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# Compact conduction band model for transition-metal dichalcogenide alloys

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ABSTRACT

Monolayer transition metal dichalcogenide (TMD) alloys, such as $Mo_{1-x}W_xS_2$, owing to the unique electronic properties of the atomically thin two-dimensional layered structure, can be made into high performance metal–oxide–semiconductor field-effect transistors. The compact conduction band model of effective mass approximation (EMA) with the second nonparabolic correction is proposed for monolayer $Mo_{1-x}W_xS_2$. The three band tight-binding (TB) method is used for calculating the band structure for monolayer TMD alloys such as $Mo_{1-x}W_xS_2$, and a compact conduction band model is precisely developed to fit the band structures of TMD alloys calculated with tight-binding methods for the calculation of electron mobility. The impact of alloys on electron mobility of monolayer $Mo_{1-x}W_xS_2$ is discussed in this study.



## 1. Introduction

Transition-Metal Dichalcogenides (TMD) and its alloy present great potential on the application to future transistor technology. TMD alloys, with the advantage of adjustable band gap, show the potential on the application to band gap engineering and could be applied to nanoscale Metal-Oxide-Semiconductor Field-Effect Transistor (MOSFET) devices. The effects of alloy concentration on TMD alloy band structure and the correspondent carrier mobility are very important in new MOSFET device development. There are two types of Transition metal dichalcogenide alloy (TMD alloy) monolayer. For the first type monolayer TMD alloys, they are atomically thin semiconductors of type $M''X_2$, with $M'' = M_{1-x}M'_x$ a transition metal atom (M(M′) = Mo, W, etc.) and X a chalcogen atom (S, Se, etc.). One layer of M″ alloy atoms is sandwiched between two layers of X atoms. For the second type of monolayer TMD alloys, they are atomically thin semiconductors of type $MX''_2$, with $X'' = X_{1-x}X'_x$ a chalcogen atom (X(X′) = S, Se, etc.) and M a transition metal atom (Mo, W, etc.). One layer of M atoms is sandwiched between two layers of $X_{1-x}X_x'$ alloy atoms. The first type of monolayer TMD alloys, such as $Mo_{1-x}W_xS_2$, is a very promising two-dimensional material for future transistor technology. The $Mo_{1-x}W_xS_2$ layer structure exhibits similar performance to graphite, such that $Mo_{1-x}W_xS_2$ could be used for a high performance transistor device. $Mo_{1-x}W_xS_2$, with its two-dimensional super-thin atomic structure and uniquely optical and electronic properties, has been broadly studied in past years. Experimental effort has been made on TMD alloys. The 2D layered transition-metal dichalcogenide alloys may have better inter miscibility and are predicted to be stable [1]. Several layered TMD bulk alloys, such as $Mo_{1-x}W_xS_2$ and $Mo_{1-x}W_xSe_2$, have been synthesized [2], suggesting good thermodynamic stability for the corresponding TMD alloys.

In 2012, Prof. Ying-Sheng Huang's research team [3] from Taiwan obtained the statistics of the homo- and heteroatomic coordinates in monolayer $Mo_{1-x}W_xS_2$ from the atomically resolved scanning transmission electron microscope images and successfully quantified the degree of alloying for the transition metal elements (Mo or W). In their work, they performed the direct visualization of the atomic species Mo and W in the $Mo_{1-x}W_xS_2$ compounds, clearly showing how the two elements could be mixed in a monolayer [3]. Recently, Dr. Liming Xie's group from China exfoliated the first family of atomic monolayer $Mo_{1-x}W_xS_2$ and observed the composition-dependent photoluminescence from the monolayer $Mo_{1-x}W_xS_2$ (1.82 to 1.99 eV) [4]. Prof. Zigang Shuai's research group [5] investigated the composition-dependent electronic properties of monolayer $Mo_{1-x}W_xS_2$ based on first-principles calculations by applying the supercell method and effective band structure (EBS) approximation [6]. Their results released that the tunable electronic properties of monolayer TMD alloys made them attractive for electronic and optoelectronic applications. Above are the motivations of this work. To our knowledge, current effective mass approximation (EMA) band model could not accurately fit the band structure of monolayer TMD and its alloys. For this reason, it is necessary to develop the correct compact band model of monolayer TMD alloys for carrier mobility calculation. The compact conduction band structure and electron mobility of monolayer $Mo_{1-x}W_xS_2$ as a potential channel material in future transistor devices are investigated in this study. In Section 2, calculation method for band structure from TB method and compact model and electron mobility calculations of monolayer $Mo_{1-x}W_xS_2$ are presented. The results of

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this work are discussed in Section 3. Section 4 presents a conclusion of this work.

## 2. Calculation method

### 2.1. Tight-binding (TB) method

Theoretical Calculations of the structure for TMD alloys are based on the framework of a linear combination of atomic orbitals and virtual crystal approximation. The three band tight-binding (TB) atomic basis set consists of three d orbitals per atom, according to previous theoretical work of Prof. W. Yao's research group from Hong Kong [7]. Therefore, the final matrix is of size 3 × 3. Three atomic d orbits such as $d_{z2}$, $d_{xy}$, and $d_{x2-y2}$ are considered in three band TB band model of TMD alloys. TB band model considering the first nearest-neighbor (NN) interaction is shown as Eq. (1)

$$H^{NN}\left(\vec{k}\right)=\begin{bmatrix} H_0 & H_a & H_b \\ H_a^* & H_{aa} & H_{ab} \\ H_b^* & H_{ab}^* & H_{bb} \end{bmatrix},\ \vec{k}=(k_x,k_y) \tag{1}$$

where five independent matrix elements in Eq. (1) are shown in the following

$$\begin{aligned} H_a &= -2\sqrt{3}I_2\ \sin\alpha\ \sin\beta+2iI_1(\ \sin2\alpha+\ \sin\alpha\ \cos\beta)\\ H_b &= 2I_2(\ \cos2\alpha-\ \cos\alpha\ \cos\beta)+2\sqrt{3}iI_1\ \cos\alpha\ \sin\beta\\ H_{aa} &= 2I_{11}\ \cos2\alpha+(I_{11}+3I_{22})\ \cos\alpha\ \cos\beta+E_2\\ H_{bb} &= 2I_{22}\ \cos2\alpha+(3I_{11}+I_{22})\ \cos\alpha\ \cos\beta+E_2\\ H_{ab} &= \sqrt{3}(I_{22}-I_{11})\ \sin\alpha\ \sin\beta+4iI_{12}\ \sin\alpha(\ \cos\alpha-\ \cos\beta) \end{aligned} \tag{2}$$

and important parameters used in Eq. (2) are defined as below

$$(\alpha,\beta)=\left(\frac{1}{2}k_x\alpha,\frac{\sqrt{3}}{2}k_y\alpha\right) \tag{3}$$

where $k_x$ and $k_y$ are components of $\vec{k}$vector as shown in Eq. (1) and a is lattice constant of the monolayer $Mo_{1-x}W_xS_2$. TB band model considering the third nearest-neighbor (TNN) interaction is shown as Eq. (4)

$$H^{TNN}\left(\vec{k}\right)=\begin{bmatrix} V_0 & V_a & V_b \\ V_a^* & V_{aa} & V_{ab} \\ V_b^* & V_{ab}^* & V_{bb} \end{bmatrix} \tag{4}$$

Matrix elements in Eq. (4) are shown in the following

$$V_0=E_1+2I_0(2\ \cos\alpha\ \cos\beta+\ \cos2\alpha)+2\eta_0(2\ \cos3\alpha\ \cos\beta+\ \cos2\beta)+2\mu_0(2\ \cos2\alpha\ \cos2\beta+\ \cos4\alpha) \tag{5}$$

$$\begin{aligned} \mathrm{Re}[V_a] &= -2\sqrt{3}I_2\ \sin\alpha\ \sin\beta+2(\eta_1+\eta_2)\ \sin3\alpha\ \sin\beta-2\sqrt{3}g_2\ \sin2\alpha\ \sin2\beta\\ \mathrm{Im}[V_a] &= 2I_1\ \sin\alpha(2\ \cos\alpha+\ \cos\beta)+2(\eta_1-\eta_2)\ \sin3\alpha\ \sin\beta+2g_1\ \sin2\alpha(2\ \cos2\alpha+\ \cos2\beta) \end{aligned} \tag{6}$$

$$\begin{aligned} \mathrm{Re}[V_b] &= 2I_2(\ \cos2\alpha-\ \cos\alpha\ \cos\beta)-\frac{2}{\sqrt{3}}(\eta_1+\eta_2)(\ \cos3\alpha\ \cos\beta-\ \cos2\beta)+2g_1(\ \cos4\alpha-\ \cos2\alpha\ \cos2\beta)\\ \mathrm{Im}[V_b] &= 2\sqrt{3}I_1\ \cos\alpha\ \sin\beta+\frac{2}{\sqrt{3}}\ \sin\beta(\eta_1-\eta_2)(\ \cos3\alpha+2\ \cos\beta)+2\sqrt{3}g_1\ \cos2\alpha\ \sin2\beta \end{aligned} \tag{7}$$

$$V_{aa}=E_2+(I_{11}+3I_{22})\ \cos\alpha\ \cos\beta+2s_{11}\ \cos2\alpha+4\eta_{11}\ \cos3\alpha\ \cos\beta+2\left(\eta_{11}+\sqrt{3}\eta_{12}\right)\ \cos2\beta+(g_{11}+3g_{22})\ \cos2\alpha\ \cos2\beta+2g_{11}\ \cos4\alpha \tag{8}$$

$$\begin{aligned} \mathrm{Re}[V_{ab}] &= \sqrt{3}(I_{22}-I_{11})\ \sin\alpha\ \sin\beta+4\eta_{12}\ \sin3\alpha\ \sin\beta+\sqrt{3}(g_{22}-g_{11})\ \sin2\alpha\ \sin2\beta\\ \mathrm{Im}[V_{ab}] &= 4I_{12}\ \sin\alpha(\ \cos\alpha-\ \cos\beta)+4g_{12}\ \sin2\alpha(\ \cos2\alpha-\ \cos2\beta)\\ V_{bb} &= E_2+(3I_{11}+I_{22})\ \cos\alpha\ \cos\beta+2I_{22}\ \cos2\alpha+2\eta_{11}(2\ \cos3\alpha\ \cos\beta+\ \cos2\beta)+\frac{2}{\sqrt{3}}\eta_{12}(4\ \cos3\alpha\ \cos\beta-\cos2\beta)+(3g_{11}+g_{22})\ \cos2\alpha\ \cos2\beta+2g_{22}\cos4\alpha \end{aligned} \tag{9}$$

### 2.2. EMA conduction band model with the second Nonparabolic correction

The band structure of monolayer $Mo_{1-x}W_xS_2$ is calculated with a three-band tight-binding model [7,8] as mentioned in previous subsection. As one can see in Fig. 1, the conduction band is perfectly parabolic in the K valley in small energy region owing to their isotropic and parabolic effect in small energy region. Note that the part of the conduction band relevant to the electron mobility can be described by effective mass approximation (EMA, refer to Eq. (10)) band as reported in Ref. [9].

$$E=\frac{\hbar^2\left(k_x{}^2+k_y{}^2\right)}{2m^*} \tag{10}$$

However, as you know that current EMA band model could not accurately fit the band structure of monolayer TMD alloys in larger energy and k-space regions. For this reason, it is necessary to develop the more correct compact band model of monolayer TMD alloys for electron mobility calculation, and current SPICE model [10] applied to transistor devices with 2D semiconducting materials is restricted to monolayer TMD materials. It is therefore necessary to develop SPICE model with correct compact band model applicable to transistor devices with monolayer TMD alloys. Recently, Prof. David Esseni's research group from Italy [11] proposed the EMA with the first order nonparabolic factor, α correction as shown below.

$$E(1+\alpha E)=\frac{\hbar^2\left(k_x{}^2+k_y{}^2\right)}{2m^*} \tag{11}$$

In this work, we follow higher order correction for EMA mode as discussed in the text book [12] edited by Dr. Riedly to propose EMA compact conduction band model for monolayer TMD alloys considering

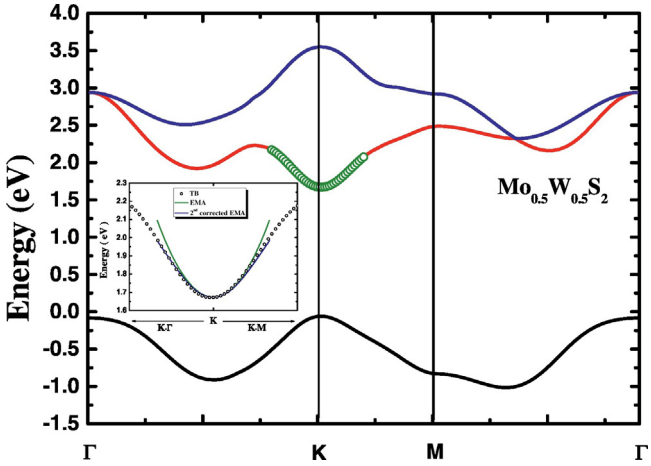


**Fig. 1.** Band structures for monolayer $Mo_{0.5}W_{0.5}S_2$ from Tight-binding method and conventional EMA model and EMA model with the second nonparabolic correction, respectively. Note that the solid line is from Tight-binding method and the symbol is from the compact EMA model with the second nonparabolic correction. Result from the compact EMA model with the second nonparabolic correction is in agreement with the one from tight-binding method. EMA model with the second nonparabolic correction is better than conventional EMA model as shown in the zoom in plot.

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