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Editor's Choice

Mechanical responses of pristine and defective C_3N nanosheets studied by molecular dynamics simulations

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ABSTRACT

The purpose of this study is to investigate the mechanical properties of a new two-dimensional graphene like material, crystalline carbon nitride with the stoichiometry of C_3N. The extraordinary properties of C_3N make it an outstanding candidate for a wide variety of applications. In this work, the mechanical properties of C_3N nanosheets have been studied not only in the defect-free form, but also with critical defects such as line cracks and notches using molecular dynamics simulations. Different crack lengths and notch diameters were considered to predict the mechanical response at different temperatures under the uniaxial tensile loading. Our simulation results show that larger cracks and notches reduce the strength of the nanosheets. Moreover, it was shown the temperature rise has a weakening effect on the tensile strength of C_3N. Our study can provide useful information with respect to the thermo-mechanical properties of pristine and defective graphene like C_3N 2D material.

1. Introduction

Single layered materials, so-called two dimensional (2D) materials have captured the interest of researchers of different fields since the isolation of graphene from graphite reported in 2004 [1–5]. Graphene is among the lightest and strongest materials with unique mechanical and thermal properties and therefore has been used in numerous applications [6–8]. Graphene can withstand a tensile strength of 130.5 GPa which is hundred times of the strength of high strength metals [9]. In-plane mechanical properties of graphene are much better than those for diamond [10]. Graphene has shown the highest measured thermal conductivity among all the materials ever known [11]. Due to the exceptionally high strength, thermal conductivity and light weight, graphene has been widely employed in the fabrication of advanced polymer composites with enhanced mechanical and thermal conduction properties [12–23]. Graphene has an extremely high ratio of surface area to mass [24] which makes it ideal for energy conversion and storage [25]. Furthermore, it is suitable in super-capacitors as conductive plates [26]. Such a super-capacitor can store more energy per unit volume than all other types of capacitors. The graphene's fascinating properties can be tailored for the special applications such as nanoelectronics, mechanical robust components, optoelectronics, thermal management systems, energy storage and energy conversion [27]. The surface of the graphene can be modified by the foreign atoms such as nitrogen and oxygen which can be used to modify the properties [28,29]. However, graphene as a semimetal has a zero band gap which makes it difficult to be used in electronic circuits as a transistor [30]. Semiconductors can carry the electrical charge when excited by an external thermal or electrical field. The zero band gap in graphene can be modified by the chemical doping or fabrication of 2D heterostructures in which another 2D materials are used [31–36].

Recently a new 2D material with the stoichiometry of C_3N has been fabricated by polymerization of diaminophenazine. The nitrogen atoms are uniformly distributed in the structure of the pristine C_3N which is analogous to graphene [37]. The 2D polyaniline C_3N shows the characteristics of a semiconductor with a small band gap [38]. Hence, it can solve the limitation of graphene which has zero band gap. It has been shown that monolayer C_3N has a band gap of 1.09 eV and is an indirect semiconductor [39]. The surface of the pristine C_3N can be engineered through functionalization with nonmetallic and semimetallic elements. The adsorption of foreign adatoms can tune further properties of C_3N [40]. Ab inito molecular dynamics simulation show that C_3N can be stable at a temperature up to 4000 K. Density functional theory (DFT) calculations showed C_3N as an extremely stiff material with a Young's modulus of 1090 GPa [38].

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The properties of the newly synthesized graphene like C_3N have not been entirely explored. There exists only limited research on the mechanical characteristics of C_3N and to the best of our knowledge the effects of defects and temperature on the mechanical properties have not been explored so far. As a common fact, in the commercially available materials there exist always defects in various forms. These defects can drastically reduce the ultimate tensile strength of the material [41–44]. Therefore, it is critical to study the mechanical properties of the materials in presence of defects such as cracks and notches [45–47]. The temperature effect on the properties of the C_3N is also a very worthy issue to be explored since it withstands high temperatures up to 4000 K. In the current study, we investigate the mechanical properties of the C_3N with defects such as cracks and notches. We study the propagation of the crack and notch for different crack lengths and different notch diameters at different temperatures up to 900 K. The comprehensive insight provided by this study can be very useful for the design of nano-devices employing the semiconducting C_3N nanosheets.

2. Molecular dynamics modelling

Classical molecular dynamics simulations were used to predict the mechanical properties of C_3N nanosheets with various cracks and notches. The molecular dynamics simulations were performed with the open-source software of LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [48]. The optimized Tersoff potential was used to define the carbon atoms interactions [49]. The Tersoff potential parameters for the nitrogen-carbon atoms interactions were taken from the work of Kinarci et al. [50]. The post processing of the results were performed through the open-source visualization software called OVITO [51]. The calculated stresses, strains, and the atomistic positions through the uniaxial tension were recorded. The top-view of the single layer C_3N is illustrated in Fig. 1. Each nitrogen atom is surrounded by three carbon atoms in a hexagonal network through strong polar covalent bonds. This structure is very similar to graphene and one can imagine the nitrogen atoms are doped in the graphene structure and occupy the place of carbon atoms in pristine graphene in a regular layout.

Similarly to graphene, monolayer C_3N has two major orientations of armchair and zigzag. The mechanical properties of pristine C_3N nanosheets under uniaxial tension loading were calculated. The simulations were performed for a nanosheet which contains 33,600 atoms. The boundary conditions are periodic along the in-plane directions. First, the simulation box was relaxed via Nosé-Hoover barostat and thermostat (NPT) method to obtain a stress free condition for the model. Then, a strain rate of 10^8 s^{-1} with time step size of 0.25 fs was applied in the MD simulations. In order to avoid the void formation during the simulation process, the atomic positions were remapped according to the size of the simulation box. The stress in values were calculated based on Virial theorem at each time step [52]. The calculated stresses for all atoms were averaged over the time steps of the simulation. To provide the uniaxial loading condition, the periodic simulation box along the structure width was adjusted using the NPT method to ensure negligible stress in this direction [53,54].

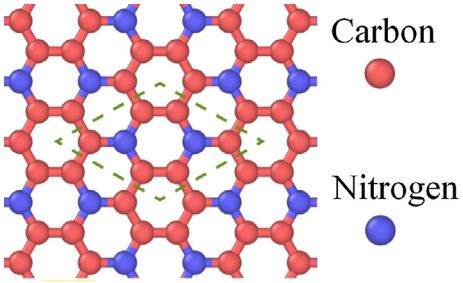

Fig. 1. Atomic layout of C_3N with a honeycomb structure including both carbon and nitrogen atoms. Each nitrogen atom is surrounded by three carbon atoms. The unit cell is shown in the structure of C_3N that contains two nitrogen atoms and six carbon atoms.

3. Results and discussion

In the current study, the molecular model was verified by comparison with molecular dynamics simulation results of Mortazavi [38]. At a temperature of 300 K, the nanosheet showed an ultimate tensile strength of 128 GPa in armchair direction and 125 GPa in zigzag direction. These results agree well to those reported in [38]. A pristine nanosheet with dimensions of 300 × 300 Å was used to study the influence of the temperatures (200, 300, 500, 700, and 900 K). Since the applied boundary conditions were periodic and we constructed a large super-cell, the acquired results are convincingly size independent. The models were stretched in the zigzag orientation and the resulting stress-strain curves of the pristine C_3N nanosheet is depicted in Fig. 2. It is worthy to note that in the stress calculations, we considered the volume of the structure using a thickness of 3.2 Å [38] for the single-layer C_3N.

At higher temperatures, the ultimate tensile strength decreases which in turn also decreases the modulus of elasticity as the temperature rises. At 300 K, the ultimate stress is 128 GPa at a strain of 0.17. The tensile stress is 82 GPa when the temperature is increased to 900 K which is about 36% lower than the ultimate stress at 300 K. The maximum tensile stress occurs at 200 K at a strain of 0.18 while the strain at the highest simulated temperature is 0.11, which is about 38% less than the maximum strain at the 200 K. At the higher temperatures, the nanosheet can be less elongated as compared to that at the room temperatures in which there

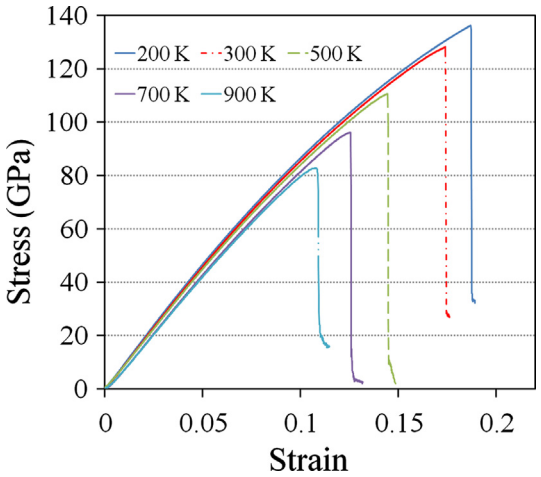

Fig. 2. The stress-strain response of the pristine C_3N nanosheet under the uniaxial tension at the temperatures of 200, 300, 500, 700, and 900 K.

Table 1
Young's Modulus (E) of the pristine nanosheet at the 200, 300, 500, 700, and 900 K.

T (K)	200	300	500	700	900
E (GPa)	953	939	911	885	867