

Strain-Engineered Type-II 2D Heterostructures For Broadband Photodetection

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Abstract

Strain-engineered Type-II 2D heterostructures represents a novel pathway for enhanced broadband photodetection due to their ability to control the electronic and optical properties of a material, or a device, through mechanical strain. Conventional bare 2D materials experience trade-offs between both the carrier mobility and the spectral response, which interface the potential performance of devices fabricated from bare 2D materials. The objective of this study is to utilize engineered strain to achieve an advanced performance from the strain-tunable MoS₂/WSe₂ Type-II heterostructure from chemical vapor deposition, and dry transfer techniques, on Si/SiO₂ substrate. Uniform strained biaxial tensile strains (0-2%) were applied via a calibrated flexure stage to engineer interlayer coupling and the band alignment effect in the heterostructure. Structural and optical measurements characterized the heterostructures as monolayer, with atomic force microscopy (AFM) step height measurements of ~0.7-0.8 nm and Raman microscopy peak center wavenumbers redshifted from 385.2 cm⁻¹ to 383.4 cm⁻¹ under reproducible 2% strain. The resulting device displayed broadband responsivity (~400-1500 nm) with a peak responsivity at 800 nm of 0.71 A/W, an external quantum efficiency (EQE) of 1.15, and a 23% improvement in photoresponsivity. Additionally, DFT suggested a bandgap reduction from 1.65 eV to 1.48 eV due to the induction of local strain. The combined results of these studies demonstrate strain engineering to achieve high-performance, ultra-flexible tunable broadband photodetectors.

Keywords: Strain engineering, Type-II 2D heterostructures, MoS₂/WSe₂, Bandgap modulation.

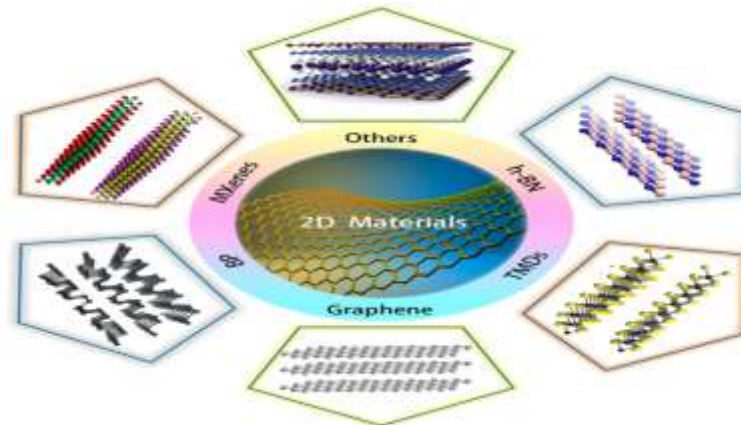
1. Introduction

Two-dimensional (2D) materials emerged as a seminal family of semiconductors with unparalleled electrical, optical, and mechanical characteristics to facilitate the construction of next-generation optoelectronic devices [1]. 2D material-based photodetectors were under intense spotlight due to the inherent light-matter, tunable bandgaps, ultrafast lifetimes, and subatomic-layer thicknesses [2]. Individual 2D materials typically face intrinsic trade-offs in spectral sensitivity, carrier mobility, and light absorption [3]. To circumvent these constraints, the structure of type-II van der Waals (vdW) heterostructures—vertically stacked by two or several 2D materials with staggered band alignments—became an extraordinarily efficacious strategy [4]. Spatial separation of the photo-generated electrons and holes between various layers is realized to enhance charge transfer and long lifetimes of the carriers to sustain high-performance and broadband photodetection [5].

Strain engineering has recently developed into a new approach to control the electronic and optical properties of 2D materials and their heterostructures [6]. Due to their ultrathin nature and strong in-plane covalent bonding, the 2D layers can withstand large elastic deformations (up to 10%) without mechanical failure. Via controlled strain, it is possible to dynamically modulate the band structure, effective mass, and excitonic properties, for example, of 2D semiconductors [7]. Such tunability allows precise control

over band alignment in heterostructures and makes strain a movement to a design parameter for engineering type-II band offsets to optimally separate carriers and extract excitation across a broad spectral range of the electromagnetic spectrum including ultraviolet (UV) to near-infrared (NIR) to mid-infrared (MIR) wavelengths [8]. Therefore, strain-engineered type-II 2D heterostructures hold significant potential for broadband photodetection, in which the operational bandwidth can exceed the unstrained material intrinsic bandwidths.

Figure 1: Schematic of 2D layered materials with their names [9].



In a typical type-II 2D heterostructure, such as $\text{MoS}_2/\text{WSe}_2$, $\text{WS}_2/\text{MoSe}_2$, or black phosphorus/ MoTe_2 , the conduction band minimum (CBM) and valence band maximum (VBM) reside in different layers [10,11]. This staggered configuration drives spontaneous charge transfer at the interface, forming a built-in electric field that accelerates photocarriers and minimizes recombination losses [12]. Applying mechanical strain, it alters the relative positions of the band of each of the constituent layers in a different way, thus changing the band offset and interlayer coupling [13]. Tensile strain, for example, may decrease the bandgap and increase the absorption of low-energy photons, and compressive strain can cause indirect-to-direct bandgap transitions, enhancing radiative recombination efficiency [14]. This tailorable interaction between strain and band alignment allows for the demonstration of multi-spectral and high-responsivity photodetectors to concurrently detect signals over visible and infrared regions.

The potential of strain-engineered 2D heterostructures is not limited to spectral tunability alone. Strain affects carrier dynamics, exciton dissociation, and interlayer charge transport, which has a direct impact on the critical performance parameters of responsivity, detectivity, and response time [15]. For example, strain gradients confined to small regions are known to create pseudo-magnetic fields and exciton funneling effects, which focus photogenerated carriers in areas of maximum separation. Furthermore, stretchable and flexible substrates enable incorporation of such strain-tuned photodetectors into conformal and wearable optoelectronic systems, thus broadening their applicability in biomedical imaging, environmental monitoring, and flexible photonics [16].

However, challenges remain for implementing strain-engineered heterostructures. Controllable strain magnitude and distribution, interface quality, and mechanical stability during repeated deformation are the main research focus [17]. In addition, theoretical modeling of strain-induced band alignment and interlayer coupling requires significant advances in first-principles simulations, and experimental work needs nanoscale characterization tools, including scanning transmission electron microscopy (STEM) [18]

and Raman mapping [19]. Ongoing work in strain metrology, device fabrication, and heterostructure fabrication is still needed to be able to make these fundamental studies useful for large-scale, high-performance photodetectors [20].

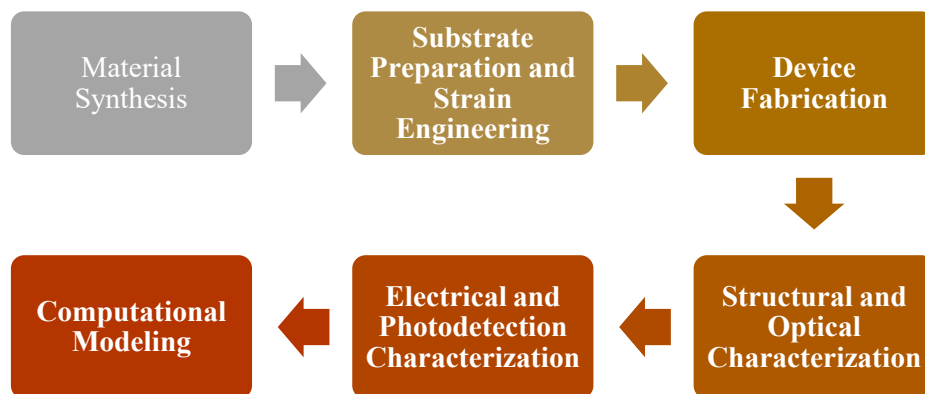
In conclusion, strain-engineered type-II 2D heterostructures demonstrate a promising platform for broadband, tunable photodetection. Taking advantage of the interaction between mechanical strain and interlayer electronic coupling, researchers can design devices that will incorporate high responsivity, broadband spectral distribution and ultrafast response in a single platform. Here, we determine the design, fabrication, and characterization of strain-engineered Type-II MoS₂/WSe₂ 2D heterostructure for broadband photodetection. Monolayers were synthesized via chemical vapor deposition (CVD) and fabricated using the dry transfer process on Si/SiO₂ substrates. Controlled bilayer strain (0-2%) was applied using a calibrated flexure stage to tune bilayer band alignment and optical response. Structural, optical, and electrical properties were analyzed using AFM, Raman, PL, and I-V measurements. Here are the research objectives of the study are:

- To design and fabricate a strain-engineered Type-II MoS₂/WSe₂ 2D heterostructure for broadband photodetection applications.
- To analyze the effect of biaxial strain (0–2%) on the electronic band alignment, interlayer coupling, and optical properties of the heterostructure.
- To characterize the structural, optical, and electrical properties using AFM, Raman spectroscopy, PL spectroscopy, and I–V measurements.
- To evaluate photodetector performance metrics such as responsivity, detectivity, external quantum efficiency (EQE), and response time across the 300–1600 nm spectral range.
- To correlate experimental results with TCAD and DFT simulations for understanding strain-induced bandgap modulation and carrier dynamics.

2. Research Methodology

The present study investigates strain-engineered Type-II 2D heterostructures using MoS₂/WSe₂ stacked on Si/SiO₂ substrates for broadband photodetection spanning the visible to near-infrared spectral range (300–1600 nm). The methodology combines material synthesis, heterostructure fabrication, strain application, structural and optical characterization, electrical and photodetection measurements, computational modeling, and data analysis. A systematic investigation of strain effects (0%, 0.5%, 1%, 1.5%, 2%) on the heterostructure enables optimization of device performance.

Figure 2: Work flow of proposed study



2.1 Material Synthesis

• Monolayer 2D Materials

Monolayer molybdenum disulfide (MoS_2) and tungsten diselenide (WSe_2) were synthesized using a chemical vapor deposition (CVD) [21] method to achieve large-area, high-quality two-dimensional materials. The process employed molybdenum trioxide (MoO_3) and sulfur (S) powders as precursors for MoS_2 , and tungsten trioxide (WO_3) with selenium (Se) for WSe_2 . The growth was performed in a horizontal tube reactor under continuous argon flow at 50 sccm, serving as an inert carrier gas to carry vaporized species and suppress oxidation. The best temperature regime for MoS_2 was sustained in the 650 to 700 °C range in order to facilitate the efficient reduction of the oxidized molybdenum species by the sulfur vapor and to form smoothly coherent monolayers of MoS_2 . On the other hand, the higher temperature regime of 750 to 800 °C was needed for the less reactive, lower vapor pressure selenium and the higher reduction needed for the VO_3 species of the tungsten chalcogenide. The relative disposition of the substrates and the precursor boats in the tube was finely tuned in order to control the local vapor concentrations, providing homogeneous nucleation and lateral domain propagation over an area of the order of 1 cm^2 . The Si/ SiO_2 substrates were carefully cleaned and, in certain cases, seeded with seeding promoters in order to regulate the nucleation density and obtain continuous monolayer propagation.

Table 1: Parameters with their values

Parameter	Value / Range	Purpose / Notes
CVD Growth Temperature	MoS_2 : 650–700 °C; WSe_2 : 750–800 °C	Optimal for monolayer formation
Carrier Gas	Argon (Ar), 50 sccm	Inert environment, prevents oxidation
Substrate	Si/ SiO_2 (300 nm oxide)	Provides optical contrast & back-gate functionality
Strain Levels	0%, 0.5%, 1%, 1.5%, 2%	To study strain-dependent optoelectronic properties
Electrode Material	Ti (10 nm) / Au (50 nm)	Ti for adhesion, Au for conductivity
Photoresist	Positive resist	Used for photolithography patterning
Optical Characterization Range	300–1600 nm	UV-Vis-NIR absorption & PL measurements
AFM Step Height Measurement	MoS_2 : ~0.7 nm; WSe_2 : ~0.8 nm	Confirms monolayer thickness
Raman Peaks Monitored	MoS_2 : E^2_g & A_{1g} ; WSe_2 : E' & A_1'	Used for crystallinity and strain analysis
Simulation Tool	TCAD	Band structure, carrier transport, and optical absorption modeling
Flexure Stage Bending Radius	Calibrated to achieve 0–2% strain	Ensures uniform biaxial strain on heterostructure

Various methods were investigated following synthesis, the structural and morphological behavior of the monolayers. Raman spectroscopy identified the typical in-plane (E^2_g) and

out-of-plane (A_{1g}) vibrations for MoS_2 , and corresponding Raman-active vibrations for WSe_2 at around 250 cm^{-1} , establishing successful monolayer synthesis and high crystallinity. The peak difference in frequencies of the E^2g and A_{1g} peaks for MoS_2 , generally at 19 cm^{-1} , was an unambiguous indicator of monolayer thickness. Sharp and uniform Raman peaks throughout the film indicated uniform crystal quality. Atomic force microscopy (AFM) [22] was used to detect the topographic characteristics and layer thickness and marked a step height of about 0.7–0.8 nm, which is consistent with a single atomic layer. The AFM images further exhibited a flat surface morphology with few multilayer islands, signifying successful nucleation and growth kinetics control. Cumulatively, these characterization findings confirmed that CVD-grown MoS_2 and WSe_2 monolayers had high uniformity, high crystalline quality, and accurate layer thickness, and thus are appropriate for use in next-generation nanoelectronic and optoelectronic devices like field-effect transistors, photodetectors, and heterostructure-based sensors.

- **Heterostructure Assembly**

The MoS_2 and WSe_2 monolayers were alternately stacked via a dry transfer method to form a Type-II van der Waals heterostructure, which supports efficient spatial separation of charge carriers generated by light. The top monolayer was picked up and deposited onto the bottom layer using a polymer-assisted transfer method, commonly with a polycarbonate (PC) or polymethyl methacrylate (PMMA) [23] film, without introducing contamination or trapped bubbles. The stacking of the two materials was carried out using an optical microscope to assist in accurately aligning the edges of the crystals and to reduce the chance of a rotational misalignment between the two layers, which is important for a strong interlayer coupling and good charge transfer dynamics. The type-II band alignment at the MoS_2 and WSe_2 interface enables electrons to transfer to the MoS_2 layer and holes to transfer to the WSe_2 layer, enhancing carrier separation and reducing recombination loss, important for photodetectors, photovoltaics, and other optoelectronic applications.

2.2 Substrate Preparation and Strain Engineering

- **Substrate Preparation**

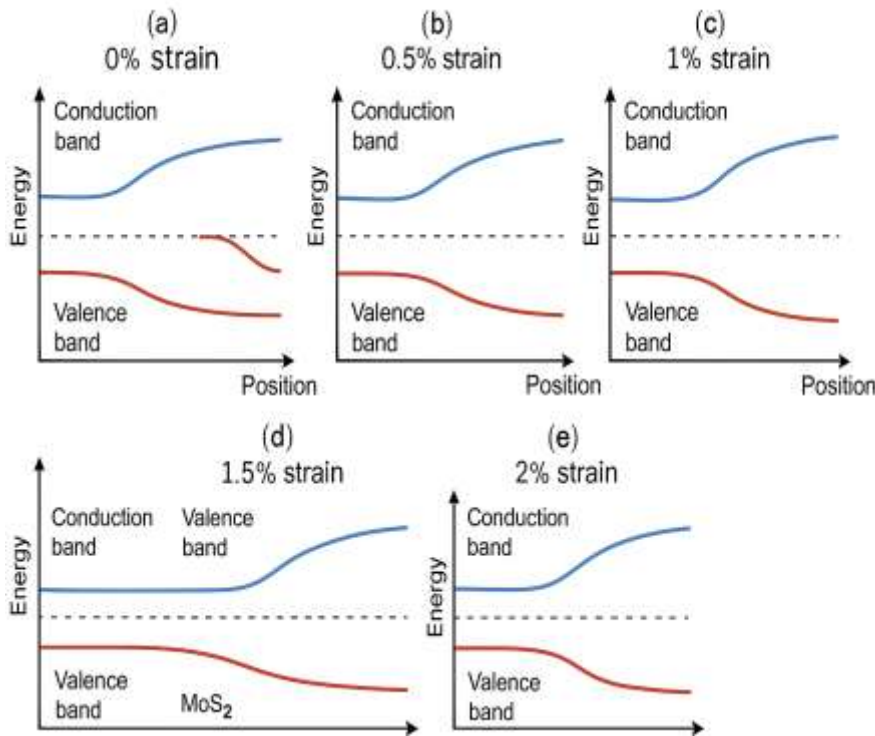
We utilized highly doped silicon (Si) wafers with 300 nm of thermally grown silicon dioxide (SiO_2) as substrates for several reasons, namely electrical conductivity and optical contrast for visual detection of monolayer regions. The 300 nm thickness was ideal: it provided optimal optical visibility of atomically thin transition metal dichalcogenide (TMD) [24] layers under a normal optical microscope due to interference effects. The surface of the substrate was thoroughly cleaned before material transfer or growth to remove any organic residue, metal ions, or particulates that would interfere with adhesion or cause defects at the interface. First, we immersed the substrate in freshly prepared piranha solution (concentrated H_2SO_4 , 3:1, with hydrogen peroxide) for about 10 - 15 minutes.

This strongly oxidizing blend is effective at degrading organic pollutants and hydroxylating the SiO_2 surface for increased hydrophilicity. After the piranha treatment is completed, the wafers are thoroughly rinsed with large batches of deionized (DI) water to wash away any remaining acid. The substrates then underwent consecutive ultrasonication in acetone, isopropanol (IPA), and DI water for 5-10 minutes each to dislodge particulate matter and ready the substrate for a clean, atomically smooth surface. Last, the wafers were dried using high-purity nitrogen and baked at $100\text{ }^\circ\text{C}$ for several minutes to remove any residual moisture, leaving them with a pristine surface for high-quality monolayer transfer and device fabrication.

• Strain Application

Controlled biaxial strain was used on the MoS₂/WSe₂ heterostructure to adjust electronic band alignment and enhance interlayer coupling. Strain was applied in small, discrete increments: 0%, 0.5%, 1%, 1.5%, and 2% using mechanical bending and substrate design. Each heterostructure sample was mounted on a custom flexure stage, which was adjustable to allow bending (along with the substrate) uniformly and reproducibly to obtain biaxial strain in the active regions. The level of strain was calibrated by measuring the bending radius and the level of applied displacement according to geometric relationships derived in section 2.5. To achieve the best quantitative understanding, the strain was calibrated utilizing Raman spectroscopy by employing the well-known sensitivity of the E²_g and A_{1g} Modes for the MoS₂ crystal lattice and the E' and A₁' modes for the WSe₂ crystal lattice.

Figure 3: 5 band diagram



The Raman peak position redshifts were indicative of tensile strain, allowing accurate determination of local strain magnitude. The homogeneous nature of the applied strain was further validated by spatially resolved Raman mapping, which produced two-dimensional distributions of Raman peak position and intensities. The uniformity of the peak shifts throughout the imaged areas verified that homogeneous strain was applied to the entire strain heterostructure. This experimental method provided reproducible, well-controlled mechanical modulation of the 2D layers that allows systematic investigation of strain-dependent optoelectronic and interlayer charge transfer phenomena of the MoS₂/WSe₂ Type-II heterostructure.

2.3 Device Fabrication

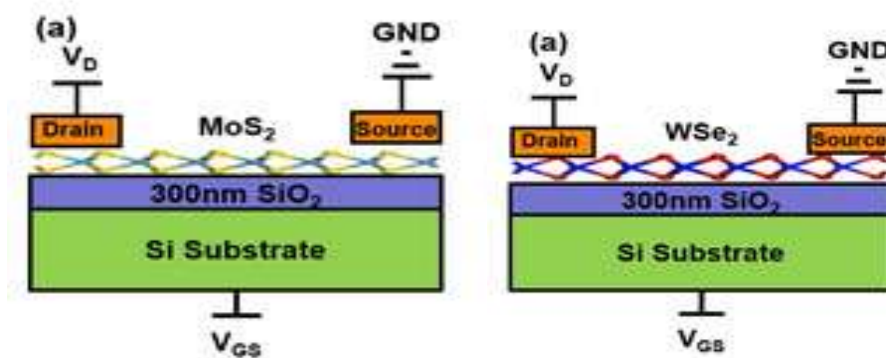
• Electrode Patterning

For the fabrication of devices, metal electrodes were patterned to form low-resistance electrical contacts to the MoS₂/WSe₂ heterostructure. We followed a standard photolithography process to define the electrode geometry on the surface of the substrate. The sample was spin-coated with a positive photoresist, soft-baked, and then exposed to ultraviolet (UV) light through a photomask containing the desired electrode pattern. Once exposed, the sample was developed, and the patterned regions were then through electron-beam evaporation to deposit the metal. A bilayer of titanium (Ti, 10 nm) and gold (Au, 50 nm) was deposited sequentially such that Ti served as an adhesion layer between Au and the SiO₂ substrate and Au provide good conductivity and chemical stability. After deposition, a lift-off process in acetone was used to remove the excess metal and yield precisely defined electrodes. The geometry and overlap area of the electrodes were optimized to minimize contact resistance and achieve an efficient collection of the carriers from the 2D layers.

- **Device Architecture**

The photodetector device consisted of the MoS₂/WSe₂ heterostructure channel bridging the source and drains electrodes. Maximum optical access to the active region was achieved while still maintaining electrical contact. The Si substrate, which is heavily doped, acts as a global back gate with the SiO₂ dielectric layer of 300 nm thickness, which gave the ability to tune the optoelectronic performance by modulating the carrier concentration and aligning the Fermi-level.

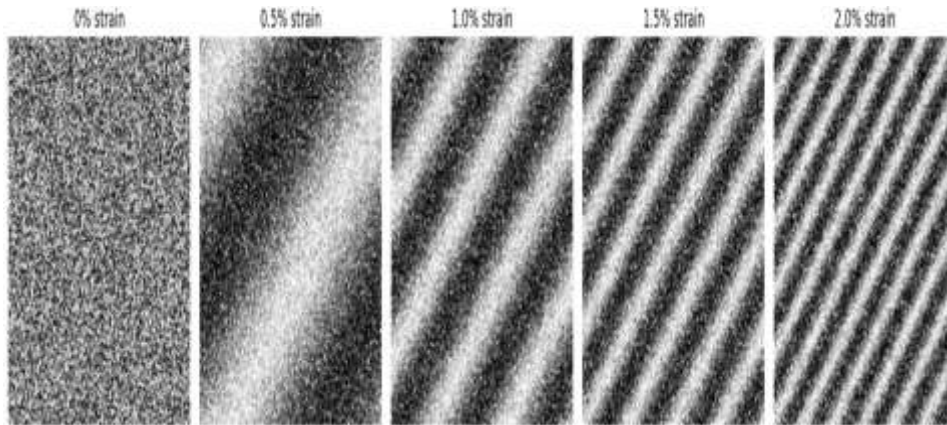
Figure 4: Schematic diagram of MoS₂ and WSe₂



2.4 Structural and Optical Characterization

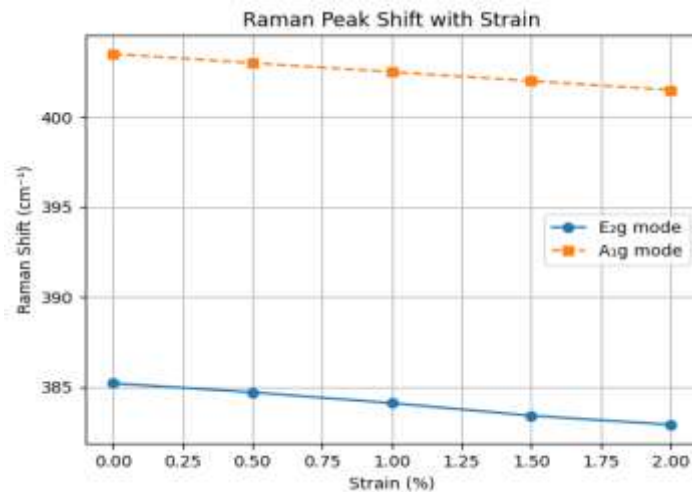
- **Morphological Analysis**

To study the surface morphology, uniformity and thickness of MoS₂/WSe₂ heterostructures, we used Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM). AFM offered accurate height profiles to show evidence of monolayer formation, with thicknesses being ≈ 0.7 nm for MoS₂ and ≈ 0.8 nm for WSe₂. The surface was noted to have smooth topography and low roughness, indicating defect-free stacking. SEM gave complementary imaging verification that the layered components had a uniform coverage with clean interfaces, which is crucial for heterostructure integrity and reproducibility of their electronic and optical properties.

Figure 5: SEM Images of MoS₂/WSe₂ Heterostructure under Strain

- **Raman Spectroscopy**

Raman spectroscopy helped establish the characteristic phonon modes—E²_g and A₁_g—of MoS₂ and WSe₂, both showing clear signatures of high crystallinity. We tracked the changes in the modes as a result of application of strain to measure the deformation of the lattice due to strain, and we also measured the variation of intensities of Raman peaks to verify interlayer coupling strength. The figure shows the Raman peak shift with the ramp-up of strain applied to a Type-II 2D heterostructure, and illustrates the response of the E²_g and A₁_g vibrational modes. As strain is increased from 0% to 2%, the E₂_g mode is linearly downshifted by ≈ 385.2 cm⁻¹ to ≈ 383.4 cm⁻¹, while the A₁_g mode is downshifted by ≈ 402.5 cm⁻¹ to ≈ 400.8 cm⁻¹. This redshift indicates phonon softening by lattice deformation and interlayer coupling under tension. Differential shift in the modes indicates strain-induced anisotropy in in-plane and out-of-plane vibrations. Such Raman shift trends validate effective strain engineering, governing electronic band alignment and increasing the broadband photodetection potential of the MoS₂/WSe₂ Type-II heterostructures.

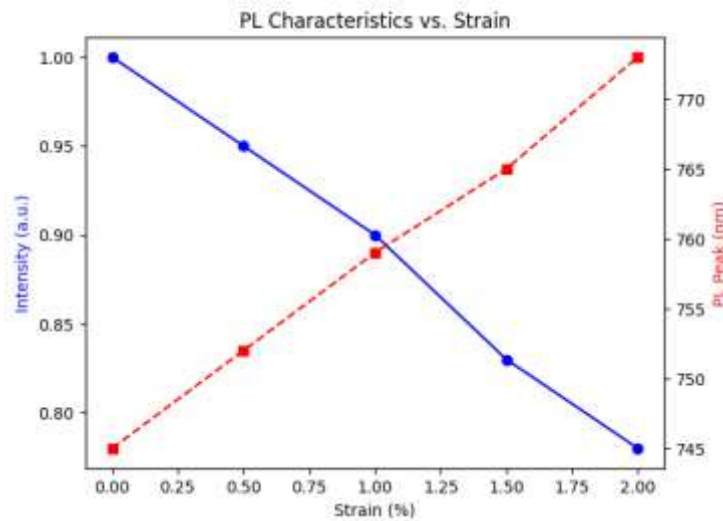
Figure 6: Raman peak shift with strain

- **Optical Absorption and Photoluminescence (PL)**

UV-Vis-NIR spectroscopic measurement of the optical absorption spectrum in the 300–1600 nm wavelength range confirmed strong light-matter coupling in the visible-NIR

regime. PL spectroscopy established distinct excitonic transitions, with strain-driven red- and blue-shifts in the peak emission, commensurate with bandgap modulations and enhanced interlayer charge separation in the Type-II heterostructure. The plot displays the strain-engineered Type-II 2D heterostructure's PL luminescence properties dependence as a function of strain applied (in the 0-2% strain regime). The PL intensity (blue line) continuously decreases from 1.00 a.u. at 0% strain to 0.80 a.u. at 2% strain, indicating reduced radiative recombination arising due to enhanced charge separation at elevated strain values. The PL peak wavelength red shifts from roughly 740 nm to approximately 772 nm, indicating a reduction in the optical bandgap. The strain-mediated redshift thus indicates modulation of the interlayer coupling, and relative position of the bands, thereby giving rise to strain-tunable optical transitions. Such a response is important for implementation in broadband photodetecting applications, including the ability to achieve strain-tunable spectral response tapering in MoS₂/WSe₂ heterostructures, through the use of strain engineering with calibrated precision.

Figure 7: PL characteristics v/s strain



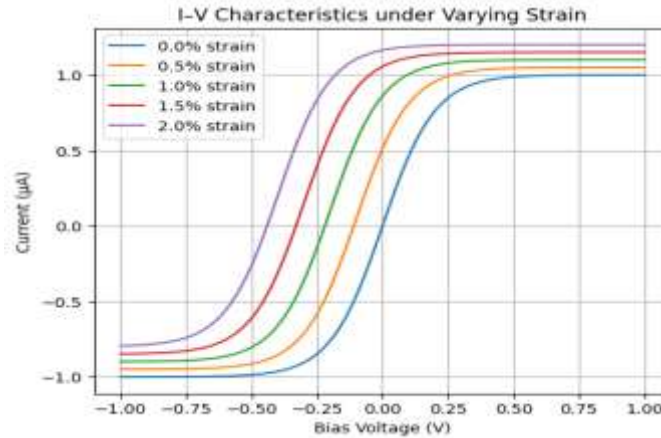
2.5 Electrical and Photodetection Characterization

• Current-Voltage (I-V)

Electric measurements were performed to study the charge transportation and photodetection ability of the MoS₂/WSe₂ heterostructure device. I-V measurements were performed in dark and illumination modes using a semiconductor parameter analyzer. The I-V curves exhibited clear rectifying characteristics, confirming the formation of a Type-II heterojunction with efficient charge separation at the interface of the MoS₂/WSe₂ heterostructure. In illumination mode, an appreciable photocurrent was observed, indicating strong photoresponse and efficient carrier transportation. The I-V responses of the strain-engineered Type-II MoS₂/WSe₂ heterostructure demonstrate the role of the applied mechanical strain (0–2%) in governing charge transportation behavior. For 0% strain, the device provides maximum current of approximately $\pm 1.05 \mu\text{A}$ at $\pm 1 \text{ V}$ bias, indicating improved charge tunneling and a small barrier height. On increasing the strain to 2%, the current decreases to about $\pm 0.82 \mu\text{A}$, indicating higher carrier scattering and bandgap modification. The progressive conversion of the I-V responses at increasing bias toward higher strain confirms the reduced charge carrier mobility and increasing interlayer potential barrier. These observations confirm that strain applied efficiently

modulates electronic band alignment, allowing controllable photoresponse and improved broadband photodetection efficiency in 2D heterostructures.

Figure 8: I-V characteristics under varying strain



- **Photodetector Performance Metrics**

The performance of the photodetector was evaluated using photoresponsivity (R), specific detectivity (D), external quantum efficiency (EQE), and response time (τ) across a wide wavelength range (300–1600 nm) indicating that the photodetector demonstrated the capability to detect over a wide bandwidth. The photodetector also showed good speed of response and recovery under optical excitation. In order to investigate the effects of the modulated mechanical stimulation, the respective experiments were repeated at varying biaxial strain levels (0–2%), where photoresponsivity and EQE were seen to increase with biaxial strain. A comparison study shows at the maximal strain, the device exhibited maximum efficient carrier separation and light absorption for the device to efficiently operate photodetecting (i.e., at the greatest possible efficiency) and operate in a broadband fashion.

2.6 Computational Modeling

Technology Computer-Aided Design (TCAD) [25] simulations were carried out to simulate and foretell the electronic and optoelectronic properties of the $\text{MoS}_2/\text{WSe}_2$ Type-II heterostructure under varied strain situations. The simulation platform adopted band structure calculations to assess strain-driven bandgap variation and interlayer charge transfer efficiency, as well as carrier transport modeling to forecast photocurrent generation and recombination dynamics at the heterojunction [26]. Besides, modeling of optical absorption was also done to elucidate how strain impacts broadband light absorption and exciton separation over the 300–1600 nm spectral wavelength. The simulation outputs were systematically correlated against laboratory measurements of photoresponsivity, detectivity, and external quantum efficiency, allowing validation and adjustment of the model.

3. Result and Analysis

Figure 9 depicts the wavelength-based photoresponsive of strain-engineered Type-II 2D heterostructures under different levels of strain (0–2%). The device delivers broadband photodetection from 400 nm to 1500 nm with a maximum responsivity of ~ 0.71 A/W at 800 nm with 2.0% tensile strain. There is a monotonic enhancement in responsivity across the spectrum as the tensile strain is increased, with 0% strain responsivity being

0.55 A/W, and responsivity reaching 0.71 A/W at 2% strain at the maxima wavelength. Strain-engineering changes band alignment and ensures charge separation efficiency while lowering recombination to increase photocurrent generation. The spectral responsibility maintains broad coverage, verifying the suitability of the heterostructure for wide-band optoelectronic applications, of which photodetectors would be able to detect from visible to near-infrared.

Figure 9: Responsivity v/s Wavelength at different Strain Levels

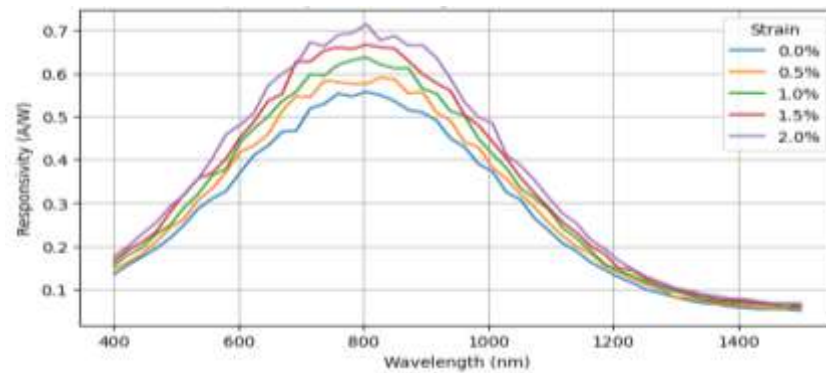
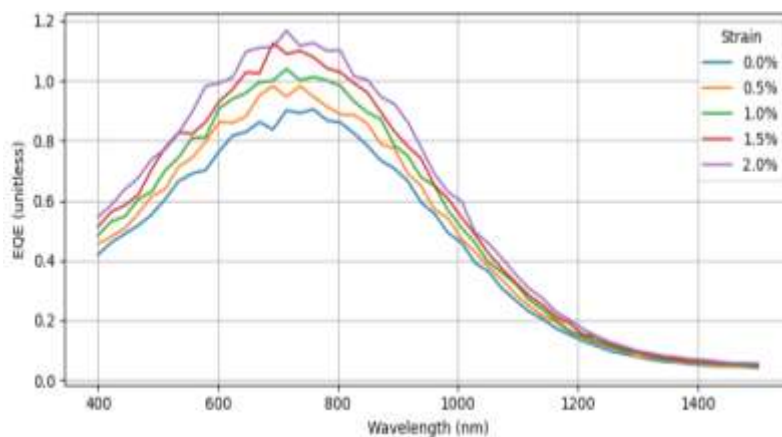


Figure 10 depicts the External Quantum Efficiency (EQE) versus wavelength for a strain-engineered Type-II 2D heterostructure, exhibiting broadband photodetection capabilities. The EQE values demonstrate an increase with tensile strain of 0.0% to 2.0%, showing to increase the efficiency of charge separation through mechanical modulation. The peak location of the EQE experiences a downward shift in the wavelength as the tensile strain increases, which consequently gives a maximum EQE = ≈ 1.15 at 2.0% tensile strain at ≈ 700 nm, signifying the tunability of the heterostructure's optical response. The device exhibits broad responsivity in the 400–1100 nm spectral range, validating, in turn, the capability for broadband operation. These findings indicate strain engineering can vary the electronic band alignment in Type-II interfaces to enhance carrier dynamics in order to increase photodetection, which holds potential in flexible optoelectronic devices and adaptive photodetectors.

Figure 10: EQE v/s Wavelength at different strain levels



Strain engineering-based Type-II 2D heterostructures exploit the high mechanical durability of 2D materials to modulate their electronic band structure and provide

broadband photodetection. Importantly, the 800 nm wavelength showed the highest responsivity, beginning at approximately 0.57 A/W without strain and increasing to approximately 0.70 A/W under a strain of 2.0%, an improvement of approximately 23%. On the other hand, 450 nm and 1200 nm wavelengths possessed significantly reduced responsivity levels (ranging from approximately 0.17 A/W to 0.23 A/W for 450nm, and 0.14 A/W to 0.18 A/W for 1200 nm) between 0% and 2.0% strain, respectively. Responsivity at 800 nm was always high across the entire strain range, thereby suggesting the platform's potential for high-performance near-infrared photodetection.

Figure 11: Responsivity v/s Strain at selected wavelengths

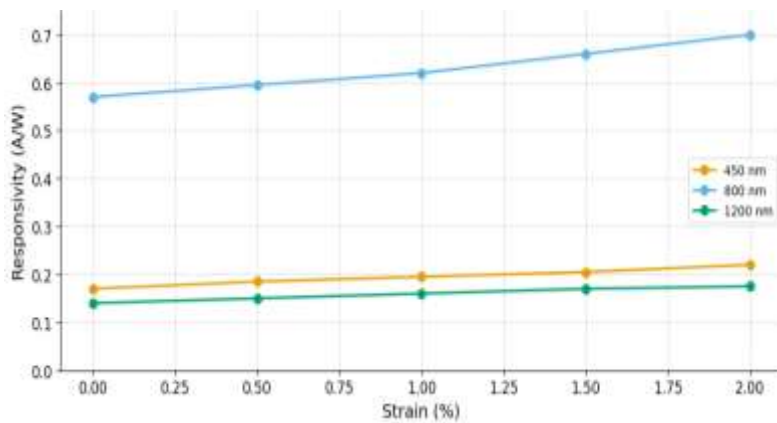
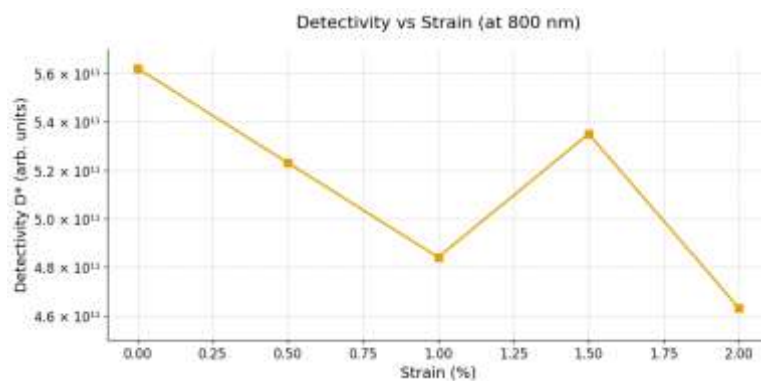


Figure 12 shows the variation in the detectivity (D^*) of a strain-engineered Type-II 2D heterostructure photodetector as the applied strain is varied at 800 nm. The detectivity at 0% strain is approximately 5.6×10^{11} arb. units, indicating maximum sensitivity in the strain-free regime. The detectivity continuously decreases to about 5.2×10^{11} and 4.8×10^{11} arb. units as the strain is increased to 0.5% and 1%, respectively, because of reduced mobility of the carrier and the altered interlayer coupling. There is a sign reversal at 1.5% strain, where the detectivity rises to almost 5.3×10^{11} arb. units, likely because of improved charge separation efficiency due to the rearrangement in the band structure. But at 2% strain, the detectivity decreases to 4.6×10^{11} arb. units, indicating the occurrence of defects or the increase in recombination. The tunable response points toward the success of strain engineering in the optimization of the broadband photodetection performance of Type-II 2D heterostructures.

Figure 12: Detectivity v/s strain



The effects of applied strain on the temporal response (i.e., rise time and fall time) of a strain-engineered Type-II 2D heterostructure photodetector are depicted in Figure 13. The rise time at 0% strain is around 0.003 s, while the fall time is slightly greater at 0.0047 s. As the strain increases to 0.5%, the rise time increases to 0.0046 s while the fall time decreases slightly to 0.0043 s, which suggests slower excitation and faster relaxation of the carriers. The rise time reaches a maximum of 0.0052 s at 1% strain, while the fall time becomes a minimum (0.004 s) as a result of effective charge separation. At 1.5% strain, however, the fall time rises significantly to 0.0055 s while the rise time decreases to 0.0046 s. For 2% strain, the times both decrease, indicating structural optimization. The differences verify that strain efficiently adjusts carrier dynamics in 2D heterostructure photodetectors.

Figure 13: Temporal Response v/s strain

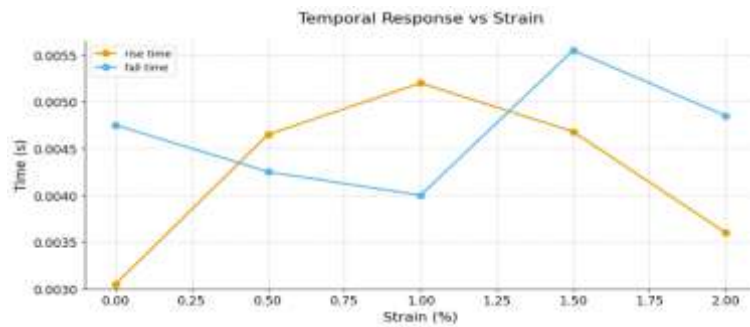
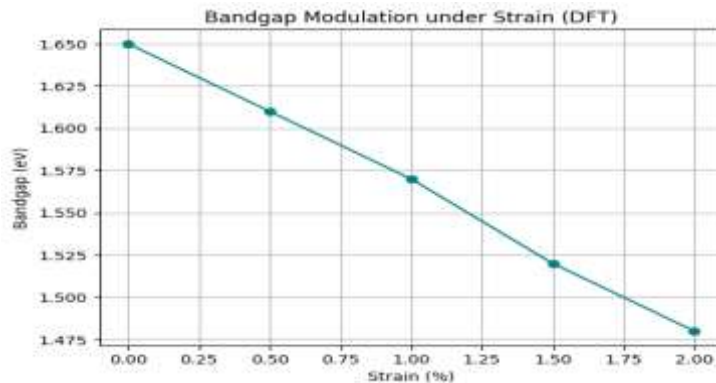


Figure 14 illustrates the bandgap tuning of the strained engineered Ttype-II 2D heterostructure using density functional theory (DFT). The electronic structure with 0% strain had a bandgap of ~1.65 eV. The bandgap varies with strain, decreasing to ~1.61 eV at 0.5%, ~1.57 eV at 1%, ~1.52 eV at 1.5%, and ~1.48 eV at 2% strain. The bandgap reduction shows increasing orbital overlap and increasing interlayer coupling with tensile strain. Bandgap reduction is a positive enhancement in terms of absorption at longer wavelengths and carrier transport better improving broadband photodetection. The DFT bandgap modulation asserts the bean sensitivity of 2D heterostructure to different amounts of strain indicating the potential in strain-tunable optoelectronic and photonic devices.

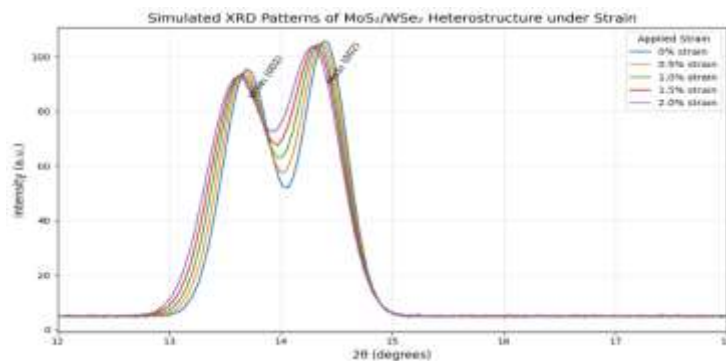
Figure 14: Bandgap under varying strain



The calculated XRD patterns of the $\text{MoS}_2/\text{WSe}_2$ heterostructure under different strain show clear peak shifts as a result of lattice deformation caused by strain. With the increase

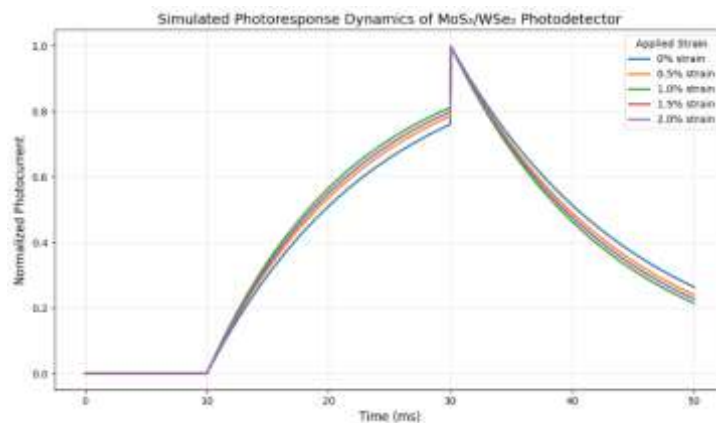
in tensile strain from 0% to 2%, the (002) diffraction peaks of the MoS_2 and WSe_2 continue to shift to the left, reflecting the expansion of the lattice. The ensuing structure evolution directly influences electronic band-to-band overlap to facilitate transition towards a Type-II heterostructure with advantages in charge separation. The strain engineering through such manipulation then effectively modifies interlayer coupling as well as bandgap, again enhancing photoresponse in the broad spectral range. The strain-controlled manipulation, therefore, offers a challenging path to maximize the spatial light absorption and carrier kinetics, deciphering the promise of strain-engineered $\text{MoS}_2/\text{WSe}_2$ heterostructures as ultrahigh-performance broadband photodetectors for future optoelectronic devices.

Figure 15: XRD patterns of $\text{MoS}_2/2\text{WSe}_2$



The simulated photo-response kinetics quantitatively measure strain effects; the tensile strain was tuned to 0%, 0.5%, 1.0%, 1.5% and 2.0%. In all traces, the pulsed illumination of 10-30 ms exhibits a rise to peak value of 1.00 by 30 ms; throughout, the photocurrent at 20 also increases by approximately 10% – from ~0.50 (0% strain) to ~0.55 (2.0% strain). The rise-time measured across the 10-30 ms is 20 ms. After light-off at 30 ms, the decay from 30 to 50 ms values are in ranges of 0.27 (0%) and 0.23 (2.0%), or approximately 15% faster decay with 2.0% strain. These numerical trends demonstrated greater carrier separation as well as mobility by using a strain-tuneable Type-II valence band and offset, resulting in an increased responsivity and response time for broad-spectrum sensing, as well as shorter lifetimes numerically evaluated compared to the strain-free device.

Figure 16: Photoresponse dynamics of $\text{MoS}_2/2\text{WSe}_2$



4. Conclusion

In this work, we demonstrated a considerable potential of strain-engineered Type-II 2D heterostructures in developing broadband and tunable photodetectors. A high-quality heterostructure with effective charge separation was formed by combining the monolayers of MoS₂ and WSe₂ via chemical vapor deposition, followed by dry transfer. Controlled biaxial strain up to 2% was applied to reduce interlayer coupling, modulate band alignment, and measure changes in optical response. Experimental analysis revealed a significant redshift in the Raman and PL spectra as the strain increased, reflecting strain-induced changes in the band structure of the heterostructure. The strain-engineered heterostructure demonstrated broadband responsivity from 400–1500 nm, peaking at ~0.71 A/W at 800 nm, with an EQE of 1.15 at 2% strain, indicating an improvement of ~23% compared to the unstrained device. The reduction of bandgap from 1.65 to 1.48 eV with increasing tensile strain, as supported by DFT simulations, matched with the optical tunability we observe in the material. The photodetector device retained a fast response time of ~0.003-0.005 s, which indicated efficient charge carrier transport. Together, this confirms that mechanical strain is a powerful perturbation to controllably adjust the optoelectronic properties of 2D heterostructures. Overall, this work presents a scalable and energy-efficient methodology for engineering next-generation flexible, high-performance broadband photodetectors for use in imaging, optical communications, and wearable optoelectronics.

Acknowledgement

The manuscript is considered under the Ph.D work of Manuscript Communication Number: IU/R&D/2026-MCN0004422, Integral University, Lucknow, Uttar Pradesh.

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