

Physical models for MoS₂ and their application to simulations of MoS₂ MSM device

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Abstract. MoS₂ 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 MoS₂. 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 simulat the MoS₂ 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 MoS₂ is a typical materials. The bandgap of MoS₂ can be modified by changing its thickness or applying stress and interesting optoelectronic properties of MoS₂ have also been demonstrated because of the direct bandgap behavior of monolayer films[1]. Comparing to one-dimensional materials, MoS₂ materials are easy to fabricate complex structures and attractive for using in next-generation electronic devices.

In order to analyze the performance of MoS₂-based devices, the mobility of MoS₂ need to be studied. Recently, Sunkook Kim[2] has obtained the mobility by measuring the Ids - Vgs curve of MoS₂ FET at room temperature. Others like J.M. Gonzalez-Medina[3] has theoretically calculated the mobility of MoS₂, which are in good agreement with Sunkook Kim's data. In this paper, the analysis model of MoS₂ carrier mobility will be established and investigated by comparing with other groups experimental and theoretical result. Further, the MoS₂ 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 MoS₂ 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]:

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

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 MoS_2 , ρ (g/cm^2), is given by

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

Where ρ_{bulk} is the mass density (g/cm^3) of MoS_2 and Z_{av} is the effective thickness of the inversion layer. Z_{av} was assumed to be independent of temperature and normal electric field. Here, Z_{av} adopts the approximation suggested by Schwarz and Russek[6]

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

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

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

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

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

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

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

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 V/cm and 1cm^{-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].

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

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

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:

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

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:

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

Where N₁ is the constant with a value of 1cm⁻³, T is the temperature, Z and c are the empirical constants, respectively. In the calculations, Z^{1-α₁} ≅ 1, the paramant α₁ 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:

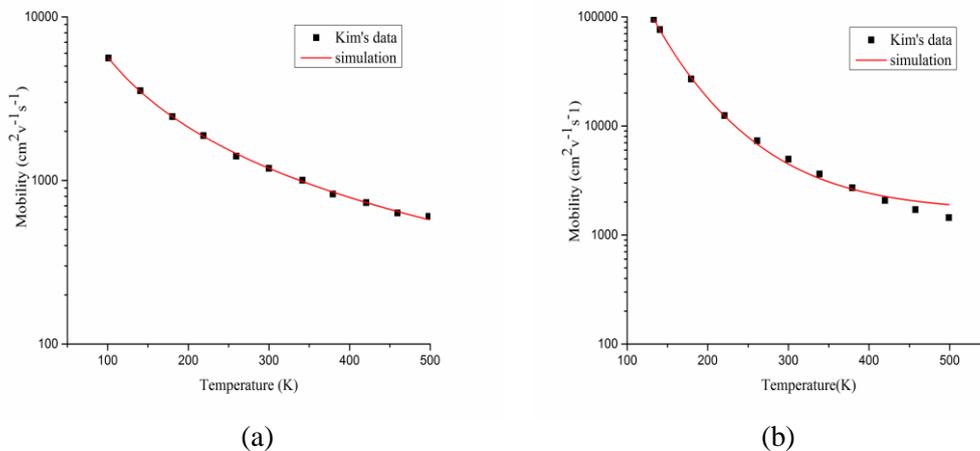
$$u_{im} = \frac{a^2}{a-b} \times \left(\frac{T_L}{300} \right)^{(3xc-1)} \tag{14}$$

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 MoS₂ 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.



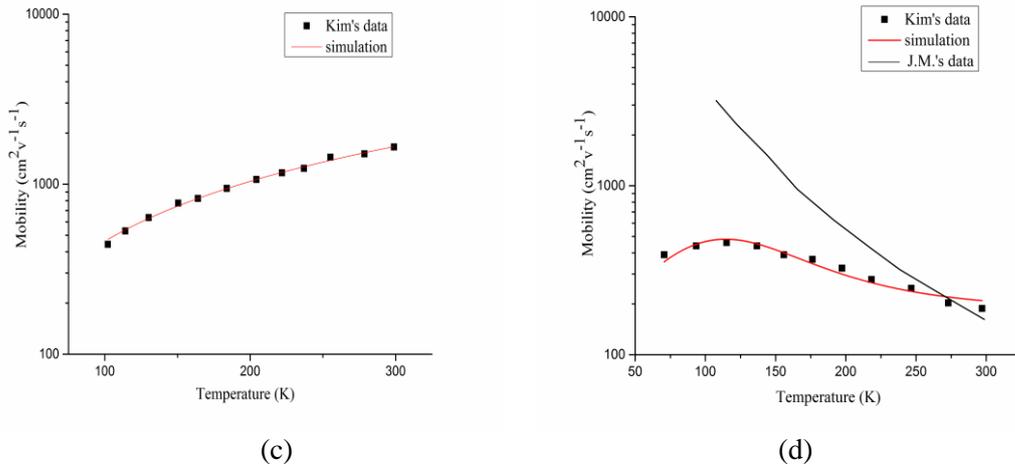


Figure 1 the simulation results of MoS₂ mobility model, (a) acoustic phonon mobility (b) optical intervalley phonons (c) impurity scattering and (d) comparison of the combined mobility.

3.2. Mobility model test

The MSM device adopted Ni electrodes with Hexagon MoS₂/Al₂O₃ 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.

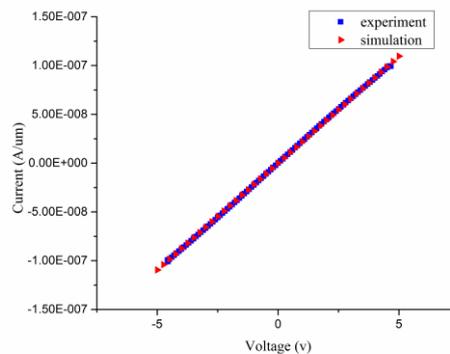


Figure 2. MSM simulation used the mobility model.

4. Summary

Physical models for MoS₂ 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 is can be seen that u_{ac} , u_b and u_{im} is the important part of the MoS₂ mobility. Finally, the MoS₂ 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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Acknowledgments

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