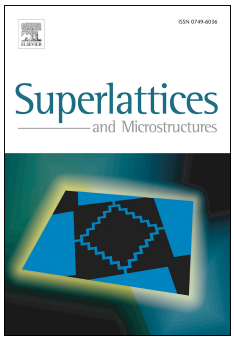
Accepted Manuscript



Effect of ripples on the finite temperature elastic properties of hexagonal boron nitride using strain-fluctuation method

Siby Thomas, K.M. Ajith, M.C. Valsakumar

PII: S0749-6036(17)31439-8

DOI: 10.1016/j.spmi.2017.06.051

Reference: YSPMI 5100

To appear in: *Superlattices and Microstructures*

Received Date: 12 June 2017

Revised Date: 14 June 2017

Accepted Date: 14 June 2017

Please cite this article as: S. Thomas, K.M. Ajith, M.C. Valsakumar, Effect of ripples on the finite temperature elastic properties of hexagonal boron nitride using strain-fluctuation method, *Superlattices and Microstructures* (2017), doi: 10.1016/j.spmi.2017.06.051.

Effect of ripples on the finite temperature elastic properties of hexagonal boron nitride using strain-fluctuation method

Siby Thomas [1], K M Ajith *[1] and M C Valsakumar[2]

[1] *Computational Physics Lab, Department of Physics, National Institute of Technology Karnataka (NITK), Surathkal, Mangalore, India - 575025.*

[2] *Department of Physics, Indian Institute of Technology Palakkad (IIT-PKD), Ahalia Campus, Kozhipara, Palakkad, Kerala, India - 678557.*

Abstract

This work intents to put forth the results of a classical molecular dynamics study to investigate the temperature dependent elastic constants of monolayer hexagonal boron nitride (h-BN) between 100 and 1000 K for the first time using strain fluctuation method. The temperature dependence of out-of-plane fluctuations (ripples) is quantified and is explained using continuum theory of membranes. At low temperatures, negative in-plane thermal expansion is observed and at high temperatures, a transition to positive thermal expansion has been observed due to the presence of thermally excited ripples. The decrease of Young's modulus, bulk modulus, shear modulus and Poisson's ratio with increase in temperature has been analyzed. The thermal rippling in h-BN leads to strong anharmonic behaviour that causes large deviation from the isotropic elasticity. A detailed study shows that the strong thermal rippling in large systems is also responsible for the softening of elastic constants in h-BN. From the determined values of elastic constants and elastic moduli, it has been elucidated that 2D h-BN sheets meet the Born's mechanical stability criterion in the investigated temperature range. The variation of longitudinal and shear velocities with temperature is also calculated from the computed values of elastic constants and elastic moduli.

Keywords: Hexagonal boron nitride, strain-fluctuation, molecular dynamics, ripples, anharmonicity, elastic constants

Email address: sibythomas1989@gmail.com, ajith@nitk.ac.in, valsa@iitpkd.ac.in (Siby Thomas [1], K M Ajith *[1] and M C Valsakumar[2])