Crystal structure and properties of thin 1D boron structures

Nevill Gonzalez Szwacki

Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland

Nanowires are being studied as mechanical components for a range of potential devices. Both crystalline and amorphous boron nanowires have been synthesized with diameters from several to hundreds of nanometers and exhibit promising properties as sensor materials [1].

We review our recent work on the structure prediction and properties of boron 1D periodic structures using a density functional theory (DFT) based genetic algorithm (GA) approach [1]. We focus our attention on the structure of thin 1D boron structures given the lack of previous experimental and theoretical work on this topic. Based on our simulations, we have identified three groups of structures: stripes with triangular motifs, nanowires with an open quasitubular shape, and regular nanowires. The binding energies of the structures are plotted in Fig. 1 as a function of the number of atoms in the simulation unit cell. The most stable thin structures are fully planar stripes with boron triangular motifs. However, thicker stripes tend to form tubular-like structures that can be viewed as precursors of nanotubes [2] or nanowires. Several 1D structures are more stable than the boron 2D honeycomb sheet. High metallic character is the usual property of borophenes (2D boron crystals). We show that the thinnest 1D boron nanostructures are also metallic.

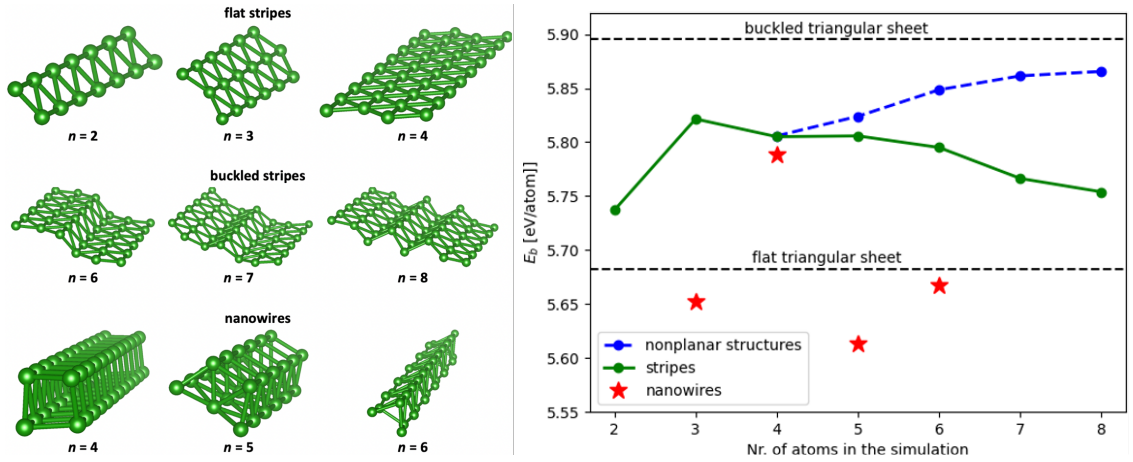

Figure 1: The structure of boron stripes with triangular motifs, nanowires with an open quasitubular shape, and regular nanowires (left). Binding energies of the 1D structures plotted as a function of the number of atoms in the simulation unit cell (right).

The work is supported by the National Science Centre, Poland, through project UMO-2021/43/O/ST3/03280. The use of supercomputers at ICM (University of Warsaw) is also acknowledged.

[1] T. Tarkowski and N. Gonzalez Szwacki, Solid State Sciences **142**, 107241 (2023).

[2] T. Tarkowski and N. Gonzalez Szwacki, Crystals **13**, 19 (2022).