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Nanoparticle mass detection by single and multilayer graphene sheets: Theory and simulations

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ABSTRACT

The discovery of graphene opened up a new field of research and led to the development of various nanosensors and actuators that form new classes of nano electro mechanical systems (NEMSs) called graphene based nano resonators (GBNRs). Recently, GBNRs have been used in mass detection applications. In such applications and others, single-layer graphene sheets play a fundamental role. However, the synthesis of monolayer graphene is usually challenging and expensive. This makes the commercial use of multilayer graphene systems more attractive and necessary. Moreover, it is now more possible to control the number of layers in large-size graphene systems, and thus the theoretical design tools could help the engineers develop more efficient graphene-based sensors for everyday applications. This paper introduces a non-local elasticity theory for the general configurations of carbon atoms that could form carbon nanotubes (CNTs), nanosheets (graphene) and nanospheres (fullerenes) by means of the laminated plate theory. The problem is solved by the generalized differential quadrature element method (GDQEM). Then, a molecular dynamics approach is used in conjunction with the operational modal analysis (OMA) to perform a nano metric modal analysis. Several comparisons are presented to validate the introduced approaches; and finally, the effects of the number of layers and of nanoparticle mass and position on the frequency shift and sensitivity of the designed sensors are studied. It is demonstrated that the frequency shift decreases slightly and the sensitivity increases by increasing the number of graphene layers. It is also demonstrated that, depending on the positions of nanoparticles in a senor, various mode shapes of a graphene sheet could be excited; and consequently, the shift of the first natural frequency may not be appropriate for particles far from the middle of graphene sheet.

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1. Introduction

Although, before 2004, the carbon ad-layer was investigated in terms of film passivation or catalyst poisoning and was more seen as an unwanted side-effect, graphene, a monolayer of sp^2 hybridized carbon atoms arranged in a honeycomb lattice, has been extensively studied in the last several years, despite the fact that it was first discovered only 11–12 years ago [1]. Andre Geim and Konstantin Novoselov won the 2010 Nobel Prize in Physics for this amazing discovery. This discovery opened up a new field of research and led to the development of various nanosensors and actuators that form some new

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classes of nano electro mechanical systems (NEMSs) called graphene-based resonators (GBRs). Apart from its nano-electro-mechanical abilities, graphene has many other sensing capabilities. The high conductivity and transparency of graphene enable it to be used as transparent electrodes in touchscreens [2] and solar cells [3]. Its conductivity and large surface area could find use in electric batteries [4]. Applications of graphene sheets in optoelectronics [5] and photo catalysts [6] have also been proposed. Some nanocomposite configurations of graphene, which could considerably improve their efficiency, have also been reported. As an example, an efficient and novel method of functionalizing graphene nanosheets with vinyl triethoxysilane (VTES) has been report in [7], in which the treated nanosheets have been successfully blended with low density polyethylene (LDPE) to prepare nanocomposites. These studies and some other useful research have been listed in the work of Wang [8], in which he has introduced and reviewed a variety of nano-resonator sensors made of carbon nanotubes and graphene sheets for the detection of atoms/molecules based on the vibration and wave propagation analyses from experimental studies, atomic simulations, and continuum mechanics.

Mass detection is an important application of GBRs [9]. The low resolution of commonly-used sensors is a great challenge for both the manufacturers and customers. The ultimate aim of any detection method is to achieve a level of sensitivity by which the individual quanta of a measured entity can be resolved [10]. In the case of nano mass detectors, a quantum is considered as one atom or molecule. Such a resolution has so far been beyond the reach of any detection device, including solid-state gas sensors hailed for their exceptional sensitivity. The fundamental reason for the limited resolving power of such sensors is the fluctuations due to the thermal motion of charges and the existing defects [10]; which lead to an intrinsic noise that exceeds the noise of a sought-after signal from each molecule, usually by many orders of magnitude. The researchers have recently demonstrated that micro meter size sensors made from graphene are capable of detecting individual events when a gas molecule attaches to or detaches from graphene's surface. The adsorbed molecules change the local carrier concentration in graphene one electron at a time, which leads to step-like changes in resistance. The achieved sensitivity is due to the graphene's being an exceptionally low-noise material electronically, which makes it a promising candidate not only for chemical detectors but also for other applications where local probes sensitive to external charges, magnetic fields or mechanical strain are required [10].

On the other hand, the synthesis of monolayer graphene sheets is usually more challenging and expensive than multilayer ones. The properties of graphene are a function of the number of layers (NOL). Controlling the NOL in large-area graphene sheets is now plausible [11]. By using a picosecond (ps) laser and applying an appropriate pulse threshold energy, the thinning removal of graphene layers from multi-layered graphene sheets and the obtaining of the desired NOL were demonstrated in [11].

Presenting an approach for measuring the vibrational properties of graphene and then developing such techniques for the detection of very small masses can be very helpful in future research works. If the offered tools are based on common developed methods, which have been thoroughly studied, and whose shortcomings have been extracted and resolved, they will certainly be more reliable; and it won't be necessary to pursue new and unfamiliar techniques for solving the problem. Using the common approaches based on modal analysis at the nanoscale can greatly help with mass detection works at these dimensions. This is one of the most important innovations of this paper.

Regarding the use of graphene in the mass detection technology, the following valuable works can be cited. Jiang [12] performed classical molecular dynamics simulations to investigate the enhancement of the mass sensitivity and resonant frequency of graphene nanomechanical resonators; which he achieved by driving them into the nonlinear oscillation regime. In addition to the experimental works in [10,13], some simulations have been performed to investigate the mass detection capability of graphene. Adhikari and Chowdhury developed a mathematical framework for using single-layer graphene sheets as nanoscale label-free mass sensors. They assumed the graphene resonators to have a cantilevered configuration [14]. Jalali and Naei studied the application of single-layered graphene sheets (SLGSs) as resonant sensors in the detection of ultra-fine nanoparticles (NPs) via molecular dynamics (MD) and non-local elasticity approaches [15].

This paper addresses two distinct subjects; it introduces a modal analysis technique for nanoscale domains, and it applies the MD and non-local elasticity approaches to bilayer graphene sheets in order to achieve sufficient resolution and sensitivity at a low cost of synthesis.

When the usual modal analysis method is used for small dimensions and the molecular dynamics technique is exploited as a tool, a basic problem that arises is the very small time step in the simulation of molecular dynamics. This problem has been solved in this paper, and the use of modal analysis at small scale has been made possible.

The optimal number of layers in graphene sheets, and the optimal GBR dimensions and boundary conditions, which lead to adequate resolution and sensitivity, reduce the production costs and improve the performance of GBRs, are some of the parameters that can be studied. In this paper, a continuum-based approach is employed in conjunction with an MD investigation and operational modal analysis (OMA) for designing the parameters of GBRs. After describing the problem, some theories are introduced for both models and then the presented approaches are validated. At the end, some valuable and practical simulations are performed.

2. Problem description

Based on the requirements mentioned in the previous section, a laminated GBR containing several nanoparticles on its surfaces should be considered. Recently, a simple and upward-scalable method has been presented for producing repaired graphene oxide sheets with a large surface area by introducing spherical multilayered graphene balls with empty interiors

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