Mechanical properties of $1T$, $1T'$, and $1H$-MX$_2$ monolayers and their $1H/1T'$-MX$_2$ (M = Mo, W and X = S, Se, Te) heterostructures

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ABSTRACT
Mechanical properties of two-dimensional (2D) transition-metal dichalcogenides (TMDCs) are of vital importance in any practical applications to flexible devices and nano-electromechanical systems. Thus, the mechanical properties of monolayer TMDCs, a stoichiometric formula MX₂ in which M = Mo, W and X = S, Se, Te, are investigated by using density functional theory. More importantly, based on the different atomic arrangement, all three chemical isomers, such as 1T, 1T′, and 1H phases, are compared in detail. We found that their 2D Young’s moduli and Poisson’s ratios display a strong dependence not only on the atomic species but also on the atomic arrangements. For the same structural phase, monolayer TMDCs with the W (S) atom are found to be much stiffer in each chalcogenide (metal) group. Due to the threefold rotation symmetry of the hexagonal lattice, 1T- and 1H-TMDC monolayers belong to the isotropic structures, while the strong anisotropic Young’s moduli and Poisson’s ratios are observed in the 1T′ phase, i.e., 2D Young’s moduli along the armchair direction are nearly 50% larger than those along the zigzag direction for tellurides. Interestingly, 1T-TMDC monolayers show negative Poisson’s ratios. Furthermore, their in-plane 1H/1T′ heterostructures could be constructed, and the corresponding mechanical properties are explored. We found that the influence of the 1H/1T′ interface on the mechanical behavior is detrimental, which reduces the in-plane stiffness normal to the 1H/1T′ interface as compared with 1H and 1T′ structures. However, in comparison with the 1T′ phase, a remarkable strength of these novel heterostructures is along the 1H/1T′ interface direction. In brief, the present first-principles results constitute a useful picture for the mechanical properties of 2D TMDCs and their in-plane heterostructures.

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I. INTRODUCTION
Transition-metal dichalcogenides (TMDCs) are a family of two-dimensional (2D) materials with a chemical composition of MX₂, where M is a transition metal and X = S, Se, Te. Especially, due to the presence of a direct bandgap electronic characteristic, monolayer 1H-TMDCs such as MoS₂, MoSe₂, WS₂, and WSe₂ have great interest as the ideal candidates for flexible electronic/optoelectronic applications and nano-electromechanical system (NEMS) devices. Thus, it is a necessary prerequisite to understand the mechanical properties of monolayer TMDCs, further predicting their response upon incorporation into NEMS devices.

For homogeneous materials, the mechanical properties can be described by two independent constants, Young’s modulus and Poisson’s ratio. For TMDCs with monolayer or few layers, their Young’s moduli have been experimentally determined by employing nanoindentation techniques with an atomic force microscope or a nanoscopic bending test. Besides, micro-Brillouin light scattering is used to study Young’s modulus and residual stress of polycrystalline MoS₂ membranes in a simple, contact-less, nondestructive manner.

Experimentally, it was found that 2D Young’s moduli of monolayer and bilayer 1H-MoS₂ were 180 ± 60 N/m and 260 ± 70 N/m, respectively. For monolayer 1H-WS₂, a high elastic modulus...
…that along the Young’s moduli and Poisson’s ratios of monolayer 1T-MX₂ (M = Mo or W) are also reported. Besides, Young’s moduli of multilayered 1H-WS₂ were measured, and they were 596 ± 23, 690 ± 25, and 1411 ± 61 N/m for 5-, 6-, and 12-layer thick membranes, respectively. Furthermore, these experimental results could be well understood within a nonlinear elastic constitutive equation. In addition, more theoretical results were also reported on the in-plane stiffness of 1H-MoS₂, 1H-MoSe₂, 1H-WS₂, and 1H-TeS₂.36-39 Note that the extensive studies just focus on the 1H phase. A single-layer TMDC is comprised of three atom-thick layers where a layer of transition metal cations is sandwiched between two layers of chalcogen anions. In the 1H phase, each metal atom is prismatically coordinated by six surrounding chalcogen atoms, with the chalcogenide atoms in the upper layer lying directly above those of the lower layer, as shown in Fig. 1(a).

Besides, TMDCs could usually reveal 1T structures. As shown in Fig. 1(b), transition metal atoms of the 1T phase are also coordinated to six neighboring chalcogen atoms with one hexagonal layer of chalcogen anions in one hollow site on one surface and the other layer in the other hollow site at the other surface.Surprisingly, negative Poisson’s ratios are predicted in 1T-MX₂ (M = Mo and W) monolayers, while Poisson’s ratio is ∼0.29 for monolayer 1H-MoS₂.40-43 However, the 1T phase is known to be metastable and will undergo a distortion with the zigzag chains between transition metals along the β axis [1T′, as shown in Fig. 1(c)].43 In comparison to the 1H phase, 1T′ geometries of monolayer TMDCs could be stabilized by argon plasma, Re-doping, and so on.41,42 Due to the three-fold symmetry of the crystal structure, the 1H phase belongs to the isotropic structure and shows the elastic isotropy at small strains. If the indentation depth is large enough, they begin to develop a six-fold rotation symmetry. However, when the 1T phase is transformed into a 1T′ structure, the isotropy will be broken. In the case of 1T′-MoTe₂, the resistivity along the ß direction is higher than that along the α direction.43 Similar to their electronic behaviors, 1T′-MX₂ exhibit rather anisotropic elastic properties, which are less studied.44,45

In this manuscript, we present a detailed investigation of 2D Young’s moduli and Poisson’s ratios of monolayer 1T- and 1T’-MX₂ (M = Mo, W and X = S, Se, Te) and compare them with those of the 1H phase in detail by conducting extensive density functional simulations. Contrasting with the pristine TMDCs, in-plane heterostructures made from different structural phases in seamlessly stitched forms will further show novel mechanical properties.46 In this context, several TMDCs-based heterostructures have been experimentally realized by using selectively decorated molecules or electrostatic doping. Consequently, some in-plane heterostructures between the stable 1T’ and 1H phases are constructed. Finally, their corresponding mechanical properties are investigated in order to inspect the trend of mechanical properties in TMDCs.

The remainder of this paper is organized as follows. Section II describes the computational details. The main results on the mechanical properties along the armchair or zigzag directions of pristine MX₂ (M = Mo, W and X = S, Se, Te) monolayers and their in-plane 1H/1T’ heterostructures are given in Secs. III A, III B, and IV, respectively. Finally, Sec. V provides a short summary.

II. TECHNICAL DETAILS

We performed first-principles density functional theory (DFT) calculations based on the Vienna *ab initio* simulation package (VASP).50 To describe the electron-ion interaction, the projector augmented wave (PAW) pseudopotentials from the standard distribution were employed.51,52 The exchange-correlation interaction was treated using the generalized gradient approximation (GGA) proposed by Perdew-Burke-Ernzerhof (PBE).53 The plane wave was expanded to an energy cutoff of 420 eV. The Monkhorst-Pack grid for the Brillouin zone was sampled by a Γ-centered 21 × 1 × 1 k-point mesh for pristine TMDCs and 10 × 1 × 1 for their in-plane 1H/1T’ heterostructures.44 In order to avoid the image-image interactions, a vacuum region larger than 15 Å along the sheets normal direction was set. All geometries with different structural phases are fully optimized within the conjugate gradient method until the self-consistence field energies differ below 10⁻⁶ eV with a convergence threshold of 10⁻² eV/Å in the atomic force.54

III. PRISTINE MONOLAYERS

A. Armchair direction

1. Young’s moduli

The thickness of a 2D material is indeterminate because its out-of-plane configuration may change as a function of the deformation states. Hence, 2D Young’s moduli are defined intrinsically as the force per length within the elastic limit and obtained by the strain-energy method by applying a set of suitable in-plane uniaxial deformations in a multistep procedure to the rectangular cell of 1H-, 1T-, and 1T’-MX₂ (M = Mo, W and X = S, Se, Te, as shown in Fig. 1) along the zigzag or armchair directions, respectively.14,36,37 When the strain applied to one lattice constant is fixed, the other lattice constant and the atomic coordinations are fully optimized into the minimum potential energy configuration both in and out of the plane. Then, 2D Young’s moduli could be derived with a least-squares curve fit of the strain-energy data.

As shown in Fig. 2(a), the calculated 2D in-plane Young’s moduli along the armchair direction (Y_{armchair}) are less than the experimental data in the literature studies but agree well with the theoretical results.24,9,11-18,38-42 For example, our calculated Y_{armchair} value of monolayer 1H-MoS₂ is 131.28 N/m, which is comparable to the reported results (experimental values: 171 N/m, 185 N/m, and...
129 N/m,

DFT calculations: 122 N/m,

123 N/m,

124 N/m,

131 N/m,

135 N/m,

136 N/m,

146 N/m. A molecular dynamics simulation of the indentation process in 1H-MoS\(_2\) yields a larger Young’s modulus of 170 N/m. No matter what kinds of structural phases of monolayer MX\(_2\) are, all of \(Y_{\text{armchair}}\) for the same structural phase decrease monotonically as the atomic numbers of chalcogen atoms increase in each transition metal group due to the reduction in the bonding energy. Furthermore, this is because that the charge transfer will decrease, while the lattice constant will increase during switching from S to Te. The second common characteristic is that in each chalcogenide group with the same atomic arrangement, WX\(_2\) compounds become much stiffer than MoX\(_2\) compounds. Note that this trend is also independent of the structural phases and is in well agreement with the previous results. In addition, for the same MX\(_2\) compounds, \(Y_{\text{armchair}}\) in the 1T phase are minimum. When the metastable 1T’ geometries are distorted into the relatively stable 1T’ phases, all Young’s moduli along the armchair direction will be strongly enhanced. However, our results do not match the previous results that the elastic modulus along the armchair direction is 82 N/m and 66 N/m for the 1T- and 1T’-MoTe\(_2\), respectively. In comparison to \(Y_{\text{armchair}}\), between the 1T’ and 1H phases, for monolayer MoS\(_2\), MoSe\(_2\), and WS\(_2\), \(Y_{\text{armchair}}\) for 1H structures are larger than those for 1T’ structures. On the contrary, \(Y_{\text{armchair}}\) for 1H structures of telluride are less than those for 1T’ structures, which is in agreement with the calculated results in 1T’-WTe\(_2\). For monolayer 1H- and 1T’-WSe\(_2\), \(Y_{\text{armchair}}\) are nearly the same and 125.44 N/m and 125.28 N/m for 1T’ and 1H phases, respectively. In general, the calculated in-plane stiffness of MX\(_2\) which is smaller than that of graphene (\(~335\) N/m) and hexagonal boron nitride (\(~267\) N/m) indicates that the latter is more flexible than the former. This is because the elastic modulus correlates reasonably well with the B–N and M–X bonding energies using the sp\(^2\)-hybridized carbon bond. However, monolayer 1H-WS\(_2\) has a direct band gap of suitable size (\(~1.90\) eV), so it is the promising substrate material for flexible electronic/optoelectronic devices.

2. Poisson’s ratios

Poisson’s ratio is used to describe the lateral deformation and can be calculated by \(v_{\text{ab}} = \frac{\epsilon_{\text{a}}}{\epsilon_{\text{b}}}\). Here, \(\epsilon_{\text{a}}\) and \(\epsilon_{\text{b}}\) are the uniaxial strains along the \(\vec{a}\) (zigzag) and \(\vec{b}\) (armchair) directions, respectively. Thus, Poisson’s ratio along the armchair (\(\vec{b}\)) direction (\(P_{\text{armchair}}\)) is defined as \(\epsilon\) will occur along the zigzag (\(\vec{a}\)) direction when a certain \(\epsilon\) is first applied along the armchair (\(\vec{b}\)) direction. As shown in Fig. 2(b), negative \(P_{\text{armchair}}\) are observed in the 1T phase. Thus, 1T-MX\(_2\) monolayers can be categorized as auxetic materials. Moreover, the absolute \(P_{\text{armchair}}\) will decrease for monolayer 1T-MoX\(_2\) while increase for 1T-WX\(_2\) monolayers when the chalcogenide elements become heavier and heavier. On the contrary, 1T’- and 1H-MX\(_2\) monolayers have positive \(P_{\text{armchair}}\). Our calculated \(P_{\text{armchair}}\) for monolayer 1H-MoS\(_2\) and 1H-MoTe\(_2\) are \(-0.258\) and \(-0.227\), which is well consistent with the previous results. Except for 1T’-WS\(_2\), their \(P_{\text{armchair}}\) are larger than that of monolayer graphene (\(-0.16\)). When the atomic numbers of chalcogen atoms become larger and larger in each transition metal group, \(P_{\text{armchair}}\) will decrease for 1H structures, while they will increase for the 1T’ phase. In each chalcogenide group with the same structural phase (1H and 1T’), the MoX\(_2\) compounds have better lateral contraction properties than WX\(_2\) compounds. Comparing 1T’-MX\(_2\) with 1H-MX\(_2\) for monolayer MoSe\(_2\), MoTe\(_2\), and WTe\(_2\), \(P_{\text{armchair}}\) for 1H structures are less than those for 1T’ structures. On the contrary, \(P_{\text{armchair}}\) for 1H structures of sulphide are larger than those for 1T’ structures.

B. Zigzag direction

1. Young’s moduli

The 2D in-plane Young’s moduli along the zigzag direction (\(Y_{\text{zigzag}}\)) for the pristine 1H-, 1T-, and 1T’-MX\(_2\) (M = Mo, W and
FIG. 3. (a) Two-dimensional in-plane Young's moduli along the zigzag direction ($Y_{zigzag}$) and (b) the ratios of $Y_{armchair}$ to $Y_{zigzag}$ for pristine 1H-, 1T-, and 1T'-MX$_2$ (M = Mo, W and X = S, Se, Te) monolayers.

FIG. 4. Poisson's ratios along the zigzag direction ($P_{zigzag}$) for the pristine 1H-, 1T-, and 1T'-MX$_2$ (M = Mo, W and X = S, Se, Te) monolayers. The dashed line represents Poisson's ratio of graphene (~0.16).

X = S, Se, Te) monolayers are shown in Fig. 3(a). Similar to $Y_{armchair}$, $Y_{zigzag}$ will monotonously decrease as the chalcogen atoms switch from S to Se, and then to Te in the same metal group and will increase when the transition metal anions change from Mo to W in the same chalcogenide group. Differing from $Y_{armchair}$, the distortions between 1T' and 1T'' phases will lead to the slight reduction in $Y_{zigzag}$ for monolayer MX$_2$ except for WS$_2$ and WSe$_2$. Comparing 1T'' with 1H phases, $Y_{zigzag}$ for 1H structures are larger than those for 1T'' structures. Taking WTe$_2$ as an example, interestingly, Young's modulus in the 1T'' phase along the armchair direction is larger, while Young's modulus in the 1T'' phase along the zigzag direction is less than that in the 1H phase. In general, 1H-WS$_2$ has the strongest 2D in-plane stiffness along the zigzag direction.

In order to discuss the isotropy/anisotropy of 2D in-plane Young's moduli, the ratios of Young's moduli along the armchair direction ($Y_{armchair}$) to those along the zigzag direction ($Y_{zigzag}$) are calculated and shown in Fig. 3(b). Since monolayer 1H- and 1T-MX$_2$ have the threefold rotation symmetry, all of them belong to isotropic structures. Thus, the ratios ($Y_{armchair}/Y_{zigzag}$) for 1H- and 1T-MX$_2$ are ~1. For 1T'-MS$_2$ and 1T'-MSe$_2$ monolayers, $Y_{armchair}/Y_{zigzag}$ are slightly greater than ~1.2. Especially for 1T'-MoTe$_2$ and 1T'-WTe$_2$ monolayers, $Y_{armchair}/Y_{zigzag}$ are about 1.53 and 1.51, respectively, which are in good agreement with the reported ratios (1.54 for 1T'-MoTe$_2$ and 1.47 for 1T'-WTe$_2$). Thus, the in-plane stiffness is anisotropic and direction dependent in the 1T'' phase because that the 1T'' ~ 1T'' distortion results in the symmetry breaking by
the dimerization of the transition metals along one of the lattice directions.24

2. Poisson’s ratios

Poisson’s ratios ($v_{ba} = -\varepsilon_b/\varepsilon_a$) along the zigzag direction ($P_{\text{zigzag}}$) for pristine $1H$, $1T'$, and $1T''-\text{MX}_2$ (M = Mo, W and X = S, Se, Te) monolayers are shown in Fig. 4. Except for monolayer $\text{MoTe}_2$, all $1T$ structures still show negative Poisson’s ratios along the zigzag direction. Interestingly, if a certain tensile strain is first applied along the armchair ($b$) direction in monolayer $1T'$-$\text{MoTe}_2$, the optimum lattice constant along the zigzag ($a$) direction will be slightly enhanced, while the optimum lattice constant along the armchair ($b$) direction will be reduced when a certain tensile strain is applied along the zigzag ($a$) direction. When the chalcogenide atoms become heavier and heavier in each metal group, $P_{\text{zigzag}}$ still drastically increase for the $1T'$ phase, while they will slightly decrease for the $1H$ phase. In each chalcogenide group with the same $1H$ or $1T'$ structures, MoX$_2$ compounds still have better lateral contraction properties than WX$_2$ compounds. Moreover, for the common $1H$-$\text{MX}_2$, $P_{\text{zigzag}}$ are less than those of graphene.25 In addition, $P_{\text{armchair}}$ are much larger than $P_{\text{zigzag}}$ in $1T'$ and $1H$ phases. This is in agreement with the previous results on bulk $1T'_2$-$\text{MoTe}_2$ where in-plane Poisson’s ratios are found to be anisotropic and $-0.19$ ($-0.31$) for a tensile strain along the $a$ ($b$) axis.25

IV. IN-PLANE HETEROSTRUCTURES

Finally, we analyze Young’s moduli and Poisson’s ratios of monolayer in-plane $1H/1T'$-$\text{MX}_2$ (M = Mo, W and X = S, Se, Te) heterostructures. Top and side views of in-plane $1H/1T''-\text{MX}_2$ heterostructures studied in this manuscript are depicted in Fig. 5(a). To build the interface between $1H$- and $1T''-\text{MX}_2$ monolayers which exists on the middle of the constructed structure is exactly on the basis of experimental observation by Lin et al.25–27 Parallel to the $1H/1T''$ interface, five repeated cells are taken into consideration for $1H$ (red shadow) and $1T''$ (green shadow) phases. Perpendicular to the $1H/1T''$ interface, one unit cell (blue box) is included in density functional calculations. Therefore, a cell of in-plane $1H/1T''-\text{MX}_2$ heterostructures includes 20 transition metals and 40 chalcogenide atoms, respectively. Moreover, as observable in the side view of $1H/1T''-\text{MX}_2$ shown in the lower half of Fig. 5(a), a slight buckling occurs as a result of existing interfaces. Transition metals at the $1H/1T''$ interface have one less coordinated chalcogenide atoms than regular transition metals. Then, lattice constants of monolayer $1H$, $1T''$, and $1H/1T''-\text{MX}_2$ are listed in Fig. 5(b). For ease of comparison, the $1H/1T''-\text{MX}_2$ lattice constant perpendicular to the $1H/1T''$ interface is divided by 10. Obviously, the $1H/1T''-\text{MX}_2$ lattice constants along the armchair direction are always in between $1H$-$\text{MX}_2$ and $1T''$-$\text{MX}_2$ lattice constants. For lattice constants along the zigzag direction, they are larger in $1H/1T''-\text{MS}_2$ and less in

![Fig. 5.](image-url)
1H/1T'-MSe₂ than the corresponding monolayer disulfides and diselenides. Nevertheless, the difference is numerical artifacts caused by the inaccuracy of the DFT calculations.

A. Young’s moduli

By conducting the uniaxial strain simulations along the normal or parallel directions of the 1H/1T' interface, the Young’s moduli of the 1H/1T'-MX₂ heterostructure are illustrated in Fig. 6(a). In the Mo group, Young’s moduli increase and then decrease when the chalcogenide atoms switch from S to Se, and then to Te. Moreover, these changes are drastic along the parallel direction of the 1H/1T' interface, while they are small along the normal direction of the 1H/1T' interface. For 1H/1T' heterostructures, Young’s moduli perpendicular to the 1H/1T' interface are about 40.26%, 28.25%, and 21.29% less than Young’s moduli along the armchair direction for 1H-MoS₂, 1H-MoSe₂, and 1H-MoTe₂, respectively. In comparison to Young’s moduli along the armchair direction in the 1T' phase, Young’s moduli perpendicular to the 1H/1T' interface are reduced by 33.13%, 22.79%, and 25.28% for MoS₂, MoSe₂, and MoTe₂, respectively. For MoS₂, the 1H/1T' interface simultaneously reduces Young’s moduli along the zigzag direction (parallel to the 1H/1T' interface) by 35.73% and 14.41% in 1H and 1T' phases, respectively. Nevertheless, Young’s moduli along the zigzag direction decrease by 8.71% (13.46%) in comparison with 1H-MoSe₂ (1H-MoTe₂) while increase by 22.12% (28.55%) as compared with 1T'-MoSe₂ (1T'-MoTe₂). These preliminary observations can be counted as signs that in the constructed heterostructure.¹³

In the W group, when the chalcogenide atoms switch from S to Se, and then to Te, Young’s moduli normal to the 1H/1T' interface increase first and then decrease while Young’s moduli parallel to the 1H/1T' interface monotonously decrease. In 1H/1T'-WX₂ in-plane heterostructures, Young’s moduli normal to the interface are significantly reduced. Comparing to the pristine 1H(1T')-WX₂ monolayers, the in-plane stiffness of the corresponding 1H(1T')-WX₂ reduces to more than 42.77% (45.17%), 72.87% (72.78%), and 77.22% (66.70%) in sulfide, selenide, and telluride, respectively. If loading a strain parallel to the 1H/1T' interface, the obtained Young’s moduli of 1H/1T'-WX₂ heterostructures are higher than those of the native 1T' phase while are less than those of the native 1H phase along the zigzag direction. In short, these calculated results accordingly confirm the remarkable mechanical degradation perpendicular to the interface in 1H/1T'-MX₂ in-plane heterostructures.

B. Poisson’s ratios

In 1H/1T'-MX₂ in-plane heterostructures, all Poisson’s ratios are positive and larger than those of graphene. That is, the heterostructures have the tendency to compress in one direction when they are expanded in the perpendicular direction. In 1H/1T' in-plane heterostructures, Poisson’s ratios perpendicular to the 1H/1T' interface are close to the values along the armchair direction in the pristine 1H and 1T' monolayers. Moreover, Poisson’s ratios parallel to the 1H/1T' interface are slightly larger than those of the 1H phase, which indicates the stronger ability of preserving the equilibrium area of 1H/1T' in-plane heterostructures.

V. SUMMARY

An exciting fact about the emerging two-dimensional transition-metal dichalcogenides (TMDCs) is their polymorphism nature, which may play critical roles in their appealing physical properties and practical aspects. Therefore, in this study, we present a detailed density functional theory calculations to investigate the mechanical properties of two-dimensional TMDCs associated with 1T, 1T', and 1H phases. Our results clearly indicate that all the TMDCs considered in this study are less stiff than graphene, which makes them attractive substitutes or alternatives in applications requiring flexible semiconductor materials. Furthermore, our analysis of the mechanical properties of 1H/1T'-MX₂ (M = Mo, W and X = S, Se, Te) in-plane heterostructures confirms that these novel two-dimensional
structures can yield a remarkably high strength along the 1H/1T′ interface, as compared with 1T′ structures along the zigzag direction. However, the 1H/1T′ interfaces are usually detrimental, which makes the in-plane stiffness reduced along the armchair direction. The insights provided by this study can be useful for the practical applications of various forms of TMDCs including in-plane heterostructures.

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