Single Walled Carbon Nanotubes (SWCNT) display a variety of electronic structures depending on their chirality. The structure of a SWCNT is specified by the chiral vector $(\vec{C}_t = (n,m))$. Depending on the chirality vector, SWCNTs are classified into three types, namely, armchair $(n,n)$, zigzag $(n,0)$ and chiral $(n,m)$. The armchair SWCNTs are always metallic, and the zigzag SWCNTs are only metallic when $n$ is a multiple of 3. Electrical conductivity of SWCNT may also change due to deformations such as uniaxial strain. Effect of strain on the energetics and the atomic relaxations of Cu nanowires and SWCNTs are studied in [1-3].

In this study, electronic structure of (12,0) and (14,0) zigzag SWCNTs under uniaxial strain are studied using parallel order N tight binding molecular dynamic (O(N) TBMD) simulation code designed by Dereli et al [3-6]. O(N) TBMD calculates the band structure energy in real space and makes the approximation that only the local environment contributes to the bonding, and hence the band energy, of each atom. In this case, the run time would be linearly scaled with respect to the number of atoms. We have obtain the total energy and Fermi energy levels of (12,0) and (14,0) SWCNTs are. Band gap calculated from behavior of electronic density of states near Fermi energy level for each strain values. The energy band gaps of these carbon nanotubes are modified by compressive and tensile strain and they exhibit semiconductor - metal and metal - semiconductor transitions.

The research reported here is supported through the Yildiz Technical University Research Fund Project No: 24-01-01-04. The simulations are performed at the Carbon Nanotubes Simulation Laboratory at the Department of Physics, Yildiz Technical University, Istanbul, Turkey [7].