Research progress on the application of two-dimensional layered semiconductors in optoelectronic devices

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Abstract. In recent years, traditional 2D layered materials such as graphene have been widely used in the photoelectric area. As the emerging research and development of 2D layered materials, there are more and more newly developed 2D layered semiconductors being applied to this field, such as MoS_2, phosphorene, and other nanomaterials. 2D layered MoS_2 can be utilized as sensitive elements to obtain high-performance photodetectors with high responsivity, high current response rate, and short recovery time. Moreover, because phosphorene has adjustable bandgap width and strong light absorption, it has more potential in aspects of other semiconductors, and application in photoelectric devices. This article introduced the structures of some common 2D layered semiconductors, discussed their applications in photoelectric fields, and pointed out their limitations. For example, transition metal dichalcogenide (TMDC) materials generally have low carrier mobility, and black phosphorus is prone to adsorb water molecules from the air, leading to changes in its physical and chemical properties. Finally, improvement methods of applications and prospects for future development were provided.

Keywords: 2D Semiconductors, Transition Metal Dichalcogenides, Black Phosphorous, Optoelectronic Devices

1. Introduction

As people search deeper and deeper into two-dimensional layered materials, more and more of them are widely used in the photoelectric field such as photodetectors, light emitting diodes (LEDs), etc. However, as the number of integrated components on a semiconductor chip per unit continues to increase, traditional silicon-based substrate integrated circuit components face challenges when their size is reduced to a certain level. Issues such as short-channel effects and leakage losses hinder the development of integrated circuits. However, two-dimensional layered semiconductors overcome these problems by changing the structure of integrated circuit components, such as adopting a three-dimensional structure to improve device performance.

Also, due to the poor light absorption and limited spectral response of traditional two-dimensional materials, their application has been hindered [1]. This is because their low optical response performance is caused by their thickness, and their quantum yield limits their effective use in optoelectronic devices

[1]. It has been reported that monolayer graphene, with a thickness of 0.34 nm, can only absorb 2.3% of light in the visible and near-infrared regions [2].

The representative of two-dimensional materials, MoS_2, has a structure of a hexagonal crystal system. The structure of MoS_2 is good for the accumulation of its nanosheets in 3D structures so that an interlaced grid frame can be formed, providing convenience for the transfer of protons and electrons [3]. Less-layer indium selenide materials with hexagonal structures have a band gap of 1.3 eV and a wonderful electronic performance, which is expected to have a significant impact on the development of future photoelectric devices [4].

Many kinds of 2D layered semiconductor materials, with the efforts of generations of researchers, have gradually become the essential aspect of logic optoelectronic devices and supported the research and development of the devices. 2D layered semiconductor materials, as the materials to affect the core sensitivity of sensor components, have played an irreplaceable role in the preparation process of sensor components [5].

Now the researches on this field are mainly focusing on theories, but there are still some difficulties with the application. For instance, the material synthesis technology is not mature enough, the large area and high-quality preparation of 2D layered semiconductor is still facing challenges; the device manufacturing process is waiting for further optimization, the control of interface and defect density is not ideal; convert efficiency and response speed aspects are needing improvements. The traditional methods for preparing two-dimensional layered semiconductors mainly include gas-phase methods and liquid-phase methods. The gas-phase method has the disadvantage of requiring complex and expensive reactors or vacuum systems, and it has low deposition efficiency. The liquid-phase method has mild reaction conditions, and the resulting products are often amorphous or have low crystallinity. The chemical composition is easier to control, but the post-treatment process is more complex. The solid-phase method requires high reaction temperatures, and it is prone to the formation of polycrystalline phases, with a more complex post-processing procedure. This article compared the optoelectronic corresponding mechanism of several kinds of classical 2D layered semiconductors, designed and achieved photodetector based on 2D materials, and discussed the essential factors influencing the photoelectric conversion efficiency.

2. Photoelectric properties of 2D semiconductors

2.1. Transition metal dichalcogenides (TMDCs)

TMDCs are represented by the general formula MX_2, MX, or M_2X_3 where M stands for transition metal elements and X represents chalcogen elements [6]. Each TMDC layer consists of a layer of transition metal atoms M and chalcogen atoms X. Weak van der Waals forces stack these layers together. The bonding between metal and chalcogen atoms is primarily covalent, and most TMDC materials are stable in a 2H (hexagonal) crystal structure. Among TMDCs, MoS_2 is the most extensively studied member, exhibiting impressive optoelectronic properties. Its structure is illustrated in Figure 1. It has a wide optical absorption range covering visible to infrared light, with absorption coefficients as high as 5-10%. In terms of electrical properties, monolayer molybdenum diselenide ($MoSe_2$) possesses a high charge carrier mobility, resulting in excellent electroluminescent effects. It has optical characteristics similar to MoS2 but with a light response range that extends closer to the near-infrared region. The light absorption mechanisms of these materials are akin to those of TMDCs and black phosphorus, all exhibiting high-efficiency photovoltaic conversion. The TMDC family also includes various components such as tungsten disulfide (WS_2) and $MoSe_2$. The bandgap properties of TMDCs undergo significant changes from monolayer to multilayer forms. Specifically, monolayer TMDCs have a direct bandgap of approximately 1-2 eV, whereas multilayer TMDCs exhibit an indirect bandgap with a narrower bandgap width. This is the result of the increased layer interactions, leading to changes in the electronic structure. Monolayer TMDC materials have an exceptionally high optical absorption coefficient, reaching 5-10%, far exceeding traditional semiconductor materials. This is attributed to their unique particle-hole transitions resulting in strong light absorption. The absorption peaks can be tuned

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by controlling the number of layers. Under optical excitation, electron-hole pairs in TMDCs can undergo recombination within a fraction of a picosecond. The recombination process is influenced by spin-valley interactions, resulting in a pronounced valley polarization effect. Carrier lifetime is also influenced by mechanisms such as defect trapping and phonon scattering.

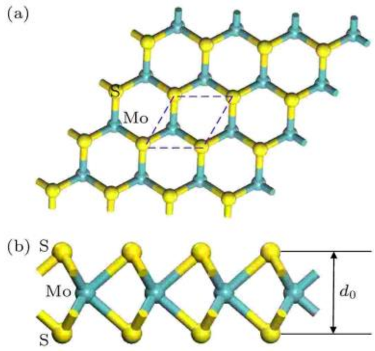

Figure 1. The structure of MoS_2 [7]

2.2. Black phosphorus

Black phosphorus is composed of single or multiple layers of phosphorus atoms. As shown in Figure 2, each phosphorus atom typically bonds with three adjacent phosphorus atoms, forming a hexagonal ring.

Phosphorus atoms are covalently bonded to each other, creating a honeycomb lattice similar to graphene. The stacking arrangement of phosphorus atoms between different layers can lead to different properties. In comparison to graphene, it exhibits a spin-orbit-split bandgap. By controlling the number of layers, the bandgap width of black phosphorus can be continuously adjusted, ranging from 0.3 eV (multilayer) to 2 eV (monolayer). This provides advantages for various optoelectronic applications. Black phosphorus demonstrates strong light absorption capability, with a single-layer absorption coefficient of up to 7.5%. Moreover, its absorption range covers visible and near-infrared light which makes it a perfect material to build a wide spectrum photodetector. Black phosphorus exhibits high-efficiency photogenerated electron-hole pairs but has a relatively short carrier lifetime. Newly prepared black phosphorus is susceptible to degradation and transformation in the presence of air, which limits its development in the field of optoelectronics [8].

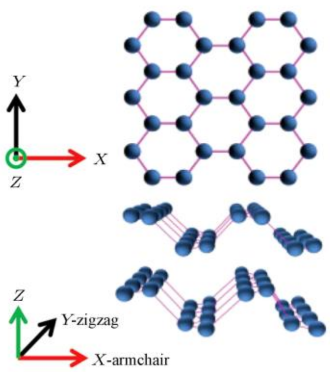

Figure 2. The structure of black phosphorus [9]

2.3. Oher 2D materials

Two-dimensional silicon carbide (2D SiC) belongs to the IV group of layered semiconductors and is a class of graphene-like materials. It is typically composed of hexagonal crystals made up of carbon and silicon atoms. It exhibits remarkable high-temperature stability, maintaining its structural integrity under extreme temperatures. This property makes it widely applicable in high-temperature electronic devices. Its optoelectronic properties are similar to TMDCs, and it has significant potential applications in

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optoelectronics and optical communication. By comparing the spectral response ranges and carrier dynamics parameters of different materials, one can select the appropriate material for achieving photodetection in different wavelength bands. Monolayer boron nitride (BN) materials are another 2D semiconductor and can also be applied in optoelectronic devices.

3. Design of optoelectronic devices with different semiconductors

3.1. MoS_2 photodetector

A MoS_2 photodetector is a photosensitive device based on two-dimensional TMDC materials, possessing unique characteristics and a wide range of potential applications. As a narrowband semiconductor, MoS_2 has good light absorption from visible to near-infrared light and has great potential in the preparation of photodetectors due to its excellent optical and electrical properties [10]. Typically, it consists of three essential components: firstly, the MoS_2 layer, which serves as the primary sensitive layer of the photodetector and is often in the form of single or multi-layers. MoS_2's two-dimensional crystalline structure grants it excellent photoelectric properties. Secondly, there are the electrodes employed to collect the generated electrons and holes. Lastly, a substrate, typically made of insulating or semiconductor materials, provides mechanical support for the MoS_2 layer. The operational principle of a MoS_2 photodetector relies on the semiconductor properties of MoS_2 and the photoelectric effect. When incident light illuminates the MoS_2 layer, photons excite electrons within MoS_2, causing their transition from the valence band to the conduction band, thereby generating electron-hole pairs. These electrons and holes are separated by an electric field and collected at the electrodes, resulting in the generation of a current signal. The size of the bandgap of MoS_2 determines the wavelength range to which it responds. This photodetector holds substantial potential across various domains. In the field of optical communication, it can be employed for receiving data signals in optical communication systems. In the biomedical field, it finds applications in medical imaging, diagnostics, and the detection of protein molecules, among others. However, as technology advances, further research and optimization of molybdenum disulfide are required to enhance its performance to meet the diverse demands of different applications.

3.2. MoS_2 field-effect transistors (FETs)

In the fields of electronics and semiconductors, MoS_2 FETs have found extensive use as alternatives to traditional silicon-based devices. Key applications encompass logic gates, amplifiers, oscillators, and memory units, all of which play pivotal roles in integrated circuits and electronic devices. MoS_2 FETs hold tremendous potential in high-performance electronic devices owing to their high electron mobility, low power consumption, rapid response times, and excellent conductivity. The structure of MoS_2 FETs typically comprises several essential components: firstly, the MoS_2 thin layer serves as the semiconductor channel. Beneath it, there is an insulating layer or substrate providing mechanical support and electrical isolation. Additionally, source and drain electrodes are used to control the flow of electrons within the device. The two-dimensional nature of this structure allows MoS_2 FETs to excel in micro and nanoscale electronic devices. The operational principle of MoS_2 FETs is grounded in field-effect control. When a voltage is applied between the source and drain electrodes, it modulates the carrier concentration of electrons and holes within the MoS_2 thin layer. By adjusting the gate voltage, the electron concentration within the channel can be controlled, thereby regulating the current flow. This field-effect control grants MoS_2 FETs outstanding electron mobility and rapid switching speeds. MoS_2's unique material properties are paramount to its successful applications. As a two-dimensional semiconductor, MoS_2 boasts exceptional electron mobility, photoelectric performance, and mechanical strength. It also possesses a sizable bandgap, facilitating lower leakage currents and higher switching speeds.

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3.3. Monolayer BN Photodetectors

Photodetectors are crucial optoelectronic devices playing a pivotal role in various applications. Monolayer BN materials can be prepared using the Chemical Vapor Deposition (CVD) method. Through CVD, it is possible to grow monolayer BN on a gold substrate, ensuring the material's single-crystalline structure and high quality. The resulting monolayer BN exhibits an ideal electronic structure, with a bandgap of approximately 5.5 eV. Monolayer BN possesses a relatively large bandgap, around 5 to 6 eV, and exhibits outstanding absorption characteristics within the ultraviolet (UV) spectrum range. These attributes make monolayer BN an ideal material for UV light detection. The photodetector comprises several key components, including the monolayer BN light-absorbing layer, an electron transport layer for efficient electron capture and transmission, and metal electrodes for collecting photo-generated electrons and generating current signals. A dedicated detection circuit further amplifies and processes the output current signals. The resulting photodetector demonstrates high absorption efficiency, sensitivity, and rapid response times. In addition to its primary application in UV radiation detection, this device holds potential applications across various fields, including biosensing and meteorological observations. Utilizing monolayer BN as the active material in photodetector design showcases its potential as a multifunctional platform for optoelectronic applications.

3.4. Solar cells

Solar cells are photovoltaic devices based on semiconductor materials that show the photovoltaic effect. When exposed to light, the P-N junction in a solar cell generates photo-generated electrons and holes, resulting in a potential difference. Under continuous illumination, this leads to the generation of a continuous electric current. Researchers have found that the bandgap of single-layer SiP_3, GeP3, $SiAs_3$, and $GeAs_3$ materials falls between 1.12 eV and 1.26 eV [11]. The material AX_3 (A= Si, Ge; X=P, As); exhibits high absorption coefficients in the visible light range. Additionally, $SiAs_3$, $GeAs_3$, and SiP_3 have higher mobility than silicon [11]. Based on these findings, scientists have designed a photovoltaic system based on SiP_3/ZnO, achieving an energy conversion efficiency of 22.15% [11]. They have also studied the development of layered solar cells using InSb/GaAs and InSb/InP, achieving photovoltaic conversion efficiencies of 27.8% and 30.3%, respectively [11]. These findings demonstrate the significant potential of two-dimensional III-VA materials in advancing the photovoltaic industry [11]. Future research can explore other III-VA materials for the development of improved two-dimensional semiconductor materials and optimize traditional fabrication methods such as gas-phase and liquid-phase methods to enhance material performance and reduce production costs

4. Prospects

Due to the excellent industrial stability and small size features of two-dimensional layered semiconductors, electronic products gradually shift towards low power consumption, wearable, intelligent, and miniaturized directions. Friction electronics, based on friction nanogenerators, use techniques to collect external mechanical energy or other forms of energy to power devices. Additionally, due to quantum size effects, nonlinear optical effects, and spin effects, layered two-dimensional semiconductors have become ideal materials for emerging fields such as optoelectronics, photodetectors, and hydrogen storage.

By improving the preparation methods of two-dimensional layered semiconductor materials, materials with superior performance can be obtained. For example, it is essential to avoid local damage, fractures, and wrinkles. With the rapid development of nanotechnology, new types of two-dimensional materials have gradually become a research hotspot. The production and use of a large number of related products will inevitably lead to the release of heavy metals or other pollutants into the environment through various pathways, posing potential threats to ecosystems and human health. In the future, research and development can focus on aspects such as pollution-free, efficient degradation, and low-cost solutions.

In the field of electronic devices, the contact resistance of molybdenum disulfide nanoscale transistors is currently high, and in the future, a more effective method may be needed to reduce the

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contact resistance of these transistors. In addition to transistors, two-dimensional layered semiconductor field-effect transistors have a wide development space in optimizing charge injection and transport due to surface and interface chemical research. Other ions can be used to prepare two-dimensional semiconductor composites, thereby changing their original structure and properties, and affecting their optoelectronic effects. The precise control of large-scale layered two-dimensional semiconductor growth technology and the preparation of high-quality molybdenum disulfide materials are also future research directions.

Photon energy greater than the semiconductor bandgap leads to thermalization losses due to excess energy, while photon energy smaller than the semiconductor bandgap leads to absorption losses [12]. If future research can reduce thermalization losses and achieve a balance between utilizing more photons, it may be possible to improve energy conversion efficiency and even exceed the Shockley-Queisser limit, thereby enhancing the efficiency of optoelectronic devices such as solar cells.

5. Conclusion

This study focuses on the research progress of different two-dimensional layered semiconductors, such as TMDCs and black phosphorus, and compares and analyzes their classification, structures, and properties. In addition, this study explores the structure, function, and performance parameters of some optoelectronic devices based on two-dimensional layered semiconductors. Building on existing research, this study also provides some prospects and predictions for the future application of two-dimensional layered semiconductors in optoelectronic devices.

However, they also have limitations. Due to the zero bandgap and semi-metallic properties of graphene, it cannot be used as a light-absorbing layer in solar cells. TMDC materials generally have low carrier mobility, and black phosphorus is prone to adsorb water molecules from the air, leading to changes in its physical and chemical properties, thus, affecting device stability. Two-dimensional layered semiconductor materials have atomic-level thickness and a relatively large surface area, making them prone to the adsorption of substances such as water molecules in the air, which can interfere with their optoelectronic properties. These limitations restrict their application in semiconductor optoelectronic devices. Therefore, further exploration of suitable packaging techniques is needed to improve the reliability of devices for two-dimensional layered semiconductor material sensors. As the era of intelligence approaches, the future applications of two-dimensional semiconductor optoelectronic devices can be oriented towards low power consumption and the development of flexible materials. The fabrication methods of two-dimensional layered semiconductors can be improved to address the material's intrinsic defects caused by current fabrication techniques. Furthermore, due to the widespread use of two-dimensional layered semiconductors, their properties such as degradability and environmental friendliness can be further enhanced. Lastly, researchers can explore materials from other families or innovate existing materials to enhance their performance in terms of carrier mobility, power conversion efficiency, and other properties.

Author Contribution

All the authors contributed equally to this work and their names were listed in alphabetical order.

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