

# MECHANICAL ENGINEERING & ENGINEERING SCIENCE GRADUATE SEMINAR SERIES

Tuesday, September 17, 2020

11:30AM – 12:30PM

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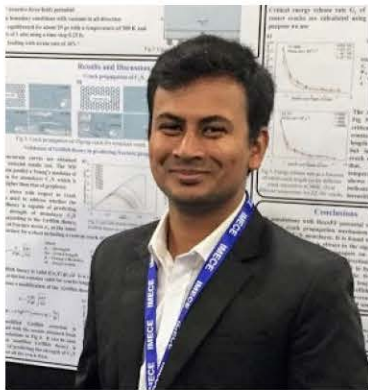
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Meeting ID: 934 3719 9501

Passcode: 951231

## A Molecular Dynamic Study of fracture properties of graphene.

Md Imrul Reza Shishir, PhD Student in Mechanical Engineering and Engineering Science  
Advisor, Dr. Alireza Tabarraei



### Md Imrul Reza Shishir

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**Abstract:** Graphene, a single layer of carbon atoms packed together in a honeycomb lattice structure, has drawn remarkable attention due to its extraordinary fundamental properties that make it a suitable material for a wide range of technological applications. Very large-scale graphene films prepared by chemical vapor deposition (CVD) are polycrystalline sheets composed of single-crystalline pristine graphene grains of varying orientation joined by grain boundaries. Grain boundaries act as defects and alter the mechanical properties of graphene. It has been reported that pristine graphene is the strongest material with Young's modulus of  $1.0 \pm 0.1$  TPa and strength of 130 GPa. However, inclusion of grain boundaries reduces the Young's modulus to 600 GPa. Reliable use of polycrystalline graphene sheet necessitates fundamental understanding of the effect of grain size and grain boundaries orientation on the mechanical and fracture properties of graphene in industrial application. Molecular dynamic (MD) simulations dominate the studies on the mechanical and fracture properties of graphene-like two-dimensional (2D) materials because it strikes a balance of computational accuracy and cost. Using molecular dynamics simulations, we have investigated the fracture properties of graphene grain boundaries with various misorientation angles. We conduct molecular dynamics simulations of the fracture of grain boundaries and express the results as continuum cohesive zone models (CZM) that embed concepts of the grain boundary toughness and strength. Cohesive zone models combine a strength-based failure criterion for the prediction of damage initiation with an energy-based fracture mechanics criterion to determine the crack propagation. An essential part of the cohesive zone models is a traction– separation law (TSL) which describes the material behavior within the cohesive zone. Using the molecular dynamics simulations, we predict the traction separation laws governing the behavior of graphene grain boundaries.

**About the Speaker:** Md Imrul Reza Shishir received B.Sc. in Mechanical Engineering from Bangladesh University of Engineering and Technology, Bangladesh in 2012 and M. Eng. in Mechanical Engineering at Inha University in 2017. Currently, He is pursuing Ph.D. in Mechanical Engineering at the University of North Carolina at Charlotte. His research interest is fracture mechanics, molecular dynamics, 2D materials, cohesive zone models, machine learning etc.