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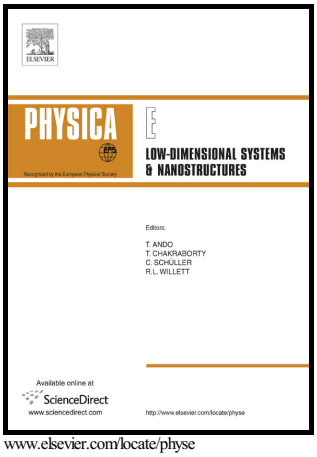

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Anomalous strain effect on the thermal conductivity of borophene: a reactive molecular dynamics study.

Bohayra Mortazavi[a,*], Minh-Quy Le[b], Timon Rabczuk[c], Luiz Felipe C. Pereira[d,*]

[a] *Institute of Structural Mechanics, Bauhaus-Universität Weimar, Marienstr. 15, D-99423 Weimar, Germany*
[b] *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*
[c] *College of Civil Engineering, Department of Geotechnical Engineering, Tongji University, Shanghai, China*
[d] *Departamento de Física, Universidade Federal do Rio Grande do Norte, Natal, 59078-970, Brazil*

Abstract

Borophene, an atomically thin, corrugated, crystalline two-dimensional boron sheet, has been recently synthesized. Here we investigate mechanical properties and lattice thermal conductivity of borophene using reactive molecular dynamics simulations. We performed uniaxial tensile strain simulations at room temperature along in-plane directions, and found 2D elastic moduli of 188 N m^{-1} and 403 N m^{-1} along zigzag and armchair directions, respectively. This anisotropy is attributed to the buckling of the borophene structure along the zigzag direction. We also performed non-equilibrium molecular dynamics to calculate the lattice thermal conductivity. Considering its size-dependence, we predict room-temperature lattice thermal conductivities of 75.9 ± 5.0 W m^{-1}K^{-1} and 147 ± 7.3 W m^{-1}K^{-1}, respectively, and estimate effective phonon mean free paths of 16.7 ± 1.7 nm and 21.4 ± 1.0 nm for the zigzag and armchair directions. In this case, the anisotropy is attributed to differences in the density of states of low-frequency phonons, with lower group velocities and possibly shorten phonon lifetimes along the zigzag direction. We also observe that when borophene is strained along the armchair direction there is a significant increase in thermal conductivity along that direction. Meanwhile, when the sample is strained along the zigzag direction there is a much smaller increase in thermal conductivity along that direction. For a strain of 8% along the armchair direction the thermal conductivity increases by a factor of 3.5 (250%), whereas for the same amount of strain along the zigzag direction the increase is only by a factor of 1.2 (20%). Our predictions are in agreement with recent first principles results, at a fraction of the computational cost. The simulations shall serve as a guide for experiments concerning mechanical and thermal properties of borophene and related 2D materials.

1. Introduction

Boron presents a wealth of possible two-dimensional (2D) allotropes, and boron sheets exhibit various structural polymorphs containing mostly hexagonal and triangular lattices [1, 2, 3, 4, 5, 6]. Low-buckled borophene sheets in the form of triangular lattices have been predicted years ago [1, 7], and have recently been synthesized on Ag substrates [5]. Electronic, magnetic, mechanical and optical properties of triangular boron sheets have recently been investigated by first-principles calculations [8, 9]. These 2D boron sheets, so-called borophene, were even predicted to exhibit superconductive behavior [10]. Recent first-principles calculations confirmed that borophene sheets can serve as an ideal anode electrode material with high electrochemical performance for Mg, Na, and Li ion batteries, which outperform other 2D materials [11]. These outstanding physical properties of borophene place it as a direct rival for graphene in a serie of applications [12, 13, 14]. Nevertheless, in spite of the promising applications of borophene, studies related to its thermal and mechanical properties at finite temperatures are still very limited. In particular, the thermal conductivity of borophene films remained almost unexplored.

*Corresponding authors
Email addresses: bohayra.mortazavi@gmail.com (Bohayra Mortazavi), pereira@fisica.ufrn.br (Luiz Felipe C. Pereira)