cm^2/V-s)	*3300(electron) *1537.5(hole)	*7700(electron) *1175(hole)	*2100(electron) *812.5(hole)
Optical – phonon energy (eV)			
Phonon mean free path Λ_0(Å)			
Specific heat (J/g-°C)	*.4075	*.505	*.6025
Thermal conductivity at 300 K (W/cm-°C)	**.11	**.083	**.085

Thermal diffusivity (cm^2/s)	*0.495	*.63	*.765
Vapor pressure (Pa)	1 at *1410°C 10^{-6} at *795	1 at *1490°C 10^{-6} at *830°C	1 at *1570°C 10^{-6} at *865°C

* value was derived through linear approximation ; ** value was derived through subjective observation of graph/diagram *** value was derived through quadratic approximation.