Uniaxial strain induced symmetry lowering and valleys drift in MoS₂

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Abstract

The uniaxial strain is an effective way to change the symmetry of a crystal and thus tuning their electronic properties. In the present work, we elucidate the physical mechanism of the symmetry-broken-induced energy valleys drift in monolayer molybdenum disulfide. When the uniaxial strain reduces the rotational symmetry of valleys from $C_3$ to $C_1$ and an in-plane electric field breaks the balance of electron distribution of valleys, the valley dipole can survive readily and quantum nonlinear Hall effect might be realized. Our work offers key insights for understanding the uniaxial strain induced valleys drift in monolayer MoS₂, which is critical to precisely control the valleytronics properties of two-dimensional materials.

1. Introduction

Valleytronic devices have great development potential in next era of microelectronics [1–13]. One of problems to study valleytronics is to endow the low-energy electrons with an additional valley degree of freedom, in other words, to create an imbalanced electron distribution between valleys [4, 9]. However, beyond the valley degree of freedom, the symmetry of valleys is an attractive problem in itself, because some properties will be revealed by symmetry lowering of the valleys. Especially, the quantum nonlinear Hall effect will appear in a system with time reversal symmetry and low symmetry of valleys when electron distribution between valleys is imbalanced [14–16]. In this work, we study symmetry change from many aspects when monolayer molybdenum disulfide (MoS₂) is stretched by an uniaxial strain.

Monolayer MoS₂ is a honeycomb-sandwich structure and consists of two hexagonal planes of S atoms and an intermediate hexagonal plane of Mo atoms coordinated through ionic-covalent interactions with the S atoms in a trigonal bipyramid arrangement [17, 18]. Based on the special crystal structure, pristine monolayer MoS₂ possess promising electronic properties as a two-dimensional semiconductor. Monolayer MoS₂ exhibits direct band gap with 1.90 eV, and the conduction band minimum (CBM) and the valence band maximum (VBM) locate at vertexes of the regular hexagonal first Brillouin zone [17–19]. Furthermore, Mo atoms provide the most part of density of states (DOS) at CBM and VBM points, particularly the $d_{z^2}$ orbitals of Mo atoms is crucial to the CBM point and continuous rotational symmetry for the $x$–$y$ plane [17, 18]. Moreover, considering the vertex angle of the first Brillouin zone is $2\pi/3$, monolayer MoS₂ have 2 nonequivalent valleys in the first Brillouin zone, namely $K$ and $K’$. Both of two valleys in the first Brillouin zone have $C_3$ rotational symmetry, which is important for valleytronics properties of MoS₂ like circularly polarized photons selectivity of the valleys [20–22].

When monolayer MoS₂ is stretched by an uniaxial strain, the size of the first Brillouin zone will be changed and the number of rotational symmetry element in both real and reciprocal space will be reduced [23, 24], which can result in the interesting phenomenon. Actually, when the uniaxial strain is applied, energy valleys of the lowest conduction band will drift away from vertexes of the deformed first Brillouin zone [24], and this drift in monolayer MoS₂ is much larger than that in graphene [23]. Since the interior
angle summation of the first Brillouin zone still maintains to $2\pi$ for not very large deformation, and there are always two nonequivalent valleys in the first Brillouin zone. The most direct result caused by the valley drift is that the symmetry of valleys will be changed, which has profound influence to valleytronics properties. Especially, the valley dipole due to symmetry lowering of valleys in deformed monolayer MoS$_2$ shows attracted great enthusiasm to men of science [14–16].

In the paper, at first, we theoretically elucidate the physical mechanism of the uniaxial strain induced drift and symmetry lowering of energy valleys in monolayer MoS$_2$, and the results exhibit that the rotational symmetry of valleys will be reduced from $C_s$ to $C_1$ for deformed monolayer MoS$_2$ with $C_1$ rotational symmetry in real space. And then, the influence of the symmetry lowering of valleys to the selectivity of the circularly polarized photons, to valley behavior under magnetic field and to valley dipole under the external in-plane electric field will be discussed. More interesting, contrary to monolayer MoS$_2$ with circularly polarized photons, to valley behavior under magnetic field and to valley dipole under the external force, the rotational symmetry of valleys will be reduced from $C_s$ to $C_1$ for deformed monolayer MoS$_2$ with $C_1$ rotational symmetry.

2. Theory and computational details

The clarification of high-symmetry points’ coordinates for the deformed first Brillouin zone is the first step to calculate the electronic properties of the deformed structure. In this work, the analytic geometry method is used to calculate the coordinate of the high-symmetry points.

There is a relation between the reciprocal lattice vectors and crystal lattice vectors [25],

$$a^* = 2\pi \frac{b \times c}{V}, \quad \text{and} \quad b^* = 2\pi \frac{c \times a}{V},$$  \hspace{1cm} (1)

where $a$, $b$ and $c$ are crystal lattice vectors, $a^*$ and $b^*$ are reciprocal lattice vectors, respectively, as shown in figure 1. $V = a \cdot (b \times c)$ is the volume of primitive cell. Because the thickness of vacuum layer is considered along vector $c$ direction, $c^*$ is senseless for two-dimensional structure, which means that only the two dimensional surface Brillouin zone should be taken into account. Obviously, if monolayer MoS$_2$ have different deformation along $b$ direction, $b^*$ will not be fixed as a constant vector, thus the rectangular coordinates will be more convenient than oblique coordinates in reciprocal space.

Considering three following crystal lattice vectors expressed in the rectangular coordinates,

$$a(x, y, z), \quad b(x, y, z) \quad \text{and} \quad c(x, y, z)$$

then, according to equation (1), we have,

$$a^*(x, y, z), \quad \text{and} \quad b^*(x, y, z).$$

Now, coordinates of the six high-symmetry points at the boundary of the deformed first Brillouin zone can be calculated as,

$$\frac{b^*}{2}, \quad \frac{a^*}{2}, \quad \frac{b^*}{2}, \quad \frac{a^*}{2}, \quad \frac{(a^* - b^*)}{2}. \quad \text{and} \quad \frac{(a^* - b^*)}{2}$$

\hspace{1cm} (4)

these six high-symmetry points are renamed as $A$, $C$, $E$, $A'$, $C'$, and $E'$, respectively in figures 1(b) and (d). The vector $(a^* - b^*)$ corresponds to the situation that the angle between $a$ and $b$ is $2\pi/3$. If one choose that the angle between $a$ and $b$ is $\pi/3$, $(a^* - b^*)$ in expression (4) should be replaced by $(a^* + b^*)$. Six equations of straight line can be written, and those six lines across the end of vector in expression (4) and are perpendicular to its direction respectively, namely,

$$l_{b^*}, l_{a^*}, l_{(a^*-b^*)}, l_{-b'}, l_{-a'}, \quad \text{and} \quad l_{-(a^*-b^*)}$$

\hspace{1cm} (5)

and the area enclosed by lines in expression (5) is the first Brillouin zone. The other six high-symmetry points are the intersections of six pairs of lines $[l_{a^*}, l_{b^*}]$, $[l_{a^*}, l_{(a^*-b^*)}]$, $[l_{(a^*-b^*)}, l_{-b^*}]$, $[l_{(a^*-b^*)}, l_{-a^*}]$, $[l_{-a^*}, l_{-(a^*-b^*)}]$, and $[l_{-(a^*-b^*)}, l_{b^*}]$, namely $B$, $D$, $F$, $B'$, $D'$, $F'$, as shown in figures 1(b) and (d). Finally, transforming the rectangular coordination of points in reciprocal space to oblique coordination with basic vectors $a^*$ and $b^*$ is the last step to use coordination of high-symmetry points in calculation of the electronic property of deformed MoS$_2$ monolayer.

In this work, the energy dispersion relation of the electron is calculated by using density functional theory that implement in Vienna ab initio simulation package program with an ultrasoft pseudopotential plane-wave basis set [26–28]. The exchange-correlation effects are treated by the Perdew Burke Ernzerhof parameterization [28]. The vacuum layer (20 Å) is added in spacing of MoS$_2$ layers to simulate monolayer case. In order to calculate three-dimensional band structure in the entire first Brillouin zone, eigenvalues of
2500 \( k \)-points are calculated, in which \( k \)-points are distributed in \([-1.5, 1.5] \times [-1.5, 1.5]\) for variable \( x \) and \( y \) in equation (3).

### 3. Results and discussion

When an uniaxial strain is applied, the rotational symmetry of monolayer MoS\(_2\) will be reduced from \( C_3 \) to \( C_1 \) rotational symmetry, as shown in figures 1(a) and (c). Meanwhile, the symmetry lowering will also occur in reciprocal space because the real and reciprocal space are related via equation (1). Owing to the symmetry lowering in reciprocal space, the first Brillouin zone will be deformed from regular with \( C_6 \) rotational symmetry to irregular hexagon with \( C_2 \) rotational symmetry, as shown in figures 1(b) and (d).

The first Brillouin zone, high-symmetry points and two-dimensional band diagram for the lowest conduction band of undeformed and deformed monolayer MoS\(_2\) are shown in figures 2(a)–(e), corresponding to monolayer MoS\(_2\) with 0%, 5%, 10%, 15%, 20% deformation along \( b \) direction, respectively. Green points in figure 2 describe the position of valleys. Figure 2(f) describes how valleys drift under different deformations along the direction of crystal vector \( b \), and the figure is the summation of green points in figures 2(a)–(e). Actually, previous study has shown that the ultimate coaxial strain which could be applied to MoS\(_2\) was 25%. And the ultimate uniaxial strain along the armchair and zigzag direction were 28% and 19%, respectively [29]. Therefore, in our work, the maximum strain of 20% is used, and in this case we have tested phonon spectrum with no virtual frequency.

In figure 2, it can be clearly seen that the symmetry of valleys will be reduced from \( C_3 \) to \( C_1 \) rotational symmetry and valleys will drift away from vertexes of the first Brillouin zone when an uniaxial strain is applied. The way of valley drift is interesting that some of valleys are almost stationary in reciprocal space, as shown in figure 2(f). This situation of valley drift of monolayer MoS\(_2\) is completely different from that of graphene stretched by the same way, where the valley drift is smaller and valleys keep close to vertexes of the deformed first Brillouin zone. In order to understand the unique way of valley drift for the lowest conduction band, one must focus on physical essence of valleys in monolayer MoS\(_2\). Actually, according to Bloch theorem and the fact that most part of DOS are provided by \( d_z^2 \) orbitals of Mo atoms, the energy valleys at vertexes of the regular hexagonal first Brillouin zone mean that there are Bloch waves with wavelength equal to half integral multiple lattice constant and the wave direction is along the nearest Mo atoms [25, 30]. In present case, the geometric configuration with periodicity along the direction of lattice vector \( a \) is fixed and will not be changed, whatever the monolayer MoS\(_2\) is stretched along the direction of lattice vector \( b \). It is the explanation for stationary behavior of some valleys in reciprocal space, that there are still Bloch waves along the direction of lattice vector \( a \) in undeformed monolayer MoS\(_2\). And then, for positions of all energy valleys in reciprocal space, they are correlated with each other by symmetric.
Figure 2. (a)–(e) The lowest conduction band in two-dimensional diagram and the first Brillouin zone of monolayer MoS$_2$ with 0%, 5%, 10%, 15%, 20% deformation along $b$ direction, respectively. From (a) to (e), the darker color, the higher energy, and green points represent the position of valleys. (f) The valley drift and its direction in reciprocal space for different deformations.

Figure 3. The highest valence band, the lowest conduction band, and electron valleys in three-dimensional diagram for (a) pristine monolayer MoS$_2$ (b) 20% deformed monolayer MoS$_2$.

requirement, which means that if an energy valley is determined according to stationary behavior of valleys in reciprocal space, one can clarify positions of all.

The reduction of band gap and direct–indirect-band-gap transition will occur when monolayer MoS$_2$ is stretched by an uniaxial strain, which is similar to the case in coaxial strained monolayer MoS$_2$ [31]. Those conclusions can be found in figures 2 and 3. In figure 2, the lighter tones mean the smaller band gap. Figures 3(a) and (b) show the three-dimensional band structure for the pristine and 20% deformed monolayer MoS$_2$, respectively, and the deformation and valley drift in the first Brillouin zone can be obviously seen. For easier and clearer display, figures 4(a) and (b) describe the band structure along high-symmetry line $K$–$\Gamma$–$K'$ and $F$–$\Gamma$–$F'$ for the pristine and 20% deformed monolayer MoS$_2$, respectively. In figures 3 and 4, valley index $K$ and $\alpha$ are used to distinguish the two situations with different symmetry properties. It should be noted that the spin–orbit coupling (SOC) effect is no essential for valley of deformed monolayer MoS$_2$ since the band structure for different spin states is degenerate at the $\Gamma$ point of the highest valence band and bottom of valleys $\alpha$ ($\alpha'$). Inserted pictures in figures 4(a) and (b) are partial charge density distribution for the bottom of valleys. It is clear that the uniaxial strain will not separate the region of electron distribution in real space for different valleys $\alpha$ ($\alpha'$), but will reduce the symmetry of the region from continuous rotational symmetry to $C_2$ rotational symmetry. Actually, one can understand the
Figure 4. (a) and (b), the band structure of pristine monolayer MoS$_2$ along $K$–$\Gamma$–$K'$ and 20% deformed monolayer MoS$_2$ along $F$–$\Gamma$–$F'$. The pictures on the right denote the enlarged view of valley bottom and their partial charge density distribution.

Table 1. The data of orbital hybridization for the bottom of valleys.

|          | $d_z^2$ | $d_x^2$ | $d_{xy}$ |
|----------|---------|---------|----------|
| Pristine | 0.771   | 0.000   | 0.000    |
| 5% deformed | 0.753 | 0.007   | 0.013    |
| 10% deformed | 0.702 | 0.028   | 0.050    |
| 15% deformed | 0.635 | 0.052   | 0.097    |
| 20% deformed | 0.568 | 0.070   | 0.146    |

symmetry lowering of partial charge distribution from orbital hybridization [24]. Table 1 exhibits the change of orbital components $d_z^2$, $d_x^2$ and $d_{xy}$ of Mo atoms for charge distribution of bottom of valleys with different deformation along $b$ direction.

As a matter of fact, pristine monolayer MoS$_2$ is $C_3$ rotational symmetry, and $d_z^2$ orbital is continuous rotational symmetry in $x$–$y$ plane and provide most part of state of valley electrons, which is the reason that the charge density distribution in real space is continuous rotational symmetry for $x$–$y$ plane. In addition, $d_{xy}$ and $d_x^2$ orbitals are $C_4$ and $C_2$ rotational symmetry in $x$–$y$ plane, respectively. Therefore, the symmetry of charge density distribution for valley electrons in real space will be reduced from continuous rotational symmetry to $C_2$ rotational symmetry as the orbital components of $d_{xy}$ and $d_x^2$ increase when monolayer MoS$_2$ is stretched by an uniaxial strain, as shown in table 1. In the inserted partial charge density in figures 4(a) and (b), the charge density distribution in real space as continuous and $C_2$ rotational symmetry for pristine and deformed monolayer MoS$_2$ are shown, respectively.

To show the energy valleys with $C_3$ rotational symmetry, we can plot wave vector of Bloch states at energy valleys as regular triangle with different color in a clearer way. Figure 5(a) schematically shows $C_3$ rotational symmetry of valleys $K$ and $K'$. The black and red arrow show the direction of wave vector for valleys $K$ and $K'$, respectively. Due to the cyclicity of the first Brillouin zone in reciprocal space, it is reasonable that only energy valleys in the first Brillouin zone should be considered. Figure 5(b) schematically shows $C_1$ rotational symmetry of valleys $\alpha$ and $\alpha'$ for deformed monolayer MoS$_2$.

The change of rotational symmetry of valleys will have profound influence to valleytronics properties. Firstly, the circularly polarized photons selectivity of valleys will be influenced by the symmetry lowering of valleys. The optical selection rule is based on the phase winding of the Bloch wave states in energy valleys with $C_3$ rotational symmetry [20, 22, 23],

$$\hat{C}_3 |u(k)\rangle = e^{i\frac{2\pi}{3}} |u(k)\rangle,$$

where $u(k)$ is periodic part of Bloch wave function for the lowest conduction band. Because the $C_3$ rotational symmetry of valleys is vanished in the deformed monolayer MoS$_2$, we expect that shine circularly
Figure 5. (a) and (b) show the $C_3$ rotational symmetry and $C_1$ rotational symmetry of valleys corresponding to pristine and deformed monolayer MoS$_2$, respectively. Black and red arrow represent the wave vector of Bloch states in different valleys.

polarized light onto monolayer MoS$_2$ will not, effectively, create a population imbalance between two valleys anymore.

Owing to the spin of electrons in energy valley, a nonuniform magnetic field can also be used to break the time-reversal symmetry of a system, and then, be used to control valleytronics properties. In the present case of reduced symmetry, the bottom of valley $\alpha$ and $\alpha'$ have a spin gap of 10.2 meV, as shown in figure 4 and this value is similar to pristine case 3.2 meV. Furthermore, although $d_z^2$ and $d_{xy}$ orbitals of Mo atoms have more influence to hybridization states of valley bottom and $d_z^2$ orbital have contrary behavior when the deformation become larger, the summation of $d$ orbitals which is still dominant is almost invariant, as shown in table 1. Therefore, a low-energy effective Hamiltonian, which can be used to describe valley electrons of the pristine monolayer, is still working for the deformed case.

The Hamiltonian can be expressed as \[ H = H_0 + H_{SOC} + H_{EX} + H_R \] (7)

and the above four parts describe orbital interactions, spin–orbital coupling effect, proximity-induced exchange, and Rashba interactions, respectively, where

\[ H_0 = v_F \left( \tau \sigma_x p_x + \sigma_y p_y \right) + \frac{m}{2} \sigma_z \] (8)
\[ H_{SOC} = \tau s_z (\lambda_c \sigma_+ + \lambda_v \sigma_-) \] (9)
\[ H_{EX} = -s_z (B_c \sigma_+ + B_v \sigma_-) \] (10)
\[ H_R = \lambda_R \left( \tau s_y \sigma_x - s_x \sigma_y \right) \] (11)

Here, the Pauli matrices $s_k$ and $\sigma_k$ ($k = 0, x, y, z$) refer to real spin and orbital pseudospins, respectively, and $\sigma_\pm \equiv 1/2(\sigma_0 \pm \sigma_z)$. $p$ is the momentum of electrons and $v_F$ is the Fermi velocity. $\tau = \pm 1$ is employed for different energy valley $\alpha$ and $\alpha'$. $\lambda_c$, $\lambda_v$, $B_c$, $B_v$, and $\lambda_R$ are coefficients to describe spin–orbital coupling effect, proximity-induced exchange, and Rashba interactions, respectively. One can find the detailed discussions about those coefficients in references [32, 33]. The electronic state vectors of valley bottom are $|\psi_{\alpha, \uparrow}\rangle$ and $|\psi_{\alpha', \downarrow}\rangle$, respectively, where $|\psi_{\alpha}\rangle$ is a superposition of $d$ orbitals of Mo atoms.

By using the Hamiltonian to the state vectors, the energy of valley electrons can be studied. We define the energy difference between valley $\alpha$ and $\alpha'$ as,

\[ \Delta_{\text{valley}} = E_{\alpha, \uparrow} - E_{\alpha', \downarrow}. \] (12)

$\Delta_{\text{valley}}$ is forced to be zero in absence of nonuniform magnetic field, which means that there are no two part $H_{EX}$ and $H_R$ in the Hamiltonian (7). However, at presence of nonuniform magnetic field, $H_{EX}$ and $H_R$ parts of Hamiltonian will generate the nonzero terms contributing to $\Delta_{\text{valley}}$. Therefore, the different energy will arise at the different valleys. Especially, from equations (10) and (11), $H_{EX}$ and $H_R$ will have different reaction for orbital $d_z^2$, $d_{z^2}$ and $d_{xy}$. In the case of symmetry lowered monolayer, situation of orbital hybridization of valley bottom state is different from the pristine monolayer, as aforementioned analysis.

Therefore, we can expect that $\Delta_{\text{valley}}$ for symmetry lowered monolayer will be larger than that for pristine one at presence of nonuniform magnetic field, and the reason is that, compared to pristine monolayer, the symmetry lowered case has an additional nonzero contribution from $H_R$ term.
Moreover, the symmetry lowering of valleys is the first step to realize quantum nonlinear Hall effect that arises from the valley dipole in the first Brillouin zone [14, 15, 25]. The expression of valley dipole moment for the lowest conduction band of two-dimensional system is [15],

\[ D_{\alpha(y)} = \frac{1}{(2\pi)^2} \int f \frac{\partial}{\partial k_{\alpha(y)}} \Omega_z \, d^2 k \]  

(13)

where \( f \) is the distribution function and the rectangular coordinates in this equation is convenient. \( \Omega_z \) in equation (13) is \( z \) component of Berry curvature [34],

\[ \Omega(k) = \nabla_k \times < u(k) | i \nabla_k | u(k) > . \]  

(14)

Because the Berry curvature is odd function for a time-reversal invariant system, that is [34],

\[ \Omega(-k) = -\Omega(k) . \]  

(15)

In combination with odd function property of Berry curvature and equilibrium distribution function of valley electrons, the valley dipole moment term in equation (13) is forced to vanish. However, an in-plane electric field along or contrary to the wave vector of valley electrons can break the equilibrium distribution of electrons in two valleys of the deformed monolayer MoS\(_2\) [15, 35, 36], thus a valley dipole occurs when the valley dipole moment term in equation (13) integrate over the first Brillouin zone. Actually, the largest symmetry, that allows to survive a nonzero valley dipole at presence of the external electric field, is \( \text{C}_{1v} \) symmetry for a two-dimensional system [15]. In our case, the deformed monolayer MoS\(_2\) in this work has \( \text{C}_1 \) rotational symmetry, that is low enough to survive valley dipole. For monolayer MoS\(_2\) with a mirror symmetry element, the mirror symmetry element requires the direction of the valley dipole must along to the mirror plane, and the expansion of the first Brillouin zone along the mirror plane demands that the direction of strain must be perpendicular to it. Therefore, in monolayer MoS\(_2\) with a mirror symmetry element, the direction of the valley dipole is forced perpendicular to the strain [15, 37]. But in our case that the deformed monolayer MoS\(_2\) have the lowest rotational symmetry without a mirror symmetry element, there is no restriction on the directional relationship, which causes the direction of valley dipole aligns with the strain.

4. Summary

In summary, we show the deformation of the first Brillouin zone, symmetry lowering, and the valley drift in the first Brillouin zone when monolayer MoS\(_2\) is stretched by an uniaxial strain theoretically. The results show that the symmetry of valleys in reciprocal space is reduced from \( \text{C}_3 \) to \( \text{C}_1 \) rotational symmetry and this valley drift is unique for monolayer MoS\(_2\). The symmetry lowering of valleys have profound influence, which depends on \( \text{C}_3 \) rotational symmetry of valleys like circularly polarized photons selectivity of valleys. Moreover, as the \( \text{C}_1 \) rotational symmetry is low enough to survive the valley dipole in momentum space at presence of the external in-plane electric field, the quantum nonlinear Hall effects arising from the valley dipole can occur in the deformed monolayer MoS\(_2\). Especially, unlike the deformed monolayer MoS\(_2\) with \( \text{C}_{1v} \) symmetry where the direction of valley dipole is perpendicular to the strain, the direction of valley dipole in the deformed monolayer MoS\(_2\) with \( \text{C}_1 \) rotational symmetry aligns with the strain.

Conflict of interest

There are no conflicts to declare.

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