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Electronic transport anisotropy of buckling graphene under uniaxial compressive strain: *Ab initio* study

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Electronic transport properties of graphene under uniaxial compressive strain are studied using *ab initio* calculations. With approximate thermal perturbation, buckling occurs when strain exceeds a threshold, comparing to flat unperturbed structures. Transmissions of flat graphene compressed along zigzag direction (ZCG) and buckled graphene compressed along armchair direction (ACG) are insensitive to strain, whereas those of buckled ZCG and flat ACG are negatively correlated to strain. Flat graphene has anisotropic resistance along the strain direction, while buckling suppresses the anisotropy by releasing the strain. The insensitivity of buckled graphene on strain direction and out-of-plane deformation makes feasible to implement flexible electronics. © *2012 American Institute of Physics*. [doi:10.1063/1.3680092]

Graphene, a single-layer hexagonal lattice of carbon atoms, has outstanding electrical, mechanical, and thermal properties.[1–3] Ripples are an intrinsic feature of graphene[4] and the mechanism of rippling was intensively discussed.[5,6] Controlled creation of periodic ripples in suspended graphene was reported using thermally generated strain.[4] Sine-wave shapes of buckled graphene nanoribbons (GNRs) were induced by compressive strain.[7] The impact of strain on morphology and instability of supported graphene was studied.[8] However, electronic properties of graphene with and without buckling, critical to flexible devices, are rarely discussed. Studies on electronic transport anisotropy of buckled graphene are relatively lacked.[9,10] In previous paper, we find transport properties of graphene are insensitive to various deformations without strain.[11] In this work, we study how buckling, induced by uniaxial strain, changes the transport properties of graphene.

Monolayer graphene compressed along zigzag or armchair direction (labeled as ZCG or ACG) is shown in Fig. 1. Based on the experimental observation in Ref. 6 and theoretical estimation in Ref. 12, an out-of-plane perturbation of 0.02 Å is applied to mimic thermal fluctuation. Unperturbed structures are also calculated as the references, which represent devices at 0 K. All structures are relaxed to obtain stable states of the devices. Bias voltage V_b is applied to investigate the transport properties based on the atomic coordinates after relaxation. Perturbed and unperturbed structures are compared under increasing strain ε to explore the generation and influences of buckling.

Our simulation is based on SIESTA package[13] and transport properties are studied using TranSIESTA module.[14] Exchange-correlation functional of Local Density Approximation (LDA) (Ceperley-Alder[15]) are used. A 200 Ry mesh cutoff is chosen. A double-ζ basis set is used. The convergence criterion for density matrix is 10^{-4}. A large spacing of 15 Å is imposed on y-axis direction to hinder interactions between adjacent supercells. Monkhorst-Pack k-meshes of $100 \times 1 \times 1$ are used to calculate the Hamiltonian for atomic relaxation. Structures are relaxed until the maximum force is less than 0.01 eV/Å. K-meshes of $800 \times 1 \times 800$ for electrodes and $800 \times 1 \times 1$ for scatting region are adopted to calculate transport properties.

To locate the threshold strain ε_T of buckling generation, total energy difference ΔE_{total} relative to non-strained structure and maximum out-of-plane displacement among all atoms ΔH_{max} with respect to flat graphene plane are depicted in Fig. 2. For Unperturbed Zigzag Compressed Graphene (UPZCG) and Unperturbed Armchair Compressed Graphene (UPACG), ΔE_{total} increases and ΔH_{max} remains near-zero versus increasing strain. This reveals that compression induced energy accumulates in C-C bonds while the unperturbed structures stay flat due to strong bending rigidity of graphene. Unperturbed flat graphene only exists at temperature of 0 K, which is regarded as a reference. When $\varepsilon > \varepsilon_T$ (2.7% for PZCG and 2.6% for PACG), ΔE_{total} has an abrupt reduction which indicates transition from an unstable state to a stable one. This is consistent with the instability of compressed graphene revealed in Refs. 7 and 8. Sharp increase of ΔH_{max} indicates that central atoms are pushed out of plane. The accumulated energy in compressing process is released by buckling. By contrast, changes of ΔE_{total} and ΔH_{max} for PACG at the threshold are notably larger than those of PZCG due to the larger length along z-axis (2.4 nm of PACG versus 1.35 nm of PZCG). In elastic mechanics, under the same strain, longer double-clamped (on electrodes) beam has larger displacement and thus is easier to generate buckling. The ε_T is larger than that in previous reports because of the smaller device length, based on the classical Euler's column equation.[7,16] The displacement-length ratios, 12.6% for PZCG and 9.4% for PACG, are close to 13.9% in Ref. 17 and 12% in Ref. 9.

To study the transport properties of graphene with or without buckling, transmission spectra at $V_b = 0.5$ V under different strains are calculated. As shown in Fig. 3(a),

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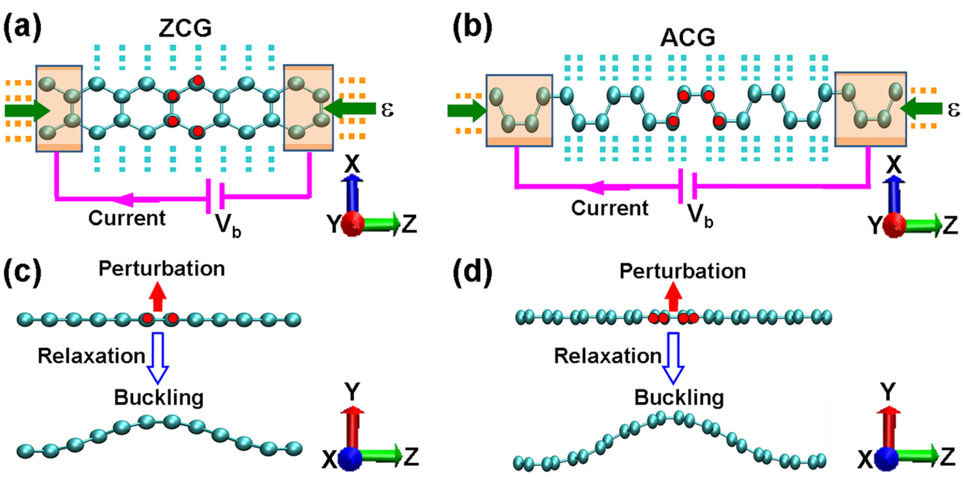

FIG. 1. (Color online) (a)-(b) Top views of ZCG and ACG. Compressive strain is labeled as ε. Periodic boundary conditions are imposed in x-axis direction. Semi-infinite electrodes (shadowed) are clamped and applied with V_b to calculate transport properties along z-axis. Thermal perturbations of 0.02 Å are applied on the middle 4 atoms overlapped with red circles. (c)-(d) Illustration of buckling generation in side views. Perturbed structures are relaxed and buckling occurs when ε exceeds the threshold strain ε_T.

transmission of UPZCG is nearly independent of strain, which resembles the zigzag GNRs that remain insensitive to high-level strain.[18] Transmission of PZCG drops considerably at ε_T of 2.7% and decreases further at strain level of 5%. Transmission difference (ΔT) between PZCG and UPZCG is negligible when $\varepsilon < \varepsilon_T$. When $\varepsilon > \varepsilon_T$, ΔT is negatively correlated to strain with the maximum of 0.007 at strain of 5%.

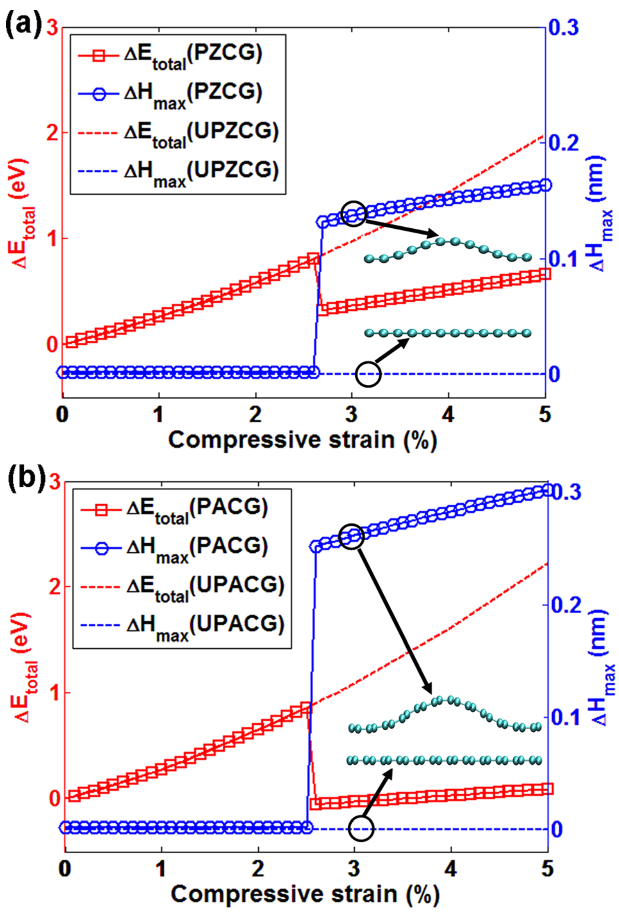

FIG. 2. (Color online) Total energy (ΔE_{total}) and maximum displacement ($\Delta H_{\max}$) of ZCG (a) and ACG (b) versus compressive strain. Perturbed or unperturbed structures are labeled with prefix "P" or "UP." Before the threshold strain is reached, ΔE_{total} and $\Delta H_{\max}$ of perturbed and unperturbed structures are identical. After the threshold is reached, abrupt changes of ΔE_{total} and $\Delta H_{\max}$ occur, indicating release of energy through bulking. Insets are the atomic positions after relaxation, which illustrate flat and buckled graphene, respectively.

The asymmetry of ΔT in positive and negative energy regions is also found in the transmission of arched GNRs in Ref. 19. It should be noted that this asymmetry does not influence our analysis. In Fig. 3(b), transmission of UPACG

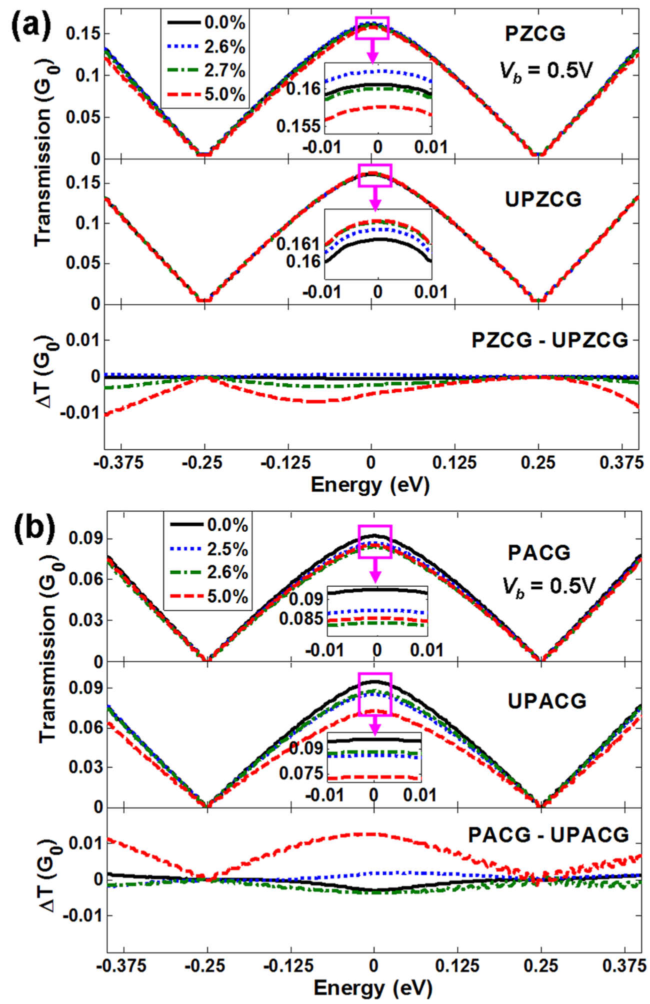

FIG. 3. (Color online) Transmission spectra of ZCG (a) and ACG (b) at $V_b = 0.5$ V under typical strain values: no strain, right before and after buckling threshold, and large strain (the percentage numbers). Insets are enlarged views near the Fermi level. Transmission differences between perturbed and unperturbed structures are represented as ΔT. Transmission of UPZCG is insensitive to strain, while that of PZCG is negatively correlated to strain when $\varepsilon > 2.7\%$. Transmission of UPACG is negatively correlated to strain, while that of PACG is insensitive to strain when $\varepsilon > 2.6\%$.

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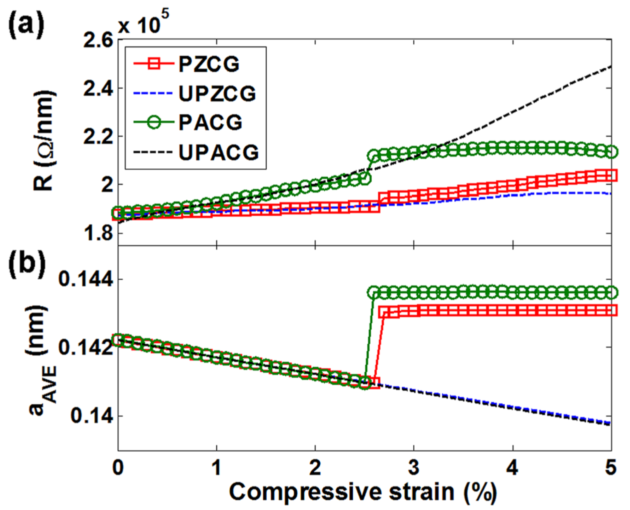

FIG. 4. (Color online) (a) Resistance per unit length (R) at $V_b = 0.5$ V versus compressive strain. UPZCG and UPACG have anisotropic R upon strain directions. While PZCG and PACG suppress the anisotropy after buckling occurs. (b) Average bond length (a_{AVE}) versus compressive strain. a_{AVE} of UPZCG and UPACG reduce linearly with strain while a_{AVE} of PZCG and PACG increase abruptly at buckling threshold. Energy stored in compression process is released through recovering bond lengths to low strain states.

decreases with increasing strain, especially near the Fermi level, which is consistent with the sensitivity of armchair GNRs upon strain.[18] Transmission of PACG is nearly unchanged when $\varepsilon > \varepsilon_T$ (2.6%). ΔT between PACG and UPACG fluctuates only within 0.003 when $\varepsilon < \varepsilon_T$. However, ΔT increases appreciably when $\varepsilon > \varepsilon_T$, with maximum of 0.012 at strain of 5.0%.

To compare ZCG and ACG with different lengths, resistance per unit length R of graphene devices versus strain is showed in Fig. 4(a). All results of R are consistent with the transmission spectra. R of UPZCG increases slightly upon strain while R of UPACG increases almost linearly by 39% at strain of 5%. The anisotropy between UPZCG and UPACG is attributed to the group velocity of π electrons. As in Ref. 10, group velocity along the strain direction changes more significantly with armchair configuration than zigzag one. Because transport current is positively correlated to group velocity, R has anisotropy on strain direction. These resemble the anisotropic *I-V* curves of arched GNRs in Ref. 19. In contrast, R of PZCG increases when $\varepsilon > \varepsilon_T$, while R of PACG changes abruptly at ε_T and then becomes insensitive to strain. With $\varepsilon > \varepsilon_T$, R of PZCG and PACG approach to each other due to that buckling releases the accumulated energy and recovers the bond lengths to less strain states. In Fig. 4(b), PACG has larger average bond length (a_{AVE}) than PZCG after buckling, confirming that PACG releases more energy. This makes R of PACG deviating from R of UPACG more pronouncedly after buckling. Comparing R of PZCG and PACG reveals that buckling can help suppressing the anisotropic resistance on strain direction. Because buckling is common in compressed graphene at room temperature, it hinders experimental measurement of the transport anisotropy. Besides, the maximum change of R through buckling is about 10% at strain of 5%. The relatively low sensitivity of resistance upon strain makes graphene an attractive material in a range of applications including flexible devices.

In summary, buckling of graphene under uniaxial compressive strain is studied. Buckling occurs when thermal perturbation is applied and strain exceeds the threshold. Transmission spectra versus strain depend on the strain value and direction. Resistance of flat graphene has anisotropy upon strain directions. However, when buckling occurs, strain-induced energy is released and reduced bond lengths recover, so that the resistances of ZCG and ACG approach to each other. The low sensitivity of transport properties on buckling makes graphene flexible devices more feasible without much concern about the out-of-plane deformations.

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