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# Tensile behavior of gallium nitride monolayer via nonlinear molecular mechanics

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ABSTRACT

The aim of the present study is the numerical prediction of the mechanical behavior of the hexagonal gallium nitride (GaN) monolayer. For this purpose, a nonlinear molecular mechanics (MM) method is developed and proposed which is based on the use of three-dimensional (3d) non-linear, spring-like, finite elements, capable of representing appropriately the interatomic interactions between the atoms of the nanomaterial. In order to establish the constitutive equations of the utilized finite elements, the Stillinger-Weber potential is adopted, which may approximate both two-body (2b) as well as three-body (3b) interatomic interactions via appropriate nonlinear functions of the bond length and the interbond angle, respectively. According to the proposed MM formulation, square-shaped, single-layered, hexagonal GaN sheets of several sizes are modelled and tested under tensional loadings in both in-plain directions to compute corresponding effective mechanical properties such as Young's modulus, Poisson's ratio, tensile strength, failure strain and fracture toughness. The numerical results are compared with other estimations which are available from the literature, where possible.



## 1. Introduction

Extensive interest has been recently devoted to the study of the GaN-based nanomaterials due to their remarkable electronic (Moradian et al., 2008; Wang et al., 2009), optic (Shokri and Ghorbani Avaresi, 2013) and electrochemical properties (Chakrapani, 2015). GaN, like carbon and boron nitride, is expected to be capable of forming interesting allotropes. GaN nanotubes (GaNNTs) have been already discovered and produced. In the near future, special GaN allotropes are expected to be key materials for high-power, high-frequency and electronic devices such as light-emitting diodes (LEDs).

The synthesis of GaN based media has attracted the interest of many researchers due to their potential to be used in a variety of applications (Li et al., 2015). Hu et al. (2003) have achieved the creation of crystalline GaNNTs in bulk by a two-stage process based on the well-controllable amorphous gallium oxide nanotube conversion. Goldberger et al. (2003) have reported the successful formations of hexagonal cross-sections of single crystalline GaNNTs of various diameters utilizing an 'epitaxial casting' approach. Han et al. (1997) have prepared GaN nanorods through a carbon nanotube-confined reaction. Xing et al. (2009) have synthesized Zn-doped GaNNTs with zigzag morphology by a chemical vapor deposition method. Jiang et al. (2013) have prepared large-area porous single crystal GaN micro/nanotube arrays by a simple method using zinc oxide arrays as the template. Suresh et al (Suresh Kumar et al., 2008) have grown GaN nanocrystals on the tip of aligned carbon nanotubes (CNTs) substrate by chemical vapor transport method. Yan et al. (2009a) have demonstrated the growth of GaN nanowires by metal organic chemical vapor deposition with CNTs as templates. Finally, Lin et al. (2010) have demonstrated the first example of the use of NiI 2-filled CNTs for the synthesis of GaN nanowires.

Many theoretical studies have been conducted in the effort to characterize the behavior of the GaN nanomaterials targeting mainly on their opto-electrochemical properties (Moradian et al., 2008; Wang et al., 2009; Shokri and Ghorbani Avaresi, 2013;

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Chakrapani, 2015) and their formation (Hao et al., 2006; Yan et al., 2009b). However, fewer are the theoretical approaches involving the contribution of their mechanical performance. Jeng et al. (2004) have adopted a classical molecular dynamics (MD) simulation with the realistic Tersoff many-body potential model to investigate the mechanical properties of GaNNTs. Wang et al. (2006, 2008a) have investigated the mechanical properties of wurtzite-type single-crystalline GaNNTs under applied tensile strains via MD methods with a Stillinger-Weber potential while in a similar attempt they have studied the tensile behavior of GaN nanowires (Wang et al., 2007). Wang et al. (2008b) have investigated the tensile mechanical behavior of GaNNTs under combined tension-torsion using MD simulations with an empirical potential. More recently, Wang et al. (2008c) have investigated the buckling responses of single-crystalline GaNNTs under torsion using an MD simulation based on a Stillinger–Weber potential. Zhang and Meguid (2015) have studied, analytically and numerically via MD simulations, the piezoelectric potential of strained intrinsic GaNNTs. Lastly, Kumar et al. (2015a) have studied the elastic properties of GaN nanotubes using the second generation REBO potential by Brenner and co-workers.

Since the production of various GaN based nanostructures and especially GaNNTs has been already accomplished, the fabrication of single layers of hexagonal GaN is considered feasible. However, despite the fact that extensive theoretical research has been made on GaNNTs mainly by utilizing MD simulations, the hexagonal GaN monolayer has not been explored to the same extent. Peng et al. (2013) as well as Sahin et al. (Sahin et al., 2009). have investigated the mechanical properties of graphene-like hexagonal GaN nitride monolayer using first-principles calculations based on density functional theory (DFT). Sharma et al. (Sarma et al., 2013) have performed classical MD simulations by employing the Stillinger-Weber potential on a system of single layer nanosheet of GaN containing single and double atomic vacancy defects. Last but not least, Kumar et al. (2015b) have calculated the frequencies of various motions of hexagonal GaN sheets and GaNNTs using simple 6-exponential potential between gallium and nitrogen atoms.

In the present study an atomistic finite element approach which is based on the use of 3d axial and torsional springs is developed for the simulation of the tensile response of hexagonal GaN monolayer. The tested GaN sheets are treated as frames of point and line spring-like, two-noded, finite elements of six translational degrees of freedom per node. In order to approximate the appearing forces and deformations within the nanostructure, a Stillinger-Weber potential (Stillinger and Weber, 1985; Lei et al., 2006) is adopted which describes effectively both 2b and 3b interatomic interactions. To describe appropriately the interatomic interactions, the one-to-one mapping is adopted within the atomic system. This leads to the use of a triple node at each atomic position which increases the computational cost. However, the present MM modelling technique provides realistic coupling of the degrees of freedom between different atomic positions while remains computationally attractive in comparison with other MD based schemes, since it does not require calculations over time. In addition, even though static MM methods do not include the effect of thermal motion, they have been proved to be efficient in estimating nanomechanical properties (Liu et al., 2008). Several sizes of almost squared-shaped GaN monolayers are tested under tensile loadings along both in-plain directions in order to demonstrate the nanosize and chirality effect on their mechanical properties. Indicative solutions from other studies are presented for comparison reasons. The computational material characterization involves only perfect sheets given that during nanostructural design, defect-free nanocomponents are naturally chosen despite the production difficulties and limitations. However, it should be mentioned that the proposed scheme may straightforwardly treat different kinds of defects due to its modelling simplicity.

## 2. Molecular mechanics formulation

The static MM approaches are now well established (Liu et al., 2008). Furthermore, the MM methods have already proved their efficiency to simulate the mechanical behavior of different tabular (Zhang et al., 2002) as well as planar (Georgantzinos et al., 2011) nanomaterials regardless of the incorporated molecular potentials. Numerous comparisons with various experimental and other theoretical data have proved the stable performance of the MM methods (Liu et al., 2008; Zhang et al., 2002; Georgantzinos et al., 2011). However, concerning the hexagonal GaN monolayer limited theoretical works may be found in the literature (Peng et al., 2013; Sahin et al., 2009; Sarma et al., 2013), mainly due to the inefficient reported relevant interatomic potentials. In the present study a spring based MM method, which uses a Stillinger-Weber potential model parameterized for GaN interactions, is applied for the first time to provide new material property evidence for the GaN monolayer, giving prospects for further future evaluation.

### 2.1. Stillinger-Weber potential energy

According to the Stillinger-Weber model (Stillinger and Weber, 1985), the total potential energy $U_{\text{tot}}$ within a hexagonal GaN monolayer may be expressed as a sum of 2b and 3b interatomic interaction terms as:

$$U_{\text{tot}} = \sum U_r + \sum U_\theta \tag{1}$$

where $U_r$ is the potential energy between two bonded atoms $i$, $p$ due to a change of the bond length $r_{ip}$ from the equilibrium bond length $r_0$ to the changed length $r_0 + \Delta r$ while $U_\theta$ is the potential energy between two linked bonds $ip$, $iq$, of the lengths $r_{ip}$ and $r_{iq}$, respectively, due to a change of the interbond angle $\theta_{piq}$ from the equilibrium inerbond angle $\theta_0$ to the modified angle $\theta_0 + \Delta\theta$.

The interatomic potentials $U_r$ and $U_\theta$, respectively, may be expressed as (Lei et al., 2006):

$$U_r = A\left[B\left(\frac{\sigma}{r_{ip}}\right)^4 - 1\right]\exp\left(\frac{\sigma}{r_{ip} - b\sigma}\right) \tag{2}$$

$$U_\theta = \lambda \exp\left(\frac{\gamma\sigma}{r_{ip} - b\sigma} + \frac{\gamma\sigma}{r_{iq} - b\sigma}\right)\left(\cos\theta_{piq} + \kappa\right)^2 \tag{3}$$

In the above equations the Ga-N bond parameters $A$, $B$, $\sigma$, $b$, $\lambda$ and $\gamma$ are taken equal to 2.801 nN × nm, 0.694, 0.17 nm, 1.8, 10.342 nN × nm and 1.2, respectively (Lei et al., 2006). Finally the parameter $\kappa$ is set equal to −0.5 so that the potential favors bond configurations with the desired ideal hexagonal geometry. Fig. 1 illustrates the variation of the potential function $U_r$ with respect to the bond length $r_{ip}$, which presents a minimum at the equilibrium length $r_0 = 0.1949$ nm. In addition, the variation of the potential term $U_\theta$ with the interbond angle $\theta_{piq}$ for $r_{ip} = r_{iq} = r_0$ is presented in Fig. 2. As observed, the specific potential function is minimized at the equilibrium interbond angle values $\theta_0 = \pm 2\pi/3$.