Mechanically and thermally tunable properties of graphene materials

Yufeng Guo[a] Wanlin Guo

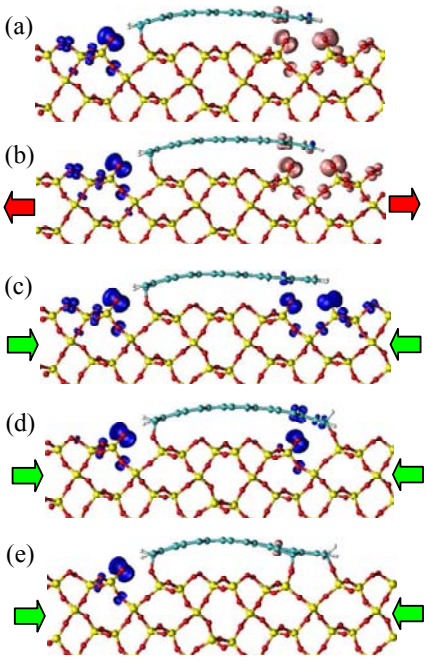
State Key Laboratory of Mechanics and Control of Mechanical Structures and MOE Key Laboratory for Intelligent Nano Materials and Devices, Institute of Nanoscience, Nanjing University of Aeronautics and Astronautics, Nanjing, 210016, China

Graphene nanoribbon (GNR), a graphene strip of nanometer in width, exhibits exceptional electronical and chemical properties because of the appearance of edge states [1, 2]. A nanoribbon of zigzag edges has a flat energy band at the Femi level and strong localized states on the edge sites, which are absent for a nanoribbon of armchair edges. This difference gives rise to distinguished electronic behaviors in zigzag and armchair nanoribbons [3, 4]. The zigzag graphene nanoribbon (ZGNR) has been predicted to have an antiferromagnetic ground state and possess edge magnetism. For actual application in nanoelectronics, GNRs will normally be put or transferred on a substrate. The edge properties and structure of GNRs are inevitably modified because of physical or chemical coupling with substrate. For instance single-layer ZGNRs bond strongly with silicon substrate at its edges and lose their semiconducting and magnetic properties, while bilayer ZGNRs on the same substrate exhibit intriguing magnetoelectric effects under a gated bias [5, 6].

In addition, the interaction between GNR and substrate might introduce novel performance to the substrate where, for example, magnetism can be induced on the surface of ZGNR adsorbed silicon substrate [7]. Silicon dioxide (SiO_2) is widely used as a dielectric medium in integrated circuits and also as an insulating substrate for graphene system. Particularly, SiO_2 plays an important role in Si/SiO_2 interface of Si based technology-the mainstream technology of present semiconductor industry. A lot of studies have been conducted concerning the effects of the underlying SiO_2 substrate on the electronic and structural properties of graphene above it. However, due to high chemical activity of GNR edges a better understanding about the influence of the adsorbed nanoribbon on the intrinsic properties of SiO_2 substrate is also necessary for GNR/SiO_2 based nanoelectronic devices.

On the other hand, nanomechanical methods such as mechanical strainand interlayer compression as well as utilizing the surface morphology of substrateare proved to be effective ways to modulate the structure, electronic band and magnetism of graphene materials, and also successfully employed in the silicon electronics industry to boost device performance. Therefore, to explore the response of GNR/SiO_2 system to structural strain will be helpful for graphene applications.

Our density functional theory (DFT) calculations show that when a ZGNR is put on (100) α-quartz SiO_2 substrate, some surface O-O bonds of the substrate are broken by bonding with the edge atoms of the adsorbed nanoribbon. This leads to an antiferromagnetic ground state in the ZGNR/SiO_2 system. Further study reveals that the spin states and magnetism of the SiO_2 surface can be effectively tuned by mechanical strain applied on the substrate, with the total magnetic moment varying from negative to positive when the strain turns from tensile to compressive, as shown in Figure 1. Moreover, the ZGNR/SiO_2 system transforms from antiferromagnetic into ferromagnetic state under compressive strain. The present results unveil some fundamental magnetic behaviors of the GNR and insulator substrate system, and suggest potential applications in mechanically tunable spintronics devices and sensors basing on the total properties of the whole system.



[a] Corresponding author. Email: yfguo@nuaa.edu.cn

Figure 1. Isosurface of the charge density difference [in unit of 0.01 e/(Å)^3] between the α-spin and β-spin states for the system under (a) 0, (b) 3.7%, (c) -0.5%, (d) -0.8% and (e) -1.9% transverse strain. The blue and pink colors represent the charge density of spin-up and spin-down, respectively.

Graphene can easily ripple and wrinkle on substrates into disordered states and show distorted properties. Our nonequilibrium molecular dynamics simulations show that on graphite substrate a wrinkle of a graphene sheet created by uniaxial compression will run toward the cold region with constant translational acceleration when the graphene is subjected to a thermal gradient. An established theoretical model demonstrates that this motion is driven mainly due to the difference of potential energy and its gradient between the hot and cold sides of the wrinkle, which is induced by applied temperature difference. The wrinkle shape and interaction with substrate significantly influence, even might halt the wrinkle translational movement.

References

[1] Novoselov K.: Mind the gap. *Nat. Mat.* **6**: 720, 2007.

[2] Han M. Y., Oezyilmaz B., Zhang Y., Kim P.: Energy band-gap engineering of graphene nanoribbons. *Phys. Rev. Lett.* **98**: 206805, 2007.

[3] Yang L., Park C., Son Y. W., Cohen M. L., Louie S. G.: Edge state in graphene ribbons: Nanometer size effect and edge shape dependence. *Phys. Rev. Lett.* **99**: 186801, 2007.

[4] Son Y. W., Cohen M. L., Louie S. G. : Energy Gaps in Graphene Nanoribbons. *Phys. Rev. Lett.* **97**: 216803, 2006.

[5] Zhang Z., Cheng C., Guo W.: Magnetoelectric Effect in Graphene Nanoribbons on Substrates via Electric Bias Control of Exchange Splitting. *Phys. Rev. Lett.* **103**: 187204, 2009.

[6] Zhang Z., Cheng C., Zeng X., Guo W.: Tuning the magnetic and electronic properties of bilayer graphene nanoribbons on Si(001) by bias voltage. *Phys. Rev. B* **81**: 155428, 2010.

[7] Zhang Z., Guo W., Zeng X.: Tunable magnetism on Si(111)-(2×1) via chemisorption of graphene nanoribbons. *Phys. Rev. B* **82**: 235423, 2010.