

# Physical models for MoS<sub>2</sub> and their application to simulations of MoS<sub>2</sub> MSM device

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**Abstract.** MoS<sub>2</sub> is a kind of two-dimensional semiconductor material with excellent electrical and optical properties, which can be used to develop new types of electronic devices and optoelectronic devices. Here, we established the mobility model of the MoS<sub>2</sub>. It is found that the simulation results agree with the experimental data. And our model are better than the theoretical results at low temperature. At the same time, we used the model to simulate the MoS<sub>2</sub> MSM device. The I – V curve are basically identical with the measurement results, which proves the practicability of the model.

## 1. Introduction

In the last few years, bidimensional materials have driven the attention of the scientific community as one of the best alternatives to the traditional Si-based technology, among which MoS<sub>2</sub> is a typical materials. The bandgap of MoS<sub>2</sub> can be modified by changing its thickness or applying stress and interesting optoelectronic properties of MoS<sub>2</sub> have also been demonstrated because of the direct bandgap behavior of monolayer films[1]. Comparing to one-dimensional materials, MoS<sub>2</sub> materials are easy to fabricate complex structures and attractive for using in next-generation electronic devices.

In order to analyze the performance of MoS<sub>2</sub>-based devices, the mobility of MoS<sub>2</sub> need to be studied. Recently, Sunkook Kim[2] has obtained the mobility by measuring the Ids - Vgs curve of MoS<sub>2</sub> FET at room temperature. Others like J.M. Gonzalez-Medina[3] has theoretically calculated the mobility of MoS<sub>2</sub>, which are in good agreement with Sunkook Kim's data. In this paper, the analysis model of MoS<sub>2</sub> carrier mobility will be established and investigated by comparing with other groups experimental and theoretical result. Further, the MoS<sub>2</sub> MSM device has been fabricated and test the analysis model.

## 2. Physical models

The mobility is affected by several scattering mechanisms, including lattice scattering, ionized impurity scattering, carrier-carrier scattering and so on. The structure of MoS<sub>2</sub> is very similar to the graphene, S and Mo atoms are covalently bonded in the monolayer. And there is no dangling bond on the surface. So we focus on three different scattering mechanisms such as acoustic phonons, optical intervalley phonons and ionization impurities, and establish the mobility models for each scattering mechanism. Further, the combined mobility, which includes the three mechanisms above, is[4,5]

$$u_T^{-1} = u_{ac}^{-1} + u_b^{-1} + u_{im}^{-1} \quad (1)$$

Where  $u_{ac}$  is the mobility from acoustic phonons interaction,  $u_b$  is the mobility from optical intervalley phonons interaction and  $u_{im}$  is the mobility from ionization impurities interaction.

### 2.1. Acoustic phonons

In the two-dimensional deformation potential theory of surface phonon scattering and for a



nondegenerate surface, the electron mobility is given by [5]:

$$u_{ac} = q\hbar\rho u_1 / m^* m_h Z_A \quad (2)$$

Where  $q$  is the elementary charge,  $\hbar$  is the Dirac constant,  $u_1$  is the sound velocity,  $m^*$  and  $m_h$  are the effective mass and the mobility mass, respectively,  $Z_A$  is the deformation potential,  $k$  is the Boltzmann constant, and  $T$  is the absolute temperature. The areal mass density of  $\text{MoS}_2$ ,  $\rho(\text{g}/\text{cm}^2)$ , is given by

$$\rho = \rho_{\text{bulk}} Z_{\text{av}} \quad (3)$$

Where  $\rho_{\text{bulk}}$  is the mass density ( $\text{g}/\text{cm}^3$ ) of  $\text{MoS}_2$  and  $Z_{\text{av}}$  is the effective thickness of the inversion layer.  $Z_{\text{av}}$  was assumed to be independent of temperature and normal electric field. Here,  $Z_{\text{av}}$  adopts the approximation suggested by Schwarz and Russek[6]

$$Z_{\text{av}} = Z_{\text{CL}} + Z_{\text{QM}} \quad (4)$$

$$Z_{\text{CL}} = 3kT/2qE_{\text{eff}} \quad (5)$$

$$Z_{\text{QM}} = \left( \frac{9\hbar^2}{4m_{\perp}qE_{\text{eff}}} \right)^{1/3} \quad (6)$$

$$E_{\perp} = E \sin \theta = E \times |J| \quad |J \leftrightarrow e f_j| \quad (7)$$

So the acoustic phonons (LA and TA) is expressed as:

$$u_{\text{ac}} = \frac{a}{(E_{\perp}/E_1)^b} + \left( \frac{c(N/N_1)^d}{(E_{\perp}/E_1)^e} \right) \cdot \frac{1}{T_n} \quad (8)$$

$$T_n = \left( \frac{T_L}{300} \right)^f \quad (9)$$

Where  $T_L$  is the lattice temperature,  $E_{\perp}$  is the perpendicular electric field.  $a$ ,  $b$ ,  $c$  and  $d$  are the empirical constants, respectively.  $f$  is the temperature dependence of the probability of surface phonon scattering and  $N$  is the total doping concentration. The  $E_1$  and  $N_1$  are the constant with a value of  $1 \text{ V}/\text{cm}$  and  $1 \text{ cm}^{-3}$ , respectively.

## 2.2. Optical intervalley phonons

At low temperature, the acoustic phonon vibration is the main influence factor to the mobility. however, when the temperature increased, optical intervalley scattering play a major role.

The mobility ( $u_b$ ) from optical intervalley phonons interaction adopts the empirical model in a slightly modified form which preserves their model parameters fitted at room temperature[5,6].

$$u_b = u_0 + \frac{u_{\text{max}}(T) - u_0}{1 + (N_A/C_r)^\alpha} - \frac{u_1}{1 + (C_s/N_A)^\beta} \quad (10)$$

$$u_{\text{max}}(T) = u_{\text{max}} \left( \frac{T}{300} \right)^{-\gamma} \quad (11)$$

Where  $T$  is the temperature,  $u_1$  is the sound velocity,  $N_A$  is the acceptor concentration. Others parameters are the empirical constants.

So this component is given by:

$$u_b = f \times e^{-\frac{h}{N}} + \frac{[g \times (T_L/300)^{-a} - f]}{1 + (N/b)^c} - \frac{f}{1 + (d/N)^e} \quad (12)$$

Here, N is the total density of impurities and  $T_L$  is the lattice temperature, a, b, c, d, e and f are the empirical constants, respectively.

### 2.3. Ionization impurities

Ionized impurities are mainly affected by temperature and impurity concentration. The mobility from ionization impurities interaction,  $u_{im}$  can be described by:

$$u_{im} = Z^{1-\alpha_1} u_{i.n} \left( \frac{T}{300} \right)^{3\alpha_1-1} \left( \frac{N_1}{Z^2 N_1} \right)^{\delta} + u_{i.c} \left( \frac{300}{T} \right)^{0.5} \left( \frac{c}{Z^2 N_1} \right) \quad (13)$$

Where  $N_1$  is the constant with a value of  $1\text{cm}^{-3}$ , T is the temperature, Z and c are the empirical constants, respectively. In the calculations,  $Z^{1-\alpha_1} \cong 1$ , the paramant  $\alpha_1$  stems from the description of the majority carrier mobility as a function of impurity concentration[7].

It can be seen that the second part plays a dominant role in the case of high doping, so the impurity scattering components is obtained using the following equation:

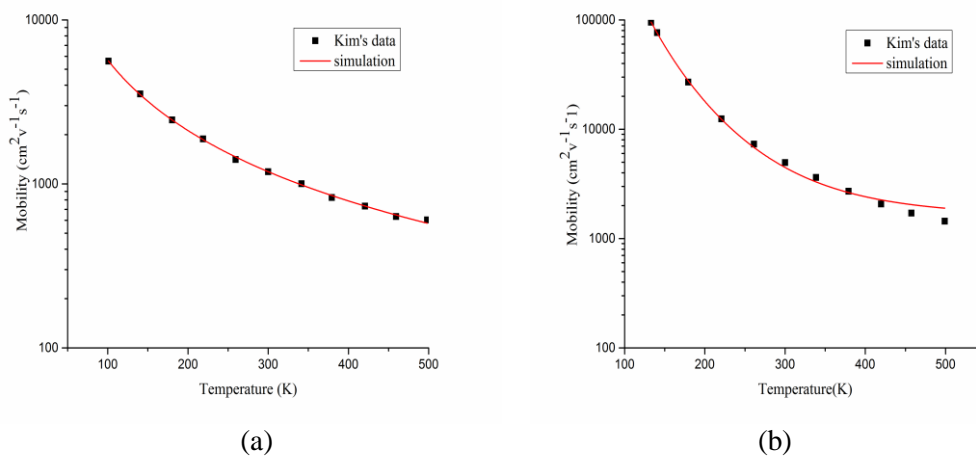
$$u_{im} = \frac{a^2}{a-b} \times \left( \frac{T_L}{300} \right)^{(3 \times c - 1)} \quad (14)$$

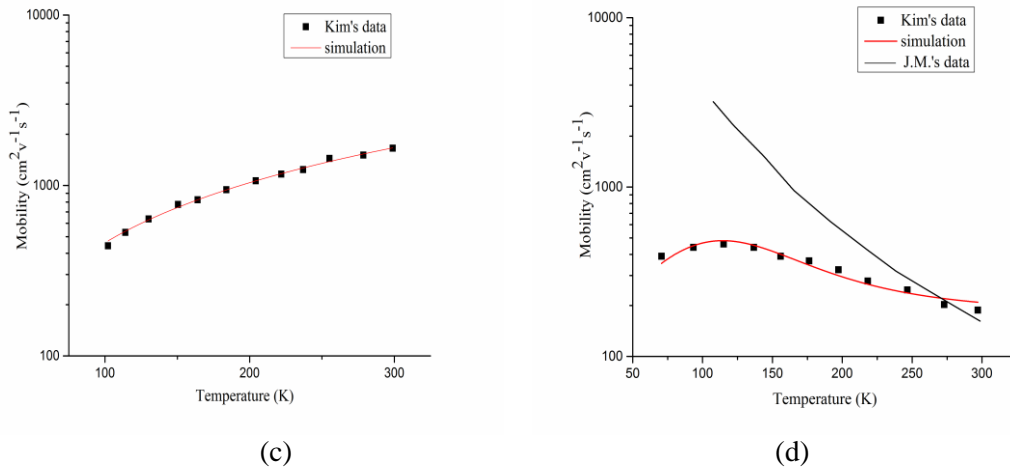
Where  $T_L$  is the lattice temperature, a, b and c are the empirical constants, respectively.

## 3. Results and discussion

### 3.1 Mobility model

Figure 1 shows the simulation results of MoS<sub>2</sub> carrier mobility model. We can see that the  $u_{ac}$ ,  $u_b$  and  $u_{im}$  fitting well with the Kim's theoretical results in Fig. 1(a), (b) and (c), which can be explained that the model is reasonable. And in Fig. 1(d), we can find that the combined mobility is very consistent with the J.M.'s experimental data. Meanwhile, the model is better than the Kim's theoretical calculation at low temperature.

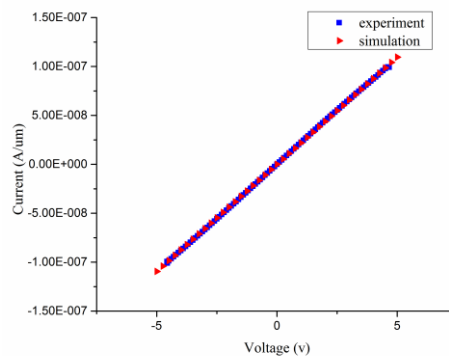




**Figure 1** the simulation results of MoS<sub>2</sub> mobility model, (a) acoustic phonon mobility (b) optical intervalley phonons (c) impurity scattering and (d) comparison of the combined mobility.

### 3.2. Mobility model test

The MSM device adopted Ni electrodes with Hexagon MoS<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> substrates and measured the I – V curve. The mobility model is applied to simulating the same structure device and compared with the experimental results in Figure 2. The results are in good agreement with the experimental data.



**Figure 2.** MSM simulation used the mobility model.

## 4. Summary

Physical models for MoS<sub>2</sub> have been established and investigated. And we have stimulated the characteristic of the model and compared with the experimental data and the theoretical calculation. According to the results, it can be seen that  $u_{ac}$ ,  $u_b$  and  $u_{im}$  is the important part of the MoS<sub>2</sub> mobility. Finally, the MoS<sub>2</sub> MSM device has been fabricated and simulated to verify this model. The results indicate that the new model is reasonable.

## 5. References

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