2D semiconductor Van Der Waals heterojunction applications

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Abstract. As the demand for new energy sources continues to grow, the market value of solar power, a key component of new energy, is also expanding. Van der Waals (vdW) heterojunctions made from two-dimensional (2D) semiconductors especially transition metal dichalcogenide (TMD), demonstrates immense potential in terms of the portability and efficiency of photovoltaic devices. Additionally, it shows great promise in the field of novel miniature high-speed photoelectric detectors. It offers multiple benefits, including high carrier mobility, tunable optical and electrical properties, enhanced optical properties and ultra-thinness, making it suitable for variant applications. This report reviewed the emerging 2D semiconductor Vdw heterojunction technologies on photodetection and photovoltaics. Summarized the advantages of MoS_2/WSe_2, WSe_2/ReS_2 and WSe_2/WS_2-based Vdw heterojunctions and their challenges. The continued research and development in this field are expected to lead to more efficient energy conversion, scalable fabrication methods, and broader commercial applications of these technologies.

Keywords: Van Der Waals heterojunction, 2D semiconductor, photodetector, solar cell, transition metal dichalcogenide.

1. Introduction

The Vdw heterojunction-based devices require junction equilibrium to maintain their stability and efficiency. Unlike the chemically combined junctions, the 2D materials used in Vdw heterojunction usually doesn't involve dopant-induced free carriers that combine within the interface - the 2D semiconductors used to form Vdw heterojunctions are usually undoped, leading to absence of depletion region. Although no ionized charge carriers exist, the built-in optional still exists due to their unique energy band alignment [1]. Materials with higher electrical affinity tend to hold more electrons towards them, and those with lower work functions can donate electrons more easily. This electron attraction difference induces a potential at the interface, defining the Vdw heterojunction's band alignment. The dynamically balanced electron attraction and built-in potential results in an equilibrium in heterojunction. Therefore, the carrier in the junction is guided like a conventional P-N junction. Besides, the equilibrium is also contributed by the balance between band alignment and internal interaction within each layers. The fermi level of two individual materials must be aligned for their combination, which requires the electrons and holes within interface to redistribute. The Vdw heterojunction is classified into: Straddling Gap Alignment (Type-I) – both valence band maximum(VBM) and conduction band minimum(CBM) of one material falls within the band gap of the other material, Staggered Gap Alignment (Type-II) - the CBM of one material lies on the other's VBM, and Broken Gap Alignment (Type-III) - VBM of one material overlaps with the CBM of the other material, creating a situation where the VBM is at a higher energy level than the CBM [2]. Depending on the energy band alignment, they each have identical carrier behaviour, making them capable for different applications. Since band gap depends on the material, the resultant energy band structure of Vdw heterojunctions is deeply relevant to the component material, resulting into tunability in electrical and optical properties.

The size of the 2D semiconductors plays a significant role in defining the properties of heterojunctions. The size tunability of 2D semiconductors is categorized into thickness and lateral size when discussing their electrical properties. Thickness refers to the number of layers within the material, and the term '2D materials' often refers to monolayer materials, where charge carriers are confined to a plane. A change in thickness causes variations in carrier confinement, which affects the band structure of the 2D material. For certain materials (e.g., Molybdenum disulfide), a direct bandgap occurs only in monolayer form, and the bandgap becomes indirect as the thickness increases. As the lateral size decreases, edge effects become more significant, influencing the material's electrical properties. A smaller lateral dimension also provides a higher relative edge area, where defects and scattering centers are more likely to be present. These defects significantly impact the carrier mobility and the optical properties of the material.

2. Vdw heterojunctions-based p-n junction for laser/photodetectors

External electrons or holes are added by introducing impurities into a semiconductor material. The transition metal dichalcogenide (TMD) Molybdenum disulfide (MoS_2) can be n-doped with Group I elements, exhibiting negligible electron mobility loss [3]. For instance, Potassium-doped MoS_2 can theoretically be n- or p-doped, depending on the sites occupied by Potassium. P-doped materials with higher electron affinity tend to attract electrons due to the sufficiency of holes, while n-doped materials with more free electrons more readily donate electrons. The dynamically balanced electron attraction and built-in potential result in equilibrium in the p-n junction. Therefore, aligning the Fermi levels of materials is necessary for their combination, requiring electrons and holes at the interface to redistribute. The nature of band gap tunability of 2D materials promises precise operating wavelength tunability in a wide range. Making the 2D semiconductor Vdw heterojunction versatile for many laser applications. The inherent thinness and flexibility of 2D materials allow for the development of compact and potentially flexible optical devices. With high carrier mobility and reduced dimensionality, the Van der Waals (vdW) heterojunction exhibits a fast response time, enabling its use in extreme high-speed laser applications (EHLAs). Many 2D semiconductors in monolayer form have a direct bandgap, allowing for efficient electron-hole recombination, which is essential for generating ultrafast laser pulses. The confined carrier configuration and high surface-to-volume ratio of 2D semiconductors enhance light-matter interactions, generating short and intense laser pulses.

Chip-scale photonic integrated circuit (PIC) is the fundamental building block of optical computing, many materials have been induced to fabricate PICs [4]. The commonly used silicon-based PICs offer large-scale production with low cost, silicon nitride PICs are capable with high operating power etc. However, monolithic integration of waveguide and photodetector is a remaining challenge. Photons are transmitted in the waveguide, and light absorption is avoided; this lack of optical signal absorption makes it impossible for them to function as a photodetector. The 2D Vdw p-n junctions enabled the possibility of integrating waveguide and photodetector on same material [4]. A waveguide-integrated BP/MoTe2 heterojunction photodetector with low dark current and fast responsibility for on-chip PICs is reported [4]. Its structure is described in Figure 1. The charge carrier transport direction in p-n junction is perpendicular to the direction of light propagation. The BP layer absorbs the light within waveguide spectrum to generate photocarriers. With the build-in potential of p-n junction, the photocarriers are quickly separated at the heterojunction's interface, thus the monolithic integration is achieved. Although BP/MoTe2 heterojunction shows promise in low dark current and fast response, it's still challenging to have low dark current while keeping high responsivity and fast response. Because it suffers from the complexity of integrating 2D materials with optical waveguides and ensuring efficient carrier extraction and transport. An advanced fabrication mechanism and 2D material combination might be further studied to solve this problem.

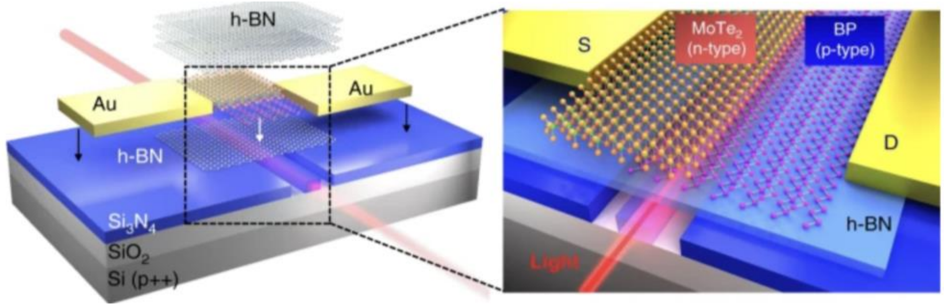

Fig 1. Schematic of BP/$MoTe_2$ heterostructure [4].

3. Solar cells

The 2D semiconductor Vdw heterojunction is expected to enable ultralight and ultrathin efficient solar cells [5] [6]. It benefits from the nature of 2D semiconductor materials and its Vdw heterostructure, which is competitive to conventional silicon optoelectronic technologies [7]. The enhanced light-matter interaction of many 2D semiconductors within the spectrum region of sunlight enables their high carrier transport. Moreover, the absence of chemical bonding of Vdw heterojunction offers the possibility of integration for a wider material selection. Because the lattice mismatch between component materials less influences the quality of heterojunction. However, there are certain challenges for 2D semiconductor Vdw heterojunction photovoltaic and photodetection applications.

A reported device model which is capable of simulating the current-voltage behavior of type-II Van der Waals heterojunctions when exposed to light was used to investigate the physical properties of 2D TMDs Vdw heterojunction-based solar cell devices 2018 [8]. As shown in Figure 2, a MoS2/WSe2 heterojunction is grown upon a SiO2/Si platform, both layers represent a thickness in monolayer level. The device behaves as p-n junction via electrostatic doping of back-gate voltage to the platform [9]. The strong optical absorption of 2D semiconductors in the solar spectrum region makes them exceptionally efficient at absorbing energy from the sun. The enhanced electrical mobility theoretically promises an expected power conversion efficiency (PCE) which exceeding 25% with relatively low energy loss during conversion. However, the device model exhibits a reduced external quantum efficiency (EQE) while the light intensity increases – 1% at ~1 kWm-2 green light with a wavelength of 532 nanometre due to an insufficient carrier extraction. It reveals that while these heterojunctions demonstrate efficient spatial charge transfer, they also face significant carrier recombination losses. These losses arise from inadequate electrical transport, resulting in a substantial accumulation of photogenerated carriers within the interface of heterojunction. This accumulation consequently leads to inefficient carrier extraction. To summarize, the study induced the significance of carrier transport rate for improving the PCE of atomically thin solar cells. Also, provided a solution for challenges of carrier recombination and extraction.

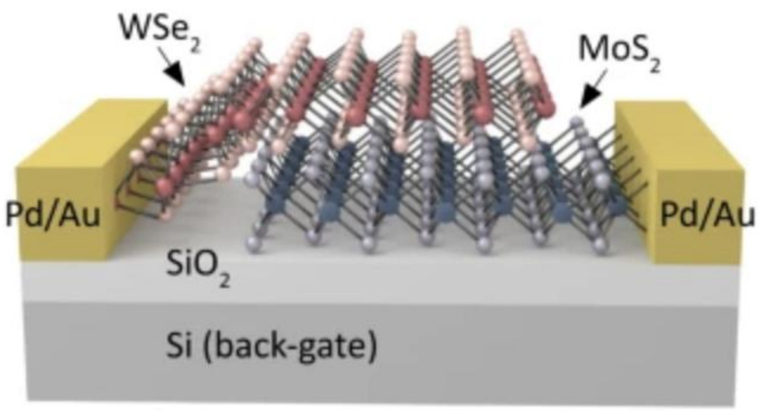

Fig 2. Schematic of MoS_2/WSe_2 heterostructure [8].

One the next year, a Type-II Vdw heterojunction consists of multiple layers of WSe2 and ReS2 was reported [10]. Such heterointerface with 4 layers of WSe2 and 6 layers of ReS2 shows a flexible near-direct band gap at 0.7 eV with an inaccuracy of 0.0175 eV to a direct band gap and is confirmed by an IR photodetector. This near-direct band gap premise is strong carrier mobility and light-matter interaction, thus enhancing carrier transfer efficiency. The thin layers exhibit a response time of 5 μs, an open-circuit current of 0.64 V, a short-circuit current of 2.6 μA and a responsivity of 3 Watt per Amper. This implies a high output power, efficient spatial charge transfer and large photocurrent generation especially in the overlap region of the heterolayers. As illustrated in Figure 3, the WSe2 and ReS2 layers were grown on heavily p-doped silicon subtract which covered by SiO2 to form the active region for self-emitting photodetector or photovoltaic devices, and it's achieved through facile single contact metal fabrication process. The sample is capable for long-term use due to its strong air resistivity. Apart from the advantages, the challenges are also curial – providing a uniform and controllable layer deposition and maintaining stability and efficiency over long-term practical applications.

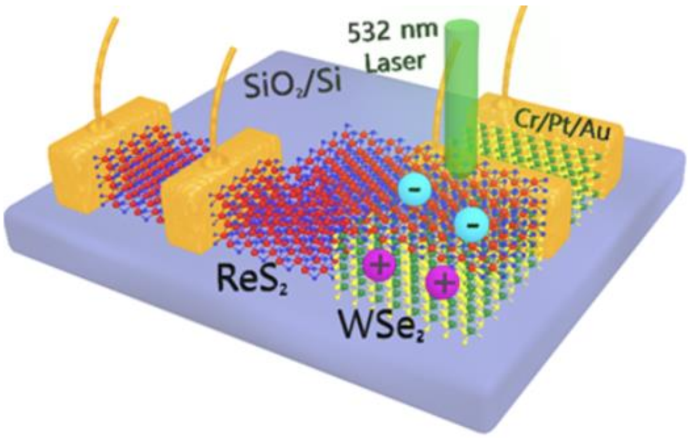

Fig 3. Schematic of WSe_2/ReS_2 heterostructure [10].

A photovoltaic response tunable WSe2/WS2 Vdw heterojunction was reported in 2020 [11]. In contrast to Vdw heterojunctions made of the other 2D semiconductor materials, the WSe2/WS2 one benefits from the ambipolar nature of WS2, which permits flexibility in charge carrier type and effective conductivity modulation. Because WS2 can be either n- or p-doped by changing carrier concentration through electrostatic doping, even in the post-fabrication stage. Thus, devices containing WS2 can operate in different conduction regime and dynamically control one's band alignment. It's also capable with modern silicon-based semiconductor technologies, which enable large-scale production. The developed junction yields a PCE of 2.4% and an open-circuit voltage of 0.58V. Besides, the nature of self-powering is a reliable solution for reducing overall energy consumption. As for photodetection devices, the self-powered diode formed by WSe2/WS2 Vdw heterojunction shows good prospect on fast-response photodetector in near-infrared spectrum region. However, these WSe2/ReS2 Vdw heterojunction-based devices still suffer from optical absorption loss and carrier scattering – a reduced thickness of 2D material leads to increased optical absorption loss and decreased EQE. The modern 2D semiconductor-silicon integration technology also suffers from high carrier scattering, which influences the performance of devices – it leads to reduced solar cell efficiency and reduced signal-to-noise ratio (SNR) as a photodetector. Especially limited its potential for imagining.

4. Conclusion

This review explored their remarkable potential in advancing photodetection, photovoltaics, and optical computing technologies. The unique properties of these heterojunctions, such as high carrier mobility, tunable optical and electrical characteristics, and enhanced light-matter interactions, underscore their significant role in next-generation semiconductor technologies. Notably, their ultra-thinness positions them as ideal candidates for chip-scale optical devices, while their absence of surface dangling bonds reduces the impact of lattice mismatches, enhancing device stability and performance. This review highlighted various types of VdW heterojunctions, such as MoS2/WSe2, WSe2/ReS2, and WSe2/WS2, discussing their respective advantages and challenges. These heterojunctions demonstrate promising capabilities in various applications, from efficient photovoltaic devices to high-speed photodetectors, owing to their efficient electron-hole recombination and robust carrier mobility. However, challenges such as carrier recombination and extraction losses, optical absorption loss, and carrier scattering remain significant hurdles. These issues often result from the inherent properties of 2D materials and their integration with existing semiconductor technologies. Addressing these challenges requires further research into advanced fabrication techniques and exploration of new material combinations that can optimize the performance and efficiency of VdW heterojunction-based devices. To summarise, 2D semiconductor VdW heterojunctions represent a frontier in material science with immense potential for revolutionizing various technological fields. Their integration into existing systems and the continued research into overcoming their limitations will undoubtedly pave the way for groundbreaking advancements in electronics and optoelectronics. The future of VdW heterojunctions is vibrant, promising a new era of highly efficient, versatile, and miniaturized semiconductor devices.

References

[1] Geim A., Grigorieva I. Van der Waals heterostructures. Nature, 2013, 499: 419-425.

[2] Ihn T. Band structure. Semiconductor Nanostructures: Quantum states and electronic transport. Oxford, 2009; online edn, Oxford Academic, 1 Feb. 2010: 19-52.

[3] Boland J. L., Conesa-Boj S., Parkinson P., Tütüncüoglu G., Matteini F., Rüffer D., ... Johnston M. B. Modulation doping of GaAs/AlGaAs core-shell nanowires with effective defect passivation and high electron mobility. Nano Letters, 2015, 15(2): 1336-1342.

[4] Tian R., Gan X., Li C., et al. Chip-integrated van der Waals PN heterojunction photodetector with low dark current and high responsivity. Light Sci Appl, 2022, 11: 101.

[5] Novoselov K. S., et al. Two-dimensional atomic crystals. Proc. Nat. Acad. Sci. USA, 2005, 102: 10451-10453.

[6] Podzorov V., Gershenson M. E., Ch. Kloc, Zeis R., Bucher E. High-mobility field-effect transistors based on transition metal dichalcogenides. Appl. Phys. Lett., 2004, 84: 3301-3303.

[7] Kang S., Lee D., Kim J., Capasso A., Kang H.S., Park J.-W., Lee C.-H., Lee G.-H. 2D semiconducting materials for electronic and optoelectronic applications: potential and challenge. 2D Mater., 2020, 7: Article 022003.

[8] Furchi M.M., Höller F., Dobusch L., et al. Device physics of van der Waals heterojunction solar cells. npj 2D Mater Appl, 2018, 2: 3.

[9] Furchi M. M., Pospischil A., Libisch F., Burgdörfer J., Mueller T. Photovoltaic effect in an electrically tunable van der Waals heterojunction. Nano Lett., 2014, 14: 4785-4791.

[10] Varghese A., Saha D., Thakar K., Jindal V., Ghosh S., Medhekar N. V., Ghosh S., Lodha S. Near-Direct Bandgap WSe2/ReS2 Type-II pn Heterojunction for Enhanced Ultrafast Photodetection and High-Performance Photovoltaics. Nano Letters, 2020, 20(3): 1707-1717.

[11] Lin P., Yang J. Tunable WSe2/WS2 van der Waals heterojunction for self-powered photodetector and photovoltaics. Journal of Alloys and Compounds, 2020, 842: 155890.