High performance self-gating graphene/MoS$_2$ diode enabled by asymmetric contacts

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Abstract

A graphene-MoS$_2$ (GM) heterostructure based diode is fabricated using asymmetric contacts to MoS$_2$, as well as an asymmetric top gate (ATG). The GM diode exhibits a rectification ratio of 5 from asymmetric contacts, which is improved to $10^5$ after the incorporation of an ATG. This improvement is attributed to the asymmetric modulation of carrier concentration and effective Schottky barrier height (SBH) by the ATG during forward and reverse bias. This is further confirmed from the temperature dependent measurement, where a difference of 0.22 eV is observed between the effective SBH for forward and reverse bias. Moreover, the rectification ratio also depends on carrier concentration in MoS$_2$ and can be varied with the change in temperature as well as back gate voltage. Under laser light illumination, the device demonstrates strong optoelectric response with 100 times improvement in the relative photo current, as well as a responsivity of 1.9 A W$^{-1}$ and a specific detectivity of $2.4 \times 10^{10}$ Jones. These devices can also be implemented using other two dimensional (2D) materials and suggest a promising approach to incorporate diverse 2D materials for future nano-electronics and optoelectronics applications.

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(Some figures may appear in colour only in the online journal)
based on 2D materials. A diode is one of the most important electronics devices with the main feature of rectifying output characteristics. Typical semiconductor diodes are mostly fabricated by selective doping techniques like diffusion or ion implantation of dopants. However, to fulfill the requirement of ultra-fast and low power modern electronics, channel size is reducing drastically, which puts severe limitations on the fabrication and doping techniques for sub-nanoscale devices. Therefore, multiple new configurations of diodes based on 2D materials have been proposed and studied. These studies include diodes fabricated using surface and plasma doping techniques [12, 13]. Liquid gates, asymmetric contacts and split gates have also been used to achieve diode operation in 2D materials [14–17]. Further, the van der Waal heterostructure of different 2D materials have also shown diode like properties. These heterostructures include BP/MoS2 [18], MoS2/WSe2 [19], InAs/WSe2 [20], and graphene/MoS2 (GM) [21]. Because of semimetallic nature of graphene, GM heterostructure based diodes show insignificant rectification ratio [20, 21], which is one of the most important parameter to determine the performance of a diode. This is because graphene form better contact with MoS2 as compared to high barrier metal contact and the device operates like Schottky diode due to this asymmetry in contacts. As both graphene and MoS2 are the most attractive 2D materials due to their interesting electrical, optical and energy band characteristics, therefore improving the performance of GM diode would find wide applications in electrical and optical devices. In this work, we have fabricated a GM diode by using different contacts materials to MoS2 flake i.e., graphene contact on one side and the metal contacts on the other side. The performance of the fabricated diode is further improved by incorporating an asymmetric top gate (ATG) to modulate the barrier height in sync with the polarity of the applied bias. After the incorporation of an ATG structure, the rectification ratio of the device increases from 5 to 105 and also affects the relative photo current, which shows a selective improvement of two orders of magnitude in this ATG-GM diode. The proposed configuration can also be implemented to improve the characteristics of diodes based on other 2D materials and heterostructures.

2. Results and discussions

Figure 1(a) is the schematic drawing of GM self-gating diode in which graphene contact is used on one side of MoS2 while metal (Cr/Au) contact is used on the other side. The device is fabricated by first exfoliating MoS2 from a commercial bulk crystal on a silicon substrate capped with 300 nm SiO2 using the standard mechanical exfoliation method. Similarly graphene is also exfoliated and suitable flakes are selected using optical microscope and transferred on top of MoS2 using the polymer assisted transfer technique. Electrodes pattern is made by electron beam lithography followed by metal (Cr/Au 10/30 nm) deposition in electron beam deposition chamber. Similar procedure is adopted to transfer h-BN on top of the device and the top metal gate, ATG, is deposited in such a way that it is connected with metal contact of MoS2 as well, as illustrated in figure 1(a). Graphene and MoS2 flakes were characterized by Raman spectroscopy using a 532 nm laser under ambient conditions as shown in figure 1(b). MoS2 Raman spectrum comprise of signature MoS2 peaks: E2g and A1g at frequencies of 383 cm−1 and 405 cm−1, respectively [22]. The difference of peak frequencies (22 cm−1) indicates that MoS2 thickness is more than four layers, [22] which is further confirmed by atomic force microscopy (AFM) and comes out to be 4.2 nm (six layers) as shown in figure S1, available online at stacks.iop.org/NANO/29/395201/mmedia. Likewise, the Raman spectrum of graphene is comprised of signature graphene peaks G and 2D, at frequencies of 1582 cm−1 and 2680 cm−1, respectively [23]. Graphene and h-BN thickness is also confirmed by AFM and comes out to be 1.5 nm (five layers) and 22 nm, respectively, as shown in figure S1. Further, MoS2 channel length and width are 7 μm and 3 μm, respectively.

Figure 1(c) is the output characteristics of GM device after h-BN transfer and before the deposition of the top gate at different back gate voltages, Vbg and a rectification ratio of ~5 can be seen in the current–voltage characteristics. This rectification is due to presence of asymmetric contacts to MoS2 layer, as the graphene contact exhibits less contact resistance compared to metal contact because of low barrier at the GM interface [24, 25]. However, after the deposition of top gate, GM device exhibits significantly higher asymmetry (Ion/Ioff) of 105 in the output characteristics, where Ion is the device current at Vd = −2 V and Ioff is the device current at Vd = 2 V as seen from figure 1(d). This increase in the rectification ratio after the deposition of top gate can be explained with the help of schematics in figures 2(a) and (b).

Figure 2 explains the mechanism behind the asymmetric transport based on the fact that under high drain voltage, the device current is mainly affected by the barrier at injection contact (source electrode only) [26, 27]. During forward bias, as shown in figure 2(a), the injection of electrons in MoS2 is from the graphene side, as the graphene electrode is negative while the other metal electrode is positive. The ATG will generate positive electric field to accumulate electrons in the MoS2 near the drain electrode, thus making it highly conducting. This accumulation of electrons in MoS2 combined with the injection of electrons from the less resistive graphene contact results in high channel current as shown in figure 2(a). During reverse bias, graphene electrode is positive while the metal electrode and ATG is negative. In this case, the injection of electrons in MoS2 is from metal electrode, however, because of negative bias, the ATG will generate negative electric field which leads to the depletion of electrons in MoS2. This depletion not only makes the channel more resistive but also results in increased effective Schottky barrier height (SBH) for electron injection. Although, for a particular metal and semiconductor, SBH is fixed, however, effective SBH can vary with the change in carrier concentration. This change in carrier concentration in the channel can vary the depletion width at metal–semiconductor interface which affects the injection of carriers. The carrier injection consists of three main components: thermionic emission, thermionic field emission and tunneling component, of which, the last two components vary exponentially with change in depletion width. This variation leads to an observed change in
Figure 1. (a) Schematic of the GM self-gating diode, (b) Raman spectra of MoS$_2$ and graphene, (c) output characteristics of GM diode before the incorporation of ATG (semi-logarithmic scale), (d) output characteristics of GM diode after the deposition of ATG (semi-logarithmic scale).

Figure 2. (a) Schematic and band diagram showing contacts polarity and electron accumulation in MoS$_2$ during forward bias, (b) schematic and band diagram showing contacts polarity and electron depletion in MoS$_2$ during reverse bias.
the measured SBH also known as effective SBH. Therefore, during reverse bias, resistive channel combined with increased effective SBH at metal–MoS2 interface results in highly reduced channel current as seen in figure 1(d).

We have further validated this explanation of variable SBH from the temperature dependent measurement by extracting the effective SBH during forward and reverse bias. The output characteristics of the device were measured at different Vbg, in a temperature range of 230–350 K. Equation (1) has been used to extract the effective SBH [26, 28]:

\[
I = A^* T^{3/2} \exp \left( - \frac{q\phi_b}{k_B T} \left( \exp \left( \frac{qV_d}{k_B T} - 1 \right) \right) \right). \tag{1}
\]

In this equation, \( I \) is the total current, \( A^* \) is the modified Richardson constant, \( \phi_b \) is the effective SBH, \( V_d \) is the drain voltage, \( q \) is the electron charge, \( k_B \) is Boltzmann constant and \( T \) is temperature in Kelvin. We measured the device current at different temperatures and the effective SBH is extracted from the slope of linear fit of \( \ln(I/T^{3/2}) \) versus \( 1/T \). The extracted values of effective SBH at different Vbg is shown in figure 3(a).

It can be seen from figure 3(a) that effective SBH for forward bias is much less than that of the reverse bias. This difference in effective SBH validates the previous explanation where rectification in the \( I-V \) characteristics has been attributed to the accumulation and depletion effect of ATG on the carrier concentration and thus the effective SBH. Another important observation in figure 3(a) is that effective SBH of forward as well as reverse bias reduces with an increase in Vbg. However, the rate of change for forward bias is less than that of reverse bias and therefore, the difference between the two also reduces with increasing Vbg. The difference in effective SBH for forward and reverse bias at Vbg = 0 V is around 0.22 eV, which reduces to around 0.12 eV at Vbg = 14 V. This is due to the fact that the increase in electron concentration in the channel with Vbg cancels out the increment in the effective SBH due to ATG, therefore the effective SBH decreases at a higher rate in the reverse bias (at the metal–MoS2 contact) as compared to forward bias (GM contact).

This trend also appears in figure 3(b), where the on/off ratio of the device substantially changes with variations in both temperature, as well as Vbg. The increase in either Vbg or temperature results in an increased electron concentration in the channel and subsequently, reduction of effective SBH. As shown in figure 3(a), an effective SBH in reverse bias is more sensitive to carrier concentration and reduces at a rate faster than that of forward bias. Therefore, the on/off ratio of the device also reduces with increasing temperature as well as Vbg, as seen in figure 3(b). This unique dependence of on/off ratio on the carrier concentration modulated by both ATG and back gate can also be utilized to improve the opto-electrical characteristics, where the carrier concentration is modulated by the photo-generated electron–hole carriers.

Figure 4 presents the relative photo current of device, which is an important parameter to evaluate the performance of any optical sensor. The GM device is illuminated by a light source of 655 nm and the relative photo current is obtained by first subtracting the dark current from total current under laser illumination and then dividing the difference with the dark current (\( I_{ph} = I_{laser} - I_{dark} \), where \( I_{laser} \) is total current under illumination). Before deposition of top gate, as shown in figure 4(a), relative photo current is of the order of 10^3. However, after the deposition of ATG, as shown in figure 4(b), relative photo current is increased to 10^5. As the illumination of laser results in the generation of electron–hole pairs in the MoS2, therefore, the carrier concentration in the channel increases under illumination and as discussed earlier, under high carrier concentration, the asymmetric gating effect of top gate becomes less effective. This results in high current flowing in device under reverse bias as well, which ultimately leads to higher value of relative photo current. This increase in relative photo current by 100 times in the same device after deposition of ATG, reflects the advantage of the proposed device for optoelectronics applications. Further, we have

**Figure 3.** (a) Effective SBH obtained from temperature dependent measurement at different back gate voltages during forward and reverse bias, (b) plot between rectification ratio of device and temperature at different back gate voltages.
calculated the responsivity and specific detectivity of our ATG-GM device, which are the key features of any optical sensor. The maximum obtained value of responsivity is 1.90 A W$^{-1}$ at $V_d = -2$ V, which is obtained from the ratio of the photo current to the incident laser power, $R = I_{ph}/P_{in}$ [12, 16, 20]. Specific detectivity is mostly used to determine optical sensor sensitivity and the maximum obtained value of detectivity is $2.4 \times 10^{10}$ Jones, calculated by using $D^* = A^{1/2}/\text{NEP}$, where $A$ is the illuminated area and NEP is the noise equivalent power, $\text{NEP} = (2qI)^{1/2}/R$.

3. Conclusions

In conclusion, we have demonstrated the operation of a doping free self-gating diode where high rectification ratio is achieved by asymmetric modulation of carrier concentration and effective SBH by the top gate. The rectification ratio of the device varies with carrier concentration in MoS$_2$ and can be controlled by changing temperature and back gate voltage. The ATG-GM device also evinces a strong opto-electric response, when illuminated by light source, and a 100 times improvement has been observed in relative photo current compared to the pristine GM heterostructure.

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