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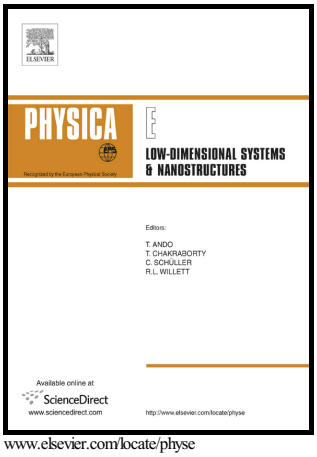

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The bond force constants and elastic properties of boron nitride nanosheets and nanoribbons using a hierarchical modeling approach

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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/rad^2 for in-plane rotation and 1.32×10^{-19} Nm/rad^2 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.