Strain-engineered growth of two-dimensional materials

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The application of strain to semiconductors allows for controlled modification of their band structure. This principle is employed for the manufacturing of devices ranging from high-performance transistors to solid-state lasers. Traditionally, strain is typically achieved via growth on lattice-mismatched substrates. For two-dimensional (2D) semiconductors, this is not feasible as they typically do not interact epitaxially with the substrate. Here, we demonstrate controlled strain engineering of 2D semiconductors during synthesis by utilizing the thermal coefficient of expansion mismatch between the substrate and semiconductor. Using WSe₂ as a model system, we demonstrate stable built-in strains ranging from 1% tensile to 0.2% compressive on substrates with different thermal coefficient of expansion. Consequently, we observe a dramatic modulation of the band structure, manifested by a strain-driven indirect-to-direct bandgap transition and brightening of the dark exciton in bilayer and monolayer WSe₂, respectively. The growth method developed here should enable flexibility in design of more sophisticated devices based on 2D materials.
Two-dimensional (2D) transition metal dichalcogenides (TMDCs) have been the subject of focused research owing to their potential applications in optoelectronics and sub 10 nm transistors. The primary attraction of TMDCs such as MoS$_2$ and WSe$_2$ for both applications is their naturally terminated surface, which allows them to be scaled down to the atomic limit without the concern of surface dangling bonds. Furthermore, in many 2D materials, a number of desirable properties emerge at the monolayer limit, the most notable of which being the presence of a direct bandgap. Many studies based on mechanical bending of exfoliated 2D TMDCs have been conducted on flexible substrates, and they have shown that the application of strain can tune the properties of this new class of materials. For example, it has been demonstrated that in multilayer WSe$_2$, particularly in nominally indirect-gap bilayer WSe$_2$, application of tensile strain can result in a transition from an indirect-to-direct bandgap. However, studies on the effects of strain in TMDCs have been limited to mechanical bending of samples, and there has yet to be a technique, which can directly realize built-in tensile and compressive strains.

Traditionally, strain engineering of semiconductors has been leveraged to tune the electronic band structure of high-performance devices, the most notable of which being to reduce intervalley scattering, increase mobility in Si transistors, and reduce the hole effective mass in III–V semiconductor lasers. Growth on epitaxial substrates with a controlled lattice constant is typically utilized to establish built-in strain in three-dimensional semiconductors. However, due to the relatively weak interaction between 2D materials and substrates, this established method of strain engineering is likely not applicable for the strain-engineered growth of TMDCs. Therefore, a route toward development of large-area strained TMDCs on a practical substrate is highly desirable. Significant research efforts have been made to realize large area TMDCs, with the majority of efforts focusing on chemical vapor deposition (CVD) routes. Interestingly, a number of studies employing CVD growth of 2D materials have reported apparent strain in the synthesized samples.

However, growth of high-quality 2D materials with controllable built-in strain has not been realized. Hence, properties that are difficult to probe via mechanical bending experiments, such as low-temperature optical measurements and electrical performance, have yet to be explored.

In this work, we demonstrate strain engineering of 2D materials directly via CVD growth while simultaneously maintaining high material quality, by utilizing the thermal coefficient of expansion (TCE) mismatch between the TMDC and the growth substrate. Electron diffraction of strained monolayers grown directly onto transmission electron microscopy (TEM) windows is utilized to unambiguously quantify strain. Using WSe$_2$ as a model system, we show that it is possible to obtain both tensile (of ~1%) and compressive (0.2%) strained 2D semiconductors over large areas on rigid substrates. Furthermore, in the WSe$_2$ model system we show indirect-to-direct optical transition in tensile strained WSe$_2$ bilayers as well as removal of dark exciton quenching in WSe$_2$ monolayers.

**Results**

**TCE-mismatch induced strain.** Owing to the high growth temperatures used to synthesize TMDCs, the TCE mismatch between the substrate and the 2D semiconductor can be utilized to control the strain in the synthesized 2D material, as shown schematically in Fig. 1. The theoretical upper limit for the strain, assuming no relaxation, can be calculated using the difference in lattice constant of the substrate and 2D semiconductor at room temperature and synthesis temperature:

$$\varepsilon(T_g) = \frac{a_{2D}(T_g) - a_{2D}(25 \degree C)}{a_{2D}(25 \degree C)} - \frac{a_{Sub}(T_g) - a_{Sub}(25 \degree C)}{a_{Sub}(25 \degree C)}$$

where $a_{2D}$ is the in-plane lattice constant for the 2D material being grown, $a_{Sub}$ is the in-plane lattice constant of the substrate, and $T_g$ is the growth temperature. More generally, this can be calculated using the temperature dependent thermal expansion coefficient for the 2D material ($\alpha_{2D}$) and substrate ($\alpha_{Sub}$).

![Fig. 1](image1.png) Strain-engineered growth of WSe$_2$ using TCE-mismatch. Schematic of the process through which strain is realized during the growth of 2D materials via mismatch in substrate and TMDC thermal expansion coefficient. a. Tensile strain is achieved when the TCE of the substrate is less than that of the 2D material, b. relaxed samples are achieved when the TCE of the substrate and 2D material match, and c. compressive strain is achieved when the TCE of the substrate is greater than that of the 2D material.
van der Waals forces to an amorphous substrate.

Experimentally, Frenkel strain upon cooling. To estimate the magnitude of the corrugation strains of this magnitude to arise during epitaxial growth, it is necessary to maintain the nonslip condition that transmits strain to the layer. Although one expects bonding between the 2D layer and the substrate must be efficiently strong and corrugated to maintain the nonslip condition that transmits strain to the layer. Although one expects strains of this magnitude to arise during epitaxial growth, it is difficult to see how a similar strain can arise for van der Waals forces to an amorphous substrate. Experimentally, the corrugation in the film must be large enough to retain the strain upon cooling. To estimate the magnitude of the corrugation necessary to sustain the strain, we analyzed a 2D Frenkel–Kontorova model, shown in Supplementary Note 1 and Supplementary Fig. 1. This model suggests that atomic binding energy variations of as little as 14 meV over the range of the unit cell are capable of retaining strains of the magnitude of those observed experimentally. This variation is \( \epsilon \) 1% of a typical covalent bond strength, and very near to the typical strength of a van der Waals bond. Though a more detailed theory needs to be developed, especially to understand the surface chemistry immediately prior to growth to determine the nature of the bonding, this simple analysis suggests that thermal-expansion mismatch can strain a film, even in the case of weak binding between the film and the substrate. It should be noted that in a previous study, local heating of MoS\(_2\) using a laser was used to generate strains of up to 0.2% arising from the TCE-mismatch of MoS\(_2\) with the substrate\(^\text{17}\). Although this method does not generate built-in strains (strain is released once the laser is turned off), it suggests that the MoS\(_2\)-substrate bonding is strong enough to enable TCE-mismatched induced strain engineering\(^\text{17}\).

To demonstrate strain-engineered CVD growth of WSe\(_2\), four substrates were chosen, which have a range of TCEs. Fused silica and aluminum nitride (AlN) have a TCE of 0.55 and 5.5 ppm, respectively, much smaller than that of WSe\(_2\) (9.5 ± 3.2 ppm), and would be expected to induce tensile strain\(^\text{5, 18-22}\). In contrast, sapphire has a TCE closely matched to WSe\(_2\) and would be expected to produce relaxed samples and strontium titanate (STO) with a TCE of 12 ppm should yield compressively strained samples\(^\text{20, 23, 24}\). The sample was rapidly quenched after growth to limit relaxation in the WSe\(_2\). It is important to note that the rapid quenching process was found to be important in maintaining the presence of strain, and delay of the quenching step can result in partial relaxation of the 2D material.

Characterization strain and material quality. To characterize the strain present in the as-grown material, multiple characterization methods were utilized. First, electron diffraction was performed on WSe\(_2\) as-grown on SiO\(_2\) TEM grids and WSe\(_2\) transferred to SiO\(_2\) TEM grids. The resulting diffraction patterns are shown in Figs. 2a–c. In all TEM diffraction measurements on WSe\(_2\), the camera length and lens aberrations of the imaging systems were calibrated using polycrystalline aluminum and single crystal aluminum calibration samples (Ted Pella), and the microscope lens settings were left constant for all subsequent measurements. Corresponding images and photoluminescence (PL) spectra of the samples in Figs. 2b, c are shown in Supplementary Fig. 2. By comparing the lattice constant extracted from the diffraction patterns of strained (as-grown) and unstrained (transferred) WSe\(_2\), and utilizing the center of mass for 75 diffraction spots from each sample, we calculate that a 1.39 ± 0.28% tensile strain is present in the as-grown sample. The
calculated error represents the standard deviation in lattice constant value over 75 measured diffraction spots. Raman spectrum shown in Fig. 2d reveals a shift of the E’ in-plane Raman mode of $1.5 \pm 0.2$ cm$^{-1}$ between as-grown and transferred WSe$_2$. We note that the strain measured here is biaxial, not uniaxial, in contrast to mechanical bending studies and thus we do not observe splitting of the E’ mode. Therefore, the theoretically calculated value for the Gr"uneisen parameter ($\gamma$) of WSe$_2$ is used to calculate the expected peak shift according to: $\omega(\epsilon) = \omega_0 + \omega_1 \chi$, which is consistent with the approximately 1% tensile strain measured via diffraction$^{[25-27]}$. It should also be noted that after transfer the E’ mode shows no shift relative to samples prepared either by exfoliation or as-grown on sapphire. High resolution Raman mapping was performed and is shown in Figs. 2e, f for WSe$_2$ crystals as-grown on fused silica and transferred to a new fused silica substrate, respectively. We observe a uniform Raman shift throughout the full WSe$_2$ domain for both samples indicating that the strain is uniformly distributed within the sample on the scale of the Raman spot size. In addition, PL and atomic force microscopy images of as-grown WSe$_2$ on fused silica are shown in Supplementary Fig. 3.

PL measurements were employed to measure the bandgap as a function of strain. Figure 3a shows PL spectra of samples grown on all substrates investigated in this work as well as an exfoliated reference. There is a large spectral shift of 120 meV between samples grown on fused silica with near zero TCE and STO, which has the highest TCE of all substrates investigated in this work. Figure 3b shows the estimated strain from the PL peak shift as a function of predicted strain in WSe$_2$, vs. the lattice mismatch between the substrate and TMDC lattice constant. Strain values are determined from the experimentally measured PL peak position (measurement error was calculated using the standard deviation of strain measured from fifteen different crystals) and theoretically calculated bandgap as a function of strain extracted from refs $^{[3, 27]}$. It is important to note that we utilized the difference in peak position relative to an unstrained sample to eliminate effects from absolute bandgap error relative to theoretical calculations. We performed an analysis of the expected strain due to lattice parameter misfit (Supplementary Table 1 and Supplementary Note 2) to rule out the influence of epitaxial strain between the substrate and WSe$_2$. From this calculation, the expected strain from the lattice mismatch shows the opposite trend as compared with what we observe experimentally. We find that our experimentally realized strain per $\Delta$TCE of $-0.10 \pm 0.01\%$ per ppm K$^{-1}$ is in excellent agreement with the theoretical value of $0.09\%$ per ppm K$^{-1}$. To verify that the substrate does not affect the PL peak shape or position of monolayer WSe$_2$, samples were transferred to the four substrates used in this study (Supplementary Fig. 4) and no shift of the PL peak was observed. The impact of growth temperature to tune the strain was also studied using fused silica as the substrate. Figure 3c shows the tensile strain in monolayer WSe$_2$ grown at different temperatures, estimated using PL peak position. We are able to tune the strain from $0.94 \pm 0.06\%$ to $0.67 \pm 0.05\%$ as the growth temperature is changed from 900 to 673 °C. PL spectra corresponding to Fig. 3c is shown in Supplementary Fig. 5.

**Tensile strain engineering of mono- and bilayer WSe$_2$.** Calibrated PL measurements were used to provide a gauge of material quality. We find that strained WSe$_2$ monolayers as-grown on fused silica show comparable PL intensity to exfoliated WSe$_2$, demonstrating that strain engineering of 2D materials can be achieved without compromising material performance. Specifically, as exfoliated samples show a typical quantum yield (QY) of $2.3 \pm 0.4\%$, while samples grown on fused silica show a typical QY of $1.9 \pm 0.6\%$. Upon transfer, the strain within the as-grown material is released and its emission peak shifts to 1.65 eV, closely matching that of exfoliated samples, as shown in Fig. 4a. In addition to emission, the absorption spectrum of the as-grown monolayer was measured and is shown in Fig. 4b. The absorption spectra clearly shows that the A and B exciton resonances are re-
shifted with the presence of tensile strain, and are consistent with the observed shift in the emission. Interestingly, the absorption of the C exciton peak shows no shift between the as-grown and exfoliated samples, which is consistent with previously reported mechanical bending experiments on exfoliated monolayers, although it should be noted that in these experiments the strain was uniaxial\(^\text{28}\).

More interestingly, it has been previously demonstrated using bending experiments that under the application of a uniaxial strain of ~1.5%, bilayer WSe\(_2\) undergoes an indirect-to-direct bandgap transition\(^7\). This effect is caused by an increase in the energy level of the indirect valley at the \(\Sigma\) point as well as a corresponding decrease in the energy level of the direct valley at the \(\text{K point}\}\(^6\). While it is important to note these results are obtained under uniaxial strain, similar trends between uniaxial and biaxial strain have been observed in theoretical studies on other 2D material systems\(^29\). Figure 4c depicts the PL spectra of as-grown, exfoliated and transferred bilayer WSe\(_2\). In the as-grown strained bilayer, we observe a single sharp PL peak, as oppose to a broader spectrum corresponding to emission from both the indirect and direct bandgaps observed in the unstrained exfoliated and transferred samples. Moreover, the intensity of the PL is reduced by approximately 50 times upon transfer and exfoliated samples. In contrast to the indirect and direct bandgaps observed in the unstrained sample, we observe a single sharp PL peak, as oppose to a broader spectrum corresponding to emission from both the indirect and direct bandgaps observed in the unstrained exfoliated and transferred samples.

To further characterize WSe\(_2\) monolayers, we performed low-temperature PL measurements. Numerous studies have experimentally observed that the PL of monolayer WSe\(_2\) is quenched at reduced temperatures. This behavior is unusual for a direct bandgap semiconductor and has been attributed to the formation of dark excitons with an energy level ~30 meV below the bright state\(^30, 31\). It has been hypothesized that at low temperatures the bright exciton is allowed to relax to the lower energy level resulting in a reduction of the PL QY. Conversely, both theoretical and experimental studies have suggested that unstrained monolayer WSe\(_2\) is an indirect-gap semiconductor and has been attributed to the formation of dark excitons with an energy level ~30 meV below the bright state\(^30, 31\).

Discussion

In summary, we have demonstrated controlled and stable strain engineering of 2D materials by growth, realized through TCE mismatch between the substrate and 2D material. The demonstrated strain engineering allows for dramatic modulation of the physical properties of 2D materials using WSe\(_2\) as a model system, we have achieved a strain induced indirect-to-direct
Materials growth

**WSe$_2$** was grown on several substrates with varying thermal expansion coefficients using CVD. Specifically, growth was performed on fused silica (amorphous), aluminum nitride (c-plane), Sapphire (c-plane), or strontium titanate (<100>); all substrates were electronic grade and have a root mean square surface roughness of <10 Å. Substrates were first cleaned by sonication in acetone and isopropl alcohol for 10 min. The growth was carried out using a two-heating-zone furnace (Daepoong Industry, 50602); a schematic of the growth setup is shown in Supplementary Fig. 7. The cleaned substrates were loaded into the downstream zone, and a ceramic boat containing mixture of WO$_3$ and potassium bromide (KBr) was then placed next to the substrates. KBr was mixed with WO$_3$ at a ratio of 1:2, with the KBr acting as a promoter for the growth. This is similar to methods described in ref. 36. However, we found that several salts can be used and the choice of promoter has a significant role in determining the ultimate sample morphology (this is further discussed in the Supplementary Methods). It should be noted that regardless of the promoter used, the strain present in the sample was unaffected as shown in Supplementary Fig. 8. A ceramic boat containing 500 mg Se powder was placed in the center of the upstream zone. After loading, the quartz tube was evacuated and Ar was introduced at 60 sccm resulting in a pressure of 2.6 Torr. The temperature of upstream zone was then ramped to 100 °C and the downstream furnace was subsequently ramped to a setpoint of 825 °C. The set point of the upstream zone was adjusted such that the residual heat from the downstream zone results in vaporization of Se. Once the temperature of downstream furnace was stabilized, hydrogen was introduced at a flow rate of 40 sccm (total pressure of 3 Torr). This initiates the growth as the presence of hydrogen is required to decompose and vaporize WO$_3$. The growth time used was 15 min. Once the growth is complete, hydrogen flow was stopped, and the furnace was opened to rapidly cool the sample. The influence of the H$_2$/Ar ratio, growth time and growth pressure is discussed in the Supplementary Methods and are shown in Supplementary Figs 9–11. Optical microscope images of samples grown on various substrates is shown in Supplementary Fig. 12. Specific growth conditions were tuned to optimize the PL QY of the as-grown samples and to either promote growth of bilayer or monolayer domains (discussed in Supplementary Methods). It should be noted that for growths where the substrate temperature was varied the WO$_3$/KBr boat was placed in the center of the first heating zone and the Se boat was placed at the edge of the first heating zone. The substrates were placed in the center of the second heating zone. The position of Se boat was adjusted to control the temperature. Transfer of growth WSe$_2$ is done using a HF based wet transfer technique with PMMA as the transfer medium using the specific procedure described in ref. 11. The electrical performance of CVD WSe$_2$ grown on fused silica and transferred to Si/SiO$_2$ is also compared to that of exfoliated samples, and is shown in Supplementary Fig. 13.

**Transmission electron microscopy.** WSe$_2$ monolayers were directly grown and transferred on 8 nm thick SiO$_2$ membranes (Ted Pella) for electron diffraction measurements in order to directly measure the lattice constant of the strained and unstrained samples, respectively. Electron diffraction measurements were...
performed at the National Center for Electron Microscopy at LBNL using a FEI Titan 60–300 microscope operated at 80 kV with parallel beam illumination.

Optical characterization. The PL data presented in this work was obtained using a custom built micro-PL instrument described in detail in ref. 9. In brief, measurements were performed using the continuous wave 514 nm line of an Ar+ laser (Lexel 95) and the laser power was adjusted using neutral density filters. The laser was focused on the sample using an 80 x objective lens (NA = 0.9). The PL signal was measured using the same objective lens, passed through a 550 nm dielectric longpass filter, dispersed by a f = 340 mm spectrometer with a 150 mm x 1 grating, and detected using an Si CCD camera (Andor iDus BEX2-DD). Prior to each measurement the CCD background was obtained and subsequently subtracted from the PL acquisition. The sensitivity of the instrument as a function of wave-length (instrument function) was determined through measurement of a virtual Lambertian blackbody source under the objective, created by imaging the illumination from a temperature stabilized lamp (ThorLabs SLS201) on a diffuse reflector (SpectraL). The system efficiency was determined by measuring the response of the excitation laser focused onto a diffuse reflector (SpectraL), with the 550 nm longpass filter removed. The measured external quantum efficiency was converted to QY using sample absorption at the pump wavelength and the fraction of light, fL, which is able to escape the sample (1/4−fL), where n is the refractive index of the medium. All measurements shown in this work were performed at an incident power of 1.5 mW cm−2 (corresponding to a laser power of 200 nW). This laser power is significantly below the onset of birefringent recombination in WSe2.18. Low temperature measurements were performed using a long working distance 50 x objective lens in a micro-cryostat (Janis) with an infrasil window. The procedure described previously was used to calculate the sample PL efficiency. PL imaging was performed on the samples to determine their uniformity. Measurements were performed using a florescence microscopy setup using a 470 nm light emitting diode as the excitation source and a CCD detector (Andor Luca). Raman measurements and high-resolution mapping were performed to characterize the strain in the WSe2. Raman spectra were obtained using a WITec Alpha 300R equipped with a piezo electric scanning stage. The sample was excited using the 532 nm line of a frequency-doubled Nd:YAG laser as the excitation source and focused on the sample using a 100 x objective.

Data availability. The data that support the findings of this study are available from the corresponding author on request.

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Author contributions

G.H.A., M.A. and A.J. conceived the idea for the project and designed the experiments. G.H.A., M.A. and A.J. wrote the manuscript. J.P.M., D.C.C., J.W.A., M.D. and A.J. analyzed the data. Additional information Supplementary Information accompanies this paper at doi:10.1038/s41467-017-00516-5.
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