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Explicit expressions describing elastic properties and buckling load of BN

nanosheets due to the effects of vacancy defects

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Abstract

In this study, effects of the presence of vacancy defects in a hexagonal nanosheet on Young's modulus, effective Poisson's ratio, buckling loads and buckling modes, regardless of its constituent atoms, have been studied. Explicit expressions are proposed in order to define these characteristics considering a defect distribution term as a modifying parameter. Molecular structural mechanics concepts and FEM simulation are utilized in order to obtain these expressions and results. Different sizes and shapes of defects as well as random distribution of vacancies have been considered. The results for perfect Boron Nitride, Silicon Carbide and graphene nanosheet as well as defected Boron Nitride nanosheets are in a good agreement with those available in literature. Linear degradation behavior of Young's modulus and linear increase of effective Poisson's ratio in terms of defects distribution are observed in obtained results. A second order behavior is also observed in decreasing buckling load in terms of increasing vacancy distribution. Moreover, buckling mode characteristics due to the percentage of defects distribution has been investigated.

Keywords: Boron nitride, Nano sheets, Vacancy defects, Elastic properties, Buckling load

1. Introduction

Boron Nitride (BN) nanotubes and nanosheets have been attracted lots of attention since the discovery of BN nanotubes through extensive local density function and quasi-particle calculations in 1994 [1] and synthesizing BN

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