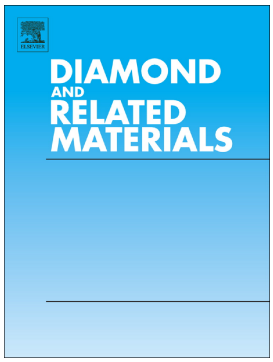

Reactive force field based atomistic simulations to study fracture toughness of bicrystalline graphene functionalised with oxide groups

Akarsh Verma, Avinash Parashar

PII: S0925-9635(18)30256-5
DOI: doi:10.1016/j.diamond.2018.07.014
Reference: DIAMAT 7163

To appear in: *Diamond & Related Materials*

Received date: 11 April 2018
Revised date: 11 June 2018
Accepted date: 18 July 2018

Please cite this article as: Akarsh Verma, Avinash Parashar , Reactive force field based atomistic simulations to study fracture toughness of bicrystalline graphene functionalised with oxide groups. Diamat (2018), doi:10.1016/j.diamond.2018.07.014

Reactive force field based atomistic simulations to study fracture toughness of bicrystalline graphene functionalised with oxide groups

Akarsh Verma and **Avinash Parashar***

Department of Mechanical and Industrial Engineering, Indian Institute of Technology, Roorkee, India
*Email: drap1fme@iitr.ac.in; Ph: +91-1332284801

Abstract

The aim of this article was to study the effect of oxide functionalisation on the fracture toughness of bicrystalline graphene. Molecular dynamics based simulations in conjunction with reactive force field were performed to study the fracture toughness of functionalised bicrystal of graphene. Separate studies were performed with hydroxyl and epoxide functionalisation, and later on the same simulations were extended over graphene oxide (GO) as a whole. Failure morphologies depict that epoxide groups tend to boost the fracture toughness, via altering the failure path and transforming the fracture mode from mode-I to mode-II. In addition to the transformation, epoxide-to-ether conversion also played significant role in enhancing the fracture toughness of bicrystalline graphene. On the other hand, steric hindrance exhibited by the hydroxyl group mitigates the fracture toughness of GO. Overall, certain spatial sandwich configurations of epoxide groups concluded an enhanced fracture toughness for bicrystalline graphene; which further opens new avenues for the application of these graphene sheets in nanodevices, nanomembranes and nanocomposites.

Keywords: Bicrystalline graphene, Grain boundaries, Oxygen functionalisation, Fracture toughness, Molecular dynamics