

Mechanical behavior of planar borophenes: A molecular mechanics study



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ABSTRACT

The aim of the present work is to provide numerical data regarding the in-plane tensile mechanical response of two-dimensional boron sheets known as borophene sheets or borophenes. The proposed theoretical approach is grounded in a molecular mechanics method which utilizes the equilibrium atomistic structure of the nanomaterials under investigation. In addition, it incorporates special spring-like finite elements to approximate the interatomic force field. The computational approach is mainly based on the modified Morse interatomic potential. Some of the relevant force field parameters concerning boron element are estimated according to the universal force field. Four different atomistic configurations of borophene monolayers are analyzed, i.e., an ideal perfect sheet exclusively made from regular triangular motifs, a sheet made from the ideal structure of the B36 molecule, a sheet known as “ α ” containing uniformly distributed regular hexagonal holes, and a sheet known as “ β ” having hexagonal holes distributed in lines. The four tested sheets are selected to have an almost square shape of the same size. Based on the computed tensile stress-strain curves, several mechanical properties along the zigzag and armchair directions are estimated. The Young’s modulus, Poisson’s ratio, tensile strength and failure strain of the borophenes are illustrated with respect to the hexagonal hole density. Comparisons are made where possible.

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1. Introduction

The field of two-dimensional (2D) nanomaterials has grown significantly over the last decade due to the requirement for new materials for specialized applications in nanotechnology [1]. Monolayer nanomaterials, due to their exceptional properties, have attracted most of the relevant research. The one-atom thick materials demonstrate a vast array of unique chemical and physical properties. Graphene, a single-layer sheet of carbon atoms arranged in a hexagonal pattern, has been on the list of the world changing materials for the last few years [2], mainly due to its superior mechanical behavior.

Boron due to its similar chemical nature with carbon is expected to play a significant role in the development of novel monolayer nanomaterials. It is now well known that boron may form bonds nearly as strong as carbon. It may develop with itself a variety of planar [3], quasi-planar [4,5], tabular [6] and spherical clusters [7]. Many of these boron based structures [8,9] have been found to present several interesting properties such as a significant mechanical strength, a very high melting point and a fully metallic

behavior. These unique characteristics of boron allotropes make them potentially useful in a variety of composite, high-temperature, energy and electronic applications in nanoscale.

Generally, few experimental studies associated with borophene sheets have been reported. The reason is that their laboratory synthesis is very difficult. The existence of planar boron has already been confirmed via photoelectron spectroscopy [4,10]. Recently, experimental evidence has been provided for the viability of novel boron nanostructures with hexagonal vacancies [11]. Specifically, the experimental isolation of the B36 molecule has been achieved. The specific molecule consists of 36 boron atoms which are triangularly arranged in a layer with a hexagonal hole in the middle. More recently, the synthesis of atomically thin boron sheets on silver surfaces has been experimentally confirmed [12,13].

The isolation of boron monolayers combined with their promising properties has motivated research in developing theoretical approaches for characterizing the crystalline order and basic material properties of borophenes. In this scientific effort, first principle calculations, mainly based on density functional theory (DFT), have been played the most significant role. Early ab initio studies have pointed out the remarkable structural stability of quasi-planar boron clusters [5,6]. A new class of stable, planar boron sheets, composed of triangular and hexagonal motifs, has been thoroughly

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analyzed by using DFT calculations [14–20]. Furthermore, the significant effect of the hexagonal hole density, also referred as vacancy concentration, on boron sheets has been investigated by several researchers via the DFT and the cluster expansion method [21,22]. In some very recent DFT based studies, the growth process [23], the optical behavior [24] and the metallic nature [3] of borophenes has been investigated. In other more focused ab initio works, the potential application of B36 borophene sheet as a sensor for HCOH [25] and the dissociative adsorption of ammonia onto its surface [26] has been explored. The mechanical properties of borophene such as tensile strength and critical strain have been also estimated using DFT [27]. Even though molecular dynamics (MD) method is commonly used for the investigation of 2D materials, very few are the reported MD simulations concerning borophenes. Characteristic relevant studies are associated with the feasibility of using borophene as an anode material for sodium-ion as well as sodium-oxygen batteries [28] and for lithium-ion batteries [29]. Very recently, the anisotropic in-plane tensile properties and structural stability of borophene sheets have been studied by using solely MD [30].

The characterization of the mechanical performance of borophenes is pre-required in order to advance their implementation in modern applications. However, the mechanical behavior of borophenes has not been studied to a very large extent [12,18,27,30]. Thus, new relevant evidence is required to establish better understanding of their performance. A computational efficient molecular mechanics (MM) method is formulated here, to approximate the characteristic anisotropic mechanical properties of flat borophenes.

Sheets of different structural configurations regarding the inner distribution and density of the hexagonal holes are investigated. To the author's best knowledge, this is the first attempt of adopting a MM numerical scheme to study the mechanical response of borophenes. The interactions between bonded boron atoms are represented via the nonlinear modified Morse potential [31] while specific force field parameters associated with boron are determined by the universal force field (UFF) model [32]. The bond length change and interbond angle bending interactions are simulated by utilizing appropriate line, spring-like finite elements. These elements interconnect appropriate boron atoms and are described by nonlinear stiffness matrices. Some comparisons between the present predictions and relevant mechanical property data found elsewhere are provided where possible.

2. Structural characteristics of investigated borophenes

Four borophene structures are analyzed in the present study. In order to describe effectively the atomistic geometry of the tested borophene sheets, it is convenient to define a hexagonal hole density parameter as [14]:

$$\eta = \frac{\text{No of hexagonal holes}}{\text{No of atoms in the perfect sheet version}} \quad (1)$$

The first borophene sheet under investigation consists exclusively from planar triangular boron lattices as Fig. 1a depicts while evidently corresponds to $\eta = 0$. The specific borophene sheet, hereafter

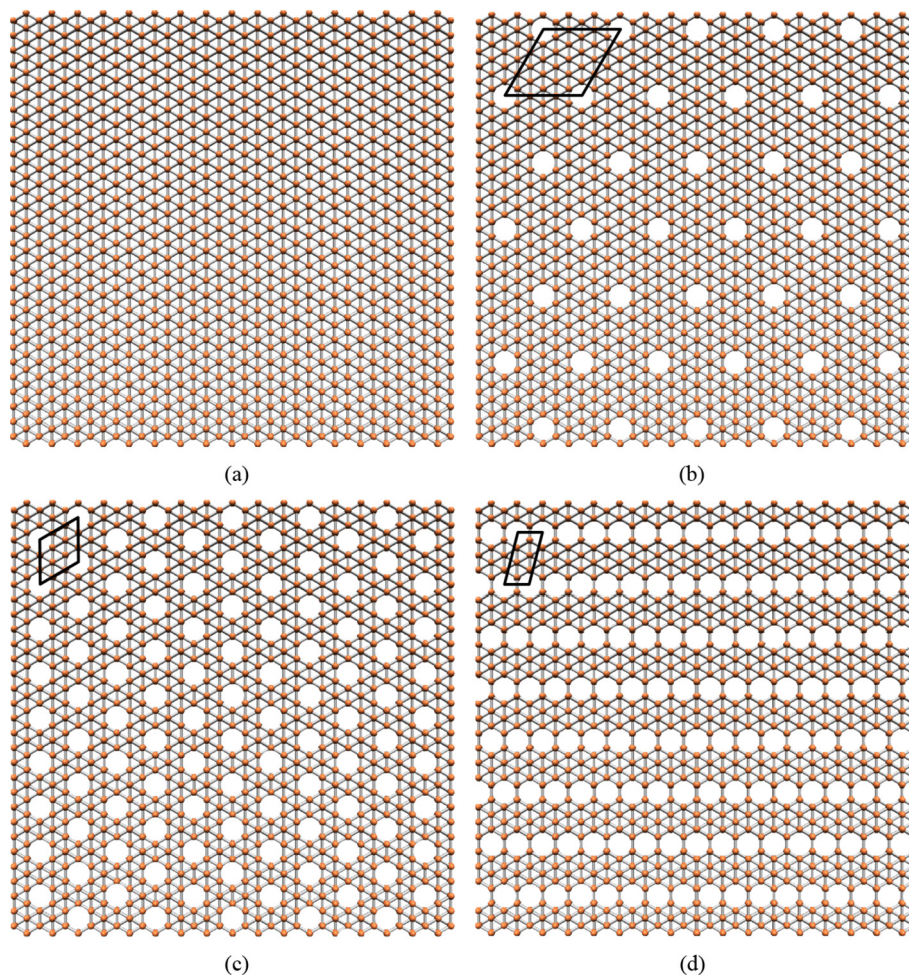


Fig. 1. Nanostructures of planar borophenes under investigation: (a) Perfect sheet, (b) B36 sheet, (c) α sheet, and (d) β sheet.

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