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Abstract

Despite numerous theoretical investigations on the mechanical properties of graphene, an accurate identification of its material behavior is still unattained. One hypothesis for this uncertainty is that modeling graphene as a static membrane cannot describe the strong coupling between mechanics and thermodynamics of this structure. Therefore, characterization methods built upon static models could not capture these effects. In this paper, we propose a new method for building a reduced order model for the dynamics of thermalized graphene membranes. We apply the proper orthogonal decomposition algorithm on time responses obtained from molecular dynamics simulations. As a result, a set of orthogonal modes is obtained which are then employed to build a reduced order model. The proposed model can describe the motion of the suspended graphene membrane over the whole spatial domain accurately. Moreover, due to its computational efficiency, it is more versatile for exploring the nonlinear dynamics of the system. This model is then employed for studying the nonlinear dynamics of graphene membranes at large amplitudes to extract Young's modulus. The obtained Young's modulus incorporates the effects of nano-scaled thermally induced dynamic ripples and hence, is temperature and size dependent. Our proposed atomistic modal order reduction method provides a framework for studying the dynamics and extracting the mechanical properties of other nano-structures at the molecular level.

Keywords: Graphene, Idenification, Nonlinear Dynamics, Molecular Dynamics, Proper Orthogonal Decomposition, Reduced order modeling, Elasticity.

1. Introduction

The fabrication of graphene as a single atom thick membrane has been a promising step towards down-scaling of Nano Electro-Mechanical Systems (NEMS) with potential applications in pressure sensing [1], mass sensing [2, 3], and electronics [4–6]. The proper modeling and characterization of graphene is a crucial step towards the development and commercialization of these advanced applications. For this reason many experimental, theoretical, and computational studies have been performed to investigate the limit of intrinsic mechanical properties of pristine graphene [7–14]. However, there is still a large variation in the experimentally measured Young's modulus of graphene as compared to its theoretical limit [13]. For instance, Atomic Force Microscopy (AFM) measurements have shown a large variation in the values of the Young's modulus from 0.43-1.2 TPa [13, 14], respectively. On the other hand, theoretical methods have resulted in a range of 650 to 1240 GPa for the Young's modulus of graphene depending on the load direction, temperature, the size of the structure [7, 8, 13].

Among others, *ab initio* calculations, Density Functional Theory (DFT), Molecular Mechanics (MM), and Molecular Dynamics (MD) are the most commonly used algorithms for obtaining the material properties of graphene, and in particular its elastic modulus, numerically [15, 16]. These methods are usually based on static approaches, i.e. following the changes in the energy of the system due to a stepwise static displacement at the boundaries of the membrane. By fitting a static continuum based model to the response of such simulations, the Young's modulus is identified.