



Strain gradient polarization in graphene



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ABSTRACT

Flexoelectricity phenomenon is the response of electric polarization to an applied strain gradient and is developed as a consequence of crystal symmetry in all materials. In this study, we show that the presence of strain gradient in non-piezoelectric graphene sheet does not only affect the ionic positions, but also the asymmetric redistribution of the electron density, which induce strong polarization in the graphene sheet. Using quantum mechanics calculations, the resulting axial and normal piezoelectric coefficients of the graphene sheet were determined using two loading conditions: (i) a graphene sheet containing non-centrosymmetric pores subjected to an axial load, and (ii) a pristine graphene sheet subjected to a bending moment. Particular emphases were placed on the role of edge and corner states of pores arising due to the functionalization. We also investigated the electronic structure of graphene sheet under different in-plane strain distributions using quantum mechanics calculations and tight-binding approach. The findings of our work reveal that the respective axial and normal electromechanical couplings in graphene can be engineered by changing the size of non-centrosymmetric pores and radii of curvature. Our fundamental study highlights the possibility of using graphene sheets in nano-electromechanical systems as sensors or actuators.

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1. Introduction

Recent advances in nanoscale technologies have renewed interest in flexoelectricity. Large strain gradients present at the nanoscale level may lead to strong electromechanical coupling. Piezoelectricity - electrical polarization induced by a uniform strain (or vice-versa) - is the most widely known and exploited forms of electromechanical coupling that exists in non-centrosymmetric crystals. In centrosymmetric crystals, the presence of the center of inversion results in the absence of bulk piezoelectric properties. In contrast to piezoelectricity, flexoelectricity can be found in any crystalline material, regardless of the atomic bonding configuration [1]. The symmetry breaking at surfaces and interfaces in nonpolar materials would allow new forms of electromechanical coupling, such as surface piezoelectricity and flexoelectricity, which cannot be induced in bulk materials. The first step towards a theoretical

understanding of flexoelectricity was due to Kogan [2]. It is worth mentioning that the term “flexoelectricity” for crystalline materials was coined by a similar phenomenon in liquid crystals [3]. Piezoelectric materials are commonly used where precise and repeatable controlled motion is required, such as atomic force microscopy probes, smart structures [4–6], piezotronic devices [7], sensors and actuators, and nanogenerators [8]. The conventional piezoelectric ceramics are heavy, brittle, and some pose significant environmental risk due to the inclusion of high lead content [9]. Piezoelectric polymers, on the other hand, are light and environmentally benign, but typically display considerably smaller piezoelectric response in terms of actuation. Piezoelectric single-layer hexagonal boron nitride is a promising nanomaterial for nano-electromechanical system (NEMS), but its synthesis is much harder which has been a major issue for more than a decade.

The successful synthesis of 2D single layer graphene sheet [10] has attracted considerable attention from both academia and industry. This is due to its unique scale-dependent electronic, mechanical, and thermal properties [11–14]. It is widely considered to be one of the most attractive materials of the twenty-first century. Remarkably, high electron mobility and other striking features, such as anomalous quantum hall effect, pseudomagnetic field, and

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spin transport [15], have made graphene an intensely studied material from both basic science viewpoint as well as advanced applications in micro- and nano-electronics [7], spintronic devices, electron lenses, energy storage systems [16], and gas separation membranes [17]. In view of its unique 2D structure and electrical properties with zero bandgap, graphene is most suitable for NEMS applications.

The flexoelectric effect in carbon nanotubes was observed by White et al. [18] for the first time in 1993. In their study, the bond symmetry breaking due to curvature was visible in the electronic properties of carbon nanotubes (CNTs). A homogeneous mechanical deformation of graphene cannot induce polarization due to the symmetry of its lattice. However, second-order electronic flexoelectric effect in graphene can be induced by the presence of a strain gradient. The strain gradient changes the ionic positions as well as leads to asymmetric redistribution of the electron density. Contrary to 3D systems, graphene are also able to sustain large strains up to 25% [13] and, thus can exhibit exceptional forms of electromechanical coupling [19]. Zeinalipour-Yazdi and Christofides [20] determined the size-dependent Young's modulus and C–C binding energy in graphene nanoribbons via electron first principles computations. They reported linearity between the C–C binding energy and Young's modulus, which was explained by the decrease in the molecular polarizability due to deformations within the proportional limit of the graphene nanoribbons. Dumitrică et al. [21] investigated the normal polarization induced by bending of graphite shells, which microscopically occurs because of a shift in sp^2 hybridization at each atomic site. Using density functional theory (DFT) calculations for bent nanographitic ribbons made of up to 400 atoms, Kalinin and Meunier [22] predicted the electromechanical coupling, in agreement with the prediction of linear theory for flexoelectric coupling in quantum systems. Note that the stability of planar carbon materials is higher than their curved nanostructures (e.g. Fullerenes and CNTs) and this is associated to the existence of the energy requirements to bend a graphene sheet. Based on average bond-dissociation-enthalpies, Zeinalipour-Yazdi and Loizidou [23] applied physical sphere-in-contact models to elucidate the cap geometry of single walled CNT with sub-nanometer width (i.e., (3,3), (4,4) and (5,5)-SWCNTs). Their DFT calculations reveal that these new carbon geometries have similar stability to carbon found in other ball-capped zigzag and arm-chair nanotubes (i.e., (5,5), (6,6), (9,0) and (10,0)). Recently, experimental and theoretical investigations reported that creating nanoscale non-centrosymmetric pores in graphene nanoribbons would lead to

apparent piezoelectric behavior [24,25]. These exceptional and highly desirable electromechanical properties have motivated our interest in this work. To the best of the authors' knowledge, the axial and normal flexoelectricity coefficients of graphene have not yet been reported. In this study, we first examined the band structures of graphene sheet subjected to different in-plane strain distributions using quantum mechanics calculations and tight-binding (TB) approach. Then, we focused our attention to determining the induced piezoelectric coefficients of graphene with and without non-centrosymmetric pores of different sizes using quantum mechanics calculations. The outcome of this work should lead to a greater insight into strain-induced electric polarization in graphene sheets that would allow exploring the essence of their strong piezoelectric response through different loadings.

2. TB modeling of electronic structure of graphene

Graphene has unique electronic properties evolving from its hexagonal honeycomb lattice structure, which makes electrons in graphene behave as massless relativistic fermions that satisfy the Dirac equation [26]. In-plane strain distributions in graphene sheet significantly modify its band structure around the Fermi level, which break the inversion symmetry [27]. Theoretically, both the TB model and ab initio approaches have been widely adopted to investigate the effect of strain on the band structure of graphene and graphene nanoribbons [28,29]. In this research, we first study the electronic structure of graphene sheet under different in-plane strain distributions using quantum mechanics calculations and Hückel TB model [29,30]. If the inversion symmetry breaking is confirmed with particular planer strain distribution case, then the flexoelectric effect in graphene sheet with non-centrosymmetric pore is examined.

We define x-direction to be along the unstrained graphene axis and y as the transverse direction, as shown in Fig. 1.

The following changes occur in the x-component of the coordinate of the i th atom when the graphene sheet is subjected to uniaxial or shear strains:

$$\left. \begin{aligned} x_i &\rightarrow (1 + \epsilon_A)x_i \\ x_i &\rightarrow (1 + \epsilon_Z)x_i \end{aligned} \right\} \text{Uniaxial strains} \quad (1a)$$

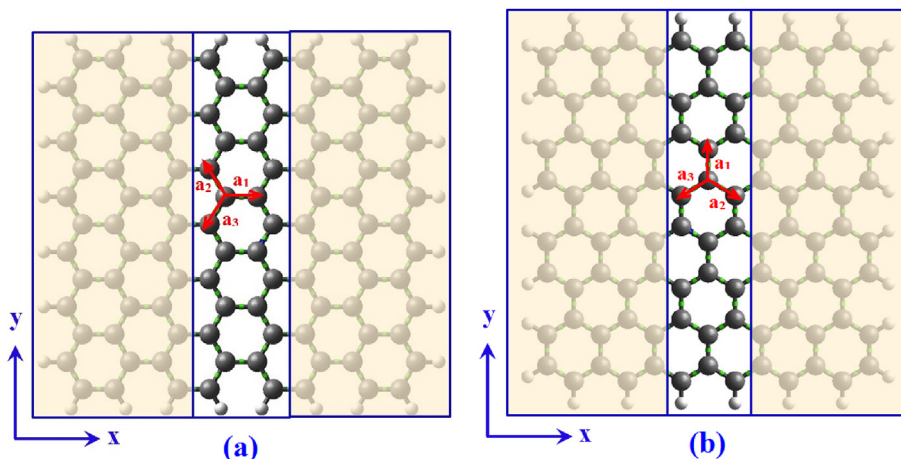


Fig. 1. The unit cells of (a) armchair graphene sheet, and (b) zigzag graphene sheet. a_1 , a_2 and a_3 are the bond vectors. (A colour version of this figure can be viewed online.)

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