Current Applied Physics 17 (2017) 1323–1328

Contents lists available at ScienceDirect

Current Applied Physics

journal homepage: www.elsevier.com/locate/cap

Molecular dynamics study of the shear strength and fracture behavior of nanoporous graphene membranes

Te-Hua Fang [a], Zhe-Wei Lee [a], Win-Jin Chang [b, *]

[a] Department of Mechanical Engineering, National Kaohsiung University of Applied Sciences, Kaohsiung 807, Taiwan
[b] Department of Mechanical Engineering, Kun Shan University, Tainan 710, Taiwan

ARTICLE INFO

Article history:
Received 9 April 2017
Received in revised form
4 July 2017
Accepted 5 July 2017
Available online 6 July 2017

Keywords:
Graphene
Nanoporous
Shear strength

ABSTRACT

We perform molecular dynamics (MD) simulations to study the structural response and fracture characteristics of nanoporous graphene (NPG) membranes subjected to shear loading. The effects of porosity, temperature, and shear velocity on the mechanical responses of NPG membranes are examined. The results show that the wrinkling of the membrane becomes more obvious with increasing strain. Fractures occur around holes on the long diagonal of the NPG parallelogram, and fracture stress in the NPG membrane decreases with increasing porosity. In addition, the effect of shear velocity on the shear modulus decreases with increasing porosity. The fracture strain of NPG membranes with different porosities obviously decreases with increasing temperature. The results enhance our understanding of the shear mechanical properties of NPG membranes and are helpful for the design and application of high-performance NPG membranes.

1. Introduction

In the last decade, graphene [1,2] has been widely investigated because of its high mechanical strength [3], good chemical stability [4], and excellent electronic properties [5]. Recently, graphene with nanopores has attracted considerable attention. It has become a promising material for different potential applications in many technological fields such as water purification [6–9], gas separation [10,11], and DNA sequencing [12,13].

In recent years, some researchers have studied the fabrication and application of nanoporous graphene (NPG) using experimental techniques [14–20]. For example, Bai et al. [14] first reported the fabrication of NPG membranes with variable periodicities and neck widths using block copolymer lithography. Kostoglou et al. [16] synthesized a NPG-based material with large surface area via the wet chemical reduction of graphene oxide in combination with freeze drying. NPG can be used for hydrogen adsorption and gas separation. Furthermore, Qin et al. [17] synthesized continuously hierarchical NPG films by combining the low-temperature chemical vapor deposition growth of a hydrogenated graphite (HG) coating on nanoporous copper with the rapid catalytic pyrolysis of HG at high temperature. They showed that the resulting films can be used as flexible, solid-state supercapacitors with excellent performance.

In addition, there are some reports on the mechanical properties and vibration analysis of NPG using theoretical methods. For example, Carpenter et al. [21] studied the elastic response of graphene nanomeshes based on molecular statics and molecular dynamics (MD) simulations of uniaxial tensile deformation tests. They found that the elastic moduli were independent of pore lattice arrangement, and the elastic moduli became more sensitive to porosity with increasing temperature. Liu and Chen [22] performed MD simulations to investigate the mechanical properties of NPG membranes under tensile testing and obtained the relationship between the stress-strain curve and porosity. A similar study was also reported by Hu et al. [23]. Recently, Lee and Chang [24] analyzed the vibration behavior of a NPG using an atomic-scale finite element method. They examined the effects of pore location and porosity on the vibrational behaviors of armchair and zigzag NPG layers with different boundary conditions.

When in use, NPGs may be subjected to various external forces under different environmental conditions. Despite these recent theoretical studies, the mechanical properties of NPGs under shear loading have not been investigated until now. The aim of this paper

* Corresponding author.
E-mail address: changwj@mail.ksu.edu.tw (W.-J. Chang).

http://dx.doi.org/10.1016/j.cap.2017.07.003
1567-1739/

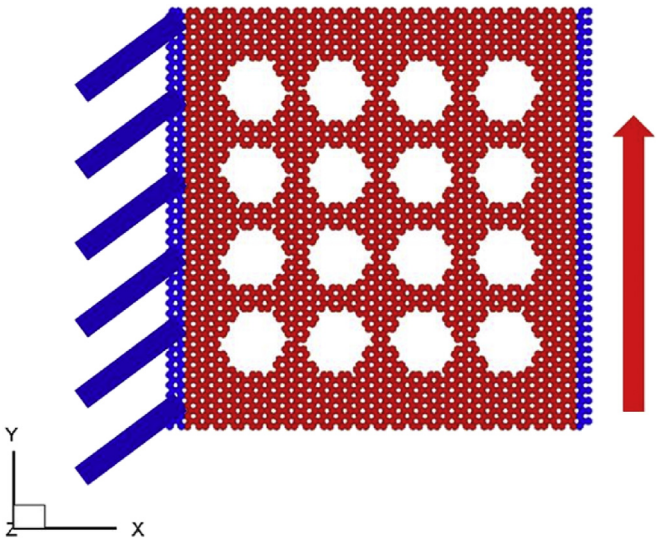

Fig. 1. The configuration of a NPG membrane under shear loading using MD simulations.

is to understand the shear behavior and explore the corresponding structural response and fracture characteristics of a NPG membrane. Toward this end, we perform MD simulations using a many-body interatomic potential to study the mechanical response of NPGs subjected to shear force.

2. Simulation method

The configuration of a NPG membrane under shear loading using MD simulations is illustrated in Fig. 1. The size of the NPG membrane used in the computational simulation is 10 nm by 10 nm. NPGs with five porosities (10.4%, 14.98%, 23.38%, 40%, and 50%, corresponding to 3504, 3294, 2981, 2276, and 1945 atoms, respectively) are adopted in this study. The porosity (P) is defined as the ratio of the missing atoms to the total number of atoms in pristine graphene [24].

The two edges of atoms at both the left and right ends of the membrane are fixed, while the others are free to move. Periodic boundary conditions are imposed on the x-y plane. Sixteen nanopores are uniformly distributed in the membrane to investigate the effect of porosity on the NPG membrane. In order to obtain different porosities, the distance between adjacent nanopores is varied uniformly. The system remains at a temperature of 300 K, and the time step is fixed at 0.5 fs. The left edge is fixed. A shear force with a velocity of 5 m/s in the y-direction is applied to the atoms on the right edge.

The simulations use the reactive empirical bond order (REBO) potential, which is a combination of the Tersoff potential function and Abell function [25]. The REBO potential has been used to

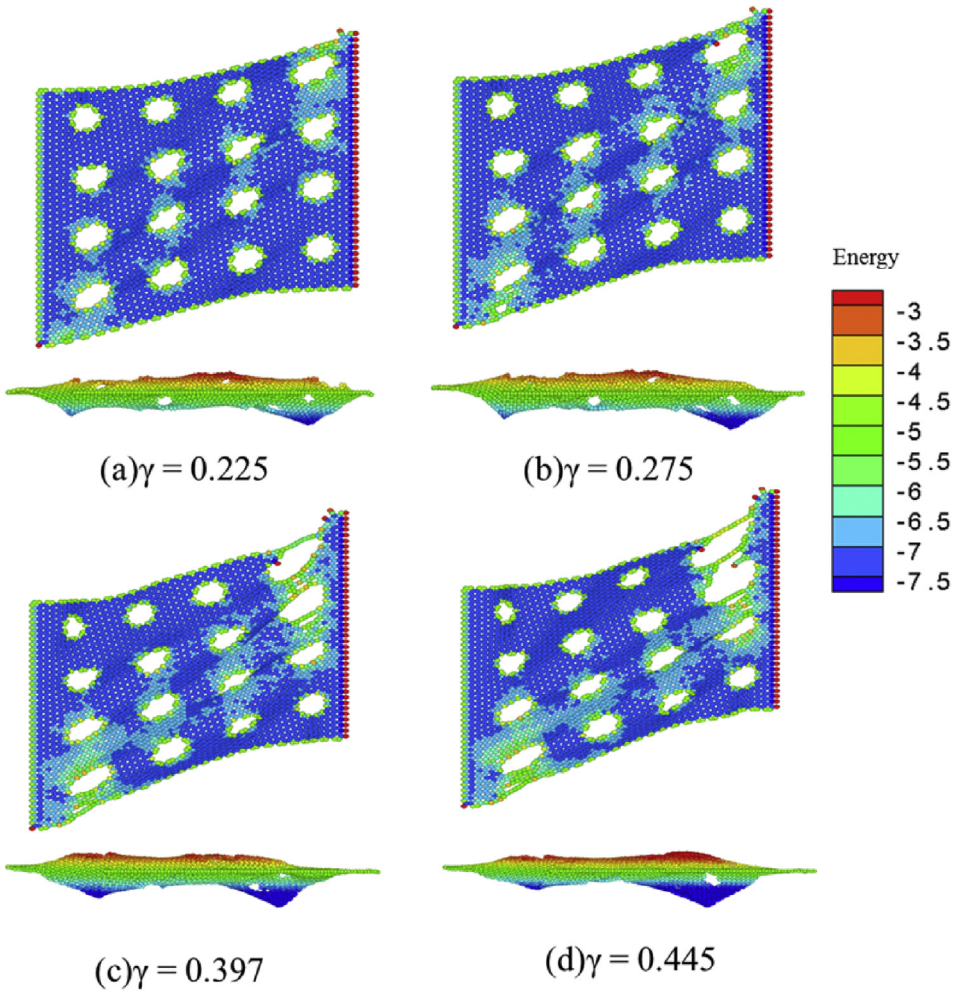

Fig. 2. The snapshots of a NPG membrane with a porosity of 10.4% under shear loading for different strains at a shear velocity of 5 m/s and 300 K. (unit:eV).