Experimental Demonstration of Electrically-Tunable Bandgap on 2D Black Phosphorus by Quantum Confined Stark Effect

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Abstract

We report that the bandgap of 2D few layer black phosphorus (BP) can be electrically tuned by applying a perpendicular electric/displacement field. The variation of bandgap is as large as 200 meV with 2V/nm displacement field. The bandgap modulation can be understood with the quantum confined stark effect within the SiO_2/BP/boron nitride (BN) sandwiched structure. This unique material property provides a new route to design and fabricate novel electronic and photonic devices based on black phosphorus.

Introduction

2D black phosphorus (BP) has recently attracted intensive research interests due to its unique properties such as anisotropic transport, high carrier mobility, and direct bandgap of 0.35-2eV, all of which are controlled by the layer thickness [1-3]. Surprisingly, a room temperature hole Hall mobility as high as 5000 cm^2/Vs is reported in BN/BP/BN van der Waals quantum well [4], which exceeds the theoretical limit [5]. Meanwhile, direct observation of its band structure modulation by angle-resolved photoemission spectroscopy experiments has shown that the bandgap of BP is tunable under strong electrical fields induced by potassium doping [6]. In this work, we are able to demonstrate the electrically tunable bandgap on BP by studying the effect of vertical displacement (D) field in BP through the dual gate devices. The variation of bandgap ($\Delta E_g=E_{g0}-E_g$) with the applied D field is investigated. A maximum ΔE_g of 200 meV has been observed with 4-8 nm thick BP, which explains the striking enhancement of BP mobility under the large gate biases.

Device Fabrication and Measurement

In order to form a 2D quantum well, few layer BP is sandwiched by global back gate (90 nm SiO_2) and local top gate (1.6 nm BN/4nm Al_2O_3, EOT ~ 4.5nm), as shown in Fig. 1. The fabrication process is similar to our previous work on high performance BP transistors [7]. In this work, BP thickness is from 2.5-8 nm with a bandgap around 0.45-0.9 eV. As shown in Fig. 2, the minimum drain current (I_{off}) is measured from I_d-V_g curves at different D field in order to extract the bandgap. The effective D field and ΔE_g can be calculated with the formula as shown in inset of Fig. 2 [8, 9].

There are two ways to apply the D field: (i) from the local top gate or (ii) from the global back gate. The difference is that the top gate can only modulate the channel region without changing the condition of source/drain contact while the back gate can modulate all regions. The band diagrams of the two measurement configuration are shown in Fig. 3 (a) and (b). Fig 4 (a) and (b) shows the transfer curves of BP FETs with D field applied by the global back gate. By electrically controlling the back gate voltage, either N or P type transport can be achieved. However, it is difficult to precisely define I_{off} and consequently E_g cannot be extracted in this measurement mode. The effect of source/drain metal (Ti, Ni, and Pt) on the transport behavior is shown in Fig. 5 and 6. The device shows entirely hole transport with Pt contacts while it becomes ambipolar transport with Ti contacts. Since the bandgap is extracted from I_{off} of the ambipolar transport, Ti is used for all devices below.

Results and Discussion

Fig. 7 shows the transfer curves of a 4 nm thick BP device with 200 nm channel length. A fixed D field is applied to the top gate when sweeping the back gate bias. The top gate voltage (V_{tg}) is from -3 to 3 V with an equivalent D field of 1 to -2 V/nm. At V_{tg} = 1V, the device shows the minimum I_{off} of 10^{-10} A/μm. At V_{tg} = 3V, the devices show the maximum I_{off} of $3.5*10^{-9}$ A/μm. Fig. 8 shows the I_{off} at different V_{tg} for devices with 4, 6, and 8 nm BP films. Generally, I_{off} increases with the increasing of the D field. Since I_{off} is reverse-exponentially dependent on E_g, it is observed that E_g decreases when the applied D field increases. Fig. 9 shows the change of ΔE_g with different D field for 4-8nm thick devices. E_g reduces more rapidly for thicker films due to the larger Stark effect coefficient (S_{nl}), i.e. $\Delta E_g/\Delta E=-e*S_{nl}$ [10, 11].

BP is known as an anisotropic material, which shows significant different electrical properties along armchair (X) and zigzag (Y) directions. Fig. 10 shows the transfer curves of a zigzag device with 7 nm thickness. It was reported that a Dirac cone can be formed only along the armchair X direction by degenerated potassium doping [6]. At small D fields, however, the anisotropic band-structure modulation induced by Stark effect is not profound. Fig. 11 shows the maximum achieved ΔE_g for thick devices, which is between 160-200 meV. For the 4 layer device, I_{off} is almost independent on V_{tg} as shown in Fig. 12. A much higher D field is required to observe the modulation of bandgap on thinner BP, which is beyond the dielectric breakdown field.

This bandgap narrowing and mobility enhancement effect on 2D BP channel can be understood with the quantum confined Stark effect [12]. As shown in Fig. 13, if the D field is applied to a quantum well, electrons and holes are pulled to the opposite sides of the quantum well, which can form bound-exciton. Due to the existence of D field, the potential energy of electrons are decreased while that of holes are increased. As a result, the effective bandgap is reduced. The band structure can even become inverted at an even larger D field as shown in Fig. 14, making BP in X direction like graphene.

Conclusion

Electrically tunable bandgap has been achieved on BP by applying an external D field to the dual gate devices. E_g can be reduced by 200 meV on 4-8nm BP devices. This unique property could be used for novel electric and photonic devices based on BP. The work is supported by AFOSR, NSF and ARO.

References

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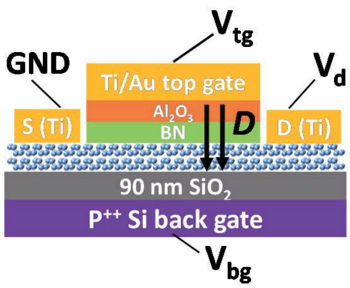

Fig. 1 Schematic diagram of the fabricated device. Few-layer BP is sandwiched between SiO_2 and BN/Al_2O_3 to form a 2D quantum well structure.

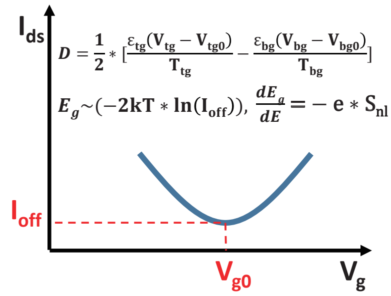

Fig. 2 Definition of I_{off} and V_{g0} in the ambipolar transport behavior. Inset shows the formula used to calculate effective displacement field and the change of bandgap.

$$D = \frac{1}{2} * \left[\frac{\varepsilon_{tg}(V_{tg} - V_{tg0})}{T_{tg}} - \frac{\varepsilon_{bg}(V_{bg} - V_{bg0})}{T_{bg}}\right]$$

$$E_g \sim (-2kT * \ln(I_{off})), \quad \frac{dE_g}{dE} = -e * S_{nl}$$

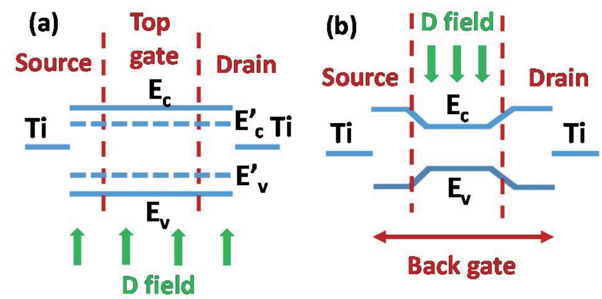

Fig. 3 Band diagram of dual gate devices with applied gate voltages: (a) the displacement field is induced by the global back gate and (b) the displacement field is induced by the local top gate. S/D region is not controlled by the top gate.

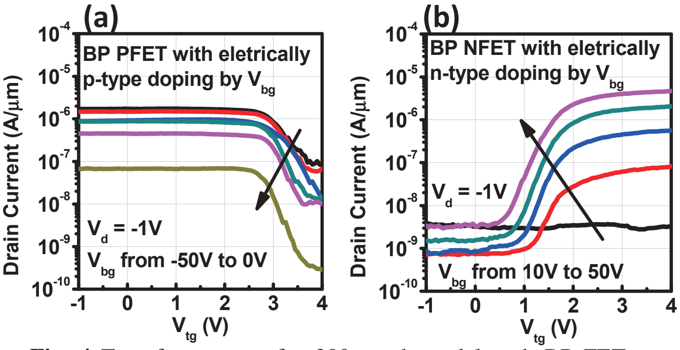

Fig. 4 Transfer curves of a 200nm channel length BP FET at different back gate bias. The device can be operated as a (a) PFET or (b) NFET. The p or n type doping is induced by the electrostatic doping from the back gate voltage.

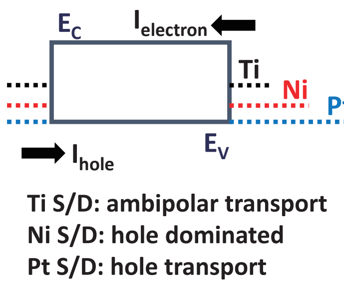

Fig. 5 Band diagram of a BP FET with different source/drain metals: Ti, Ni, and Pt.

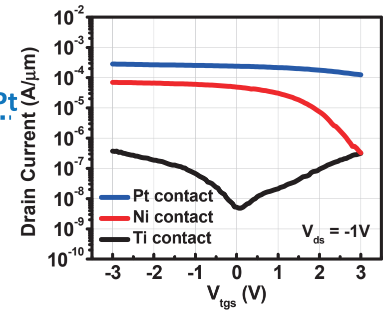

Fig. 6 I-V transfer curves of BP FETs with different contact metals: Ti, Ni, Pt. Ambipolar transport is achieved by using Ti contacts.

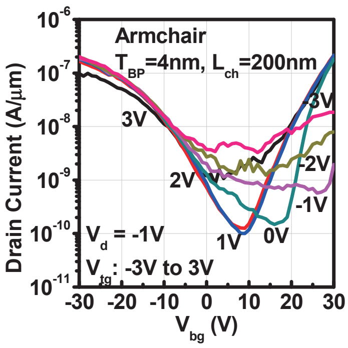

Fig. 7 Transfer curves of a 4 nm BP device at different top gate voltages. The displacement field is induced by top gate by applying a fixed top gate voltage when sweeping the back gate.

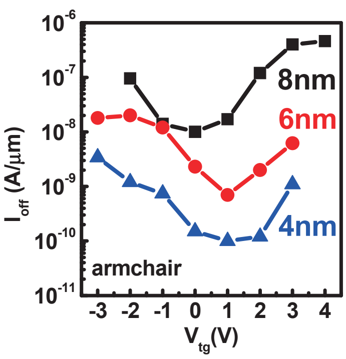

Fig. 8 Dependence of I_{off} on top gate voltage for the 4, 6, and 8 nm thick BP devices. I_{off} increases by a factor of 35-50 when the magnitude of top gate voltage (i.e. displacement field) increases.

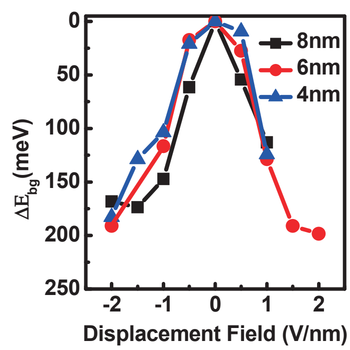

Fig. 9 The variation of bandgap at different displacement field for BP devices with thickness of 4, 6, and 8 nm. E_g reduces rapidly with electric field for thicker flakes.

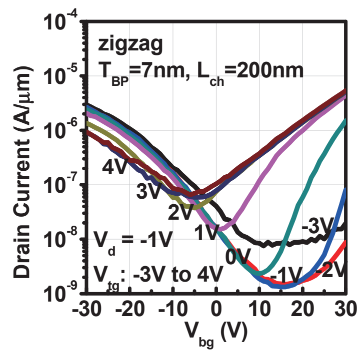

Fig. 10 Transfer curves of a dual gate BP device at different top gate voltages. I_{off} increases by a factor of 50 when the magnitude of top gate voltage

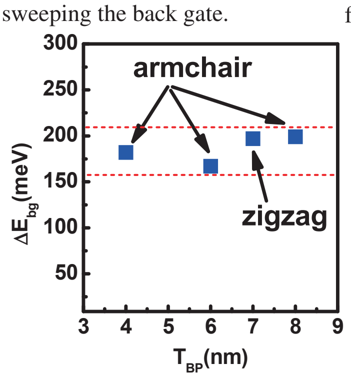

Fig. 11 The maximum variation of bandgap induced by displacement filed for devices with different thickness.

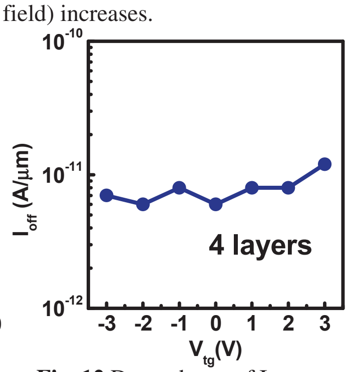

Fig. 12 Dependence of I_{off} on top gate voltage for the 4 layer (2.5nm) BP device. I_{off} is almost independent on the top gate voltage.

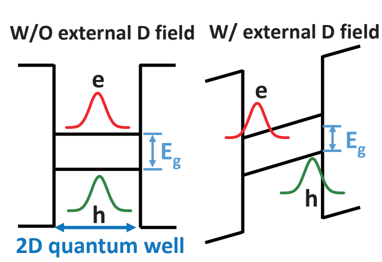

Fig. 13 Band diagram of a 2D quantum well structure with and without external displacement field. Band gap reduces due to the potential difference of electrons and holes.

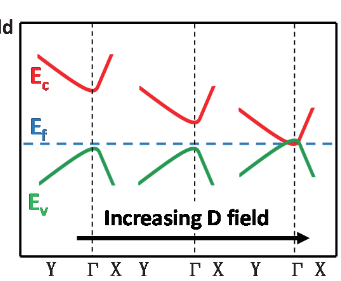

Fig. 14 Schematic of band structure evolution with the increasing displacement field. Band inversion occurs at a very large D field beyond the solid state dielectric can offer [9].