Investigation of Electronic Properties of $Mo_xW_{1-x}S_2$ Alloy by Tight-binding Method for Interband transition

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***Abstract*-Two dimensional (2D) materials have been popular recently due to their low-dimensional transport properties. And transition metal dichalcogenides (TMDCs) show a wide range of electronic and optical properties. In this paper, the electronic and optical properties of $Mo_xW_{1-x}S_2$ alloy such as band structure, bandgap, effective mass and absorption coefficient are modeled by sp^3d^5tight-binding model.**

***Keywords*- sp^3d^5tight-binding model, TMDCs, $Mo_xW_{1-x}S_2$**

I. INTRODUCTION

Recently, two dimensional (2D) materials have become popular due to its unique structural and electronic properties. They exist in bulk from stacks of layers bonded by Van der Waals force, and can be exfoliated into an individual, atomically thin layer. Graphene is one of popular 2D materials due to its excellent electronic properties, it has high carrier mobility and good conductivity. But Bulk Graphene has zero bandgap, and only opens it bandgap with nanoribbon structures. Therefore, it is difficult to directly apply the graphene to electronic and optical device. They are typically used as a role of metal. Transition metal dichalcogenides (TMDCs) show interesting electronic and optical properties which are good for electronic and optical applications and in contract to graphene that has no bandgap between conduction band and valence band. MoS_2 and WS_2 are the two of most popular TMDCs. MoS_2 monolayer and nanoribbons with strain show special electronic properties[1], they have indirect and smaller bandgap trend and lower carrier effective mass with increasing tensile strain. In the result of tight-binding model, the band structure of MoS_2 armchair nanoribbons show an intermediate band between the conduction band and valence band and when the thickness of MoS_2 armchair nanoribbons increase, the states in the intermediate band become more. The result shows that MoS_2 armchair nanoribbons have potential for solar cell applications[2].

In this work, the electronic and optical properties of $Mo_xW_{1-x}S_2$ are investigated by sp^3d^5 tight-binding model. The content of this paper is shown as followings: (1) the methodology of band structure calculation of $Mo_xW_{1-x}S_2$ alloy is shown first; (2) we will show you how to extract bandgap, effective mass and absorption coefficient of $Mo_xW_{1-x}S_2$ alloy; (3) The simulated results of $Mo_xW_{1-x}S_2$ electronic properties are presented and discussed; (4) finally, we make the conclusions.

II. METHODOLOGY

A. Alloy Tight-Binding model

Studies related to MoS_2 and WS_2 tight-binding calculation and density functional theory (DFT) calculation are still developed. But in $Mo_xW_{1-x}S_2$ alloy band structure calculation, the computing domain is larger. Therefore, the computing time of DFT calculation becomes too long. We consider tight-binding method is more suitable to calculate the band structure of $Mo_xW_{1-x}S_2$ alloy due to shorter computing time. For MoS_2 band structure calculations by tight-binding method, the earliest one[3] used the generic algorithm to fit the DFT result. In their tight-binding model, non-orthogonal first-nearest Mo (sp^3d^5) and S (sp^3d^5) were chosen and included the spin-orbit coupling and we apply this tight-binding model to calculate the $Mo_xW_{1-x}S_2$ alloy. At first, the $Mo_xW_{1-x}S_2$ alloy atom map is created by randomly placing the W and Mo atoms. The number of total metal(W, Mo) atoms in $Mo_xW_{1-x}S_2$ alloy atom map is larger than 100. We randomly created several $Mo_xW_{1-x}S_2$ alloy atom maps and calculated the band structure of them by sp^3d^5tight-binding model.

B. Electronic and Optical Properties Calculation

At first, we average all band structure results of each randomly created atom map to obtain an average band structure. We extract the bandgap and effective mass of $Mo_xW_{1-x}S_2$ from average band structure. The effective mass is given by

$$m^* = \hbar^2\left(\frac{\partial^2 E(k)}{dk^2}\right)^{-1} \quad (1)$$

, where m^* is effective mass, $\hbar$ is reduced Planck's constant, k is wavenumber, E(k) is eigenvalue. The absorption coefficient of $Mo_xW_{1-x}S_2$ alloy is calculated by Fermi's Golden rule as following

$$\alpha(\hbar\omega) = \frac{\pi e^2\hbar}{cn\epsilon_0 m_0^2}\frac{1}{\hbar\omega}\sum_{i,f,k}\left|< \psi_i|\frac{m_0}{\hbar}\nabla_k H(k)|\psi_f >\right|^2 \times \frac{J_{if}(\omega)}{L}\,\delta(E_f - E_i - \hbar\omega) \quad (2)$$

$$J_{if}(\omega) = \frac{2}{\pi^2}\frac{dk^2}{dE_i(k)+dE_f(k)} \quad (3)$$

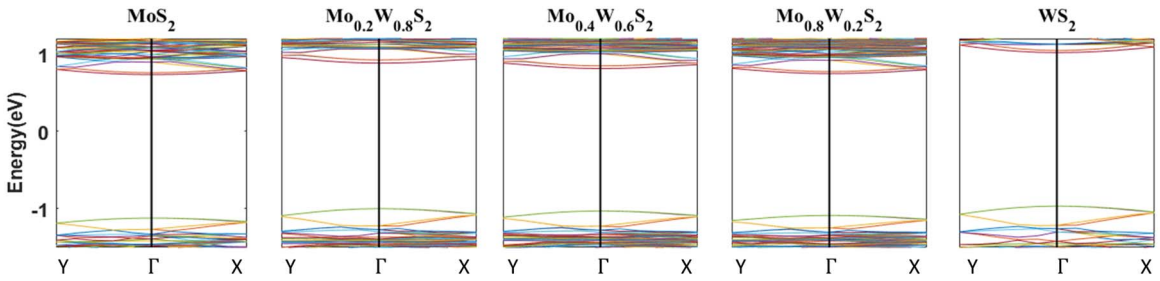

Fig. 1. The band structure of $Mo_xW_{1-x}S_2$

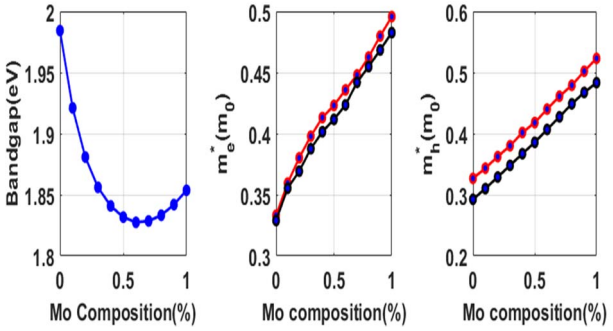

Fig. 2. (a) The bandgap o f $Mo_xW_{1-x}S_2$ with different W composition.

(b) and (c) are effective mass of electron and hole.

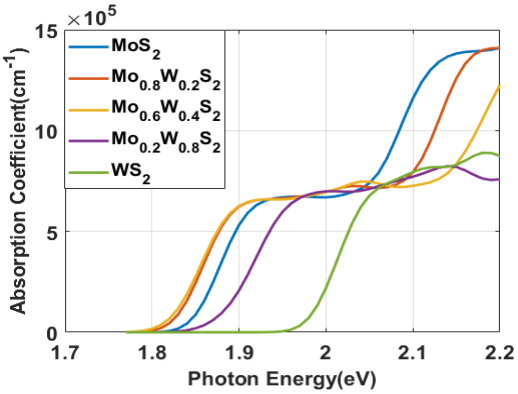

Fig. 3. The absorption coefficient of $Mo_xW_{1-x}S_2$ with different Mo composition.

where i and f correspond to the initial and final state. $\alpha(\hbar\omega)$ is absorption coefficient, $J_{if}(\omega)$ is joint density of states, $\hbar\omega$ is photon energy and L is thickness of $Mo_xW_{1-x}S_2$. The constant term contains the electron mass(m_0), permittivity(ϵ_0), photon frequency(ω), light speed in free space(c), refractive index(n). The momentum matrix element can be calculated with tight-binding Hamiltonian via the relation $p(r) = \frac{m_0}{\hbar}\nabla_k H(k)$.

III. RESULT AND DISCUSSION

The Fig. 1 shows the band structures of different Mo composition of $Mo_xW_{1-x}S_2$ alloy, and we can observe that when the composition of Mo decreases, the position of conduction and valence band becomes higher. The Fig. 2(a) shows the bandgap of different Mo composition of $Mo_xW_{1-x}S_2$ alloy. When the composition of Mo is close to 60%, the bandgap become smaller, the bandgap at 60% Mo composition is about 1.83eV, and the bandgap with different Mo composition is very close to experiment value[4]. Figs. 2(b) and 2(c) show the effective mass of electron and hole at conduction band and valence band edge. When Mo composition of $Mo_xW_{1-x}S_2$ alloy decrease, the effective mass of electron and hole become smaller, and both of curve is like linear lines. Finally, Fig. 3 shows the absorption coefficient of $Mo_xW_{1-x}S_2$ alloy with different Mo composition. The absorption coefficient of is quite large for energy larger than 0.1eV above the bandgap. The trend in different composition is similar.

IV. CONCLUSION

We have demonstrated the electronic and optical properties of $Mo_xW_{1-x}S_2$ alloy by sp^3d^5 tight-binding model. The result of bandgap is very close to experiment trend, it shows the precision of sp^3d^5tight-binding model. The result of effective mass is not small enough, it will cause $Mo_xW_{1-x}S_2$ alloy to has a smaller mobility. The absorption coefficient of $Mo_xW_{1-x}S_2$ is great, and it is suitable for photovoltaic device.

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