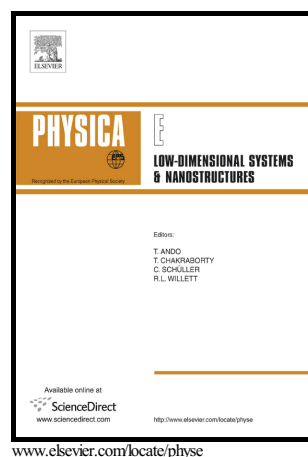


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PII: S1386-9477(16)30867-0
DOI: <http://dx.doi.org/10.1016/j.physe.2016.12.003>
Reference: PHYSE12677

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

Received date: 11 August 2016
Revised date: 22 November 2016
Accepted date: 5 December 2016

Cite this article as: A. Tapia, C. Cab, A. Hernández-Pérez, C. Villanueva, F. Peñuñuri and F. Avilés, The bond force constants and elastic properties of boron nitride nanosheets and nanoribbons using a hierarchical modeling approach *Physica E: Low-dimensional Systems and Nanostructures* <http://dx.doi.org/10.1016/j.physe.2016.12.003>

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The bond force constants and elastic properties of boron nitride nanosheets and nanoribbons using a hierarchical modeling approach

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Abstract

A hierarchical approach bridging the atomistic and nanometric scales is used to compute the elastic properties of boron nitride nanosheets and nanoribbons, examining the effect of sheet size, aspect ratio and anisotropy. The approach consists in obtaining the bond force (force field) constants by dedicated computations based on density functional theory (DFT) and using such constants as input for larger scale structural models solved by finite element analysis (FEA). The bond force constants calculated by DFT are 616.9 N/m for stretching, 6.27×10^{-19} Nm/rad² for in-plane rotation and 1.32×10^{-19} Nm/rad² for dihedral rotation. Using these constants, the elastic properties of boron nitride nanosheets and nanoribbons predicted by FEA are almost independent of the sheet size, but strongly dependent on their aspect ratio. The sheet anisotropy increases with increased aspect ratio, with nanoribbons of aspect ratios of 10 exhibiting a ratio of elastic moduli along both in-plane directions of 1.7.

Keywords: Boron nitride; nanosheets; nanoribbons; elastic properties; density functional theory; finite element analysis; bond force constant.

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