Retraction

Retraction: Effect of Stone-Thrower-Walls Defect on Mechanical Properties of Bi-layer Graphene - A Molecular Dynamics Study (IOP Conf. Ser.: Mater. Sci. Eng. 912 032084)

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It has come to the attention of IOP Publishing that this article should not have reached publication because of its substantial replication without citation of an earlier work by Suvojit Hore and Diptam Roy Choudhury, (2019), 'Characterization of Mechanical Properties of 2D Nanomaterials Using Molecular Dynamics a Project Report', (SRM University, India: Undergraduate Project Report). Consequently, this paper has been retracted by IOP Publishing. The authors disagree with this retraction.

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Effect of Stone-Thrower-Walls Defect on Mechanical Properties of Bi-layer Graphene - A Molecular Dynamics Study

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Abstract. This paper mainly focusing on the effects of topological defects like Stone-Thrower-Wales (STW) defect on the mechanical properties of bilayer graphene. The effect of STW defects on crack propagation mechanism were analyzed using Molecular Dynamics (MD) simulation. The results obtained are plotted to visualize the failure characteristics and the maximum stress that the material can withstand before undergoing fracture. These data are then validated with literature and experimentally obtained data.

1. Introduction
Nanotechnology is the branch of science that focuses on the study and development of materials on the Nano scale level [1]. The field of nanotechnology is relatively new, and extensive research work and progress is being carried out in this field. It is impossible to study atoms and molecules in the nanoscale level using the standard microscopes. Special instruments like the Scanning Tunneling Microscope (STM) [3] and Atomic Force Microscope (AFM) [4] were introduced about thirty years back which have enabled scientists to view matter at the nanoscale level. Nanotechnology is believed to have huge applications in the future as nanomaterials promise some unique properties which will help scientists create stronger materials with desirable properties compared to ordinary materials.

Graphene is a material that has gained a lot of popularity among the scientific community due to its excellent properties such as Young’s modulus value of around 1 TPa [5], ultimate tensile stress of 100 GPa and shear modulus of 280 GPa [6]. Graphene also has some interesting thermal properties which include its thermal conductivity of 5000 W/mK [7-8] and a melting temperature of 4900 K [9-14]. Other properties of graphene that has been observed to be of significance include the mobility of electrons at ambient temperature to have a value of 250000 cm2/Vs [5], a specific surface area of 2630 m3/g [15] and an optical transmittance of 97.90% [16]. These interesting properties of graphene make it useful in several applications such as nano-actuators [15], nano sensors [15], gigahertz oscillators [15], graphene based gas and bio sensors [16], energy production and storage [17], memory devices [18], transparent electrodes and battery [15], drug delivery [15] etc. It is an emerging candidate as nanofiller for manufacturing nanocomposites with excellent mechanical, thermal and electrical properties [15, 19, 20, 21] and it is often regarded to be the material of the future.
The following types of defects are generally observed in 2D nanomaterials: Stone-Thrower-Wales (STW) defects, vacancy defects, dislocations and Grain Boundaries (GBs) [22]. These defects generally occur due to chemical and heat treatment, ion beam radiation or during production processes such as Chemical Vapour Deposition (CVD) and mechanical exfoliation. The Stone-Thrower-Wales (STW) defect is caused due to the rotation of covalent bond of carbon-carbon atoms by 90° with respect to the midpoint of the bond. STW defect, yielding a transformation of four neighboring hexagonal unit cells into two heptagonal and two pentagonal unit cells, due to 2 heptagons and 2 pentagons transformations this defect is also known as 5-7-7-5 defect. STW1 defects is formed for horizontal and vertical straight bond rotation whereas STW2 is formed by rotation of slanted bond by 90 degrees [23].

![Figure 1](https://via.placeholder.com/150)

**Figure 1** Formation of (a) STW1 defect (b) STW2 defect.

These defects as shown in Figure 1 can either already exist or be engineered to exist that is, the defects can be intentionally introduced in the nanomaterial. They can also form during self-healing of graphene. The effect of such defects on the electrical and thermomechanical properties is an important research topic in the field of nanofillers [22].

2. Simulation Details

LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) software is openly sourced by the company Sandia National Laboratories (SNL) for complex Molecular dynamics simulations [23]. It can be used to model atoms, molecules, soft matter, nanomaterials, etc. on a large scale. LAMMPS has input scripts for different materials, nanomaterials like graphene, boron carbide, etc. and it runs using an input script that determines the model and simulation process parameters. The input script can be created using several parameters like temperature, strain rate, pressure, etc. and can be used to model, remove atoms, rotate atom(s), etc [24]. OVITO is a visualization and analysis software for scientific data and models at the atomic and molecular levels [25]. It is a freeware and a powerful tool that can be used for several complex analysis and visualization in the macro and nanoscale level. The software has several features such as slicing, color coding, particle selection, distance measurement, creation and display of atomic bonds, etc [26]. In this paper, OVITO is used for visualization and analysis of bilayer graphene with crack and STW defects at varying distances from the crack tip is often regarded to be the material of the future.

Molecular dynamics simulation and modelling of single and bilayer graphene was carried out in LAMMPS and the results were viewed in OVITO. STW1 and STW2 defects and cracks were introduced in bilayer graphene along the zigzag and armchair chirality at a constant rate of strain of 0.001 ps⁻¹ and at 1 K temperature at a cut off distance of 1.92 Å and AIREBO potential [27]. The validation of the modelling input script was carried out on single layer graphene using the same above mentioned parameters and the results were found to be in agreement with already available literature [27].
3. Results and Discussion.

3.1. Molecular dynamics simulation of bi-layer graphene:

Molecular dynamics simulation study was carried out on bilayer graphene using the input script model that was validated on single layer graphene with its pristine form as well as graphene sheet with STW-1 and STW-2 defects along with the zigzag and armchair directions at 300 K and at a strain rate of 0.001 ps-1. In this molecular dynamic study, Stone Thrower Wales (STW) defects were introduced near a crack of length 1.2 nm at varying distances from the crack tip and their effects on crack propagation and their failure morphology were studied. All these molecular dynamics simulation was carried out at 1K and rate of constant strain of 0.001 ps-1. In first set of molecular dynamics simulation, bilayer graphene was modeled such that a crack of 1.2 nm was placed in the top layer and two STW-1 defects were placed at ‘X’ nm from the crack tips. This simulation was carried out by applying the constant rate of strain of 0.001ps-1 in zigzag and armchair directions. The stress-strain graph obtained from the simulations are given in Figure 2.

In the second set of simulations, the same conditions were done for STW-2 defects as well, where two STW-2 defects were placed at ‘X’nm from the crack tip. The value of X was varied, and the simulations were carried out by applying 0.001 ps-1 rate of strain along with armchair and zigzag directions. The stress strain graph obtained from the results are given in Figure 3. From Figure 2 and Figure 3, we can observe that there are two peaks in the stress-strain graphs. This is caused because the failure of the top layer which has the crack and defects occur first followed by the second layer below it which is in pristine form without any cracks or defects. Thus, the graphene sample has two peaks of ultimate tensile stress.

![Figure 2](image-url)

**Figure 2** - Bilayer graphene with STW-1 defects at ‘X’ nm from crack tips in top layer only with strain being applied in (a)Armchair direction and (b) Zigzag direction.
In the third set of simulations, two STW-1 defects were placed at 'X' nm from the crack tips of the crack of 1.2 nm crack length in the top layer of the bilayer graphene sample. The value of X was varied, and the simulations were carried out by applying 0.001 ps⁻¹ rate of strain along with armchair and zigzag directions at 1K. The same crack of 1.2 nm crack length was placed in the second layer exactly below the crack in the top layer. However, no STW defects were introduced near the crack in the second layer. The stress strain graph obtained from the simulation is given in Figure 4. From the two graphs, a significant amount of difference can be seen in the average values of ultimate tensile strength which shows that zigzag direction is more favorable and stronger than armchair in this case.

![Stress-Strain Graph](image)

**Figure 3** - Bilayer graphene with STW-2 defects at 'X' nm from crack tips in top layer only with strain being applied in (a) Armchair direction and (b) Zigzag direction.

![Stress-Strain Graph](image)

**Figure 4** - Bilayer graphene with crack on both layers and STW-1 defects on top layer at 'X' nm from crack tip subjected to strain in (a) Armchair direction and (b) Zigzag direction.
In the fourth set of simulations, just like the above mentioned in the third set, two STW-2 defects were placed at ‘X’ nm from the crack tips of the crack of 1.2 nm crack length in the top layer of the bilayer graphene. The value of X was varied, and the simulations were carried out by applying the strain rate of 0.001 ps\(^{-1}\) along with armchair and zigzag directions at 1K. The same crack of 1.2 nm crack length was placed in the second layer exactly below the crack in the top layer. However, no STW defects were introduced near the crack in the second layer. The stress strain graph obtained from the simulation is given in Figure 5. From the stress strain graphs of Figure 4 and 5, it can be observed that the graphs have only one peak unlike the cases in Figure 2 and 3. In the tailored conditions of the figures, 4 and 5, the failure of both the layers of the bilayer graphene sample under simulation occurs at the same time.

In the fifth set of simulations, two STW-1 defects were placed at ‘X’ nm from the crack tips of the crack of 1.2 nm crack length in both the layers of the bilayer graphene sample. The value of X was varied, and the simulations were carried out by applying the strain rate of 0.001 ps\(^{-1}\) along with armchair and zigzag directions at 1K. The stress strain graph obtained from the simulation is given in Figure 6.

**Figure 5** - Bilayer graphene with crack on both layers and STW-2 defects on top layer at ‘X’ nm from crack tip subjected to strain in (a) Armchair direction and (b) Zigzag direction.

**Figure 6** - Bilayer graphene with crack on both layers and STW-1 defects on both layers at ‘X’ nm from crack tip subjected to strain in (a) Armchair direction and (b) Zigzag direction.
Figure 7 - Bilayer graphene with crack on both layers and STW-2 defects on both layers at 'X' nm from crack tip subjected to strain in (a) Armchair direction and (b) Zigzag direction.

In the sixth set of simulations, two STW-2 defects were placed at 'X' nm from the crack tips of the crack of 1.2 nm crack length in both the layers of the bilayer graphene sample. The value of X was varied, and the simulations were carried out by applying the strain rate of 0.001 ps-1 along with armchair and zigzag directions at 1K. The stress strain graph obtained from the simulation is given in Figure 7.

The graph in figure 7 shows failure at a slightly lower value of strain compared to the graph in figure 6. This shows that STW2 defects stress field interaction with that of the crack is slightly lower than that of STW1 defect. Moreover, in figure 7. (b) we observe a trend of increasing ultimate tensile strength as the distance of defect from the crack tip is increased. The failure in figure 7. (b), that is in zigzag direction occurs at a significantly higher strain compared to figure 7. (a) that is in armchair direction thereby implying that graphene has more resistance to failure in zigzag direction.

4. Conclusion

The vast amount of data obtained from the detailed simulation of graphene nanosheets with tailored conditions has been studied thoroughly and useful inference has been derived from the same. Research shows that tailored conditions like STW defects cause significant changes in the mechanical properties of graphene. The STW defects create a stress field that interacts with the stress field of the crack causing changes in rate of crack propagation and ultimate tensile strength. The simulations were carried out with the STW defects at several distances and thereby concluding that defects too close to the crack cause reduction in ultimate tensile strength by 5 to 10%, whereas, defects away from the crack cause minimal to no difference in the ultimate tensile strength with significant stress field interaction to restrict the propagation of the crack thereby failing at higher strain rate.

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