Properties of Different Structures of 2D MoS_2 and Their Applications in Solar Cells, Photodetectors and Transistors

Yuhang Zhou

The Chinese University of Hong Kong, Shatin NT 999077, Hong Kong
1155173844@link.cuhk.edu.hk

Abstract. Molybdenum disulfide (MoS_2) is a promising two-dimensional (2D) nanomaterial to substitute graphene, with unique adjustable bandgap and distinctive structure. Among all 2D transition-metal dichalcogenides (TMDs), MoS_2 is extremely advantageous due to its natural layered structure. High-quality 2D MoS_2 can be obtained by mechanical peeling, instead of complex chemical synthesis process. It has many applications in different fields, such as photodetectors in optical field, solar cells in energy applications, and transistors in electronics. The absorption of solar energy by monolayer MoS_2 solar cells is one order of magnitude higher than that of silicon. Photodetectors based on MoS_2 heterojunctions offer much faster charge transfer and photoresponse, with more functionality than a single detector. MoS_2 can be used to construct interband tunnel field-effect transistors (FETs) with lower power consumption. The different MoS_2 structures, including the bulk, monolayer, few layer and multi-layer, will be discussed in this work, with a focus on their applications on solar cells, photodetectors and transistors.

Keywords: Molybdenum disulfide (MoS_2), Two-dimensional (2D), Solar cells, Photodetectors, Transistors.

1 Introduction

The shrinking size of transistors based on silicon is quickly approaching to its fundamental limit. When the channel length gets closer to the depletion layer width, it faces challenges of short-channel effects in MOSFET and high heat dissipation level. Therefore, exploring new materials for channels and create new device architectures beyond classical electronics based on silicon is urgent.

Researchers were searching for alternative semiconductor materials, since silicon-based devices appear to be reaching the end of the road at the nanoscale. Silicon transistors has narrow metal interconnection lines with high density between them, which is a big problem to be solved. They increase the value of the resistance and capacitance between and lead to high latency. For thin gate oxides, tunneling problems are more serious. However, if substituted with other high-K dielectric

Y. Yue (ed.), *Proceedings of the 2024 International Conference on Mechanics, Electronics Engineering and Automation (ICMEEA 2024)*, Advances in Engineering Research 240,
https://doi.org/10.2991/978-94-6463-518-8_10

materials, the diode performance will be degraded due to poor thermal instability, channel mobility, and interface compatibility.

Compared with previous devices, MoS_2 appears to solve many of the problems faced by electronic devices. Its large band gap converts in thin thickness. The direct band in thin structures of MoS_2 allows the fabrication of electronic devices with smaller size, unlike semiconductor materials with no band gap or indirect band gap. Additionally, even with materials of high-K dielectric, MoS_2 still has high mobility, making it suitable for fabricating thin-film transistors (TFT). Furthermore, as a 2D material, MoS_2 has long-range order and anisotropy. It can be manipulated to get various shapes or sizes, and obtain unique crystal structures through surface modification. Due to its excellent switching characteristics together with the high efficiency in on/off shifting, MoS_2 also has potential for use in 1 nm gate transistors. Compared to semiconductor devices based on silicon, 2D MoS_2 has better performance for electronic and quantum properties.

2 Properties of MoS_2 of Bulk, Multi-layer, Few Layer and Single Layer

2.1 Basic Properties of MoS_2

Two-dimensional MoS_2 attracts great research interest for its exceptional properties and diverse potential. It exhibits promising applications in optoelectronics even compared to graphene. MoS_2 belongs to the family of TMDCs. The interior of each S-Mo-S layer is bonded by covalent bonds, while the layers are held together by weak van der Waals forces. Due to its robustness, MoS_2 is outstanding in the family of TMDCs. MoS_2 can be mechanical peeled to obtain high-quality 2D MoS_2 due to its natural layered structure.

2.2 Basic Property of MoS_2 Range from Bulk, Multi-layer, Few Layer and Single Layer

The energy band structure of MoS_2 varies with the number of layers. Its band gap energy has different values for different structures. There exists a crossover between the indirect gap and the direct gap. The material has a hexagonal crystal structure with closely packed S-Mo-S atoms. However, for adjacent layers, it is weak van der Waals forces hold them together. Therefore, these layers can be peeled off mechanically into several 2D monolayers.

Bandgap. MoS_2 exhibits special properties for different thickness. Significant bandgap transitions occur during the transformation from bulk to monolayer, leading to excellent photoelectric properties. When it thinned into a single layer, the band structure becomes a direct band gap, which attracted great interest in the electronic and optoelectronic field.

As a layered semiconductor material, MoS_2 has different structures and band gaps for various numbers of layers. The value of band gap ranges from 1 to 2 eV. While bulk MoS_2 has an indirect band gap of 1.29 eV, the band gap of multi-layer MoS_2 ranges from 1.29 eV to 1.90 eV: monolayer MoS_2 (1.64 eV direct bandgap), bi-layer (1.17 eV indirect gap) and trilayer MoS_2 (1.08 eV indirect gap).

Under pressure, the electronic structure of band gap is controlled by the bond angle, while interlayer coupling controls electronic structure for multilayer and bulk MoS_2. The dielectric environment can also affect the band gap of monolayer MoS_2, resulting in the band gap change from 2.8 eV to 1.9 eV. Compared to monolayer, the band gap of multilayer MoS_2 gradually decreases with the number of layers increasing, but its field effect mobility and current density increase accordingly.

Mobility. The mobility of bulk semiconductors decreases rapidly with film thickness. However, with channel width much larger than its thickness, the corresponding effect on mobility can be ignored. Therefore, 2-D MoS_2, particularly in monolayer and bi-layer cases, is still very competitive.

The synthesized MoS_2 is hexagonal or rectangular with metallic luster, with a carrier concentration at room temperature around $10^{15}cm^2$. And it typically behaves as N-type, while P-type can be obtained through doping. Compared with the mobility of bulk MoS_2 (200-500$cm^2/(Vs)$), the mobility of monolayer MoS_2 sheets are relatively low (0.5-3$cm^2/(Vs)$) [1]. Therefore, in the aspect of improving device performance, multilayer MoS_2 is a better material than monolayer MoS_2. For thin MoS_2, it has a linear relationship for transport characteristics. In contrast, thick MoS_2 has diode characteristics, which constructs p-n junction in multi-layer MoS_2 sheets [2].

Optoelectronic Properties. The intrinsic MoS_2 has different advantages in its optoelectronic properties, which are related to its thickness. Due to its large direct band gap, monolayer MoS_2 film has the ability to produce strong photoluminescence and electroluminescence. Multilayer MoS_2 behaves as the p-type in the dark, while it behaves as the n-type under light illumination [2].

Due to the outstanding thickness-dependent optoelectronic properties, MoS_2 is considered as a good material for photodetectors and transistors. The optical properties of single MoS_2 layers depends on their yield. The excitonic states in MoS_2 vary with dopant concentrations, resulting in changes in photoluminescence spectroscopy (PL) intensity under different conditions. The strong peaks in the visible range spectrum of monolayer MoS_2 indicated that it could enhance the light-capturing properties [3].

Among all structures, only monolayer MoS_2 has a direct bandgap, so semiconductors with this structure have high luminous efficiency [4]. Transistors based on monolayer MoS_2 has high on/off current ratios of 10^8 together with ultra-low standby power consumption. It also has many excellent properties for photodetection, including high broadband gain and detectivity which is up to 10^{10} $cm(Hz)^{1/2}/W$ [5]. Phototransistors based on monolayer MoS_2 exhibit high photoresponsivity (~2200 AW^{-1}) together with fast photoresponse time (~40 us), indicating an evident photovoltaic effect [5]. Few-layered MoS_2 photodetectors can satisfy harsh electronic applications, which can operate at 200°C [5].

3 Applications of MoS_2

3.1 Molybdenum Disulfide Based Solar Cells

Monolayer MoS_2 has great application potential in solar cell with effective absorption in the range of visible light (~10%). It is an order of magnitude higher than silicon at the nanoscale. The bandgap of MoS_2 changes from the bulk form into the monolayer, making it highly configurable. As the number of MoS_2 layers reducing, quantum confinement occurs, which leads to a higher band gap, resulting in improved capability of light harvesting and larger extinction coefficients.

With a promising potential for absorption and conversion of solar energy, 2D monolayer MoS_2 is ideal choice as the sunlight absorbers in ultrathin photovoltaic (PV) devices. MoS_2 monolayers can capture most of the incoming sunlight in the range of visible light with subnanometer thickness. Monolayers of MoS_2 can absorb up to 5-10% of sunlight it receives, even if it is less than 1 nm thick, which is equivalent to silicon with the thickness of 50 nm [6]. Monolayer MoS_2 has high carrier mobility (~200 $cm^2/(Vs)$), which can create photovoltaics having extremely low resistance in series with large voltages. Photovoltaics has near-optimal I-V curves, making them appealing for PV applications [6].

For solar cells based on MoS_2, it can achieve 1% of power conversion ratio with active layer of only 1 nm thickness consisted of two stacked monolayers like graphene or WS_2 [6]. Even with conservative assumptions, the power conversion efficiency of these solar cells can reach up to 1% within the thickness of 1nm, enabling a pretty high level of power density [6].

3.2 MoS_2 Photodetectors

The layered MoS_2 shows great properties in various optoelectronic and photovoltaic fields. It has tunable band gap together with high electron mobility. Therefore, it is suitable for the use of MoS_2 in photodetectors and photovoltaics applications.

MoS_2 holds great promise in optoelectronic applications for its optical activity in the visible light range. In the monolayer limit, optical absorption of MoS_2 for visible light is dominated by direct transition. The optical property of the materials is determined by exciton formation. When MoS_2 is exposed under illumination with photon energies greater than its bandgap, it absorbs photons and generates electron-hole pairs that can move under electric field. MoS_2 exhibits a strong light-matter interaction, resulting in a high absorption coefficient that can reach approximately 10^6/cm. This superior light absorption, combined with its good mobility and the ability to fabricate very thin layers, makes it a suitable material for building photodetectors based on very thin layers. Meanwhile, it still maintains high light conversion efficiency.

3.3 Molybdenum Disulfide Transistor

Monolayer MoS_2 has a direct band gap that enables the construction of interband tunnel FETs with reduced power consumption. Moreover, its thinness, transparency, and semiconducting properties make it a promising material for several fields such as mesoscopic physics, optoelectronics, and energy harvesting. Additionally, MoS_2 can be used alongside graphene for the requirement of thin transparent semiconductors, like the field of optoelectronics and energy harvesting. Organic conductors are easy to process, but their performance figures are lower than silicon-based electronics. However, MoS_2 monolayers offer comparable mobility to graphene nanoribbons, with even higher bandgap and smaller thickness than the thinnest silicon films that have been made so far. The direct gap of monolayer MoS_2 makes it possible to create interband tunnel FETs. These transistors conduct faster than classical transistors, resulting in lower power consumption. While for silicon, as an indirect gap semiconductor, it is still challenging to create interband tunnel FETs.

2D monolayer MoS_2 has been used as a conductive channel in a FET, with a thickness of only 6.5 Å. This transistor has a high mobility (200 $cm^2V^{-1}s^{-1}$) under room temperature, which is comparable to the mobility in thin silicon films [7]. Additionally, it has a large switch current ratio (over 1×10^8), making it an excellent candidate for future electronic devices. It is an important step towards realizing the integrated circuits with low standby power based on 2D materials.

4 Challenges

The challenges faced in the development of MoS_2 are discussed below. MoS_2 has broad prospects in the electronics and optoelectronics fields in the "post-Moore" era, as a two-dimensional nanostructured material. However, MoS_2 still faces some challenges in its application. Although the MoS_2 bandgap value is good, it is still at a disadvantage when compared with silicon (1.12 eV direct bandgap). And since MoS_2 has lower mobility (30-60 cm^2/Vs) than that of silicon (~1000 cm^2/Vs), the contact resistance of CMOS based on MoS_2 is still 1 to 2 orders of magnitude higher than silicon [8]. In addition, although MoS_2 has outstanding optical, electronic and optoelectronic properties, its preparation and performance improvement still require further development. For the aspect of synthesis and manufacturing, there are two main challenges. Firstly, synthesizing MoS_2 with the largest yield without altering its chemical and physical properties is one area of study. Another challenge is how to fabricate different 2D structures with high quality and at large scale, which is critical for final industrial application. Therefore, it is desired to further improve CVD technology to make material growth involving solid precursors more controllable [9]. We also need to gain a deeper understanding of CVD growth mechanism and further studies on crystal growth kinetics. As for the performance improvement aspect, the characteristics of semiconductor devices are one of the top priorities among all. Despite significant advances, the performance of 2D FETs based on MoS_2 still can not match their most advanced product based on Silicon. To enable the application of 2D MoS_2 in ultra-thin and ultra-short CMOS electronics, the interface engineering of 2D MoS_2 is necessary to be solved, specifically in the aspects of optimizing the contact and tuning the properties [10]. Firstly, it is highly desirable to obtain ohmic contacts with low contact resistance between metal and MoS_2, since it curbs the drain-source current and becomes a limitation for size reduction of devices based on 2D MoS_2 [10]. Secondly, it is not applicable for the classical doping techniques of CMOS logic circuits based on silicon to be applied on thin MoS_2 films with atom-thickness. This ion implantation processes used in doping has high energy, which can damage the structure and degrade performance of the fragile MoS_2 [10].

5 Conclusion

In this review, the properties of different structures for MoS_2 and their application in various fields are discussed. A comparison of the optical, electronic, and optoelectronic properties among all structures are highlighted, including band structure, bandgap energy, light absorption, light emission, and their applications. A summary of the MoS_2 applications on solar cells, photodetectors, and transistors was also made. This work will contribute to promoting the research and application of MoS_2.

References

1. Mingsheng Xu, Tao Liang, Minmin Shi, and Hongzheng Chen: Graphene-Like Two-Dimensional Materials. Chemical Reviews 113(5), 3766-3798 (2013)
2. Xuying Zhong, Weichang Zhou, Yuehua Peng, Yong Zhou, Fang Zhou, Yanling Yina, and Dongsheng Tang: Multi-layered MoS_2 phototransistors as high performance photovoltaic cells and self-powered photodetectors. RSC Advanced 5(56), 45239-45248 (2015)
3. Al-Ghiffari, Abu Dzar, Norasikin Ahmad Ludin, Matthew L. Davies, Rozan Mohamad Yunus, and Mohd Sukor Suait: Systematic review of molybdenum disulfide for solar cell applications: Properties, mechanism and application. Materials Today Communications 32, 104078 (2022)
4. Sergii Golovynskyi, Oleksandr I. Datsenko, Dan Dong, Yan Lin, Iqra Irfan, Baikui Li, Danying Lin, and Junle Qu: The Journal of Physical Chemistry C 125(32), 17806-17819 (2021)
5. Meng-Lin Tsai, Sheng-Han Su, Jan-Kai Chang, Dung-Sheng Tsai, Chang-Hsiao Chen, Chih-I Wu, Lain-Jong Li, Lih-Juann Chen, and Jr-Hau He: Monolayer MoS_2 heterojunction solar cells. ACS nano 8(8), 8317-8322 (2014)
6. Bernardi, Marco, Maurizia Palummo, and Jeffrey C. Grossman: Extraordinary sunlight absorption and one nanometer thick photovoltaics using two-dimensional monolayer materials. Nano letters 13(8), 3664-3670 (2013)
7. Radisavljevic, B., Radenovic, A., Brivio, J. et al: Single-layer MoS_2 transistors. Nature nanotechnology 6(3), 147-150 (2011)
8. Samy O, Zeng S, Birowosuto MD, El Moutaouakil A: A Review on MoS_2 Properties, Synthesis, Sensing Applications and Challenges. Crystals 11(4), 355 (2021)
9. Ye, Z., Tan, C., Huang, X. et al: Emerging MoS_2 Wafer-Scale Technique for Integrated Circuits. Nano-Micro letters 15(1), 38 (2023)
10. Liao, Wugang and Zhao, Siwen and Li, Feng and Wang, Cong and Ge, Yanqi and Wang, Huide and Wang, Shibo and Zhang, Han: Interface engineering of two-dimensional transition metal dichalcogenides towards next-generation electronic devices: recent advances and challenges. Nanoscale horizons 5(5), 787-807 (2020)