Chapter 26
Graphene-Based Sensors for Monitoring Strain: A First-Principles Density Functional Theory Analysis

M. Mirnezhad
University of Guilan, Iran

H. Rouhi
University of Guilan, Iran

R. Ansari
University of Guilan, Iran

M. Faghihnasiri
University of Guilan, Iran

ABSTRACT

The application of graphene as a nanosensor in measuring strain through its band structure around the Fermi level is investigated in this paper. The mechanical properties of graphene as well as its electronic structure are determined by using the density functional theory calculations within the framework of generalized gradient approximation. In the case of electronic properties, the simulations are applied for symmetrical and asymmetrical strain distributions in elastic range; also the tight-binding approach is implemented to verify the results. It is indicated that the energy band gap does not change with the symmetrical strain distribution but depend on the asymmetric strain distribution, increasing strain leads to band gap opening around the Fermi level.

INTRODUCTION

Nanoelectromechanical systems (NEMS) (Craigheah, 2000) have aroused enormous scientific interest in recent years and are anticipated to drastically affect many areas of science owing to their numerous potential applications in upcoming nanotechnology devices. Carbon allotropes such as carbon nanotubes and graphene are increasingly used in NEMS applications (Sapmaz et al., 2003; Poetschke et al., 2010). This is largely due to their exclusive mechanical and electronic properties over other existing materials. In terms of mechanical properties, graphene possesses high Young's modulus, low friction, extremely low density and a breaking strength 200 times higher than steel, with a tensile strength of 130 GPa (Bunch et al., 2007; Lee et al., 2008). These

DOI: 10.4018/978-1-4666-5125-8.ch026

superior mechanical properties meet the stability requirement of NEMS and therefore allow graphene to be used for NEMS applications such as pressure sensors and resonators (Frank et al., 2007). In conjunction with the mechanical advantages of graphene, its electronic properties have made it a promising candidate in many electronic components of NEMS such as nanotransistors (Westervelt, 2008). Also, experimental studies on the transport measurements reveal that graphene has high electron mobility at room temperature which is greater than $15000 cm^2 V^{-1} s^1$ (Geim & Novoselov, 2007).

Among carbon allotropes, the critical role of graphene has been emphasized by the researchers as it is the basis for the identification of the electronic properties in other allotropes. Graphene is a semi-metal or zero-gap semiconductor (Novoselov et al., 2004). As a result of the linear energy-momentum dispersion relation at low energies, electrons near the six corners of the two-dimensional hexagonal Brillouin zone behave as massless relativistic fermions that satisfy the Dirac equation (Semenoff, 1984; Avouris et al., 2007; Novoselov et al., 2005). Moreover, it has been revealed that the quantum Hall effect can be measured in the graphene even at room temperature (Novoselov et al., 2007; Gusynin & Sharapov, 2005; Zhang et al., 2005; Du et al., 2009; Bolotin et al., 2009).

The band structure of graphene was studied by Wallace (1947) for the first time and he revealed the unusual semi-metallic behavior in this material. Afterwards, the electronic structure of graphene has been the subject of many research papers and debate. A comprehensive review on the electronic properties of graphene can be found in Castro Neto et al. (2009). Gui et al. (2008) studied the electronic structure of graphene subjected to different planar strain distributions through the first-principles pseudopotential plane-wave method and the tight-binding (TB) approach. Their work showed that graphene with a symmetrical strain distribution is always a zero band-gap semiconductor and its pseudogap decreases linearly with the strain strength in the elastic regime. Using the tight-binding approach along with the ab initio calculations, the electronic and quantum transport properties of graphene are investigated in (Dubois et al., 2009). On the basis of first-principles calculations, Topsakal et al. (2010) studied the mechanical and electronic properties of monolayer hydrocarbon, graphene under elastic strain. They indicated that the band-gap can be effectively modified by applied strain in the elastic range. The atomic, electronic, and magnetic structures of graphene under elastic and plastic deformation were analyzed by Topsakal and Ciraci (2010) based on a first-principles density-functional theory.

One of the future targets in growing field of nanotechnology is to design sensors (Hierold et al., 2007) that are capable of monitoring the mechanical characteristics of nanosystems operating under hard environmental conditions through a non-contact measuring way. Based upon its unique mechanical and electronic properties, graphene can be regarded as a promising candidate for the mentioned applications. Therefore, the present study aims at investigating the relationship between the applied strain and the electronic structure of graphene based on a first-principles density functional theory (DFT) analysis and the tight-binding (TB) approach. First, DFT calculations are carried out to study the response of mechanical properties of graphene to the strain in the harmonic region which leads to obtain the in-plane stiffness and Poisson's ratio. Thereafter, the electronic structure of graphene under different planar strain distributions including symmetrical and asymmetrical ones is fully investigated in the elastic regime. The TB method is also used to verify the corresponding results. All simulations are performed using the Quantum-Espresso code (http://www.pwscf.org) on the basis of the generalized gradient approximation (GGA) together with the exchange correlation of the Perdew-Burke-Ernzerhof (PBE).