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Phase transition, effective mass and carrier mobility of MoS_2 monolayer under tensile strain

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ABSTRACT

We report a computational study on the impact of tensile strain on MoS_2 monolayer. The transition between direct and indirect bandgap structure and the transition between semiconductor and metal phases in the monolayer have been investigated with tensile strain along all direction configurations with both *x*-axis and *y*-axis components ε_{xy} (ε_x and ε_y). Electron effective mass and the hole effective mass are isotropic for biaxial strain $\varepsilon_{xy} = \varepsilon_x = \varepsilon_y$ and anisotropic for ε_{xy} with $\varepsilon_x \neq \varepsilon_y$. The carrier effective mass behaves differently along different directions in response to the tensile strain. In addition, the impact of strain on carrier mobility has been studied by using the deformation potential theory. The electron mobility increases over 10 times with the biaxial strain: $\varepsilon_x = \varepsilon_y = 9.5\%$. Also, the mobility decreases monotonically with the increasing temperature as $\mu \sim T^{-1}$. These results are very important for future nanotechnology based on two-dimensional materials.

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1. Introduction

Recently, MoS_2 monolayer, with layered honeycomb structure in which the transition metal atoms (Mo) are sandwiched between sulfur (S) atoms, is of great interest because of its extraordinary electronic, optical and mechanical properties [1,2]. These properties benefit from the direct energy bandgap (E_g) in monolayer MoS_2 ($E_g \approx 1.8$ eV). In comparison, bulk (or multilayer) MoS_2 is held together by relatively weak van der Waals forces between adjacent layers and has indirect energy bandgap ($E_g \approx 1.3$ eV) [3]. Also, two-dimensional (2D) MoS_2 monolayer can be obtained from bulk MoS_2 by using exfoliation technique which has been used to obtain graphene [2,4]. It has also been successfully demonstrated that chemical vapor deposition (CVD) method can produce 2D MoS_2 monolayer [5,6]. In addition, compared to the popular 2D graphene, the existence of the native bandgap renders MoS_2 monolayer a promising candidate for field-effect transistors with excellent current on/off ratio ($\approx 10^8$) [7], which may open a suite of applications in logic and memory integrated circuits.

In experiment, tensile strain in MoS_2 monolayer can be achieved by stretching or bending elastomeric substrate with external stress. Strain in MoS_2 monolayer can be detected by Raman spectroscopy in which the E_{2g} mode splits and shifts due to the strain [5–8]. It has been also demonstrated that strain can reduce photoluminescence and tune the polarization associated with K–K direct bandgap transition [8,9]. To date, many works have been reported on the simulations and modeling about the transformation of energy band structure activated by strain [10,11]. The strain effects on electronic, optical and magnetic properties have also been well investigated and predicted by Mahapatra et al. [12,13]. It is widely recognized that tensile strain will cause reduction in E_g. Also, the conduction band minimum (CBM) and valence band maximum (VBM) will be overlapping each other at Fermi level under sufficiently large strain [10,14]. However, the distinct transition from direct to indirect bandgap structure and the transition from semiconductor to metal phase have not yet been found. The dependence of carrier effective mass on crystal direction has not been studied. In addition, the low carrier mobility (μ) is probably one of the major barriers for the application of MoS_2 based field-effect transistor (FET) [15,16]. There have been found that the value of μ can be enhanced to about 200 $cm^2 V^{-1} S^{-1}$ by the deposition of high-dielectric HfO_2 layer [7]. In this work, we have studied

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the effect of tensile strain on the phase transitions, carrier effective mass and mobility in MoS_2 monolayer at room temperature (RT). The temperature depended mobility of electrons and holes are also investigated. The results have quantitatively demonstrated the carrier mobility enhancement by using tensile strain, this suggesting an alternative to improve the electrical performance of MoS_2 monolayer for device application.

2. Methodology

In this study, first principle calculations were carried out by using the Virtual Nanolab Atomistix ToolKit (ATK) package with density functional theory (DFT) [17]. The localized density approximation (LDA) exchange correlation with a double zeta polarized (DZP) basis is used with a mesh cut-off energy of 150 Ry [18]. The temperature is set to 300 K for our simulations on the bandstructure, charge carriers' effective mass and their mobility under strain effect at RT. For the investigation on the temperature depended mobility, we set this value to 200 K, 300 K and 400 K, respectively. A unit cell containing two Mo atoms and four S atoms was chosen with a periodic boundary condition. We used $11 \times 11 \times 1$ Monkhorst-Pack k-grid mesh in this simulation [19]. All atomic positions and lattice constants were optimized by using the generalized gradient approximations (GGA) [20] with the maximum Hellmann-Feynman forces of 0.05 eV/Å. The Pulay-mixer algorithm is employed as iteration control parameter with tolerance value of 10^{-5}. The maximum number of fully self-consistent field (SCF) iteration steps is set to 100. The result of structural optimization indicated that the simple orthorhombic lattice constant $a_0 = 5.47$ Å, $b_0 = 3.16$ Å, and the thickness of MoS_2 monolayer = 3.17 Å. a_0 and b_0 represent the lattice constant in armchair and zigzag directions, respectively. This optimized MoS_2 monolayer structure is in a good agreement with other publications [11,21].

3. Results and discussion

At first, we studied the bandstructure of MoS_2 monolayer for comparison. Fig. 1(a) shows the lattice structure of MoS_2 monolayer where the orthorhombic supercell, the smallest rectangular structure used for elastic constants calculation, is enclosed within the solid lines. The supercell is built in the orthorhombic way to demonstrate the carrier conduction along the [1,0] (armchair) and [0,1] (zigzag) directions. This has been shown to be more intuitive than the hexagonal lattice [22]. The K point, which is defined as the fractional reciprocal coordinates (1/3, 1/3) in hexagonal lattice, is equivalent to (1/3, 0), the midpoint between Γ and Y points for orthorhombic supercell [22] in this study. The bandstructure of unstrained MoS_2 monolayer is shown in Fig. 1(b) with a bandgap of 1.82 eV at RT, which is in a good agreement with the previous studies [10,23] In addition, the valence band energy at $\Gamma(0, 0)$ is slightly lower than the VBM at $K(1/3, 0)$, indicating a direct bandgap at K point.

Then, we investigated the electronic properties of MoS_2 monolayer under tensile strain for different in-plane direction configurations. The components of strain along [1,0] and [0,1] directions are noted as ε_x and ε_y, respectively. In this work, the strains are evaluated as the lattice stretching percentage. We defined $\varepsilon_x \equiv \Delta a_0/a_0$ and $\varepsilon_y \equiv \Delta b_0/b_0$, where Δa_0 and Δb_0 are the increase of lattice constants a_0 and b_0, respectively, due to the tensile strain. A wide range of strain configurations (magnitude from 0 to 18%, in all directions) has been employed in the study. For the purpose of precision and computational efficiency, a small increment of strain, $\Delta\varepsilon = 0.1\%$, has been used to study the direct–indirect bandgap transition, while a large $\Delta\varepsilon = 2\%$ has been used to study the semiconductor–metal transition. The exact transition boundaries have been found by using Newton's method with a precision of 0.0075% in strain and 0.001 eV in E_g.

The tensile strain will induce direct to indirect bandgap transition in MoS_2 monolayer [24]. However, very few studies reported the exact transition boundary on this issue with detailed information, and there is a large difference among them. For example, the study by Li [25] reported that 1% uniaxial strain is insufficient for this transition, while the study by Yun et al. [10] showed that the critical point for the transition from direct to indirect bandgap is 0.3% biaxial strain. In order to find out this transition, we carried out an explicit study: tensile strain along different combinations of [1,0] (ε_x) and [0,1] (ε_y) directions were applied on a MoS_2 monolayer. Both ε_x and ε_y range from 0 to 0.7% with a step $\Delta\varepsilon = 0.1\%$, this totally including 64 combinational configurations. In addition, the exact transition boundary is found by using Newton's method with a smaller step. Fig. 2(a) shows the bandgap as a function of tensile strain ε_{xy} (ε_x, ε_y). A clear boundary for the direct to indirect bandgap transition is found to be a straight line: ε_{xy} with $\varepsilon_x + \varepsilon_y \approx 0.66\%$, well covering the result of the aforementioned study by Yun et al. who reported that $\varepsilon_x = \varepsilon_y \approx 0.3\%$ is the critical point for this transition [10].

For the study of semiconductor to metal transition, a wide range of strain configurations ε_{xy} ($0 \le \varepsilon_x$, $\varepsilon_y \le 18\%$) with a step $\Delta\varepsilon = 2\%$ along both [1,0] and [0,1] directions has been studied, this generating a 10×10 mesh grids. Similar to the study of direct to indirect bandgap transition, the exact semiconductor to metal transition is found by using Newton's method with a smaller step. Fig. 2(b) shows the bandgap of MoS_2 monolayer as a function of ε_x and ε_y. The bandgap decreases monotonically with increasing applied strain, and becomes zero when the edges of valence

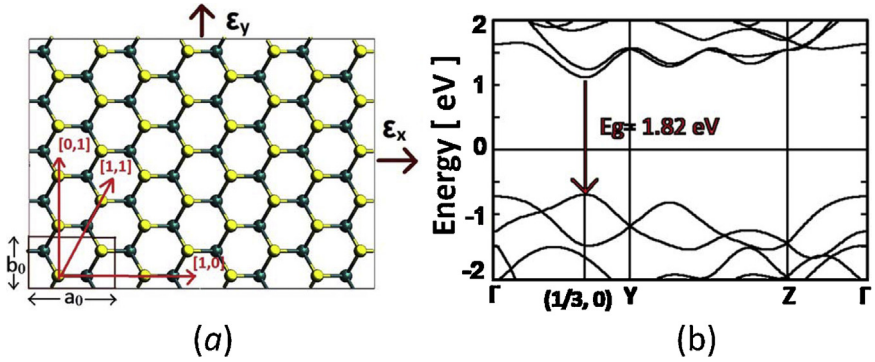

Fig. 1. (a) Atomic structure of MoS_2 monolayer: the rectangle supercell selected for the numerical simulation is within the red line. The arrows represent the lattice directions. (b) The energy band structure of unstrained MoS_2 monolayer. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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