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MOLECULAR DYNAMIC SIMULATION OF GRAPHENE WITH VOID

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ABSTRACT

Graphene is widely used in the manufacture of composite materials for aerospace applications. This study investigates the effect of temperature changes on its mechanical properties of void-graphene nanosheets (VGNs). In order to achieve this goal, PGNs samples were prepared using a recently developed computational tool called "LUNAR", which stands for "LAMMPS Utility for Network Analysis and Reactivity". The "LAMMPS" tool was also used, "LAMMPS" stands for "Large-scale Atomic/Molecular Massively Parallel Simulator", which is used to perform "Molecular Dynamics (MD) modelling "and simulate the PGNs mechanical behaviour utilizing the "Polymer Consistent Force Field (PCFF)". Other computational tools were used, such as "OVITO and QTIplot" were utilized to collect and analyse the obtained data using precise scientific techniques. The simulation was performed within a temperature range between 200 ºK to 350 ºK (-73.15 ºC to 76.85 ºC). This temperature range is commonly applied for aerospace structures. This research concludes that VGNs are only slightly affected within the proposed temperature ranges, which explains the use of graphene in space applications. Molecular dynamics simulations provide clear evidence of the mechanical and thermal stability of graphene. Graphene exhibits a slight and consistent decrease in mechanical properties with increasing temperature. Additionally, this study has demonstrated that the PCFF force field used to simulate VGNs is computationally inexpensive (fast), and possesses efficiency, accuracy, and produce reliable results. The predicted data shows that Young's modulus is ranged from 1.16TPa to 1.21TPa. Thus, the methodology used in this study can be used as a reliable computational modelling procedure to speed up the development of aerospace structures.

1. Introduction

Graphene was first introduced of nanotechnology by Andre Geim and Konstantin Novoselov in 2004 as two-dimensional layer of carbon atoms formed into repeated hexagonal shapes [1]. Due to its abundance and its unique mechanical, thermal, and electrical properties, graphene has garnered significant attention from nanotechnology scientists. This has led to its widespread use in various engineering fields, including mechanical engineering. For example, graphene is used in aerospace, solar cells, energy storage solutions, flexible structures, and many other applications [2]. As the graphite represents the raw material of graphene, scientists had a

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lot of difficulties in separating a single layer of graphene until Andre Geim and Konstantin Novoselov came up with a new method called mechanical exfoliation in 2004[1].

This method alleviates the process to produce graphene single nanosheets out of graphite layers. It opens the door for scientists and researchers to look deeper into utilizing this new material in nanotechnology [3, 4].

Molecular Dynamics (MD) is the science to study the molecular behaviours of materials throughout time intervals. And it requires a set of force fields to represent the interaction between atoms and molecules and provide computational information. using Large-scale Atomic/Molecular Massively Parallel Simulator, LAMMPS [5], which is an open-source software developed by "Sandia National Laboratories". MD relies on classical physics laws to study the movement and behaviours of molecules and atoms over time. Where MD can be used to understand and interpret the physical properties of nanomaterials, including graphene and its nanocomposites [6-11]. For a long time, MD has provided researchers with a computational tool to study and understand materials at the atomic level, but MD also suffers from limitations in terms of available computational resources. Thus, researchers have been focusing on developing efficient and less computationally expensive interatomic potentials and force fields. Polymer Consistent Force Field (PCFF) which has been developed by Hendrik Heinz et al [12]. has shown its capability to perform fast MD simulations with the required accuracy in comparison to the reactive force fields.

To best of the authors knowledge, PCFF has not yet been used to simulate graphene nanoplatelets. This research aims to provide a new computational scheme to model VGNs using MD with PCFF force field. A systematic modelling procedure to address the capabilities and effectiveness of PCFF in evaluating the mechanical behaviour of VGNs at different temperatures. The temperature range (200 - 350 ºK) was selected to match the requirements for aerospace application as graphene can be integrated in polymer-based nanocomposite of aerospace structures. The MD modelling with PCFF was relatively computationally inexpensive using a local machine. The MD outcomes were analysed using postprocessing computational tools ("OVITO" [13] and "QTIplot" v0.9.8.3). The methodology of MD modelling adopted in this work is reliable to predict the mechanical behaviour of pristine graphene nanosheets. Furthermore, it can be developed to study the effect of other key processing parameters, such as structural integrity, on the mechanical behaviours of graphene.

2. Methodology

2.1 Building VGNs MD Model

Initially, an MD model of graphene nanosheets was created in the form of a hexagonal network of carbon atoms using "LUNAR" [14].

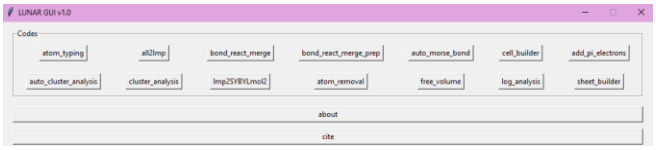


Figure 1. Main interface of LUNAR GUI v1.0.

The "sheet_builder" window contains many options for creating graphene sheets, including the "Global Inputs" option, thru which the type of atoms used in constructing the graphene nanosheets in this study was selected. The "cp" atom type (typically used for sp2 carbon structures) was selected for building GNs MD models. Based on the lattice specifications of graphene, the bond length was set to 1.42 angstrom.

The other part of the "sheet_builder" window is the "Sheet mode." From this section, you can specify the name of the file to be created, the dimensions of the sheet, the number of graphene nanosheets layers, and the distance between each layer. The type of angle and the type of stacking can also be specified. In this study, a graphene model consisting of 834 carbon atoms was used due to the limitations of computational resources. Notably, periodic boundary conditions were applied later for all MD simulations of VGNs. Providing the fact of PCFF being fast for MD simulations along with the relatively small size of VGNs MD model, all MD simulations were performed using a local PC machine.

After creating the graphene nanosheets, the "PCFF" force field was added thru the "all2lmp" option in the "LUNAR" program. It provides all required parameters for covalent bonds between two connected atoms, angle specifications for three bonded atoms, dihedral and improper specifications for four bonded atoms, which are illustrated in figure 2.

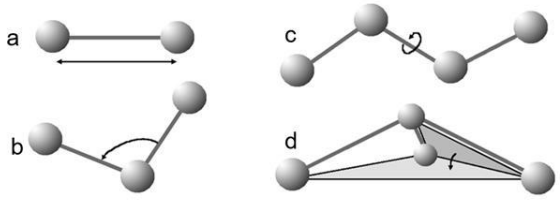


Figure 2. (a) bond stretching, (b) bond angle, (c) proper dihedral angle, (d)improper dihedral angle

The "Morse feature" was then added thru the "auto_Morse_bond" option in the main interface of the "LUNAR" program. PCFF is commonly known as fixed bonding force field in which bond breaking under stretching cannot be simulated. However, adding the Morse feature is used as a modification to the force field parameters to simulate bond scission at a certain tensile strain. Further information about LUNAR and its usage can be found in the package documentation [14].

Figure 3 shows the pristine graphene sheet that was built using the LUNAR according to the steps outlined above. This VGN consists of 834 sp2 (cp) carbon atoms. Clearly it has two edge types; the zigzag edge (top and bottom), and the armchair edge (left and right).

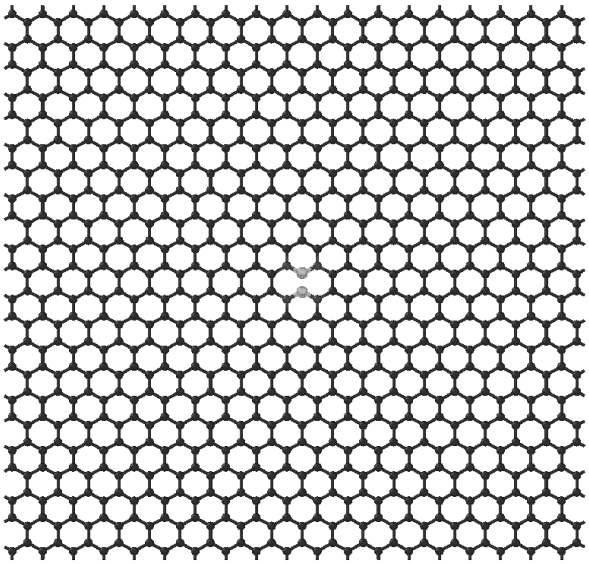


Figure 3. A void-graphene sheet composed of 834 carbon atoms.

2.2 Interatomic Potential

In the current study, the "PCFF" energy field (which is known as computationally inexpensive) was used. At the same time, the Morse potential was used as a bond energy function to simulate the breaking of the C-C bond. This feature is crucial for tensile modelling simulations and to assess the fracture strength of a stretched nanomaterial [15].

It has been proven that using the "PCFF" force field is effective in studying and describing the interactions between carbon atoms in graphene nanosheets. It is very efficient to characterize both bonding and non-bonding (e.g., Van der Walls, charge) interactions [16].

2.3 MD Simulation Steps and Settings

2.3.1 Model Equilibration

The created MD model of VGN (Figure 3), was subjected to an equilibration simulation process which was performed using LAMMPS [5]. The equilibrium simulation process is essential for reducing the potential energy in the molecular structure, which in turn reduces the residual stresses in the MD model. These stresses can affect the accuracy of the results obtained later from the simulation process. The time step used in the equilibration simulations was 1 fs (one femtosecond), and the simulation was conducted for 1,000,000 steps, which is equivalent to 1 ns (one nanoseconds). These setting are commonly used for such MD modelling and simulations [17, 18]. As mentioned above, the interactions between carbon atoms were simulated using the PCFF force field in which the possible bond breaking were implicitly predicted using Morse potentials. Angles, dihedrals, and improper in the molecular structure were described using class2 potential.

2.3.2 Loading conditions

After completing the equilibration process, the model is ready for the next step in the nanomaterial testing process. A tensile load was applied to the MD model in the form of a strain rate (2×108 ns-1). And then the simulation was redone, taking into account the temperature range (200 ºK, 225 ºK, 250 ºK, 275 ºK, 300 ºK, 325 ºK, 350 ºK). The canonical NPT ensemble was applied to maintain the required temperature value and preserve thermal stability along the simulations.

The tensile load was applied along the zigzag and armchair directions for the VGN molecular simulation models separately. The simulation was conducted until reaching the complete fracture in the molecular structure of the VGNs.

The atomic coordinates were saved every 100 steps to track the structural deformations. During the simulation, thermal and mechanical data, pressure, size of the simulation box in all direction, potential energy, stresses and strains.

2.3.3 Data collection and Analysis

"OVITO"[13], a popular program in the field of molecular dynamics, was used to display MD simulations and track the paths of atoms and molecules during the simulation. It also provides instantaneous numerical results on the stability of the simulation and includes multiple tools for analysing these results. In the current study, both equilibration and tensile simulations were watched using OVITO. VGNs waviness and its structural deformation until breakage were precisely observed under tensile loading.

Figure 4 shows the progress in crack propagation for the MD model in which complete failure occurs at true strain ratio 13% (time step = 6998000).

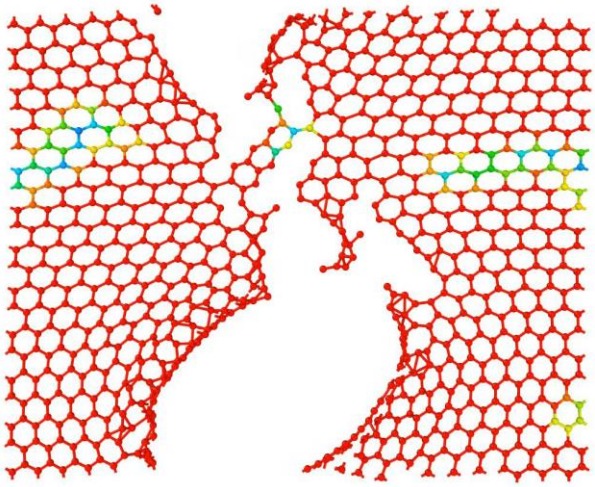


Figure 4. Representative VGN MD model shows the complete failure at true strain ratio 13% (time step = 6998000).

"QTIplot"(v0.9.8.3), was used as another tool for data processing and analysis. This tool provides the necessary flexibility to analyse and plot the computational data obtained from the simulation process. Therefore, all data curves presented in this study were plotted using QTIplot.

3. Results and Discussion

Once the MD simulations of PGNs were completed, quantitative and qualitative analysis of the obtained results were conducted. The development in stress-strain relationships, elastic modulus, fracture strength, and strain energy were plotted with the variation in temperature using QTIplot.

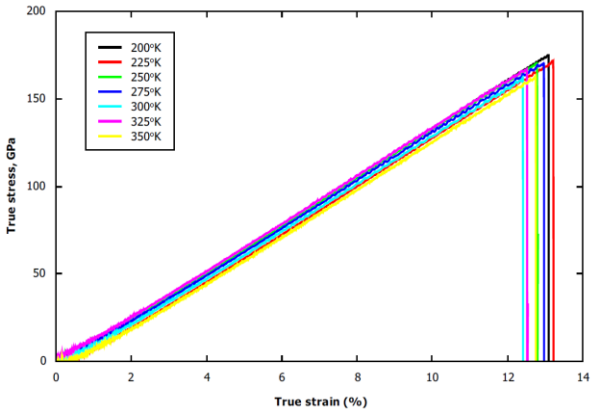


Figure 5. Stress-Strain curve of VGNs at different temp. - along armchair axis.

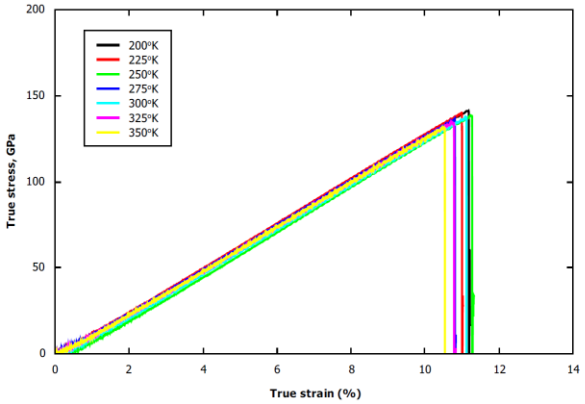


Figure 6. Stress-Strain curve of VGNs at different temp. - along zigzag axis.

The figures 5 and 6 illustrate the stress-strain curves of the VGNs MD models at various temperatures along the armchair and zigzag axes. All curves demonstrate a linear relationship within the defined temperature range of 200 to 350 K, signifying a consistent elastic response. The findings indicate a distinct variation between the two loading directions. The tensile strength along the chair axis exceeds that along the zigzag axis by approximately 35GPa [19]. This can be attributed to the varying fracture paths along the two axes. Failure occurs abruptly at a specific stress level, indicating the brittle failure characteristics of graphene [20]. The initiation of this failure typically occurs at the peripheries of the voids, attributed to the fragility of the atomic bonds.

The results showed that the lowest strain along the armchair direction was 12.41% and the highest was 13.22%, while the lowest stress was 162GPa and the highest stress was 175GPa. On the other hand, the results were less in the zigzag direction, where there was less strain was 10.53% and the highest was 11.27%, Meanwhile, the stress ranged from 131GPa to 142GPa.

The results demonstrate that the graphene sheet with voids shows decreased stiffness and tensile strength relative to pure graphene, attributable to stress concentration at the edges of the voids. Nonetheless, the sheet demonstrates the ability to endure considerable stresses, indicating the advantageous properties of graphene. The findings indicate a distinction between the two axes; however, the variation in strain is relatively minor, thereby reinforcing the validity of the current modelling employing PCFF.

Figure 7 shows that the Young's modulus of graphene is in sensitive to the change in temperature. This means that pristine graphene is mechanically stable within the suggested range of temperature. The predicted data shows that Young's modulus is ranged from 1.16TPa to 1.21TPa. This indicates that the presence of the void did not lead to a significant deterioration in the overall stiffness of the graphene due to the high strength of the covalent bonds within the graphene. The results also show a slight difference between the two axes resulting from the influence of the void location and the tension direction.

In overall, the current findings show reliable prediction methodology using MD modelling with PCFF. These findings support that pristine graphene has good mechanical stability within the suggested temperature range, and that PCFF is rather efficient for such purpose considering the low computational time required and availability of computing resources.

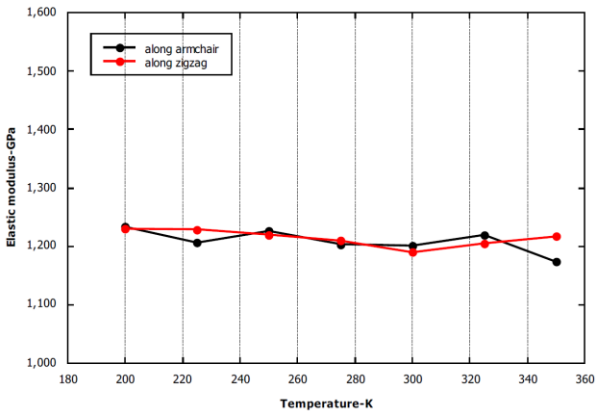


Figure 7. Elastic modulus as a function of temperature for VGNs stretched along its armchair and zigzag axes

Figure 8 shows fracture strength as a function of temperature change. The registered fracture strength ranges between 175GPa along the armchair axis, and 131GPa along the zigzag axis. Previous studies have shown similar values in the fracture strength of the armchair and zigzag axes, where it reached 110GPa [21].

These predictions support the current findings and the reliability of the adopted modelling approach using PCFF.

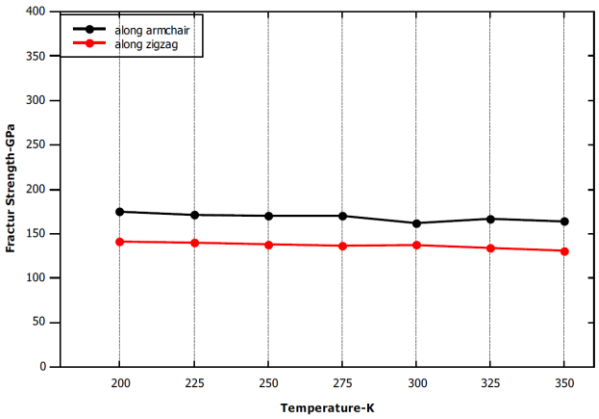


Figure 8. Fracture strength as a function of temperature for VGNs stretched along its armchair and zigzag axes

Figure 9 shows the strain energy required for a complete failure of VGNs subjected to tensile loading at different temperature ranged from 200 to 350 ºK.

the predicted strain energy evolved from 6,900-11,500 Mega Joule.

These results reflect the carbon network's ability to store mechanical energy before failure. It is observed that the

strain energy is higher around the armchair axis compared to the zigzag axis.

this is consistent to the strain energy values predicted along the zigzag and armchair axes in previous studies; 13,000 – 6,000 Mega Joule [22].

More importantly, the predicted mechanical properties obtained in this study were justified and have integrated with each other to describe the mechanical behaviours of the simulated PGNs which is subjected to tensile loading and temperature effect.

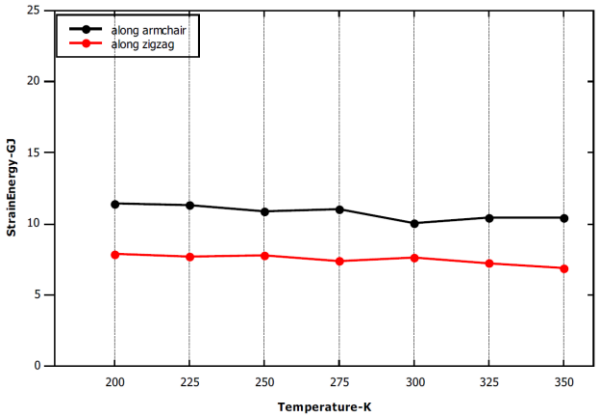


Figure 9. Energy as a function of temperature for VGNs stretched along armchair and zigzag

4. Conclusion

This research involves a new and effective methodology for modelling and testing the mechanical behaviours of nanographene sheets containing defects (voids). Molecular dynamics simulations using the PCFF force field and several other computational tools (LUNAR, LAMMPS, OVITO, QTIplot) are employed to accomplish this task. A molecular dynamics simulation of tension was conducted to predict the fracture strength and modulus of elasticity along both the armchair and zigzag directions.

Due to the extensive use of graphene in space applications, the simulation was conducted at different temperatures ranging from 200 to 350 ºK. The results show that the mechanical properties of graphene are almost stable within the range of the tested temperatures, with a slight decrease in the Young's modulus by approximately 4.5% with increasing temperatures. The analysis of the results shows a convergence between the armchair and zigzag directions, with a slight superiority of the values in the armchair direction, where the results increase by approximately 7% in this direction. In overall, the modelling scheme used in this study can be used as a reliable modelling approach considering the validated predicted mechanical properties using PCFF with previous studies from the literature.

The modelling approach used in this study can utilized for future studies to explore the mechanical properties of graphene at cryogenic temperatures. Such study can be useful for the applications fuel and gas reservoirs constructed from composite materials reinforced.

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