Reply to "Comment on 'Band structure engineering of graphene by strain: First-principles calculations' "

Gui Gui, Jin Li, and Jianxin Zhong*

Laboratory for Quantum Engineering and Micro-Nano Energy Technology, Xiangtan University, Xiangtan, 411105 Hunan, People's Republic of China and Department of Physics, Xiangtan University, Hunan 411105, People's Republic of China

(Received 10 September 2009; published 19 October 2009)

We reply to the Comment by Farjam and Rafii-Tabar [Phys. Rev. B **80**, 167401 (2009)] on our paper [Phys. Rev. B **78**, 075435 (2008)]. We show that the gap opening found in our paper is due to the use of a small number of k points in the calculation which prevents revealing the sharp contact of the two bands near K or R. Once a large number of k points is used, the density-functional theory (DFT) VASP codes give the same conclusion as obtained by Farjam and Rafii-Tabar by using the QUANTUM-ESPRESSO codes, namely, there is no gap opening in the band structure of graphene under small planar strain. We also point out that all other results in our paper remain correct, except for the conclusion of the gap opening. The results demonstrate the importance of using a large number of k points for determining the gap width of the band structure of graphene under strain as well as the validity of the DFT VASP codes for the system.

DOI: 10.1103/PhysRevB.80.167402 PACS number(s): 73.22.−f, 73.61.Wp, 72.80.Rj

We are grateful to Farjam and Rafii-Tabar for their Comment[1] on our paper[2] about the gap opening in graphene under planar uniaxial strain. It is a precious opportunity for us to present discussions about the importance of using a large number of k points for determining the gap width in the first-principles calculations of the band structure of graphene under strain as well as the validity of the density-functional theory (DFT) VASP codes for the studied system.

Using the QUANTUM-ESPRESSO codes based on the pseudopotential plane-wave method, Farjam and Rafii-Tabar[1] show that there is no gap opening in the band structure of graphene under small planar uniaxial strain. Their conclusion is in agreement with the result given by the tight-binding model[3] but is different from our previous result of the first-principles calculation using the DFT VASP codes which shows gap opening.[2] They found 0.486 and 0.178 eV for the energy splittings exactly at K and R under the strains parallel to C-C bonds and perpendicular C-C bonds, respectively. They believe that the values for the energy splittings at K and R are the gap values reported in our paper.[2] We have carefully examined our previous calculation and found that there is indeed no significant gap opening under small uniaxial strain, confirming the conclusion giving by Farjam and Rafii-Tabar. However, we want to emphasize that the gap values reported in Ref. 2 are not taken from the shift of the conduction and valence bands directly at K and R as assumed by Farjam and Rafii-Tabar in Ref. 1. We show here that the gap opening found in Ref. 2 is due to the use of small number of k points in the calculation which prevents revealing the sharp contact of the two bands near K or R. Once a large number of k points is used, the VASP codes give the same conclusion as obtained by the QUANTUM-ESPRESSO codes[1] and the tight-binding model.[3]

In our previous calculation,[2] 20 k points were used to construct the band structure. In order to systematically examine the relationship between the number of k points and the calculated band-gap width, we recalculated the band structure of the graphene under planar strain parallel to C-C bonds with $1y=0.2396$ nm (12.2% strain), which gives the maximum gap value of 0.486 eV in Ref. 2. We used nk k points between any two k points of high symmetry to calculate the band structure, where $nk=20$, 40, 80, 200, and 405. A gap of 0.486 eV occurs near K for $nk=20$ as reported in Ref. 2. The gap width turns to be 0.03, 0.0369, 0.0405, 0.0063, and 0.0003 eV for $nk=40$, 80, 200, 400, and 405, respectively, as shown in Fig. 1. From the systematic change in the value of the gap width, we conclude that there is no significant gap opening in the graphene under small planar strain parallel to C-C bonds. The gap width—strain curve obtained in Ref. 2 actually describes the change in the shift

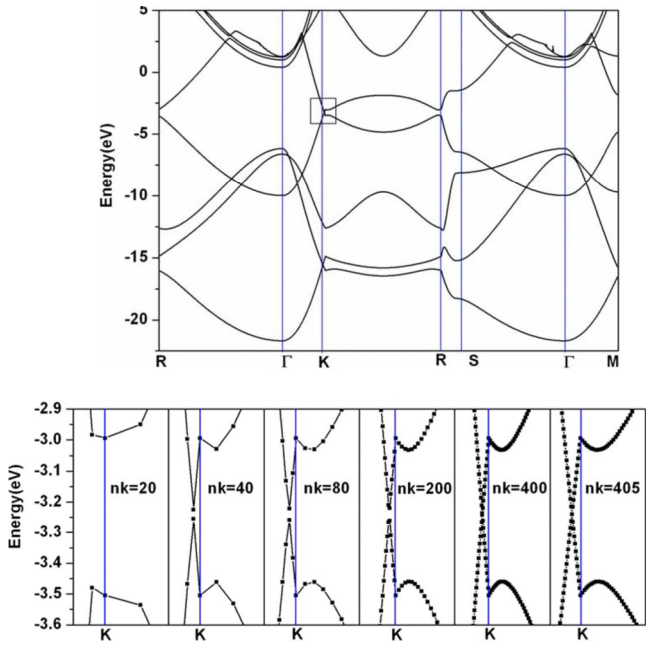

FIG. 1. (Color online) Band structure of graphene under 12.2% strain parallel to C-C bonds (top). Magnified portion of band structure near K obtained by using different numbers of k points with $nk=20$, 40, 80, 200, 400, and 405 (bottom).

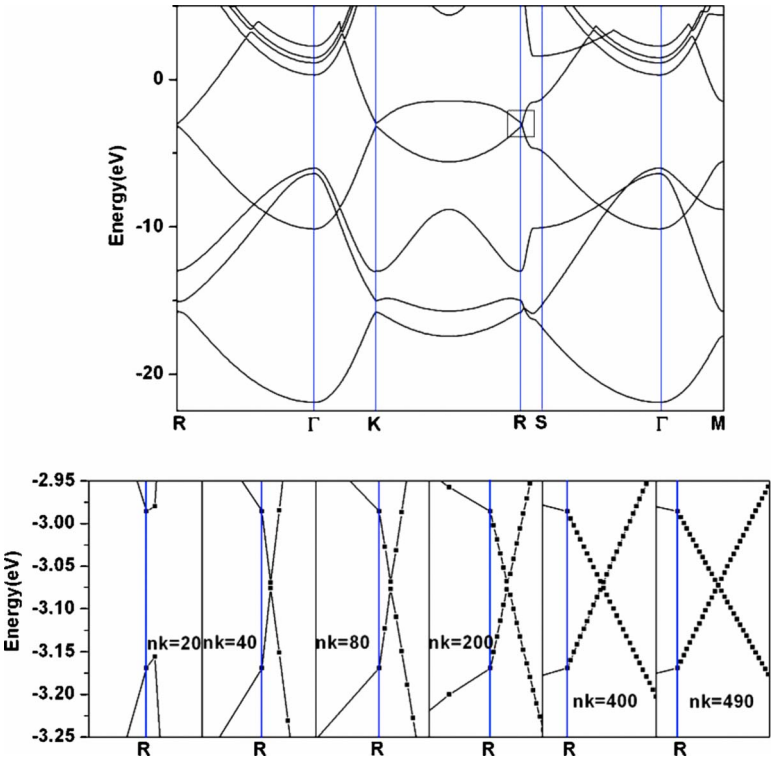

FIG. 2. (Color online) Band structure of graphene under 7.3% strain perpendicular to C-C bonds (top). Magnified portion of band structure near R obtained by using different number of k points with $nk=20$, 40, 80, 200, 400, and 490 (bottom).

of the conduction and valence bands near K, not exactly at K.

We also recalculated the band structure of the graphene under planar strain perpendicular to C-C bonds with $lx=0.1323$ nm (7.3% strain), which gives the maximum gap value of 0.170 eV in Ref. 2. We used $nk=20$, 40, 80, 200, 400, and 490 to recalculate the band structure. A gap of 0.170 eV occurs near R for $nk=20$, which turns to be 0.006, 0.0369, 0.0082, 0.0071, and 0.0095 eV for $nk=40$, 80, 200, 400, and 490, respectively, as shown in Fig. 2. The systematic change in the value of the gap width also leads to the conclusion that there is no significant gap opening in the graphene under small planar strain perpendicular to C-C bonds. The gap width—strain curve obtained in Ref. 2 actually describes the change in the shift of the conduction and valence bands near R, not exactly at R.

We conclude that the previous observation of gap opening in the strained graphene in Ref. 2 obtained by the DFT VASP codes is induced by choosing small number of k points in calculation of the band structure, which misses the exact crossing point of the bands. When a large number of k points is used, the DFT VASP codes give the same conclusion obtained by the QUANTUM-ESPRESSO codes and the tight-binding model,[3] namely, there is no gap opening in the band structure of graphene under small planar strain. Finally, we want to point out that all other results in Ref. 2 remain correct, except for the conclusion of the gap opening.

*Corresponding author.

[1] M. Farjam and H. Rafii-Tabar, Phys. Rev. B **80**, 167401 (2009).
[2] G. Gui, J. Li, and J. X. Zhong, Phys. Rev. B **78**, 075435 (2008).
[3] V. M. Pereira, A. H. Castro Neto, and N. M. R. Peres, Phys. Rev. B **80**, 045401 (2009).