MOLECULAR DYNAMICS SIMULATION OF CARBON NANO-FILM AND ITS STRESS/STRAIN USING LAMMPS (LARGE-SCALE ATOMIC/MOLECULAR MASSIVELY PARALLEL SIMULATOR)

Rjaymz L. Dela Cruz, Carlo L. De Guzman, Maxara S. Ederadan, Abraham P. Gaddi
DLSU SENIOR HIGH SCHOOL

ABSTRACT

This research investigates the stress, strain, and structure of simulated carbon nano-film through the LAMMPS software. This study also aims to create a simulation of a carbon nano-film model and have its strength tested in the simulation process. We simulated different shapes and sizes in a computer-generated environment will help us understand the material's characteristic and how the material interacts with other objects in its environment. By designing the film in the software, the strain of the carbon film can be measured. In the completion of this study, we found out that the shape that performed the highest is the block shaped nano-film and the smaller sizes perform with the same strength and endurance whether it be their Young's modulus or ultimate tensile strength. The model with the strongest structure is the block shaped nano-film with a size of 1000 cubic units, a Young's modulus of 688.67 GPa, and an ultimate tensile strength of 134.40 GPa

INTRODUCTION

Carbon is an extremely light and versatile material, which when chemically bonded with other carbon-based materials and with other elements, would produce properties that are hugely varying. Testing and experimenting on different materials can be highly expensive and very risky in the means of safety and assurance. Molecular simulations have been used by many researchers for the past decades to understand the behavior of atoms and molecules through a computer program. It has been used for methods of analysis, as a tool for chemical product designs, molecular modeling, and many more.

Carbon nanotubes and graphene sheets can be reinforced in simulations wherein their mechanical and tribological properties can be observed. A variety of simulation studies on modelling, calculation and analysis on enhanced elastic, tensile, fracture properties of carbon nanotubes and graphene sheet/polymer composites are introduced and reviewed. Strength testing the material via simulators will solve the hardship of conducting the actual experiment and help determine the optimum material quality. If the simulation is a success, the right type of carbon material to use for product applications and product applications can be determined.

Carbon-based materials can be chemically combined with other carbon-based material and other elements. This combination could potentially form strong covalent bonds, with characteristics such as high strength, high density, and high hardness. This material can potentially be utilized in various industries and disciplines.

The focus of this study is on the tensile strength and molecular modeling of carbon atoms in a simulation. The study will be utilizing the LAMMPS Parallel software. The environment would be controlled by the simulation and instill the standard temperature and pressure. Since the experiment will heavily focus on the use of Ovito and LAMMPS as the main platforms for conducting and recreating the strain of carbon films, other properties of the software will not be altered as this will only tamper with the programming setup within.

This study aims to determine the stress-strain value of LAMMPS simulated carbon with variance in conditions and its simulated environment. Specifically, this research is striving to: (1) identify the different factors that affect the strength of the simulated carbon and use it to determine the most efficient simulated carbon, and (2) pinpoint the strongest structure of the simulated carbon model that can be useful.

METHODOLOGY

RESEARCH DESIGN

The study utilizes molecular computational simulation using LAMMPS and data analytics in order to determine the strongest molecular structure of the carbon film in a virtual environment and the factors that affect the strain in the molecular structure. No ethical issues are disturbed or violated in the process of this study

DATA COLLECTION METHOD

The data collection procedure is done in LAMMPS. In creating a simulation, an input script with the given code is generated using Notepad++ and outputs a text file (.txt). LAMMPS reads the input script and goes through every command in it to simulate the atomic interaction for the virtual environment. The language of LAMMPS is run in C++ in which the commands are also formatted. The result of the simulation is the stress and strain value of the carbon film simulated. This was repeated 6 times with varying factors such as shape (block, prism, and plane) and the size of the film (1000 cubic units and 8000 cubic units). LAMMPS will simulate the deformation of the carbon film based on the three types of carbon simulation strain tests. The environment conditions are done with a constant number of atoms, constant temperature, and constant pressure. The first simulation, which is a control group, performed a normal strain test of the simulated carbon film (CS1=1000 cubic units and Block shaped). The five experimental simulations is varying in structure and amount of atoms (CS2=8000cu and Block-shaped, CS3=1000cu and prism-shaped, CS4=8000cu and prism-shaped, CS5=1000cu and plane-shaped, CS6=8000cu and plane-shaped). The output values is the strain of the carbon film with respect to the number of timesteps that have occurred in the simulation.

DATA COLLECTION MATERIALS

LAMMPS is a molecular dynamics simulation software that stands for Large-scale Atomic/Molecular Massively Parallel Simulator. LAMMPS can be installed, built, and run on any parallel computers. The language that governs in the coding of LAMMPS is C++. It is designed to be easy to modify or extend with new capabilities. LAMMPS applies Newton's equations of motions to the corresponding particles to determine their interaction with one another.

DATA ANALYSIS

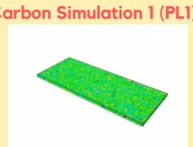
The optimum strength of each simulation was analyzed. The simulated environment applied the same force and conditions on each simulation in order to determine the strain of each simulation, which in turn indicates the strength of the carbon film simulated. The difference in distance is also noted. There are six carbon film simulations done in this study based on the two factors. These factors include the three different shapes and the two different sizes of the material. The size of the simulated carbon films was set as either 1000 and 8000 cubic units, while being shaped as either a plane, a block or a prism. The simulation showed the stress experienced by each carbon film as it moves within the change in length. The average strain of each simulation is noted in order to compare the values of each simulation's strain. The value of each simulation's strain would also indicate the carbon film's strength

STATISTICAL ANALYSIS

Descriptive statistical analysis would be used as this study's statistical analysis tool. This would be done through a table with the respective stress-strain values and calculation of the standard deviation to see how the distribution of data varies (elastic modulus and tensile strength). The values were manually extrapolated to an Excel file. The Young's Modulus (slope) and Ultimate Tensile Strength (maximum y value) of each simulation was also taken note of. The visualization of the simulations were done through the Ovito application. Ovito will import the data file generated by LAMMPS after each simulation. This software is able to output an image and video of the simulation done by an MD simulation software. Ovito will import a data/dump file generated by LAMMPS after the simulation and visualize the whole phenomenon. It will show a video of the said simulation and pictures of it will be taken as well.

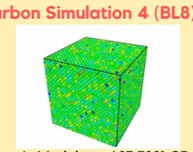
RESULTS

Carbon Simulation 1 (PL1)



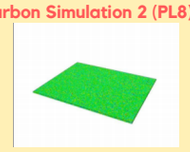
Young's Modulus = 686.7694 GPa
Ultimate Tensile Strength = 133.1933 GPa

Carbon Simulation 4 (BL8)



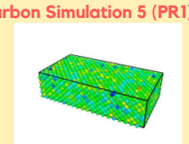
Young's Modulus = 687.7881 GPa
Ultimate Tensile Strength = 133.6443 GPa

Carbon Simulation 2 (PL8)



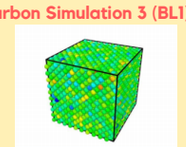
Young's Modulus = 685.6295 GPa
Ultimate Tensile Strength = 131.7392 GPa

Carbon Simulation 5 (PR1)



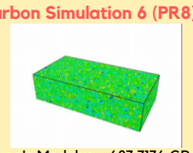
Young's Modulus = 687.9351 GPa
Ultimate Tensile Strength = 134.0518 GPa

Carbon Simulation 3 (BL1)



Young's Modulus = 688.6692 GPa
Ultimate Tensile Strength = 134.4012 GPa

Carbon Simulation 6 (PR8)



Young's Modulus = 687.7176 GPa
Ultimate Tensile Strength = 133.6094 GPa

CONCLUSION

The stress-strain test of carbon nano-films was successful and showed no errors in its results. The simulations showed that carbon is definitely a strong material and should be further studied in the field of physics, chemistry, material science, etc. The shape that showed the optimum performance in these tests is the block shaped nano-film and produced both the highest elastic modulus and ultimate tensile strength. The relationship between the size and the Young's modulus as well as the tensile strength has also been observed. The smaller the size of the nano-film material, the stronger it is and vice versa. With the given information it is also shown that the optimum material for carbon nano-film structure is the structure of carbon simulation 3 with a size of 1000 cu and a shape of a block with equal sizes.

For future research, the study of the electrical capability of the carbon nano-film in this simulation is mostly recommended because carbon can be a great asset in the electrical industry as well. It will help shape the future of more efficient batteries especially the nano batteries that could power the smallest of systems in a computer. Also, application of this structure in the macro scale is also advised so that we can see its practicality in the macroscopic world.

.