Strain-induced modulation of mechanical properties and electronic structure of edge-modification graphene nanoribbons

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Abstract—The mechanical properties and electronic structure of graphene nanoribbons (GNRs) which modified atoms or molecular groups on the zigzag edges can be tuned under the uniaxial tensile strain for application on the electronic devices. We study the elastic and plastic deformation of GNRs. The modified zigzag edges play a key role in tensile force, elastic constant, critical point (the critical point of elastic and plastic deformation) and the energy gaps. In particular, it is shown that the energy gap of edge-modification GNRs can be strongly modified under uniaxial tensile strain. This way, offer new opportunities to electronic transport and force-electronic devices for next-generation electronics.

I. INTRODUCTION

Due to the graphene nanoribbons (GNRs) have capabilities to continuously control the band gap, it can be expected the candidates for future electronic and optoelectronic devices\(^1\). However, GNRs can not be produced in the same condition, a variety of lithographic fabrication (e.g oxygen plasma) are modified with oxygen at edge. In addition, diverse atoms or molecular groups may be introduced in the manufacturing process (e.g NH\(_2\) and OH). Some theoretical and experimental studies have proved that local and uniform strain can tune the electronic properties and transport characteristics of GNRs\(^2\),\(^3\). Therefore, it is vital to study the mechanical properties and electronic structure of edge-modification GNRs by the uniaxial tensile strain.

In order to describe the pristine GNRs, we discusse the mechanical properties and electronic structure of GNRs which are modified with H, O, OH and NH\(_2\) at zigzag edges (because the zigzag interface is relatively more prone to atoms or molecular groups adsorbed). We investigate geometric and electronic properties of GNRs by the uniaxial tensile strain. We find that tension force \(F_T\), elastic constant \(C\) and critical point (the critical point of elastic and plastic deformation) of GNRs are depend on the modified edge. Furthermore, the energy gaps of GNRs change dramatically under uniaxial strains.

II. METHODS

The electronic structure calculations are performed using the density-functional theory (DFT) by PAW potentials\(^4\). The exchange and correlation effects of the electrons has been approximated by Generalized Gradient Approximation (GGA), as implemented in Vienna Ab initio Simulation Package (VASP)\(^5\). The geometry are optimized with the conjugate-gradient algorithm method. All structures are treated within supercell geometry using the periodic boundary conditions. The size of supercells are carefully tested to maintain a sufficiently large separation between adjacent nanoribbons (>12Å form nanoribbon to nanoribbon). The basis set with kinetic-energy cutoff of 400 eV has been used, and Brillouin zone have been done using a \(0 \times 0 \times 0\)-centered k-point grid for the big molecular GNRs. A representative nanoribbon (the length of 2.2 nm and the width of 0.7 nm) is shown in FIG. 1, which the edges are modified with NH\(_2\). Following the previous convention, the GNRs are defined according the number of dangling bonds on the armchair edges \(M\) and the number of dangling bonds on the zigzag edges \(N\). The deformation are added along the zigzag edge (\(X\) direction) in the 4\(\times\)9 GNRs.

Fig. 1. (I) A schematic diagram of 4\(\times\)9 GNR modified with NH\(_2\) at the 5 site at zigzag edge; (II) Local structure of edge-modification GNRs. The zigzag edge modified with O, NH\(_2\) and OH in (a), (b) and (c), respectively.
∂𝐸 respectively (the report experimental value for graphene is of GNR modified with O is bigger than those in other GNRs. The double bond between C atom and O atom, the elastic constant is also bigger than those of the graphene. Apparently, for the existence of the C-H bond, the elastic constants are liking those in graphene. However, for the existence of the C-O bond, the elastic constants are like those in graphene. The strain energy and tense force of GNRs are shown in FIG. 1. The tense force, elastic constant, critical point and energy gaps of GNRs are given along the X-axis as shown in FIG. 1. The elastic constants are listed in Table 1. The tense force, elastic constant, critical point and energy gaps of GNRs are shown in FIG. 2. Form the result we can obtain that the covalent bond parallel to the X-axis are stretched longer than those in other direction. As a result, the elastic constants of GNRs modified with H, NH2, O and OH are 278, 256, 354, and 293 N/m, respectively (the report experimental value for graphene is C=350±50[6]). Because of the similar honeycomb structure, their elastic constants are like those in graphene. However, the edge effects of GNRs, their stiffness values are smaller than those of the graphene. Apparently, for the existence of double bond between C atom and O atom, the elastic constant of GNR modified with O is bigger than those in other GNRs. This is the yielding points, where the strain energy drops suddenly. The C atom which is at the 5 site (as shown in FIG. 3) is first lose their covalent bond at the yielding points (εy) by the uniaxial tensile strain. The yielding points of elastic and plastic deformation are expecting to depend on symmetries, such as vacancy and modified. In previous reports, the εy is also depend on the temperature[7]. Just as the increase of temperature the εy is decrease. In this work, the εy of GNRs modified with H, NH3, O and OH are 0.14, 0.17, 0.18 and 0.16, respectively. The effect of vacancy is investigated by 4×9 armchair-edge GNR modified with H. Results indicate that εy in armchair-edge is bigger than those in zigzag-edge.

Depending on their crystalline defects the energy gaps of GNRs significant variations by the uniaxial tensile strain. As strain-dependent energy gap describing in FIG. 3, we find that the energy gap decreases with the increase of the strain in the elastic deformation. The energy of highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are also decrease as the increase the uniaxial strains. However, the energy of LUMO decrease speedy than those of HOMO. Energy gap increase significantly at the yielding points. Because the sp2 C-C bond of the 5 site is broken and the modified atom (or molecule) is incorporated into the C atom. This way, be able to continuously control the band gap of modified GNRs for building the next-generation electronics.

IV. SUMMARY AND CONCLUSIONS

In conclusion, we have demonstrated that the Strain-induced modulation of mechanical properties and electronic structure of edge-modification graphene nanoribbons by first-principles calculation. We found that the final structures of all atoms in GNRs are in a plane. Furthermore, strain energy, tense force, elastic constant, critical point and energy gaps of GNRs are highly dependent on the modified atoms or molecular groups. In addition, the band gaps of GNRs can be changed significantly by the uniaxial tensile strain. The above result provide us a practical method to tune the energy gap of GNRs.

REFERENCES