Two-dimensional Beyond Graphene: Applications of Atomically Thin Transition Metal Dichalcogenides

Minjeong Shin Literature Seminar October 15, 2015

The mechanical exfoliation of graphene from graphite in 2004 showed that two-dimensional materials can exist in a free-standing form.[1] Graphene, a single layer of carbon atoms, has received great interest due to its interesting properties, such as ultra-high charge carrier mobility, good thermal conductivity, and excellent mechanical strength.[2] However, graphene is a poor fit for digital electronics because of its gapless band structure. For instance, graphene-based field-effect transistors (FETs) cannot be effectively switched off and therefore have a small current on/off ratio, which makes it impractical to be used for conventional transistors or logic circuits. During the past few years, semiconducting two-dimensional transition metal dichalcogenides (TMDCs) with sizable band gaps around 1-2 eV have been extensively studied for their potential applications in digital electronic devices, optoelectronics, memory devices, and sensors.[3,4]

TMDCs are a class of materials with the formula of MX_2, where M is a transition metal element from groups IV-VII and X is a chalcogen (S, Se, or Te). TMDCs form layered structures with chalcogen atoms in the two hexagonal planes separated by a plane of metal atoms (**Fig. 1**). Adjacent layers are weakly held together by van der Waals force to form a bulk crystal. The electrical properties of TMDCs vary from metallic to semiconducting. In particular, molybdenum and tungsten-based TMDCs are semiconductors with band gaps ranging from the visible to near-infrared range of the electromagnetic spectrum.[6] In several semiconducting TMDCs, layer-dependent properties are found when the size of TMDCs reaches a two dimensional regime. For instance, the band gap of monolayer MoX_2 and WX_2 changes from an indirect band gap that is found in bulk to a direct band gap as a result of quantum confinement.[4,5] The direct band gap results in the enhancement of photoluminescence, which allows the potential use of TMDCs in optoelectronic device applications.[7]

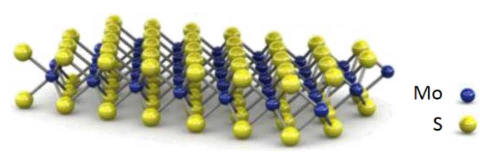

Figure 1. Lattice structure of MoS_2 monolayer, a representative example of transition-metal dichalcogenides.[12]

MoS_2 is a typical semiconductor from the family of TMDCs. Similar to graphite, the MoS_2 bulk crystal is naturally abundant and neighboring layers are weakly bound together, facilitating the mechanical cleavage when preparing atomically thin MoS_2 nanosheets.[4,8] The band gap of MoS_2 can be tuned by varying the number of layers. Bulk MoS_2 crystal has an indirect band gap of 1.2 eV, whereas monolayer MoS_2 has a direct band gap of 1.9 eV.[5] The wide band gap of monolayer MoS_2 suggests that it could be a promising material for digital electronic applications including transistors.[9] Among other TMDCs, WSe_2 is one of the most widely studied materials.[2] The study of WSe_2 is mainly focused on optoelectronic applications because it is flexible[10], nearly transparent[11], and has a direct band gap[11] therefore meeting all the criteria for next generation optoelectronic materials.

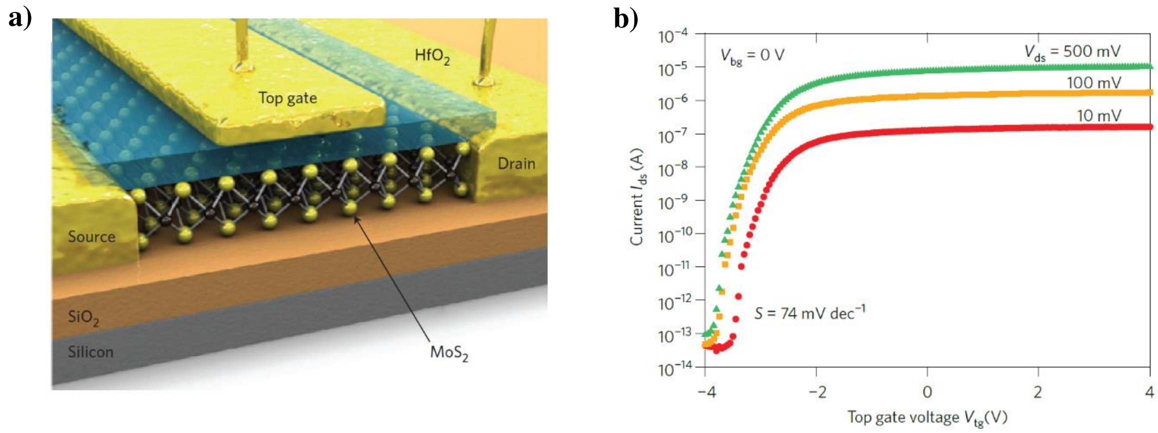

Figure 2. a) Schematic of HfO_2-top-gated monolayer MoS_2 FET device. **b)** Source-drain current (I_{ds}) versus top gate voltage (V_{tg}) curve for a bias voltage ranging from 10 mV to 500 mV.[12]

One of the most important applications of semiconductors is transistors for digital electronics. The desirable properties for digital logic transistors are high charge-carrier mobility for a fast device operation and a high on/off ratio for effective switching.[4] Unlike in gapless graphene, the large band gap of monolayer MoS_2 allows high on/off ratio to be achieved. In 2011, Kis and coworkers first reported the implementation of a top-gated field-effect transistor based on monolayer MoS_2 (**Fig. 2a**). The device exhibits an excellent current on/off ratio of 1×10^8 (**Fig. 2b**) and a room temperature electron mobility of > 200 $cm^2v^{-1}s^{-1}$, comparable to the mobility achieved in silicon films or in graphene nanoribbons.[13,14] The two-dimensional channel and a top gate dielectric coupled with a wide band gap enabled a superior gate control, achieving a small off-state current and a large on/off ratio.[12]

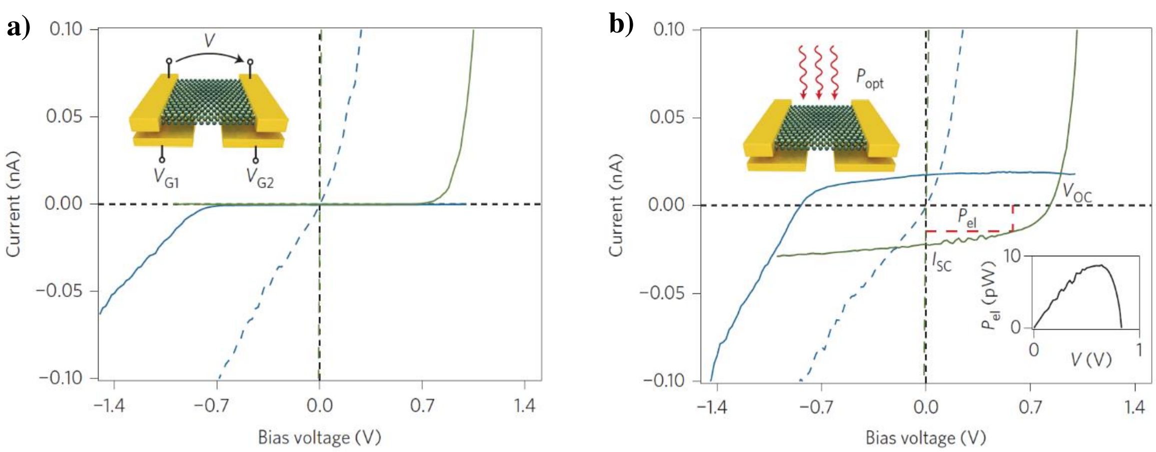

Figure 3. a) *I-V* characteristics of the device in the dark for biasing conditions as shown in the inset: p-n (solid green line; V_{G1} = - 40 V, V_{G2} = 40 V), n-p (solid blue line; V_{G1} = 40 V, V_{G2} = - 40 V), n-n (dashed green line; V_{G1} = V_{G2} = 40 V), p-p (dashed blue line; V_{G1} = V_{G2} = - 40 V). **b)** *I-V* characteristics of the device under optical illumination with 1400 Wm^{-2}. The biasing conditions are the same as in a). Lower inset: Electrical power (P_{el}) versus voltage under illumination with 1400 Wm^{-2}.[15]

Another use of the semiconductor technology is in the fabrication of optoelectronics. Optoelectronic devices are the ones that can generate, detect, and interact with light. Since the band structure of semiconductors directly influences the ability of the material to absorb and emit light, direct band gap semiconductors are desirable in optical devices due to higher absorption efficiencies. The direct band gap in monolayer TMDCs make them a great candidate for optoelectronic devices. Pospischil *et al*. have demonstrated the use of a p-n junction diode based on electrostatically doped WSe_2 monolayer in a photovoltaic solar cell, photodiode, and light-emitting diode. By applying gate biases of opposite polarity, a p-n junction diode is formed and it clearly shows rectifying behavior (**Fig. 3a**). Under optical illumination, the characteristic *I-V* curve of a p-n configuration shifts down due to the photocurrent generated (solid green line in **Fig. 3b**). As the device produces both current and voltage, electrical power (P_{el}) can be extracted. The maximum power achieved by WSe_2 is 9 pW at 0.64 V. The power conversion efficiency, which is the percentage of the incident light energy converted into electrical energy, was calculated to be $\eta_{PV} \approx 0.5\%$. The p-n junction diode demonstrates the potential of monolayer WSe_2 for novel optoelectronic applications.[15]

Through recent efforts, significant progress has been achieved in applications of two-dimensional semiconducting TMDCs. However, the factors affecting carrier mobility and device performance are not fully understood requiring more experimental and theoretical study.[16] Also, a scalable method to prepare large amounts of high purity sample is required before practical application of these devices.[17]

References

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