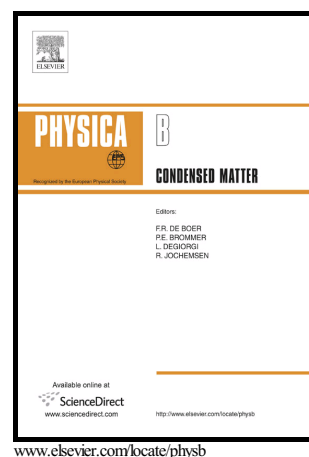


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Tawfiqur Rakib, Satyajit Mojumder, Sourav Das,
Sourav Saha, Mohammad Motalab



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Graphene and its elemental analogue: A molecular dynamics view of fracture phenomenon

Tawfiqur Rakib, Satyajit Mojumder*, Sourav Das, Sourav Saha, Mohammad Motalab

Department of Mechanical Engineering, Bangladesh University of Engineering and Technology, Dhaka-1000, Bangladesh.

*Corresponding Author. Tel.: (+880)1737434034; E-mail address: satyajit@me.buet.ac.bd

Abstract

Graphene and some graphene like two dimensional materials; hexagonal boron nitride (hBN) and silicene have unique mechanical properties which severely limit the suitability of conventional theories used for common brittle and ductile materials to predict the fracture response of these materials. This study revealed the fracture response of graphene, hBN and silicene nanosheets under different tiny crack lengths by molecular dynamics (MD) simulations using LAMMPS. The useful strength of these two dimensional materials are determined by their fracture toughness. Our study shows a comparative analysis of mechanical properties among the elemental analogues of graphene and suggested that hBN can be a good substitute for graphene in terms of mechanical properties. We have also found that the pre-cracked sheets fail in brittle manner and their failure is governed by the strength of the atomic bonds at the crack tip. The MD prediction of fracture toughness shows significant difference with the fracture toughness determined by Griffith's theory of brittle failure which restricts the applicability of Griffith's criterion for these materials in case of nano-cracks. Moreover, the strengths measured in armchair and zigzag directions of nanosheets of these materials implied that the bonds in armchair direction have the stronger capability to resist crack propagation compared to zigzag direction.

Keywords: Griffith's theory, Graphene, Silicene, hBN, Fracture Toughness, Molecular Dynamics

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