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Uni-axial Tensile loading using AIREBO Potential (Molecular Dynamics Simulation)

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Abstract - The strength of Graphene (monolayer) nanomaterial have been investigated using Molecular Dynamic simulation. Graphene is a monolayer of carbon-carbon atoms in 2 Dimensional hexagonal lattice. It is one of the strongest material with mechanical strength exceeding more than steel. In this study uni-axial tensile load is applied at graphene sheet using AIREBO potential for stress-strain curve analysis and mechanical property is compared with steel.

Key Words: Molecular dynamics; LAMMPS, uni-axial tensile loading

1. Molecular Dynamics

It is a scientific approach to investigate the atomic movement in space and its potential energy with the help of Newtons Laws of motion with specific inter-atomic potentials. MD simulation involve how the different different atoms of same as well as another elements are interacting with each other. This molecular level simulation help in predicting the trajectory of atomic particles , material's mechanical , electrical properties etc during outcomes of simulation.

1.1 LAMMPS

LAMMPS software is free and open-source software and it stands for Large-scale Atomic/Molecular Massively Parallel Simulator is a Molecular Dynamics program from sandia national Laboratories .In this software Newton equation of motion are involve for all interactive particle and helps in two or three dimensional modeling with few atoms to millions of atoms.

1.2 Modelling Software

VMD software is used to generate a protein data bank (.pdb)file in which coordinates are mentioned in a well-defined format. LAMMPS is used for simulation purposes and Ovito software is used for the visualization of the output file.

Before Deformation

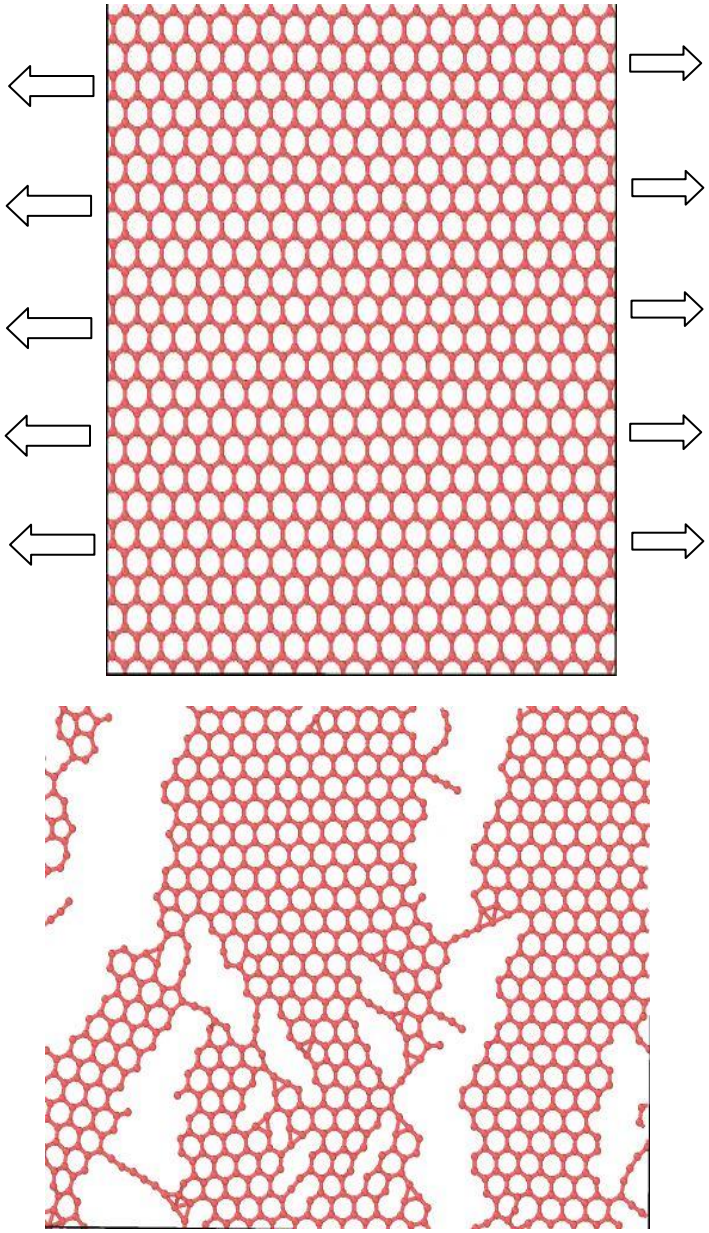

Figure-1: **Graphene Sheet under uniaxial tensile load**

2. Simulation

Initially, modeling of graphene sheet is done in VMD software and the protein data file is created for LAMMPS simulation. Periodic Boundary is used and the interatomic interactions was modeled using the (AIREBO)*Adaptive inter-molecular reactive empirical bond Order* potential [1], where its cutoff distance was modified to 2.0 Å [2]. The sample was relaxed for 25 ps with a 0.5 fs time step prior to applying strain. The simulations were performed using the (NPT) isothermal-isobaric conditions, with the temperature kept at 302 K by the NoeHoover thermostat. To aid in equilibration, carbon atoms were subjected to an initial random displacement perturbation (maximum of 0.1) in the x, y, and z directions. It should be noted that the induced out-of-plane displacement perturbations eliminate the artificial thermal expansion due to the Nośe-Hoover thermostat [3]. Now graphene sample reached an equilibrium state, the strain was applied at a rate of 0.001/ps along the y-axis. Stress and strain help in measuring of the mechanical properties of the sample during loading [4–6].

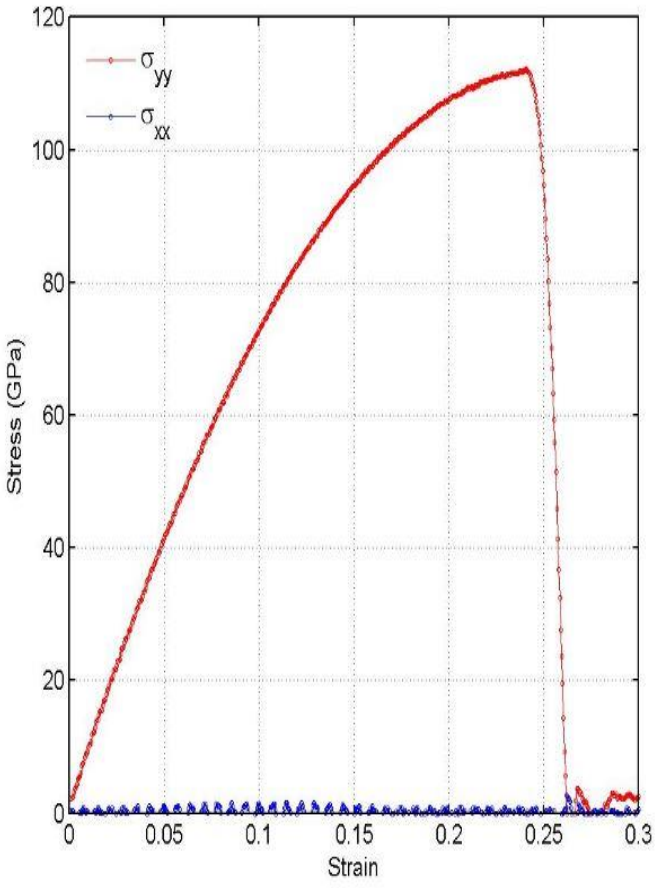

Figure -2: stress-strain curve

3. Potential Energy vs Strain Curve

In this work AIREBO potential is used for the carbon-carbon atoms interaction. The Constant strain is applied in loading direction as shown in Figure-1 . Here strain varies from 0 to 0.3 . The variation of potential Energy varies with strain as shown in the Figure - 3.

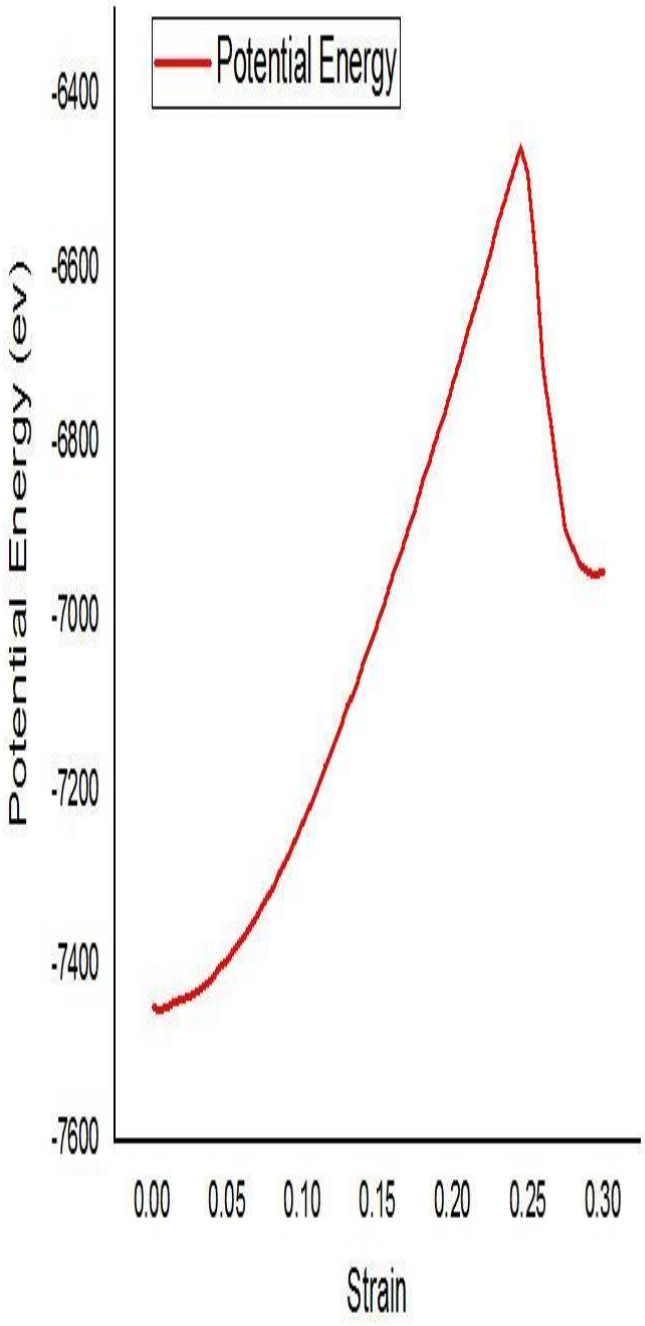

Figure -3: Potential Energy vs strain curve

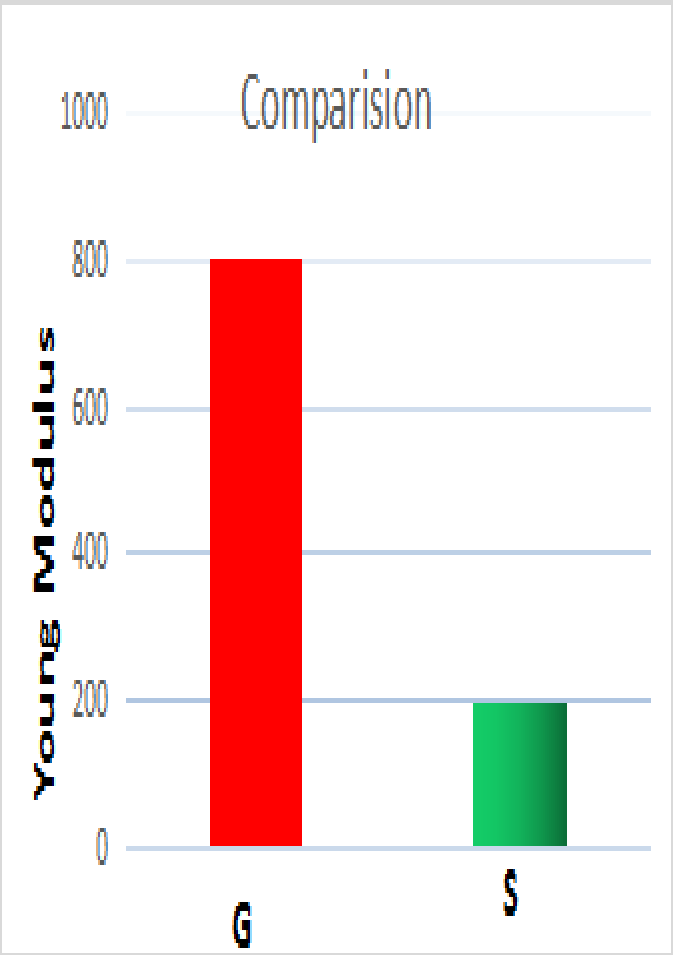

Table -1: Comparative study

Comparison			
S.No.	**Mechanical Properties**	**Graphene (G)**	**Steel (S)**
1	**Young Modulus (GPa)**	**800**	**200**

4. Conclusions

It is clear from the stress-strain curve that the elastic modulus of graphene under the elastic limit is 800Gpa which is 4 times the modulus of steel, so due to its properties it can be used as nano-filler material in the composite for the excellent mechanical property.

Acknowledgement

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References

[1] "S.J. Stuart et al"- A reactive potential for hydrocarbons with intermolecular interactions.

[2] " K.G.S. Dilrukshi,, U.G.A. Puswewala,M.A.N. Dewapriya" Size dependency and potential field influence on deriving mechanical properties of carbon nanotubes using molecular dynamics.

[3] " R.K.N.D. Rajapakse ,M.A.N. Dewapriya, , A.S. Phani, "- Influence of temperature and free edges on the mechanical properties of graphene, Modelling, and Simulation in Materials Science and Engineering.

[4] "D.H. Tsai" -The virial theorem and stress calculation in molecular dynamics.

[5] "M. Zhou, "-A new look at the atomic level virial stress on continuum-molecular system equivalence, Proceedings of the Royal Society of London. Series A: Mathematical, Physical, and Engineering Sciences.

[6]"A.K.Subramaniyan,et.al."-Continuum interpretation of virial stress in molecular simulations, International Journal of Solids and Structures.

[7] "C. Lee, X. Wei, J.W. Kysar, J. Hone"- Measurement of the Elastic Properties and Intrinsic Strength of Monolayer Graphene, Science.

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