

Strain-Dependent Electron Transport in Mono-, Bi-, and Trilayer MoS₂ and WS₂ Using Coupled First-Principles and Full-Band Semi-Classical Monte-Carlo Simulation

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Abstract—The electronic transport properties of mono-, bi-, and trilayer MoS₂ and WS₂ under various strain conditions and electric-field directions are investigated using a density functional theory (DFT)-based full-band semi-classical Monte Carlo (SCMC) simulation framework. Intrinsic phonon-limited mobility and saturation velocity at room temperature are calculated from first-principles. The results show that strain and layer number significantly modify valley configurations and effective masses, leading to substantial variations in transport characteristics. In particular, the relative ordering and energy separation of the K and Q valleys are identified as key factors governing carrier occupation, scattering processes, and overall transport performance. The study highlights the importance of accurate full-band analysis for understanding and optimizing strain-engineered multilayer Transition Metal Dichalcogenides (TMDs) devices.

Keywords — DFT, Monte-Carlo transport, TMDs, strain, mobility, saturation velocity

I. INTRODUCTION

Two-dimensional (2D) materials have attracted significant attention as beyond-silicon (Si) channel materials for field-effect transistors (FETs) owing to their atomically thin body, excellent electrostatic gate control, and dangling-bond-free surfaces. Among them, MoS₂ and WS₂ have been widely investigated for n-FETs applications because of their sizable bandgaps and favorable electronic properties. While numerous experimental demonstrations of MoS₂ and WS₂ based transistors have been reported, rigorous assessments of intrinsic transport properties, such as electron mobility and carrier velocity, remain relatively limited, particularly from a first-principles perspective.

Most previous studies have focused primarily on monolayer (transition metal dichalcogenides) TMDs due to their direct bandgap nature and unique valley-dependent electronic properties. However, practical device implementations often employ bilayer or few-layer structures rather than ideal monolayers. In fact, several experimental studies have reported enhanced carrier mobility and reduced contact resistance in multilayer MoS₂ devices compared with monolayer counterparts [1-3]. Such improvements have been attributed to stronger dielectric screening of charged impurities, reduced substrate-induced scattering, and the spatial distribution of carriers away from the dielectric interface. Furthermore, increasing the number of layers modifies the electronic structure through interlayer coupling, leading to significant changes in valley configurations, effective masses, density of states, and intervalley scattering pathways [4-6]. These layer-dependent changes can substantially influence carrier transport behavior and may

provide an additional degree of freedom for performance optimization.

Strain engineering, which has been widely adopted in advanced Si technologies to enhance carrier mobility and drive current, has also emerged as an effective approach for tailoring the electronic properties of TMDs. Previous studies have demonstrated that strain can significantly alter band structures, valley energetics, and effective masses in MoS₂ and WS₂ [7-8]. In particular, the relative energy positions of the K and Q valleys are highly sensitive to both strain and layer number, suggesting a strong interplay between strain engineering and multilayer effects. Nevertheless, despite extensive investigations of strain-induced band structure modulation, systematic studies of intrinsic transport properties incorporating both strain and layer-number dependence remain limited. Moreover, the microscopic origins of transport enhancement in multilayer TMDs have not yet been fully clarified because full-band carrier dynamics and electron-phonon scattering are often neglected.

In this work, we investigate strain-engineered electron transport in mono-, bi-, and trilayer MoS₂ and WS₂ using density functional theory (DFT)-based full-band semi-classical Monte Carlo (SCMC) simulations. By explicitly incorporating first-principles electronic structures and electron-phonon interactions, we systematically analyze the effects of strain and layer number on valley occupation, scattering mechanisms, drift velocity, and intrinsic electron mobility. Our results provide microscopic insight into the transport advantages of multilayer TMDs and establish design guidelines for the optimization of future TMD-based electronic devices.

II. METHODS

Electronic structures, phonon dispersion, and electron-phonon matrix elements were obtained from DFT calculations. Electron-phonon scattering rates were computed using Fermi's golden rule (Eq. 1), with the energy conservation condition evaluated through the linear tetrahedron integration scheme [9]. These first-principles scattering rates were subsequently employed in full-band SCMC simulations to model carrier transport. Spin-orbit-coupling effects were included because of their pronounced impact on band splitting and valley energetics, especially in WS₂. For multilayer structures, Grimme D3 van der Waals corrections with BJ damping [10] were employed to accurately describe interlayer interactions, which critically influence layer-dependent electronic structures and transport properties.

$$\Gamma_{k,k+q} = \frac{2\pi}{\hbar} |g_{k,k+q}^{n,m,v}|^2 (N_q^v + \frac{1}{2} \pm \frac{1}{2}) \delta(E_{k+q}^n - E_k^n \pm \hbar\omega_q^v) \quad (1)$$

III. COMPUTATIONAL DETAILS

First-principles calculations were performed using the Quantum ESPRESSO package [11], Wannier90 [12], and Perturbo [13]. Structural relaxations and self-consistent field calculations were carried out on a $12 \times 12 \times 1$ k-point grid using optimized norm-conserving Vanderbilt (ONCV) pseudopotentials [14] with the Perdew–Burke–Ernzerhof generalized gradient approximation (GGA-PBE) for the exchange–correlation functional. Kinetic energy cutoff of 60 Ry and a force convergence criterion of 10^{-5} Ry/bohr were used. To investigate strain effects, $\pm 2\%$ uniaxial and biaxial strains were applied to each structure. Electron–phonon interactions were initially computed on coarse $12 \times 12 \times 1$ k-point and $6 \times 6 \times 1$ q-point grids and subsequently interpolated onto fine $200 \times 200 \times 1$ grids using Wannier and Fourier interpolation, respectively. Electron–phonon matrix elements were evaluated on a $30 \times 30 \times 1$ grid and bilinearly interpolated to the fine grids. Carrier transport properties were investigated using an in-house full-band semi-classical Monte Carlo (SCMC) simulator based on the cellular Monte Carlo method [15].

IV. RESULTS AND DISCUSSION

A. Monolayer

Fig. 1 shows the electronic band structures of unstrained, biaxially compressive and tensile strained MoS₂ and WS₂. All energies are referenced to the K valley minimum of the corresponding unstrained structure, which is set to 0 eV. In both materials, the Q valley forms the second-lowest conduction-band minimum. As compressive strain is applied, the sixfold-degenerate Q valley moves below the K valley and becomes the dominant conduction-band minimum. Conversely, tensile strain stabilizes the K valley by increasing the K–Q energy separation. Because the K and Q valleys exhibit distinct degeneracies, effective masses, and scattering pathways, the strain-induced valley reordering is expected to play a critical role in determining the electron transport properties of these materials.

Fig. 2 shows the electric-field dependence of drift velocity under various strain conditions for MoS₂ and WS₂. Tensile strain improves low-field mobility, while compressive strain leads to mobility degradation in both materials. The observed trend originates from strain-induced changes in valley energetics and carrier effective masses. Specifically, compressive strain lowers the sixfold-degenerate Q valley below the K valley, increasing carrier occupation in heavier-mass states and reducing transport efficiency. Conversely, tensile strain increases the K–Q valley separation and maintains the K valley as the conduction-band minimum, resulting in enhanced low-field mobility. At higher electric fields, however, intervalley scattering becomes increasingly important, leading to velocity saturation even with strain.

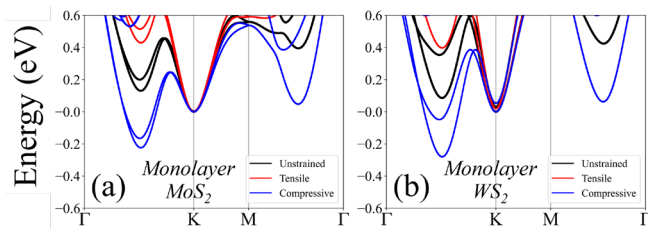


Fig. 1. Electronic band structures of monolayer (a) MoS₂ and (b) WS₂. The K valley minimum is taken as a reference of energy.

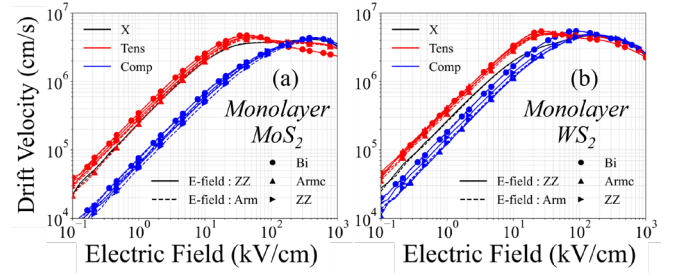


Fig. 2. Electric field vs. drift velocity for monolayer (a) MoS₂ and (b) WS₂

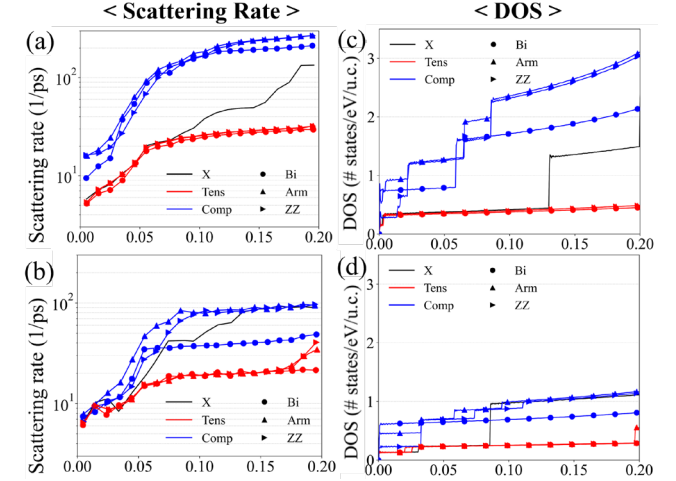


Fig. 3. Scattering rates of monolayer (a) MoS₂ and (b) WS₂. Density of states of monolayer (a) MoS₂ and (b) WS₂.

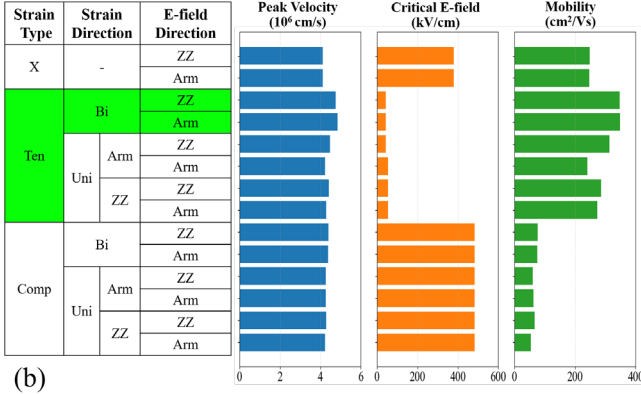
This behavior is consistent with the scattering rates shown in Fig. 3(a) and (b) and can be understood from the strain-dependent evolution of the conduction-band valleys. Under compressive strain, the sixfold-degenerate Q valley shifts below the K valley and becomes the CBM. The resulting increase in density of states (DOS), shown in Fig. 3(c) and (d), enlarges the available phase space for electron–phonon scattering, thereby increasing scattering rates and reducing carrier mobility. Conversely, tensile strain increases the K–Q valley energy separation and maintains the K valley as the dominant transport valley. This reduces the DOS near the conduction band edge and suppresses electron–phonon scattering, leading to improved mobility and drift velocity.

Table 1 summarizes the peak drift velocities, critical electric fields, and low field mobilities under various strain conditions. As discussed previously, tensile strain improves carrier transport, while compressive strain reduces mobility due to enhanced occupation of the Q valley and increased electron–phonon scattering. Among the tensile strain conditions, biaxial tensile strain generally yields the highest mobility because it maximizes the energy separation between the K and Q valleys, thereby reducing the density of states near the conduction band edge and suppress scattering.

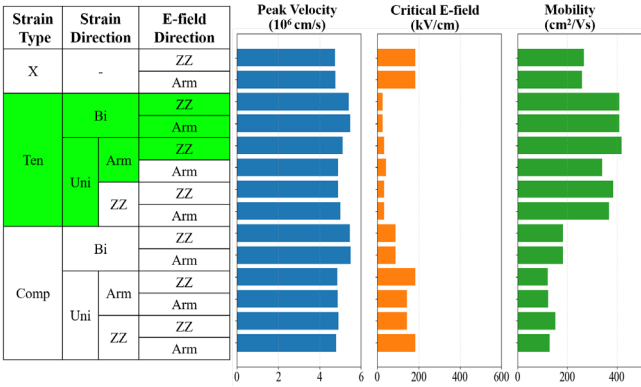
For both uniaxial tensile armchair and zigzag strains, transport along the zigzag direction consistently exhibits higher mobility than transport along the armchair direction. This behavior is primarily attributed to the smaller transport effective mass along the zigzag direction, which leads to higher carrier velocity and improved transport efficiency.

Fig. 4 further supports the transport trends discussed above by illustrating the valley population under different strain conditions. Under compressive strain, a significantly larger fraction of electrons occupies the Q valleys as the Q valley

(a)

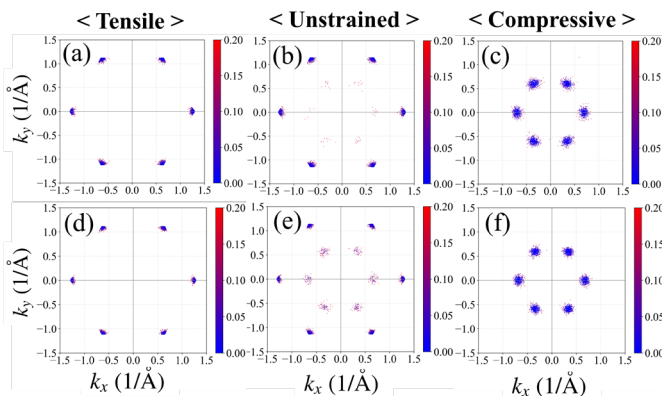


(b)


 Table 1. Peak velocities, critical electric fields, and mobilities of monolayer (a) MoS₂ and (b) WS₂ under different strain conditions.

becomes energetically favorable. Because the Q valleys possess a larger density of states and heavier effective masses than the K valley, increased occupation of these valleys enhances electron-phonon scattering and reduces mobility. In contrast, tensile strain suppresses Q valley occupation by increasing the K–Q energy separation, thereby promoting transport through the lighter-mass K valley and resulting in improved mobility.

It is noteworthy that the peak drift velocities listed in Table 1 remain within a relatively narrow range across different strain conditions. Unlike low-field mobility, which is highly sensitive to valley ordering and scattering rates, the peak velocity is primarily determined by carrier dynamics under strong electric fields. At high electric fields, electrons occupy a much broader region of the Brillouin zone and are no longer confined to states near the conduction band minimum (CBM).


 Fig. 4. Electron distribution in k-space for monolayers without electric fields for ((a)-(c)) MoS₂ and ((d)-(f)) WS₂ under unstrained and biaxial strain conditions.

Consequently, transport becomes less sensitive to the detailed valley configuration and more dependent on the overall band dispersion. Since MoS₂ and WS₂ possess similar conduction-band characteristics originating mainly from transition-metal d orbitals hybridized with chalcogen p orbitals, comparable carrier velocities are obtained over a wide range of k-space. As a result, the peak drift velocities exhibit only weak dependence on strain and material type.

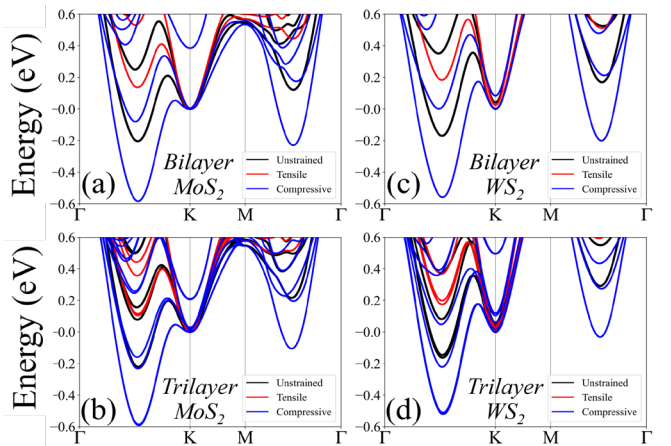
B. Bilayer & Trilayer

Fig. 5 shows the electronic band structures of bilayer and trilayer MoS₂ and WS₂ under unstrained, biaxially compressive, and biaxially tensile strain conditions. In contrast to the monolayer case, the sixfold-degenerate Q valley forms the CBM in both bilayer and trilayer structures even in the absence of strain. The resulting increase in density of states near the conduction band edge and the larger effective mass associated with the Q valley contribute to the lower mobility observed in multilayer structures compared with their monolayer counterparts.

Similar to the monolayer case, the relative energies of the K and Q valleys are strongly affected by biaxial strain. Under tensile strain, the Q valley shifts upward in energy while the K valley becomes energetically favorable CBM. Conversely, compressive strain further lowers the Q valley, increasing the K–Q valley separation. Consequently, tensile strain promotes carrier transport through the lighter-mass K valley, leading to enhanced mobility, whereas compressive strain increases Q valley occupation.

Fig. 6 provides further evidence for the relationship between valley ordering and transport properties through the electron distributions in k-space. For both MoS₂ and WS₂, electrons are primarily concentrated in the Q valleys under unstrained conditions, reflecting the Q valley CBM in multilayer structures. Under biaxial tensile strain, the upward shift of the Q valley relative to the K valley drives a significant redistribution of carriers toward the K valleys. Because the K valley exhibits a smaller effective mass and lower density of states than the sixfold-degenerate Q valleys, this strain-induced carrier redistribution suppresses electron-phonon scattering and leads to improved transport performance.

Fig. 7 shows the electric-field dependence of drift velocity under biaxial tensile and compressive strain for bilayer and trilayer MoS₂ and WS₂. In the absence of strain, both bilayer


 Fig. 5. Electronic band structures of (a) bilayer and (b) trilayer MoS₂. Electronic band structures of (c) bilayer and (d) trilayer WS₂. The K valley minimum is taken as a reference.

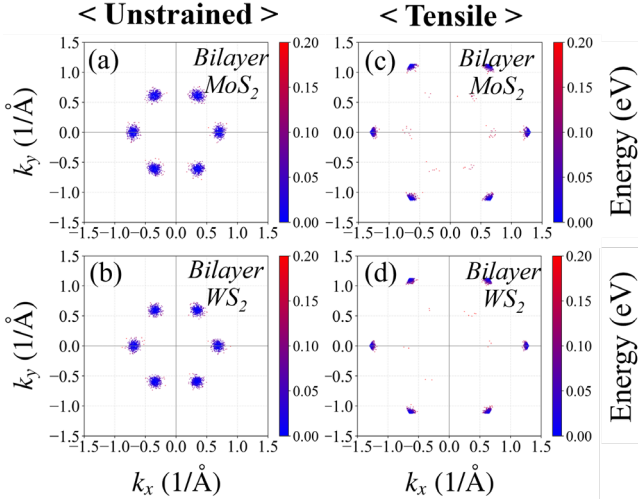


Fig. 6. Electron distribution in k-space for bilayers without electric fields for (a), (c) MoS₂ and (b), (d) WS₂, under unstrained and biaxial tensile strain conditions.

and trilayer structures exhibit lower mobility than their monolayer counterparts because the Q valleys are significantly populated and contribute to enhanced electron-phonon scattering. Biaxial tensile strain substantially enhances the mobility of both bilayer and trilayer MoS₂ and WS₂. In bilayers, the mobility increases from approximately 61 cm²/V·s to 267 cm²/V·s and 60 cm²/V·s to 478 cm²/V·s for MoS₂ and WS₂, respectively. Similarly, trilayer mobilities increase from 71 and 83 cm²/V·s to 290 and 417 cm²/V·s. The mobility enhancement originates from the transition of the CBM from the Q valley to the K valley, which suppresses Q valley occupation and reduces scattering. Interestingly, compressive strain also leads to a slight mobility enhancement in bilayers despite the increased Q valley population. This behavior can be attributed to the reduced DOS under compressive strain, as shown in Fig. 8. The lower DOS reflects a reduced effective mass, which consequently weakens scattering. This trend contrasts with that observed in monolayers, where compressive strain degrades mobility. The difference arises because the Q valleys are already lower in energy than the K valley in the unstrained bilayers.

For multilayer WS₂, tensile strain additionally reduces the critical electric field by nearly one order of magnitude, while preserving the peak drift velocity. This combination of enhanced mobility, reduced critical field, and saturation velocity highlights the effectiveness of strain engineering for improving transport performance in multilayer WS₂.

V. CONCLUSIONS

This work reveals that valley ordering is the primary factor governing electron transport in MoS₂ and WS₂. By increasing the K-Q valley separation and restoring the K valley as the CBM, tensile strain significantly enhances carrier mobility in both monolayer and multilayer structures. In particular, the intrinsic Q valley CBM in bilayer and trilayer TMDs results in degraded transport performance, making strain engineering an effective and potentially necessary approach for achieving high-mobility multilayer TMD devices.

VI. ACKNOWLEDGEMENT

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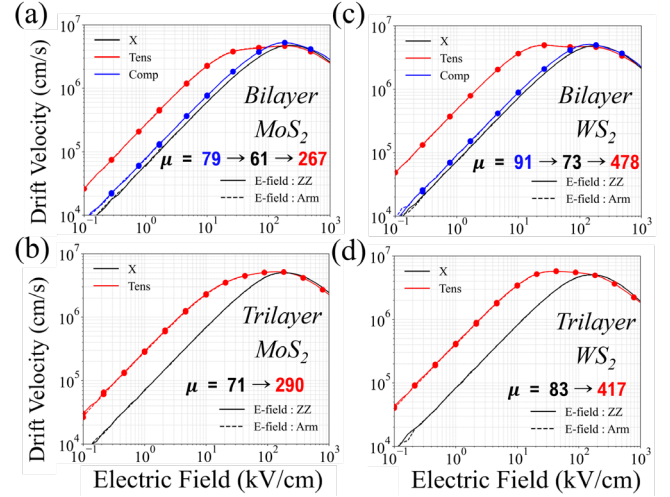


Fig. 7. Electric field vs. drift velocity for bilayer, trilayer MoS₂ and WS₂.

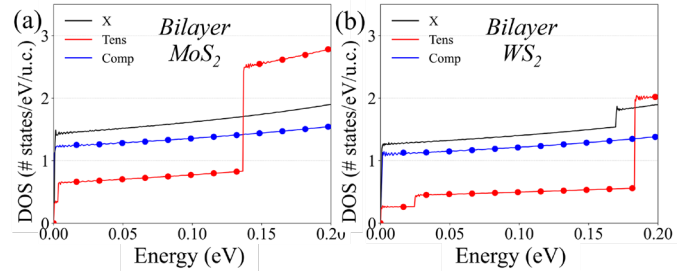


Fig. 8. Density of states of bilayer MoS₂ and WS₂.

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