Strain-induced vibrational properties of few layer black phosphorus and MoTe$_2$ via Raman spectroscopy

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Abstract
We studied and compared the effect of tensile strain on the Raman spectra of black phosphorus (BP) and molybdenum ditelluride (MoTe$_2$) crystals by using a simple custom strain device. In-situ Raman spectroscopy on BP revealed clear red shifting of all three phonon modes, $A_{1g}$, $B_{2g}$ and $A_{2g}$, under tensile stress. From our theoretical analyses, we found that such red shifting strongly depends on the direction of the strain exerted on the system even within the elastic deformation limit (i.e. strain $\leq$ 1 %). In particular, calculated results for the strain along the armchair direction are consistent with our experimental data, confirming that the strain applied to the sample acts effectively along the armchair direction. In a comparative study, we found that the effect of strain on the Raman shifting is larger for BP than that for MoTe$_2$, presumably due to the smaller Young’s modulus of BP. We also see a remarkable resemblance between donor-type intercalation induced vibrational properties and tensile stress-induced vibrational properties in BP. We anticipate that our method of in-situ Raman spectroscopy can be an effective tool that can allow observation of strain effect directly which is critical for future flexible electronic devices.

Supplementary material for this article is available online

Keywords: 2D materials, strain, strain device, black phosphorus, Raman spectroscopy

(Some figures may appear in colour only in the online journal)
1. Introduction

Strain engineering is a powerful technique for tuning the band structure of various two-dimensional (2D) materials in order to enhance the performance of opto-electronic devices [1–6]. In recent years, 2D materials such as black phosphorus (BP) and transition metal dichalcogenides (TMDs) have attracted a great deal of interest due to their remarkable properties [7–11]. Strain in 2D materials induces the modifications in electronic structure which provides an opportunity for engineering of novel devices [12].

Most TMDs are low dimensional materials consisting of stacks of one atomic layer of transition metal atoms (M = Mo, W) between two single layers of chalcogen (X = S, Se) [13]. An intriguing finding is that small amounts of strain can induce the long-known semiconductor-metal transition in thin MoS\(_2\) and MoTe\(_2\) [14]. Based upon this, it may be possible to easily engineer desirable 2D TMD phases based on the application of in-plane tensile strain. This would make strain a very attractive tuning parameter for material properties and electronics applications.

Graphene based transistor with high mobility have a low on/off ratio due to the absence of its intrinsic band gap in contrast to TMDs materials (monolayer with direct band gap but two or more layers with indirect band gap) having high on/off ratio with low mobility [15–18]. Few-layer of BP possessing a direct gap regardless of layer number, has the thickness dependent band gap which fits between the band gap of TMDs and graphene. Black phosphorus is an interesting candidate for strain engineering because of its ability to sustain a high strain and the intensive theoretical studies performed in strain-induced tuning of its mechanical, electronic, and optical properties [19, 20]. BP is a layered structured material in which each atomic layer of the puckered honeycomb lattices are stacked by van der Waals interactions, resulting in a wide range of anisotropic properties [19, 21]. Better understanding of the strain effects on the anisotropic properties of the phosphorene will be beneficial in various technologies, such as flexible electronics.

Despite the unique properties of BP, there are some limitations of using this material because of its environmental instability when exposed to an ambient environment. Degradation of black phosphorus is commonly observed as the formation of liquid droplets on the BP flake [22]. For the effective passivation of BP flakes several techniques have been proposed and tested including surface functionalization and coatings. It has been reported that air-stable BP devices can be made by covering them with double-layer Al\(_2\)O\(_3\) and hydrophobic fluoropolymer [23]. Gamage, et al have studied the effectiveness of suppressing of BP degradation by boron nitride (BN) encapsulation followed by Al\(_2\)O\(_3\) coating [24].

The ability to tune the electronic and thermal properties of 2D materials are highly desired in order to engineer new thermoelectric devices. As such, strain engineering in 2D materials can be employed in tuning the electronic and thermal properties [25]. For example, a small amount of strain in borophene causes the tuning of transport and I–V characteristics suggesting its application for future electronic devices [26]. Strain in 2D materials induces modification in the atomic bond configurations (bond angles, bond lengths and bond strength), which in turn, leads to a considerable change in the lattice vibration (phonon). These shifts in the phonon frequency can be detected by Raman spectroscopy. In this paper, we conducted a comparative strain dependent study on various 2D materials, namely BP, 1T’-MoTe\(_2\) and 2H-MoTe\(_2\) via Raman spectroscopy.

2. Experimental

2.1. Crystal growth

BP crystals were synthesized via the short chemical vapor transport (CVT) method [27]. In short, crystals of pure black phosphorus were obtained by CVT method by annealing an evacuated quartz tube loaded with a mixture of red phosphorus, tin and tin (IV) iodide, where tin and tin (IV) iodide served as mineralization additives. An ampule with precursor powders was evacuated down to 10\(^{-6}\) Torr and sealed afterward using an oxy-acetylene flame torch. Sealed tubes were placed in a three-zone furnace (MTI OTF-1200X) for annealing in such a way that the hot end of the tube was placed toward the centre of the furnace. Sample was heated from room temperature to 650 °C in 3 hr 10 min and left there for 20 mins and rapidly cooled back to 600 °C in 5 min and ramped down the temperature from 600 °C to 550 °C in 7 hr 30 min and finally cooled back to room temperature in 5 hr. Temperature gradient of 50 °C was maintained between hot end and cold end during the entire process. Crystals of 1T’- and 2H-MoTe\(_2\) used in this study were purchased from hq graphene company.

2.2. Sample characterization

The morphology, crystallinity and the details of the crystal structure of BP, 1T’-MoTe\(_2\) and 2H- MoTe\(_2\) samples were analysed using transmission electron microscopy (TEM). TEM specimens were prepared by drop-casting dispersions of samples onto commercial holey carbon-coated TEM grids. TEM measurements were performed using a 200 kV filed emission gun FEI Tecnai F20 instrument, equipped with a nanoprobe and scanning transmission electron microscopy (STEM) capabilities. The microscope was also equipped with analytical capabilities, including an EDAX TEAM\textsuperscript{™} Energy Dispersive x-ray Spectroscopy (EDX) analysis system with an Octane silicon drift detector. Figure 1 shows TEM and high-resolution TEM (HRTEM) images of typical particles of the studied BP, 1T’-MoTe\(_2\), and 2H-MoTe\(_2\) samples. Typical selected area electron diffraction (SAED) ring patterns and corresponding radial intensity profiles obtained from these samples from regions containing several particles are also included in figure 1. For the BP sample, the particles had the form of multilayer flakes and in-plane diameter of around 10 \(\mu\)m, or more (figure 1(a)). The flakes were mostly single-crystalline. HRTEM images of these flakes usually showed two sets of lattice fringes, characterized by the d-spacing values of either, both equal to 0.26 nm (figures 1(b) and (c)) or
one equal to 0.33 nm and the other one to 0.44 nm. These d-spacing values were consistent with the structure of BP. Similarly, the electron diffraction ring pattern from this sample can be indexed to the phase of BP, described by the ICDD PDF # 00–047-1626 (figures 1(d) and (e)). The particles of the MoTe\textsubscript{2} samples were significantly smaller, typically with diameters of around 1 \(\mu\text{m}\). In the case of 2H-MoTe\textsubscript{2}, the particles had also a multilayer flake morphology. HRTEM images confirmed that they were primarily single crystals and showed a hexagonal lattice with a d-spacing of 0.35 nm (figures 2(g) and (h)) which agrees with the structure of the 2H-MoTe\textsubscript{2}. The SAED ring pattern for this sample can be indexed to the 2H-MoTe\textsubscript{2} phase, described by the ICDD PDF # 00–015-0658 (figures 1(i) and (j)). As expected, all strong diffraction rings observed for this sample are of the (hk0)-type (figure 1(i)). In the case of the 1T’-MoTe\textsubscript{2}, the particles did not show a clear flake morphology. Instead, they were rather heavily distorted, defected flakes with their edges split into long fiber-like structures (figure 1(k)). HRTEM images of the flake-like sections showed d-spacing values and the symmetry of the lattice fringes consistent with the crystal structure of 1T’-MoTe\textsubscript{2}. The SAED ring patterns of this sample showed predominantly polycrystalline nature, in big part due to all those randomly oriented fiber-like segments, and could be indexed to the 1T’-MoTe\textsubscript{2} phase, described by the ICDD PDF # 01–071-2157 (figures 1(n) and (o)). This is consistent with previous reports concerning 1T’-MoTe\textsubscript{2} phase [28]. The chemical composition of all three samples was analysed using EDX. The EDX spectra were continuously collected while the nanoprobe was scanned across selected particle in each of the three samples. This allowed for the acquisition of representative elemental maps. Figure 2 shows such example maps along with the corresponding high-angle annular dark field scanning TEM (HAADF-STEM) images and EDX spectra for all three samples. The analysis confirmed the nominal composition of these samples and homogenous distribution of elements.

3. Methods

3.1. Experimental method

Figure 3 shows a schematic diagram of the setup used for strain dependent Raman experiment. The setup includes the strain mount and subminiature linear variable differential transformer (LVDT). The magnified image (within the orange circle) shows the part of the sample at which Raman spectra were collected. The strain mount design has the form of a standard C-frame; the horizontal advancing screw is used to push apart the frame arms. Located at the end of the arms are two shims held by screws. In order to secure samples to the shims, double sided tape is used for adhesion. Construction of the frame utilized 6061-T6 aluminum due to its higher yield strength compared to other aluminums. The shims were cut from 1100-H18 aluminum; the #0-80 UNF shim screws and the #2-56 UNC actuator screw were all 7075-T6 aluminum.

Crystals of BP and MoTe\textsubscript{2} were exfoliated and mounted on the shims within the strain mount device using double-sided scotch tape. Mounted samples were strained by advancing the actuator screw in order to displace the frame arms. Depending on how far the screw was advanced, the amount of tension applied could be adjusted. The displacement of the frame arms moved the shims farther apart which in turn placed the samples under tension.
Figure 2. Chemical composition analysis of BP (top row), 2H-MoTe$_2$ (middle row) and 1T’-MoTe$_2$ (bottom row). HAADF-STEM images (left panels), elemental maps (middle panels), and EDX spectra (right panels). The small concentration of oxygen detected in the spectrum of BP may originate from air exposure and residual surface contamination.

Figure 3. Schematic diagram of the setup used for strain dependent Raman study. The legend indicates the components of the setup.

A rigidly positioned torque actuator (DID-4 A Digital Torque Screwdriver) was used to turn the advancing screw, and measure applied torque to ensure the displaced arms remained with the materials proportional limit. Staying within this limit meant general elastic stress-strain relationships remained applicable. This also allowed sample strain to be calculated by measuring frame arm displacement at the tip of the arm. Displacement was measured by using a sub-miniature linear variable differential transformer (LVDT). Since the frame arms possessed the same dimensions, shared similar Young’s moduli, and were loaded within their elastic range the assumption was made that differences between the two arms displacements were negligible due to differences being significantly smaller in value than the torque actuator and LVDT’s resolution.

In order to conduct strain dependent Raman studies, strain mount setup was placed in a Raman spectroscopy stage (Renishaw inVia™ micro-Raman/PL spectrometer with a 632 nm He-Ne laser). Raman spectra at various strain values were recorded in-situ using a 50x objective lens with an exposure time of 10 sec and accumulations of 10 times.

BP samples used were stored inside a nitrogen filled glove box. We were able to mount the BP sample and perform the strain dependent Raman experiment in about 30–40 min. In order to minimize the degradation of BP in air during the strain experiment, we maintained a flow of nitrogen over the sample.

3.2. Theoretical method

The theoretical calculations were carried out using the first principle method based on the density functional theory (DFT) [29, 30], as implemented in the Vienna Ab-initio Simulation Package (VASP) [31]. The electron-ion interactions were described by the Projector Augmented Wave (PAW) [32],
while electron exchange-correlation interactions were treated by the generalized gradient approximation (GGA) \cite{33} in the scheme of Perdew Burke Ernzerhof (PBE) \cite{34}. For a full structural relaxation, the Congregate-Gradient algorithm \cite{35} implemented in VASP was applied. An energy cut-off was set to be 500 eV for the plane wave basis in all calculations, and the criteria for the convergences of energy and force in relaxation processes were set to be $10^{-5}$ eV and $10^{-4}$ eV Å$^{-1}$, respectively. A $1 \times 1$ primitive cell containing 4 phosphorus atoms was chosen to study the behaviour of black phosphorus and phosphorene under certain strain, respectively. The Brillouin zones (BZ) were sampled by $9 \times 9 \times 9$ (for black phosphorous) or $9 \times 1 \times 9$ (for phosphorene) k-point meshes generated in accordance with the Monkhorst-Pack scheme \cite{36} in the calculations. In the processes of investigating the vibration modes of black phosphorus/phosphorene under uniaxial strain, a stress was introduced (see figure 6(a)), either along the armchair direction or along the zigzag direction. Then, a fully relaxation under the strain was performed. The vibration modes at $\Gamma$ point were calculated from Hessian matrix implemented in VASP code \cite{31}.

4. Results and discussion

Here, we present strain dependent Raman spectra collected for BP, 1T′-MoTe$_2$, and 2H-MoTe$_2$. All the Raman measurements were done at the edge of each sample, since edge was subjected to more stress compared to the middle regions.

4.1. Black phosphorus under strain

We performed the strain dependent Raman experiment in order to investigate the Raman shift as a function of uniaxial tensile strains. Figure 4(a) shows the Raman spectra of few layer black phosphorus with different strain values ranging from 0.0 to 1.08%. We observed three active phonon modes $A_{1g}$, $B_{2g}$ and $A_{2g}$ at 365.4 cm$^{-1}$, 441.2 cm$^{-1}$ and 468.7 cm$^{-1}$, respectively for a as-prepared few-layer BP sample before the strain is applied. Here $A_{1g}$ mode corresponds to the vibration along the out-of-plane with the phosphorus atoms in the top and bottom sub-layers vibrating in opposite directions, whereas the $B_{2g}$ and $A_{2g}$ mode correspond to the vibration along the in-plane zigzag and armchair directions with adjacent atoms vibrating out of phase, respectively. As the strain was applied, all the three phonon modes were observed to red shift progressively up to the strain value of $\sim 1.0\%$. The phonon modes $A_{1g}$, $B_{2g}$ and $A_{2g}$ were red-shifted by 2.9 cm$^{-1}$, 4.1 cm$^{-1}$ and 4.3 cm$^{-1}$, respectively at the highest applied strain values. If a crystal is subjected to a tensile stress, the process can be envisioned that the atoms being pulled apart by lengthening the chemical bonds relative to their normal positions and lengths in the unstressed crystal. As the chemical bond length increases, the force constant decreases (for a given stress), hence the vibrational frequency decreases (frequency is proportional to the square root of the force constant). Hence shifts of the Raman peaks to lower frequencies are observed for materials that have been subjected to a tensile stress. Conversely, when a compressive stress is applied, the

![Figure 4](image_url)

Figure 4. (a) Strain dependent Raman spectrum of black phosphorus. (b) Raman shifts with quadratic fits of the phosphorene sample. (c) Unstrained Raman spectrum of BP with arrow showing the relative change in phonon modes. (d) Relative change in the Raman shift of phonon modes $A_{1g}$ and $B_{2g}$ with respect to $A_{1g}$. 

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Figure 5. The changes in $A_{2g}^1$ and $B_{2g}$ Raman modes against the change in $A_{1g}^1$ due to in-situ Li-intercalation as well as strain (shaded region) experiments.

Figure 6. (a) Schematic illustration of the uniaxial strain exerted on the black phosphorus. (b) Calculated vibration modes of BP under uniaxial strain along the armchair direction (left panel) and zigzag direction (right panel), respectively. (c) Calculated vibration modes of phosphorene under uniaxial strain along the armchair direction (left panel) and zigzag direction (right panel), respectively. The corresponding number denotes the decreasing slope for each mode. (d) Comparison of uniaxial tensile strain experimental (open circle) and theoretical (closed stars) Raman shifts for three phonon modes of BP. Phonon modes $A_{1g}^1$, $B_{2g}$ and $A_{2g}^1$ are represented by blue, black and red colours.
atoms in a crystal move closer to each other by shortening the chemical bonds, which leads to the Raman peaks shifting to higher frequencies [2, 37–39]. Hence, compressive and tensile strains induce corresponding stress in the crystal that can be observed as shifts of Raman peaks to higher or lower frequencies, respectively. The magnitude of the Raman peak shift depends on the stress and corresponding strain induced in the material. The degree to which the Raman band shifts depends on the elastic constants such as Young’s modulus of that material and the specific crystallographic axes being probed.

In order to avoid unreliable strain response measurements, we limited the Raman measurements to applied strains levels that produced a proportional response. At higher strain values however, we observed the peaks to be shifted back (see Figure S1 (available at stacks.iop.org/NANO/31/425707/mmedia)) because of the relaxation of the stress. This behavior (shown in the shaded regions of Figure S1) could be due to the poor adhesion of the sample to the tape or decoupling of the top layer from the lower layers within the few-layer BP.

We also noticed that these phonon modes ($A_{1g}^1$, $B_{2g}$ and $A_{2g}^2$) red-shifted at different rates with respect to the strain, i.e. they had different sensitivities, $\Delta \omega / \Delta \sigma$, where $\omega$ is the Raman shift and $\sigma$ is the strain. Our observation on the different shifting rates, $\Delta \omega / \Delta \sigma$ of $A_{2g}^2$, $B_{2g}$ compared to $A_{1g}^1$ is consistent with previously reported results on the comparison of polarization Raman spectroscopy between near armchair and near zigzag strain-red shift calculations [19, 40]. For any intermediate direction, it is also reported to have a red shift even though the in-plane modes are insensitive to near armchair strain while the zigzag strain has more prominent effect on these in plane modes. The $A_{2g}^2$ and $B_{2g}$ modes show higher shifts in comparison to $A_{1g}^1$ mode presumably due to the Raman tensor element ratio $c/a$ [19]. Compared to our stretching experiment under tensile strain, a slightly more sensitive shift in $A_{1g}^1$ mode has been reported under bending condition. This results from the vibrations of the opposing P atoms of the top and bottom with respect to each other within the same layer. Under stretching conditions this effect was not observed [2].

**Figure 7.** The strain dependent Raman spectra of (a) 1T’-MoTe$_2$ and (c) 2H-MoTe$_2$. (b) The Raman shifts of the two modes of 1T’-MoTe$_2$ against the strain with linear fits. (d) The Raman shift of the single mode of 2H-MoTe$_2$ against strain with a linear fit.
Figure 4(b) shows the peak position of all three phonon modes with respect to the strain where the blue line showing the quadratic fit of the measured data points. Figure 4(c) shows how the relative change in the peak position is defined. Figure 4(d) shows the relative change in the peak position of phonon modes $A^2_g$ and $B_{2g}$ with respect to the relative change in phonon mode $A^1_g$. It was observed that rates of the change of phonon modes $A^2_g$ and $B_{2g}$ against $A^1_g$, $\Delta \omega(A^2_g)/\delta \omega(A^1_g)$, $\Delta \omega(B_{2g})/\delta \omega(A^1_g)$ to be 1.40 and 1.38 respectively.

Next, we compare the effect of tensile stress with the donor type intercalation (alkali metals, etc.) on the Raman shift of BP. Similar to tensile stress, donor type intercalation leads to an increase in the electron density of a crystal and hence increase in the bond lengths eventually causing a decrease in the vibrational frequencies. Conversely, acceptor type intercalation leads to a decrease in the electron density causing a decrease in the bond length (increase in the force constant) and hence an increase of the vibrational frequencies. In the case of intercalation, one can make a direct comparison between $\Delta \omega(\delta q)$, where $\omega$ is the Raman shift and $q$ is the charge transfer, and $\Delta \omega(\Delta \sigma)$ in the case of strain. Figure 5 shows the changes in $B_{2g}$ and $A^2_g$ Raman modes against the change in $A^1_g$ from in-situ Li-intercalation from our recent study [41] and strain (shaded region) experiments in this study. It is interesting to note that the Raman shifts of $B_{2g}$ and $A^2_g$ against $A^1_g$ due to the measurable strain values follow the same linear behaviour of the data resulting from much larger shifts due to Li+ intercalation. This is not surprising as both intercalation and strain effects cause bond length stretching of BP.

We also performed first-principle calculation on the Raman shifts of black phosphorus and phosphorene (i.e. monolayer) under uniaxial strain along armchair and zigzag direction. As shown in figure 6, the red shift of Raman spectra on both BP and phosphorene strongly depends on the direction of the strain exerted on the system even within the elastic deformation limit (i.e. strain $\leq$ 1 %). In the case of black phosphorus, $A^1_g$, $B_{2g}$ and $A^2_g$ modes decrease slowly along the armchair direction with increasing strain with the slopes 3.3 cm$^{-1}$, 0.35 cm$^{-1}$, and 0.8 cm$^{-1}$, respectively (the left panel of figure 6(b)). While they decrease faster with increasing strain along the zigzag direction with the slopes 6.7 cm$^{-1}$, 8.5 cm$^{-1}$, and 1.2 cm$^{-1}$, respectively (the right panel of figure 6(b)), indicating the anisotropic behaviour of black phosphorus under strain. Such trend is also found in phosphorene under uniaxial strain (figure 6(c)). By comparing our theoretical calculations (open triangles in figure 6(d)) with our experimental results (solid circles in figure 6(d)), we found that the theoretical results for the strain along the armchair direction (left panels in figures 6(b) and (c)) are consistent with our experimental results (figure 4(b)) for the strain less than 1 %. This confirms that the strain applied to the sample acts effectively along the armchair direction.

4.2. 1T’ & 2H-MoTe2 under strain

In a comparative study, we have investigated the tensile strain effects of Raman spectra in two different phases of MoTe2 as shown in figure 7. Raman spectra of 2H-MoTe2 shows one peak at 232 cm$^{-1}$ and we detected two peaks of 1T’-MoTe2 at position 142 cm$^{-1}$ and 124 cm$^{-1}$. In both of these samples, upon increase of the strain from 0 to 5 %, we saw a downshift in each peak position (as shown in figure 7) by a peak shifting of 2.05 cm$^{-1}$ (first peak) and 1.15 cm$^{-1}$ (second peak) for 1T’-MoTe2 and by 1.23 cm$^{-1}$ for 2H-MoTe2, respectively at the highest strain value.

Finally, figure 8 shows the comparison of phonon mode shifting of BP (3 modes), 1T’-MoTe2 (2 modes) and 2H-MoTe2 (1 mode). It is observed that peak shifting ratio, $\Delta \omega(\Delta \sigma)$ of black phosphorus is much higher than that of MoTe2. For BP, we observe that phonon mode $A^1_g$ and $B_{2g}$ are downshifted by an amount that is 1.6 times larger than that of $A^1_g$ (5.50 cm$^{-1}$ vs 3.4 cm$^{-1}$). For, 1T’-MoTe2, $\Delta \omega(\Delta \sigma)$ for the two phonon modes are 0.70 cm$^{-1}$ and 0.40 cm$^{-1}$ while 2H-MoTe2 shows the smallest shift with strain with $\Delta \omega(\Delta \sigma) \sim 0.25$ cm$^{-1}$.

5. Conclusion

In summary, we studied and compared the strain dependent Raman behaviour of black phosphorus and 2 phases of MoTe2 crystals, 1T’-MoTe2 and 2H-MoTe2. We employed a custom strain mount which allowed variable reproducible strains to be applied to these materials. Our result shows that the strain induced Raman peak shifting of black phosphorus is more pronounced than that of both phases of MoTe2, which can be understood as due to the lower Young’s modulus value of BP. We also see a resemblance between donor-type intercalation induced vibrational properties and tensile stress induced vibrational properties in BP as both mechanisms result in bond length increase in BP. Therefore, peak shifting of the phonon mode is a good means for understanding the strain behaviour of 2D materials. Such methods could be beneficial for manufacturing future flexible electronic devices.
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References

[1] Guinea F, Katsnelson M I and Geim A K 2010 Energy gaps and a zero-field quantum Hall effect in graphene by strain engineering Nanot. Phys. 6 30–33
[2] Liang S, Hasan M N and Seo J-H 2019 Direct observation of raman spectra in black phosphorus under uniaxial strain conditions Nanomaterials 9 966
[3] Zhou H, Seo J-H, Paskievicz D M, Zhu Y, Celler G K, Voyles P M, Zhou W, Lagally M G and Ma Z 2013 Fast electronics with strained silicon nanomembranes Sci. Rep. 3 1291
[4] Deng S, Sumant A V and Berry V 2018 Strain engineering in two-dimensional nanomaterials beyond graphene Nano Today 22 14–35
[5] Conley H J, Wang B, Ziegler J I, Heglund R F, Pantelides S T and Bolotin K I 2013 Bandgap engineering of strained monolayer and bilayer MoS2 Nanot. 13 3626–30
[6] Jeong R H, Lee J W, Kim D I, Yang J W, Park S and Boo J-H 2020 Black phosphorus @ molybdenum disulfide 2D nanocomposite with broad light absorption and high stability for methylene blue decomposition photocatalyst Nanot. 31 155704
[7] Akhtar M, Anderson G, Zhao R, Alrugi A, Mroczkowska J E, Sumanasekera G and Jasinski J B 2017 Recent advances in synthesis, properties, and applications of phosphorene Npj 2D Mater. Appl. 1 1–13
[8] Wang Q H, Kalantar-Zadeh K, Kis A, Coleman J N and Strano M S 2012 Electronics and optoelectronics of two-dimensional transition metal dichalcogenides Nanot. 7 699
[9] Lee J, Huang J, Sampter B G and Yoon M 2017 Strain-engineered optoelectronic properties of 2D transition metal dichalcogenide lateral heterostructures 2D Mater. 4 022016
[10] Mortazavi B, Berdiyorov G R, Makaremi M and Rabczuk T 2018 Mechanical responses of two-dimensional MoTe2; pristine 2H, 1T and 1T/2H heterostructure Extreme Mech. Lett. 20 65–72
[11] Huang L, Chen C, Li Z, Zhang Y, Zhang H, Lu J, Ruan S and Zeng Y 2019 Challenges and future perspectives on microwave absorption based on two-dimensional materials and structures Nanotechnology 31 162001
[12] Jiang H, Zheng L, Liu Z and Wang X 2019 Two-dimensional materials: from mechanical properties to flexible mechanical sensors Inform 1–18
[13] Choi W, Choudhary N, Han G H, Park J, Akinwande D and Lee Y H 2017 Recent development of two-dimensional transition metal dichalcogenides and their applications Mater. Today 20 116–30
[14] Song S, Keum D H, Cho S, Perello D, Kim Y and Lee Y H 2016 Room temperature semiconductor-metal transition of MoTe2 thin films engineered by strain Nanot. Mett. 16 188–93
[15] Liu W, Kang J, Sarkar D, Khatami Y, Jena D and Banerjee K 2013 Role of metal contacts in designing high-performance monolayer n-Type WSe2 field effect transistors Nanot. Lett. 13 1983–90
[16] Das A et al 2008 Monitoring dopants by Raman scattering in an electrochemically top-gated graphene transistor Nanot. 3 210–5
[17] Liang X, Fu Z and Chou S Y 2007 Graphene transistors fabricated via transfer-printing in device active-areas on large wafer Nanot. Lett. 7 3840–4
[18] Ovchinnikov D, Allain A, Huang Y-S, Dumencio D and Kis A 2014 Electrical transport properties of single-layer WS2 ACS Nanot. 8 8174–81
[19] Wang Y, Cong C, Fei R, Yang W, Chen Y, Cao B, Yang L and Yu T 2015 Remarkable anisotropic phonon response in uniaxially strained few-layer black phosphorus Nanot. Res. 8 3944–53
[20] Zhu W, Liang L, Roberts R H, Lin J-F and Akinwande D 2018 Anisotropic electron–phonon interactions in angle-resolved raman study of strained black phosphorus ACS Nanot. 12 12512–22
[21] Wang X, Jones A M, Seyler K L, Tran V, Jia Y, Zhao H, Wang H, Yang L, Xu X and Xia F 2015 Highly anisotropic and robust excitons in monolayer black phosphorus Nanot. 10 517–21
[22] Abate Y, Akinwande D, Gamage S, Wang H, Snure M, Poudel N and Cronin S B 2018 Recent progress on stability and passivation of black phosphorus Adv. Mater. 30 1704749
[23] Kim J-S, Liu Y, Zhu H, Kim S, Wu D, Tao L, Dodabalapur A, Lai K and Akinwande D 2018 Toward air-stable multilayer phosphorene thin-films and transistors Sci. Rep. 5 8989
[24] Gamage S, Fali A, Aghamiri N, Yang L, Ye P D and Abate Y 2017 Reliable passivation of black phosphorus by thin hybrid coating Nanotechnology 28 265201
[25] Zhang G and Zhang Y-W 2015 Strain effects on thermoelectric properties of two-dimensional materials Meck. Mater. 91 382–98
[26] Shukla V, Gregoriev A, Jena N K and Ahuja R 2018 Strain controlled electronic and transport anisotropies in two-dimensional borophene sheets Phys. Chem. Chem. Phys. 20 22952–60
[27] Akhtar M, Zhang C, Rajapakse M, Khan Musa M R, Yu M, Sumanasekera G and Jasinski B J 2019 Bilayer phosphorene under high pressure: in situ Raman spectroscopy Phys. Chem. Chem. Phys. 21 7298–304
[28] Liu M, Wang Z, Liu J, Wei G, Du J, Li Y, An C and Zhang J 2017 Synthesis of few-layer 1T-MoTe2 ultrathin nanosheets for high-performance pseudocapacitors J. Mater. Chem. A 5 1035–42
[29] Kohn W and Sham L J 1965 Self-consistent equations including exchange and correlation effects Phys. Rev. 140 A1133–8
[30] Hohenberg P and Kohn W 1964 Inhomogeneous electron gas Phys. Rev. 136 B864–71
[31] Kresse G and Furthmuller J 1999 Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set Phys. Rev. B 54 11169–86
[32] Blochl P E 1994 Projector augmented-wave method Phys. Rev. B 50 17953–79
[33] Perdew J P, Chevary J A, Vosko S H, Jackson K A, Pederson M R, Singh D J and Fiolhais C 1992 Atoms, molecules, solids, and surfaces: applications of the generalized gradient approximation for exchange and correlation Phys. Rev. B 46 6671–87
[34] Perdew J P, Burke K and Ernzerhof M 1996 Generalized gradient approximation made simple Phys. Rev. Lett. 77 3865–8
[35] Gonze X 1997 First-principles responses of solids to atomic displacements and homogeneous electric fields: implementation of a conjugate-gradient algorithm Phys. Rev. B 55 10337–54
[36] Monkhorst H J and Pack J D 1976 Special points for Brillouin-zone integrations Phys. Rev. B 13 5188–92
[37] Ferralis N 2010 Probing mechanical properties of graphene with Raman spectroscopy J. Mater. Sci. 45 5135–49
[38] Yang X X, Li J W, Zhou Z F, Wang Y, Yang L W, Zheng W T and Sun C Q 2012 Raman spectroscopic determination of the length, strength, compressibility, Debye temperature, elasticity, and force constant of the C–C bond in graphene Nanoscale 4 502–10
[39] Xu Z, He Z, Song Y, Fu X, Rommel M, Luo X, Hartmaier A, Zhang J and Fang F 2018 Topic review: application of raman spectroscopy characterization in mic/mono-maching Micromachines 9 361
[40] Tokár K, Brndiar J and Štich I 2019 Raman activity of multilayer phosphorene under strain ACS Omega 4 22418–25
[41] Rajapakse M, Musa R, Abu U O, Karki B, Yu M, Sumanasekera G and Jasinski J B 2020 Electrochemical Li intercalation in black phosphorus: in situ and ex situ studies J. Phys. Chem. C 124 10710–8