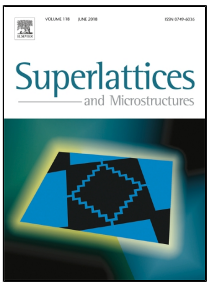
# Accepted Manuscript




The effect of defects on the fracture behavior of trilayer graphene

Minrong An, Qiong Deng, Yulong Li, Haiyang Song, Mengjia Su

| | |
|---|---|
| PII: | S0749-6036(18)31097-8 |
| DOI: | 10.1016/j.spmi.2018.07.014 |
| Reference: | YSPMI 5818 |
| To appear in: | *Superlattices and Microstructures* |
| Received Date: | 24 May 2018 |
| Accepted Date: | 06 July 2018 |

Please cite this article as: Minrong An, Qiong Deng, Yulong Li, Haiyang Song, Mengjia Su, The effect of defects on the fracture behavior of trilayer graphene, *Superlattices and Microstructures* (2018), doi: 10.1016/j.spmi.2018.07.014

# The effect of defects on the fracture behavior of trilayer graphene

Minrong An[a,*], Qiong Deng[b], Yulong Li[b,*], Haiyang Song[a,*] , Mengjia Su[b]

[a] College of Materials Science and Engineering, Xi'an Shiyou University, Xi'an 710065, Shaanxi, PR China

[b]Fundamental Science on Aircraft Structural Mechanics and Strength Laboratory, Northwestern Polytechnical University, Xi'an 710072, Shaanxi, PR China

## Abstract

The fracture behavior of trilayer graphene was investigated using molecular dynamics simulations, with the emphasis on the effect of vacancies and interlayer bonds. While both defects make the fracture happen earlier and reduce the ultimate strength, the exact details of how they change the fracture behavior are different. Interlayer bonds can make the three graphene layers fracture in a more simultaneous way by transferring and distributing load more uniformly between these layers when loaded in the zigzag direction. When loaded in the armchair direction, however, the interlayer bonds can shift the fracture plane from a bifurcating mode to a zigzag direction-dominated mode. In contrast, with increasing tensile strain, vacancies can change the fracturing manner from a catastrophic mode to a successive one, leading to a stepwise stress strain curve and the formation of carbon atom chains and polygonal rings during the fracture process. The mixture of vacancies and interlayer bonds breaks the trilayer graphene in a way coupling the effect of both defects, depending on the chirality and defect density. The results presented in this work can provide a guideline for the design and application of multilayer graphene.

*Keywords:* Molecular dynamics simulation; trilayer graphene; interlayer bond; vacancy

## 1. Introduction

Graphene is a well ranged two-dimensional atomic layer of carbon atoms in a honeycomb lattice structure. Due to its extraordinary mechanical [1-3], electronic [4-5], etc. properties [6-8], graphene has been considered as one of the most promising candidates for next-generation electronics and attracted extensive research attention since its successful fabrication [9]. Depending on the number of atomic layers, graphene can have many forms: single layer, bilayer, trilayer, etc. Single layer graphene has many superior properties such as high mobility and optical transparency, perfect flexibility and thermal stability, and

E-mails: amr_lr@163.com (M. An), liyulong@nwpu.edu.cn (Y. Li), gsfshy@sohu.com (H. Song)