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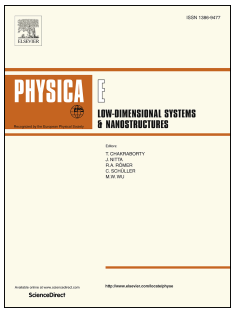

Studying the effects of longitudinal and transverse defects on the failure of hybrid graphene-boron nitride sheets: A molecular dynamics simulation

Kasra Einalipour Eshkalak, Sadegh Sadeghzadeh, Maisam Jalaly

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Studying the effects of longitudinal and transverse defects on the failure of hybrid graphene-boron nitride sheets: A molecular dynamics simulation

Kasra Einalipour Eshkalak, Sadegh Sadeghzadeh*, Maisam Jalaly

Nanotechnology Department, School of New Technologies, Iran University of Science & Technology (IUST), Narmak, Tehran, 16846-13114, Iran

*sadeghzadeh@iust. ac. ir

Abstract

At the nanoscale, various defects such as cracks and cavities can surely appear in the structure of 2D materials during their synthesis by the CVD technique. The formation of these flaws in nanomaterials can substantially alter their electrical, chemical and mechanical properties. In the present work, the effects of three types of crack defects (one along the armchair direction and two in the zigzag direction) on the mechanical properties of hybrid graphene-boron nitride (BN) nanosheets have been investigated. The obtained results indicate that hybrid nanostructures with longitudinal cracks display more desirable mechanical properties than those with the two types of transverse cracks. These greater mechanical properties can be attributed to the direction of tensile stress; when a crack in a nanostructure is aligned with the direction of tension, the defective nanostructure displays better mechanical properties. The various types of defects in a hybrid graphene-boron nitride nanostructure have a much lower effect on its Young's modulus value than its failure strength and strain. The effects of the size and location of the mentioned types of defects have also been studied. Finally, the effects of temperature and strain rate on the mechanical properties of defect-free hybrid graphene-boron nitride nanosheets and those with longitudinal cracks have been analyzed; and it has been demonstrated that in the presence of defects, the mechanical properties diminish with the rise of temperature and improve with the increase of strain rate.