Mechanical Properties of Knotted Graphene Nanoribbons

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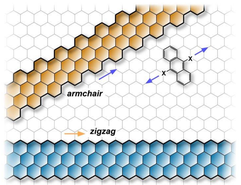
Introduction

When Andre Geim and Konstantin Novoselov discovered a way to isolate a single layer of graphite (called graphene) in 2004[1], a whole bevy of low-dimensional materials became promising to the nanotechnology sector. In the form of nanotubes, nanowires, and nanoribbons, graphene acts as a quasi-1-dimensional material which has the advantage of electron confinement, only allowing electrons to effectively move in one direction. This property allows these structures to have a wide range of mechanical and electrical properties that can be tuned by varying thickness and edge shape among other things. We focus our research on graphene nanoribbons, which are thin strips of graphene, and how knots can affect their mechanical properties.

Background

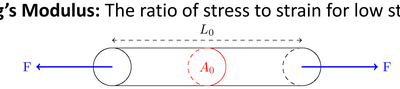
A **Graphene Nanoribbon (GNR)** is defined as a narrow strip of graphene with width less than 50 nm. GNRs can have two different edge orientations: **Zigzag (ZGNR)** and **Armchair (AGNR)**.



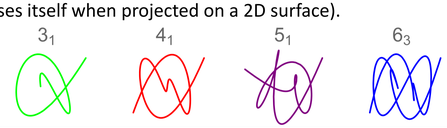
Pictured here in Orange is an AGNR and in Blue is a ZGNR. The difference is in angles of the carbon-carbon bonds on the long-edges.

Source: http://www.mpip-mainz.mpg.de/4567880/PM2016_4

The Mechanical Properties we will compute are:
-Stress: the force per unit area along the deformation direction
-Strain: the linear displacement caused by deformation
From these two quantities, we can compute:
-Young's Modulus: The ratio of stress to strain for low strains



We will stretch the GNRs that contain different knots. Knots can be classified by their crossing number (number of times the knot crosses itself when projected on a 2D surface).



Methods

We use Python to specify and calculate locations of atoms in the GNRs. The molecular dynamics program LAMMPS is used to apply uniaxial tension to the GNRs and calculate stresses and strains while VMD is used to visualize the GNRs.

Molecular Dynamics works by numerically solving for the positions, velocities, and accelerations of all the atoms at some timestep Δt later given the initial positions, velocities, and accelerations in addition to some potential function that describes the intermolecular interactions. We use the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential because it accurately describes the carbon-carbon and carbon-hydrogen interactions in graphene[2].

Data

We lay the GNRs flat and apply a fixed velocity to both ends to simulate tension. Summarized below are data retrieved from LAMMPS simulations on ZGNR and AGNR with and without knots. A higher Young's Modulus means that the GNR does not deform much for low strains. Max Stress and Strain are the stresses and strains that the GNR experiences just before breaking.

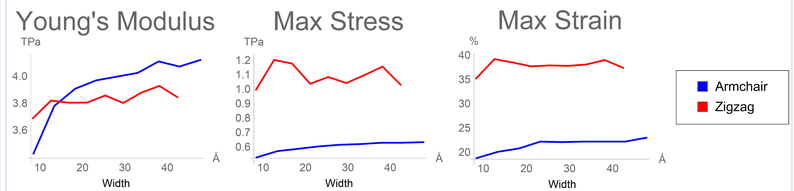


***Figure 1**: Properties plotted as a function of width for unknotted GNRs*

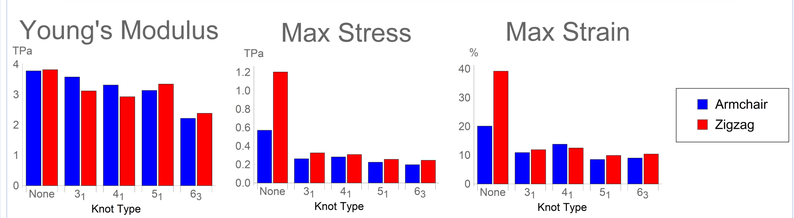
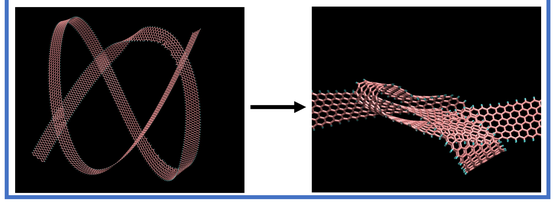


***Figure 2**: Properties plotted for GNRs with different knots at a constant width (12.56 and 13.34 Å for ZGNR and AGNR respectively)*

Visualization of Knots

These VMD images show the process of a ZGNR being tied into a 3_1 knot. The knot does not break apart when the ribbon is taut.



Conclusion and Future Work

We've shown that knots in GNRs are stable and do not break apart when tightened, which shows their immense strength. As expected, the knots significantly reduce maximum stress and strain compared to the corresponding GNR. In addition, GNR width and edge orientation make a noticeable difference in these properties which shows that edge effects cannot be ignored.

In the future we would like to test more complicated knots, ones that are known to be very strong, and see if that increases the GNR strength. Additionally, we would like to explore different mechanical properties like torsion strength, poisson's ratio, and where and when the knots are most stable.

Acknowledgements

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References

[1] Novoselov, K. S. and Geim, A. K. (2004) "Electric Field Effect in Atomically Thin Carbon Films"
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