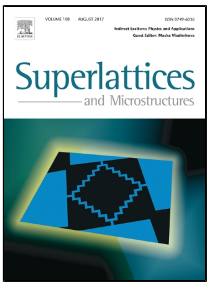
Accepted Manuscript



Synergistic effect of temperature and point defect on the mechanical properties of single layer and bi-layer graphene

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PII:	S0749-6036(17)31079-0
DOI:	10.1016/j.spmi.2017.08.040
Reference:	YSPMI 5215
To appear in:	*Superlattices and Microstructures*
Received Date:	02 May 2017
Revised Date:	11 August 2017
Accepted Date:	23 August 2017

Please cite this article as: Sanghamitra Debroy, V.Pavan Kumar, K.Vijaya Sekhar, Swati.G. Acharyya, Amit Acharyya, Synergistic effect of temperature and point defect on the mechanical properties of single layer and bi-layer graphene, *Superlattices and Microstructures* (2017), doi: 10.1016/j.spmi.2017.08.040

Synergistic effect of temperature and point defect on the mechanical properties of single layer and bi-layer graphene

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The present study reports a comprehensive molecular dynamics simulation of the effect of a) temperature (300-1073 K at intervals of every 100 K) and b) point defect on the mechanical behaviour of single (armchair and zigzag direction) and bilayer layer graphene (AA and AB stacking). Adaptive intermolecular reactive bond order (AIREBO) potential function was used to describe the many-body short-range interatomic interactions for the single layer graphene sheet. Moreover, Lennard Jones model was considered for bilayer graphene to incorporate the van der Waals interactions among the interlayers of graphene. The effect of temperature on the strain energy of single layer and bilayer graphene was studied in order to understand the difference in mechanical behaviour of the two systems. The strength of the pristine single layer graphene was found to be higher as compared to bilayer AA stacked graphene at all temperatures. It was observed at 1073 K and in the presence of vacancy defect the strength for single layer armchair sheet falls by 30% and for bilayer armchair sheet by 33% as compared to the pristine sheets at 300 K. The AB stacked graphene sheet was found to have a two-step rupture process. The strength of pristine AB sheet was found to decrease by 22 % on increase of temperature from 300K to 1073K.

Keywords: Single layer graphene sheet, AA and AB stacked graphene sheet, Molecular Dynamics simulation, Temperature effect, Point defect effect.

1. Introduction

Graphene has attracted enormous interest among the researchers since its discovery [1-23], due to its amazing mechanical and electrical properties. This makes it a potential material for a wide range of applications. Experiments on the mechanical behaviour of graphene are restricted owing to the practical complications in designing experiments at nanoscale [3, 15–16]. Therefore, atomistic methods such as MD have been extensively used to study the mechanics of graphene [11, 17–23].