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# Theoretical Investigation of Electrical Properties of $MoS_2$ FETs with Strained Channel Layer

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**Abstract**

**The electrical properties of n-type short channel molybdenite ($MoS_2$) field-effect transistors (FETs) with biaxial strain were investigated theoretically. First -principle bandstructure and density of states calculations for monolayer $MoS_2$ under strain were performed, and the results were used to calculate the $I_d$–$V_g$ characteristics of FETs under the assumption of ballistic transport. A maximum $I_{on}/I_{off}$ ratio of $1.0\times10^8$ was achieved at 1% compressive strain.**

## 1. Introduction

Two-dimensional (2D) materials are attractive for use in future electronic and optical devices. Graphene, the most commonly used 2D material, however, is not well suited for switching devices due to its zero bandgap properties [1]. More promising are some of the transition metal dichalcogenides (TMDCs), a family of 2D materials, due to their semiconducting properties and finite bandgap [2]. They are particulary promising for digital switching applications, and many experimental and theoretical studies have been made of TMDC-channel FETs in the last few years [3-6]. It is also theoretically predicted that introducing strain into monolayer $MoS_2$, one of TMDCs, modifies the bandsturucture [7, 8].

We theoretically investigated the effect of biaxial strain on the electrical properties of n-type short-channel $MoS_2$ field-effect transistors (FETs). The dependence of the on-current to off-current ($I_{on}/I_{off}$) ratio on strain was examined, and a means for increasing $I_{on}/I_{off}$ was identified.

## 2. Simulations

We investigated the bandstructure and the density of states (DOS) of monolayer $MoS_2$ under biaxial strain, which is represented by a parameter $\alpha$ (Fig. 1). First-principle calculations were performed on the basis of density functional theory (DFT) as implemented in the Atomistix Toolkit (version 12.8) [9]. The local density approximation (LDA) was used to describe the exchange-correlation potential.

The calculated bandstructure and DOS for $\alpha = -0.02$, 0, and +0.02 are shown in Figs. 2 and 3. In the unstrained case ($\alpha = 0$), both the conduction band minimum (CBM) and the valence band maximum (VBM) were at K-point, which means monolayer $MoS_2$ has a direct bandgap. In the compressive strain case ($\alpha = -0.02$), CBM moved to a point between K-point and Γ-point, leaving VBM at K-point. In the tensile strain case ($\alpha = +0.02$), VBM moved to Γ-point. This direct-to-indirect gap transition due to biaxial strain was also found by Yun *et al.* [7] and Peelaers *et al.*[8].

Figure 4 shows the dependence of the bandgap and the electron effective mass of strained monolayer $MoS_2$ on $\alpha$. The bandgap had a maximum of 1.89 eV under slightly compressive conditions ($\alpha = -0.01$), where the corresponding lattice parameter was 0.313 nm. Both large compressive and tensile strain reduced the bandgap. The effective mass showed a similar dependency: it had a maximum of 0.55 at $\alpha = -0.01$. In the area of our calculation, the smallest mass (0.42) was obtained at $\alpha = +0.05$. The large bandgap and light mass are incompatible.

The electronic properties of n-channel monolayer $MoS_2$ FETs with biaxial strain were investigated theoretically by using Rahman's ballistic short-channel FET model [10] in which the self-consistent potential at the top of the barrier $U_{scf}$ and the carrier density $N$ are first self consistently solved. Once $U_{scf}$ and $N$ are determined, the drain current $I_d$ is calculated assuming ballistic transport for electrons surmounting the top of the potential barrier:

$$I_d = \frac{q}{2}\int v_x D(E-U_{scf})[f_1(E)-f_2(E)]dE \quad (1)$$

where, $D$ is DOS, $v_x$ is electron velocity determined from the effective mass, and $f_1$ and $f_2$ are the Fermi-Dirac distribution functions at the source and drain respectively. The gate insulator thickness and permittivity were assumed to be 4 nm and 16, respectively.

Figure 5 shows the $I_d$–$V_g$ characteristic at drain voltage $V_d$ of 1 V on logarithmic (left axis) and linear scales (right axes) for an n-channel $MoS_2$ FET. An $I_{on}/I_{off}$ of $2.8\times10^7$ was attained at a 1 V logic swing. This roughly agrees with experimental $I_{on}/I_{off}$ of $10^8$ at a logic swing of about 4 V [4].

The dependence of $I_{on}/I_{off}$ on strain $\alpha$ is plotted in Fig. 6. A maximum $I_{on}/I_{off}$ of $1.0\times10^8$ was achieved for a compressive strain of −0.01. We attributed this to the large bandgap since the bandgap was also maximum at this point.

The maximum on-current was obtained at α = +0.05 since the effective mass became minimum at that point.

## 3. Conclusions

The electrical properties of monolayer $MoS_2$ FETs with biaxial strain were investigated theoretically. Strain affects FET characteristics through changes in the bandgap and effective mass. The maximum $I_{on}/I_{off}$ of $1.0 \times 10^8$ was attained at 1% compressive strain while the on-current was smaller than with larger tensile strain. This means that $I_{on}/I_{off}$ can be increased by maximizing the bandgap.


## Acknowledgements

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## References


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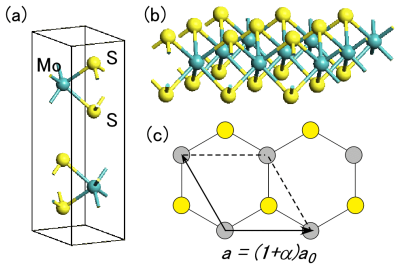


Fig. 1 (a) Bulk unit cell of $MoS_2$. (b) Monolayer of $MoS_2$. (c) Unit cell of strained monolayer $MoS_2$ with lattice constant of $a$. Parameter α defines the strain: $a_0$ is lattice constant of unstrained monolayer $MoS_2$, 0.316 nm.

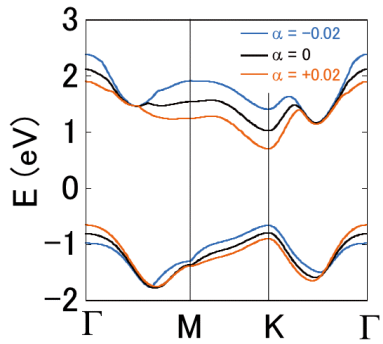


Fig. 2 Lowest conduction band and highest valence band of strained monolayer $MoS_2$ with α = −0.02, 0, +0.02.

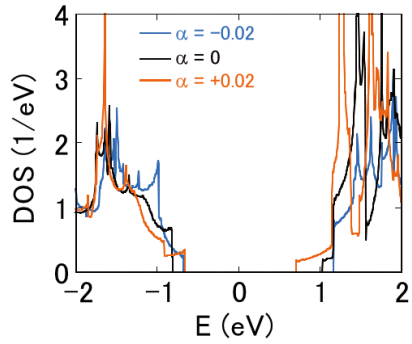


Fig. 3 DOS in unit cell of strained monolayer $MoS_2$ with α = −0.02, 0, +0.02.

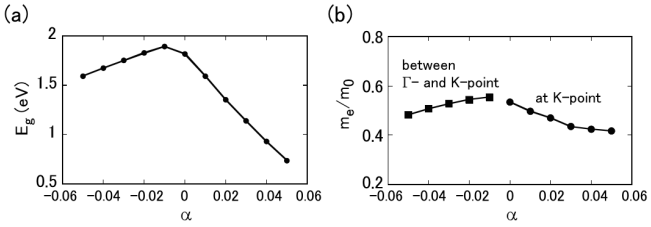


Fig. 4 (a) Dependence of bandgap of strained monolayer $MoS_2$ on α. (b) Electron effective mass of strained monolayer $MoS_2$. Circular symbols indicate conduction band minimum is at K-point; square ones indicate that it is between K- and Γ-point.

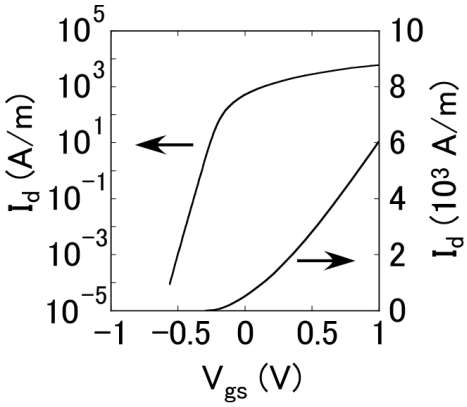


Fig. 5 Calculated transfer curve of n-channel monolayer $MoS_2$ FET for α = 0. Drain voltage, gate insulator thickness, and specific permittivity were 1 V, 4 nm, and 16, respectively.

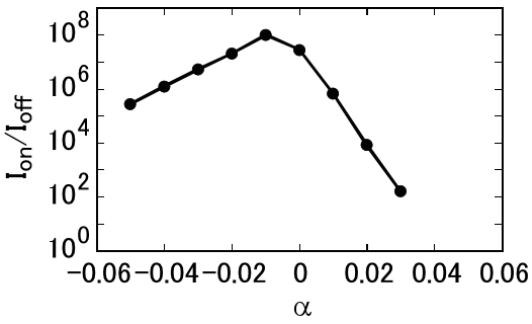


Fig. 6 On-current to off-current ratio for n-channel monolayer $MoS_2$ FET as a function of strain α.