Fracture Properties of Tetragraphene Under Mixed Mode Loading

Elnaz Haddadi[1]*, Alireza Tabarraei[1]

[1]*University of North Carolina at Charlotte, Charlotte, NC, USA*
** Presenting Author email: ehaddadi@uncc.edu*

Abstract
Tetragraphene (TG) is a quasi-2D semiconductor carbon allotrope composed of hexagonal and tetragonal rings and shows metallic or semiconducting behaviors. This study uses molecular dynamics (MD) simulations to understand fracture properties of triple-layered TG sheets with two different structures under mixed mode I and II loading using the Tersoff–Erhart potential. We investigate the effect of crack edge chirality, loading phase angle, and temperature on the crack propagation path and critical stress intensity factors.

1. Introduction

A comprehensive understanding of the mechanical behavior of the materials is critical to have a safe design in the aerospace, automobile, and electronics industries. Among various materials used in the industry, graphene is considered an excellent candidate for many applications as a result of its extraordinary features. However, pristine graphene is a semi-metal with no electronic bandgap leading to limitations in its electronic applications. Considering this issue, many studies have been focused on searching for new carbon-based two-dimensional materials which could introduce an electronic bandgap. TG is one of such newly introduced materials which has various potential applications in electronics.

While the mechanical and fracture properties of graphene have been extensively researched, more investigation is needed to comprehend the fracture characteristics of TG. Unlike graphene's flat structure, TG's atomic structure is more intricate, with a triple-layered arrangement in each sheet. Consequently, TG's failure mechanisms are more complex than those of graphene. As a result, a distinct analysis of TG's fracture properties is essential, as they may vary significantly from those of graphene.

In light of these considerations, our research aims to investigate the fracture properties of TG.

2. Results

The procedure used to analyze the fracture properties of a pre-cracked circular TG sheet was as described below:

a. Two different structures of pre-cracked circular TG sheets with different crack edge chirality are created, and their thickness is calculated separately.

b. Each structure's Young modulus is calculated using MD simulations under tensile loading.

c. Several types of loading phase angles are applied to the structures under mixed mode I and II loading at different temperatures from 0 K to 2000 K by using MD simulations.

d. The critical stress intensity factors are extracted from the MD results, and the differences in the crack propagation path are observed.

The findings indicate that the loading phase angle and crack edge chirality have an impact on the crack propagation path and critical stress intensity factor in TG. Temperature, however, does not have a significant effect on the critical stress intensity factor except for 0 K temperature with a specific loading phase angle. When subjected to mixed mode I and II loading conditions, TG sheets can experience out-of-plane deformations due to buckling induced by compressive stresses. The extent of these deformations is more pronounced when mode II loading predominates over mode I. Furthermore, the average critical stress

intensity factor is higher for mode I loading than mode II. For instance, Fig.1 depicts the critical stress intensity factor for a structure with an asymmetric crack edge, while Fig.2 shows the MD simulation of the corresponding structure under a particular loading phase angle and temperature.

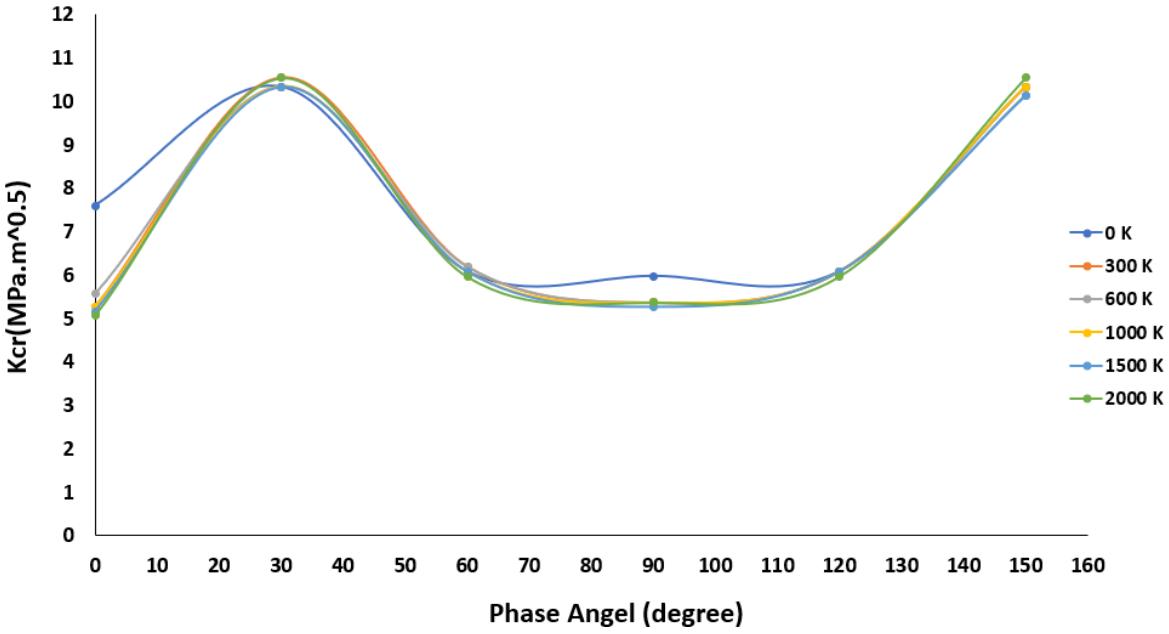
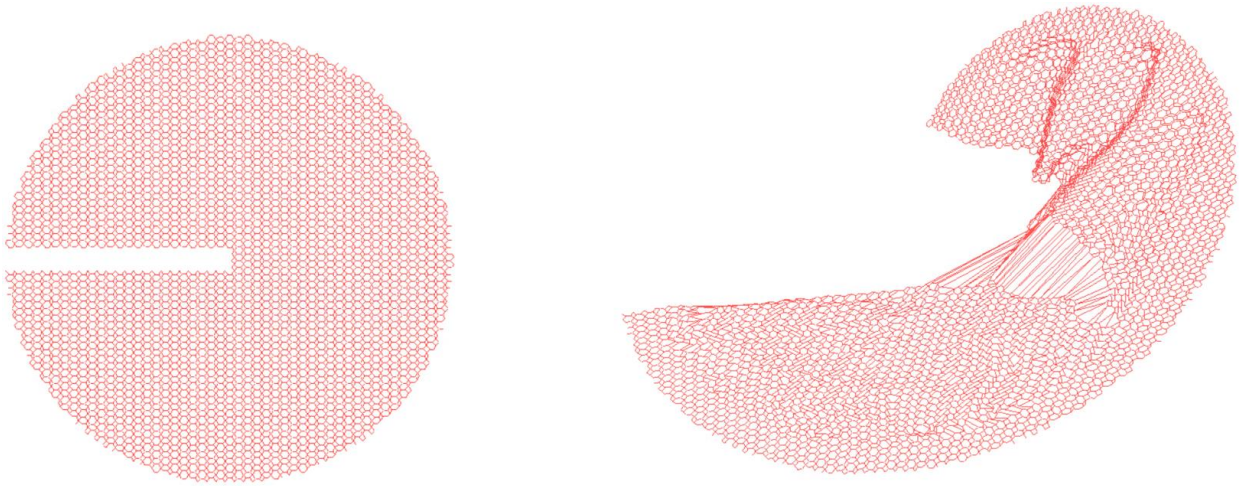


Fig.1 – Critical stress intensity factor at different loading phase angles and temperatures.



(a) (b)

Fig.2 – MD simulation of the pre-cracked circular TG sheet under mixed mode loading (a) Before applying the load (b) After applying the load.

3. Conclusions

This study demonstrates that the critical stress intensity factor and crack propagation path of TG sheets under mixed mode loading is influenced by loading phase angle and crack edge chirality; however, the temperature does not affect the critical stress intensity factor noticeably.