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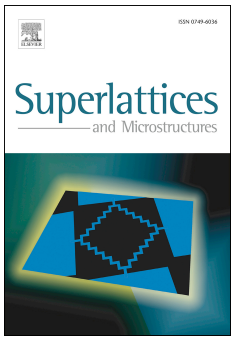

Effects of various defects on the mechanical properties of black phosphorene

Danh-Truong Nguyen, Minh-Quy Le, Van-Trang Nguyen, Thanh-Lam Bui

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Effects of various defects on the mechanical properties of black phosphorene

Danh-Truong Nguyen[1], Minh-Quy Le[1,*], Van-Trang Nguyen[1, 2], Thanh-Lam Bui[1, 3]

[1)] Department of Mechanics of Materials and Structures, School of Mechanical Engineering, Hanoi University of Science and Technology, No. 1, Dai Co Viet Road, Hanoi, Vietnam

[2)] Faculty of Mechanical Engineering, Thai Nguyen University of Technology, 3/2 street, Tich Luong ward, Thai Nguyen city, Vietnam

[3)] Faculty of Mechanical Engineering, Hanoi University of Industry, Number 298, Cau Dien Street, Bac Tu Liem Distric, Hanoi, Vietnam

Abstract – The present work investigates the effects of seven types of defects on the mechanical properties of black phosphorene. Molecular dynamics finite element method with Stillinger-Weber potential is used to simulate the uniaxial tensile tests of the pristine and defective black phosphorene sheets. Young's modulus, fracture stress, and fracture strain of the pristine and defective black phosphorene sheets are estimated. Comparison of the influence of different types of defects on the mechanical response of black phosphorene is considered. Fracture mechanism of various defective black phosphorene sheets is also analyzed. It is found that effect of the defects on Young's modulus of black phosphorene is insignificant. In contrast, due to defects fracture stress and fracture strain can reduce up to 53% and 69%, respectively. Results provide a landscape on the mechanical properties of defective black phosphorene and are useful for the design of nanodevices with black phosphorene in future applications.

Keywords: 2D material; Atomistic simulation; Phosphorene; Mechanical properties.

* Corresponding author: Tel. & fax: +84 .24. 38680103.

E-mail address: quy.leminh@hust.edu.vn