Modifying the Electronic Properties of Nano-Structures Using Strain

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Abstract. We used density-functional theory based Non equilibrium green function simulations to study the effects of strain and quantum confinement on the electronic properties of Germanium & Silicon NWs along the [110] direction, such as the energy gap and the effective masses of the electron and hole. The diameters of the NWs being studied in a range of 3-20 Å. On basis of our calculation we conclude that the Ge [110] NWs possess a direct band gap, while Si [110] NWs possess indirect band gap at nanoscale. The band gap is almost a linear function of strain when the diameter of Ge NWs D < 10 Å while shows parabolic behaviour for, D > 15 Å; & for Si it is linear in behaviour. On doping silicon wire we found that the bandgap shows parabolic behaviour for change in strain. We also concluded that the band gap and the effective masses of charge carries (i.e. electron & hole) changes by applying the strain to the NWs. Our results suggested that strain can be used to tune the band structures of NWs, which may help in design of future nanoelectronic devices.

1. Introduction
One-dimensional nanostructures, such as NWs, and nanotubes have attracted extensive research [1-4] efforts since early 90s. They are expected to play important roles as a functional component in nano & flexible electronics [3-5]. Therefore, it is of great importance to study their electronic properties. One of the key for such an application is the electrical response, which monitors the change of environment caused by external factors [5-8]. It is thus important to understanding the electron transport and the effect of external properties on nano structures. Several work [4-9] have actually been carried out to study the electron transport in NWs. Various aspects such as I-V curve, conductance, nanocontact, surface defect, disorder, doping, band gap, density of state, effective mass of charge carriers, and structural effects have been explored [6-12]. Researchers [1-8] found that the band gap, conductance, etc of NWs depends on several factors such as, size, crystalline orientation, surface chemistry, doping, etc. It is well known that strain is not avoidable during epitaxial growth if there is a lattice mismatch, in many applications NWs are usually embedded in some materials within the coatings brings strains to the wires and in the field of microelectronics, strain has become a routine factor to engineer band gaps of semiconductors [9-12]. Thus we studied the effect of strain on band structure of Ge and Si NWs of different diameter having [110] orientation.

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2. Modelling & Simulations
We are using a two-probe model, and the approach we used is employed successfully in many theoretical studies for calculating the electron transport properties in NWs, or nanotubes [12-17]. We focus on the effects of length, and strain on the electronic properties of the NWs. The largest system studied contains 512 (NW) + 200 (electrodes) atoms. Geometry optimization is performed using Gaussian until the absolute value of force acting on each atom is less than 0.04 eV/Å. The transport calculations are performed using NEGF [12-14], combined with DFT. The Landauer [18] formalism is implemented in ATOMISTIX TOOLKIT [18-19] and $I$-$V$ characteristics are calculated by,

$$I = \frac{2e^2}{h} \int T(E,V_b)\{f_L(E) - f_R(E)\}dE$$

where $e$, $h$, and $f_L$, $f_R$ are electron charge, Planck’s constant, and the Fermi distribution functions at left(right) electrode, respectively. $T(E,V_b)$ is the transmission coefficient at energy $E$ and bias voltage $V_b$. The core electrons are described using ultrasoft Vanderbilt pseudo-potentials. The dangling bonds in the NWs surface are saturated by hydrogen atoms. Valence electrons are expanded in double $\zeta$-plus polarization (DZP) and single-$\zeta$ plus polarization (SZP) basis sets for the NWs (Si and H/Ge and H atoms) and metal electrodes (Au atom), respectively. The band gap of wires is defined by the energy difference between the bottom of the conduction band (conduction-band edge (CBE) and the top of the valence band (valance-band edge (VBE). The effective masses of the electron and hole can be readily calculated using equation 2 from the band structure of the wire,

$$m^* = \hbar^2(d^2E/dk^2)$$

3. Results & Conclusions
In the present work we have used Ge and Si whose electrical properties as a bulk at room temperature is given in table 1

| Table 1. Electronic properties of Germanium & Silicon at 300°K. |
|---------------------------------|---|---|
| **Properties**                 | **Germanium** | **Silicon** |
| Band Gap (eV)                  | 0.66 | 1.12 |
| Hole Mobility (Cm$^2$V$^{-1}$S$^{-1}$) | 1800 | 450 |
| Electron Mobility(Cm$^2$V$^{-1}$S$^{-1}$) | 3800 | 1500 |
| Intrinsic resistivity (Ω.cm)   | 46  | $3.25 \times 10^5$ |

Ge NWs show a direct band gap at $\Gamma$, in Fig. 1, we present the band gap of Ge and Si NWs with varied diameters i.e. 4 to 20 Å, as demonstrated in literature.[19] The band gap of the Ge NWs in fig 1 is decreased when the diameter of wire is increased.

![Figure 1: Bandgap of Ge, and Silicon NWs of different dimensions at room temperature](image-url)
This effect is primarily due to quantum confinement. Our predicted size dependence of the band gap in Ge NWs is in a good agreement with the reference [21-22]. In case of Si NWs the band gap also decreases with increase in diameter as shown in fig 1. The variation in band gaps as a function of uniaxial strain for several different sized Ge NWs is plotted in Fig. 2(a), for the wire with a diameter of 5 & 10 Å, the band gap variation with strain is almost linear.

![Band gap vs uniaxial strain for Ge NWs](image1)

**Figure 2:** The change in the band gap in (a) Germanium NWs, (b) Silicon NWs, as a function of uniaxial strain, positive strain refers to expansion while negative strain corresponds to compression.

The gap decreases with expansion and increases with compression. The gap variation with strain in the wire with diameter of 13 Å has a more modest change in the gap for a given strain, compared with the 10 Å wire. However, for the wire with diameter of 16 & 20 Å, the gap variation with strain, exhibits a nearly parabolic behaviour, the gap drops not only under expansion, but also under compression beyond 2%. Thus we conclude that the strain effect on the band gap in Ge wires is strongly dependent on its size. On, examining the variation in energies, of VBE, and CBE with strain, shown in fig 3 for Ge NWs having diameter 10 and 16 Å. The energies of the CBE and VBE decrease with expansion while increasing with compression. Since the band gap is given by the energy difference between the CBE and VBE, it is also a nearly linear function of strain for 10 Å curve. However, for the 16 Å wire, the energies of the CBE and VBE, are not linear functions with strain. Generally, both energies of the CBE and VBE are reduced under expansion and increased with compression. It is because once the axial strain is applied, the bonds in the x and y directions will change due to the Poisson effect. The reduction in Ge-Ge bond lengths makes the electron cloud of the VBE and CBE orbital’s more efficiently shared by Ge atoms. This effect results in an increased electron-nucleus Coulomb attraction, thus an appreciable decrease in energies of both the VBE and CBE. In addition, we found that the orbital of the CBE is more delocalized than that of the VBE.
Thus, the electron cloud of the CBE is more effectively shared by Ge atoms in compared to that of the VBE. As a result, the energy of the CBE is more sensitive to strain than that of the VBE and, similarly for case of Si nano wires as shown in fig 2(b).

![Graph showing changes in CBE and VBE energies with applied strain]

**Figure 3:** The changes of CBE and VBE energies in Ge NWs are plotted as a function of strain.

### 4. Summary

We conclude that the Ge [110] NWs possess a direct band gap, while Si [110] NWs possess indirect band gap at nanoscale. The band gap is almost a linear function of strain when the diameter of Ge NWs D < 10 Å while shows parabolic behaviour for, D > 15 Å; & for Si it is linear in behaviour. On doping Si wire we found that the bandgap shows parabolic behaviour for change in strain. We also concluded that the band gap and the effective masses of charge carries (i.e. electron & hole) changes by applying the strain to the NWs. Our results suggested that strain can be used to tune the band structures of NWs, which may help in design of future nanoelectronic devices.

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