

Thermo-mechanical properties of boron nitride nanoribbons: A molecular dynamics simulation study



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ABSTRACT

Thermo-mechanical properties of boron nitride nanoribbons (BNNRs) were computed using molecular dynamics simulation with optimized Tersoff empirical potential. Thermal conductivity (TC) and heat transport properties of BNNRs were calculated as functions of both temperature and nanoribbon's length. The results show that TC of BNNRs decreases with raising temperature by $T^{-1.5}$ up to 1000 K. The phonon-phonon scattering relaxation time, mean free path of phonons, and contribution of high frequency optical phonons in TC of BNNRs were calculated at various temperatures. TC decreases as nanoribbon size increases and it converges to $\sim 500 \text{ W m}^{-1} \text{ K}^{-1}$ for nanoribbons with length longer than 30 nm. The mechanical properties, including Gruneisen parameter, stress-strain response curves, Young's modulus, intrinsic strength, critical strain, and poisson's ratio were calculated in the temperature range of 137–1000 K. The simulation results show that Gruneisen parameter and poisson's ratio of BNNRs are -0.092 and 0.245 , respectively. The Young's modulus of BNNRs decreases with raising temperature and its value is 630 GPa at 300 K. According to the results, BNNRs duo to their extraordinary thermo-mechanical properties, are the promising candidate for the future nano-device manufacturing.

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1. Introduction

Evaluation of thermo-mechanical properties of nanostructure materials is one the hottest topics in materials science domain [1–7]. Especially, the promising performance of carbon-based structures has stimulated strong interest in isomorphous materials based on boron nitride (BN) [8]. BN is a chemical compound, consisting of equal numbers of boron (B) and nitrogen (N) atoms, which is not found in nature and is produced in the lab [9]. Boron nitride is similar to carbon in having three crystalline structures: a layered hexagonal structure (h-BN) which is similar to that of graphite, the cubic zinc-blende structure (c-BN), analogous to that of diamond, and a rare hexagonal wurtzite structure (wBN) corresponding to lonsdaleite [10]. Its bulk phase (often called white graphite) with weak inter-layer bonding permits separation into individual sheets of white graphene [11]. h-BN sheet is isoelectronic and isomorphous to the graphene honeycomb lattice. Specifically, single layer h-BN is a one-atom-thick material composed of a hexagonal network with an equal number of alternating B and N atoms in sp^2 hybridization that are bonded covalently [12]. The crystallographic parameters of

h-BN and graphite are almost equal. The in-plane lattice constants are 2.46 Å and 2.50 Å for graphite and h-BN, respectively. The inter-layer distances are also similar: 3.35 Å and 3.33 Å for graphite and h-BN, respectively [13].

Owing to the geometric similarity, h-BN has many excellent physical properties analogous to graphene, such as strong mechanical properties, good thermal conductivity and high chemical and thermal stability [14,15]. Of course, h-BN possesses numerous unique properties quite different from those of graphene. For example, h-BN exhibits intrinsic half-metallicity without any external electronic field modulation. The outstanding properties have gradually induced the research on h-BN to become one of the hottest spots in the nanoscience [15].

h-BN, like graphene for carbon-based materials, is the building block of many other low dimensional structures such as boron nitride nanotubes (BNNTs), boron nitride fullerenes, and boron nitride nanoribbons (BNNRs) [16,17]. BNNR is a narrow strips of h-BN sheet with few of nanometers in width (typically < 20 nm) [18]. BNNRs exhibit similar mechanical, thermal, and thermochemical properties to graphene nanoribbons (GNRs). On the other hand, BNNRs also possess prominent electronic, optical, and magnetic properties qualitatively different from those of GNRs arising from various edge structures and terminations [19]. BNNRs also exhibit the semiconductor behavior independence of the edge shapes, and their energy gap can be adjusted efficiently by altering the rib-

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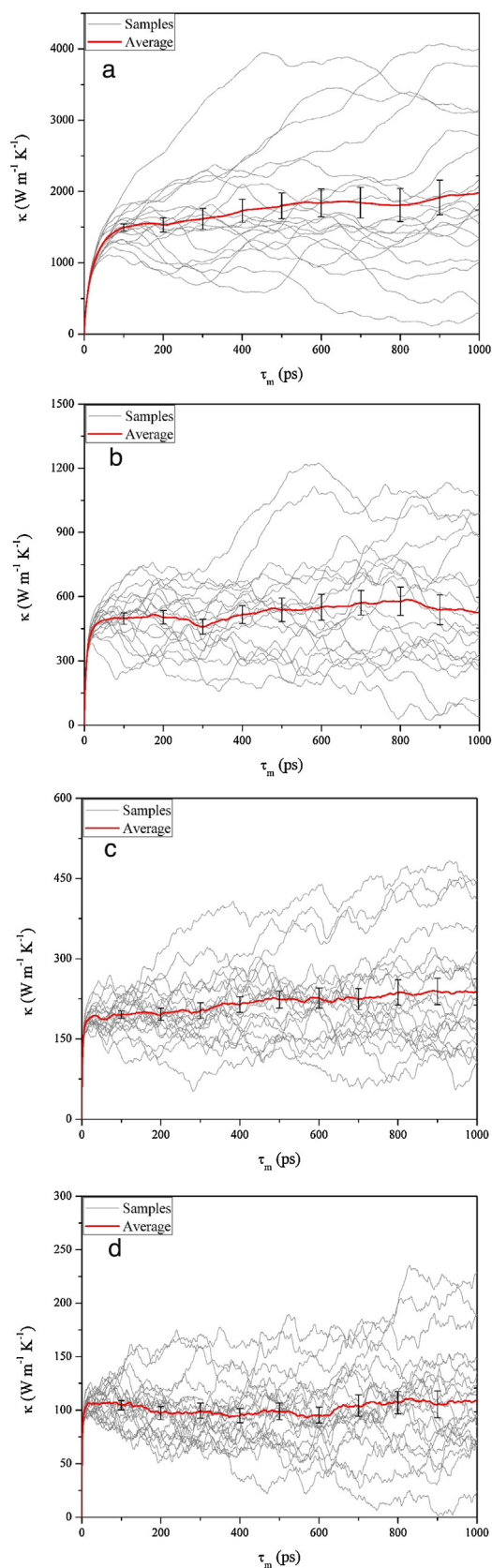


Fig. 1. Averaged TC curves (red thick line) of BNNR from twenty independent *NVE* ensembles (grey thin lines): (a) 137, (b) 300, (c) 600, (d) 1000 K. The standard error on mean is presented as error bar. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

bon width, applying external tensile strain, and/or using external electric field [20]. The properties are of great fundamental interest and also have implications for applications within various fields including spintronics and optoelectronics [19].

The preparation of such high aspect ratio nanosheets with narrow widths in BNNRs is quite challenging. To date, only a couple of approaches that use BNNTs as the starting material are currently available. In the first method, Ar plasma etching of BNNTs imbedded within a polymer was used [21]. This method will produce BNNRs with widths as narrow as 15 nm and lengths up to a few micrometre. The plasma treatment conditions could be tailored to controllably form BNNRs with defined ranges of layers down to a single sheet. In the second approach, Erickson et al. [19] found that the intercalation of vaporized potassium metal into BNNT walls was efficient enough to induce longitudinal splitting of BNNTs. High aspect ratio and few-layered BNNRs were obtained with lengths over 1 μm , widths between 20 and 50 nm, and thickness between 2 and 10 layers. Authors claimed that this route is a bulk process and might potentially be scalable if an effective purification/separation procedure could be established.

Several applications of BNNRs in thermal/mechanical nano-devices are due to their extraordinary thermo-mechanical properties. Unlike GNRs [22], limited work have been published on the transport [8,15,20,23–27] and mechanical [28–31] properties of BNNRs. Therefore, the aim of the present work is to deeply study the thermo-mechanical properties of BNNRs. For this purpose, the temperature and size dependences of thermal conductivity of BNNRs are evaluated using equilibrium molecular dynamics (EMD) simulation based on Green–Kubo (GK) method. Besides, the mechanical properties of BNNRs are studied as a function of temperature.

2. Simulation details

All simulations were performed using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) molecular dynamics code [32]. The accurate description of phonon dispersion, corresponding group velocities, and equations of state are critically important to study the thermo-mechanical properties of BNNRs. In this study, a recently optimized Tersoff potential which gives very accurate results for dynamical, mechanical, and thermal transport properties of BN nanostructures [1,8] is used.

2.1. Thermal properties

BNNRs used in the present study had a fixed 2 nm in width and different lengths of 2–50 nm. The temperature dependence of TC was also investigated by changing the temperature from 137 K up to 1000 K. The minimum value of temperature in this study ($\frac{1}{3}T_D \approx 137$ K) was chosen according to the Debye temperature, T_D , of h-BN (410 K) [33]. In our previous work, we explained in details the quantum corrections for temperature of GNR [22].

The velocity Verlet algorithm was applied to integrate the equations of motion with a fixed time step of 1 fs. The periodic boundary conditions (PBC) were applied in all three directions. All simulations were initially run for 2 ns in *NPT* ensemble (Nose–Hoover thermostat and barostat) at zero pressure and desired temperature to reach the equilibrium and then switched to *NVE* ensemble for 10 ns. The heat current was calculated after 5 ns for every 10 fs. The heat current autocorrelation function (HCACF) was calculated with correlation length (τ_m) of 1 ns. Then, the last HCACF was used to calculate the thermal conductivity (TC) using GK formalism [22]. For more information about the methodology, see the supporting information. Finally, a converged and reliable value for TC was calculated as the ensemble average of independent twenty *NVE*

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