

Simulation of the phonon-limited electron mobility in multi-layer MoS₂ field-effect transistors

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1. Abstract

We study the electron mobility in Metal-Insulator-Semiconductor Field-Effect-Transistors which use multi-layer MoS₂ as channel. The electrostatic behavior is calculated by self-consistently solving the 1D Poisson and Schrödinger equations under the effective mass approximation. Phonon-limited electron mobility is then calculated solving the Boltzmann Transport Equation under the Momentum Relaxation Time approximation for different device sizes and bias conditions.

2. Introduction

The use of 2D materials as an alternative to traditional Si-based technology has driven the attention of the scientific community during the last years. Following the trail of grapheme, transition metal dichalcogenides, and in particular MoS₂, provide interesting properties, including the capability of ultra-thin (up to atomic layer thin) body devices. Some works deal with the modeling of monolayer MoS₂ phonon-limited mobility [1]. However, its behavior for multilayer MoS₂ devices is not so well explored. Kim et al. [2] have examined the mobility of thick MoS₂ FET structures employing bulk expressions for the electron mobility, but such an approach is not accurate for thin inversion layer devices. We analyze here the phonon-limited electron mobility (μ) of MoS₂ FETs considering the confinement quantization, in an approach that can be useful for multilayer MoS₂ devices down to a few atomic layers.

3. Numerical model

The cross-section of the simulated device is depicted in Fig. 1. Wide and long-channel devices are assumed, being therefore their electrostatic behavior properly described using a 1D self-consistent Poisson-Schrödinger solution. The Effective Mass Approximation (EMA) is employed as it has been reported that, for more than 6 atomic layers, the MoS₂ band structure resembles that of bulk MoS₂ [3]. The conduction band is characterized by six equivalent valleys, distributed along the Γ -K symmetry lines (Δ points, see Fig. 1), which are here modeled using an isotropic density-of-states effective mass, different from the confinement effective mass. The values employed are extracted from [4] and summarized in Table 1. As for μ calculation, we include transversal and longitudinal acoustic phonons (TA and LA), longitudinal optical phonons (LO), homopolar phonons (HO) and polar optical phonons due to Frölich interaction (POP). The parameters employed (Table 2)

are extracted from [1], where they are calculated for monolayer MoS₂. The expressions used to model the different phonon scattering probabilities in inversion layers can be found in [5]. Once the scattering rate of each mechanism is calculated, the Momentum Relaxation Time approach is used to solve the linearized Boltzmann Transport Equation.

4. Results

We have first calculated the scattering rate due to each scattering mechanism for two devices with thickness $T_{sc}=10\text{nm}$ and $T_{sc}=2\text{nm}$, respectively (Fig. 2). As can be seen, POP is the main scattering mechanism. This conclusion is consistent with the results presented by Kim et al. for thick devices in [2]. On the other hand, homopolar phonons do not seem to play a very relevant role regardless of the device size. For the smaller device, the influence of acoustic phonons is more noticeable, in particular in the region close to $E_c=0$. Again, this behavior is consistent with the conclusions achieved in [1] for monolayer MoS₂ FETs. Then, we have analyzed the behavior of μ for devices with three different T_{sc} values (2nm, 5nm and 10nm) as a function of the inversion charge (N_i). As shown in Fig. 3, μ remains almost constant in the whole N_i range for the three different semiconductor thicknesses. There is however a strong influence of the MoS₂ thickness on the electron mobility, as a non-monotonic tendency is found. This behavior is analyzed in detail in Fig. 4, where μ is depicted as a function of T_{sc} for $N_i=5\times 10^{12}\text{cm}^{-2}$, and a maximum is observed around $T_{sc}=5\text{nm}$. The mobility associated to each scattering mechanism has also been plotted, showing that POP and LO phonons cause the non-monotonic mobility trend, while acoustic phonons monotonically grow with T_{sc} .

5. Conclusion

This work presents a simulation study of the electron mobility in FETs with a multi-layer MoS₂ channel. The electrostatic behavior is described through the self-consistently solution of the 1D Schrödinger and Poisson equations, under the EMA. The results obtained for the phonon-limited electron mobility depicts an almost independent behavior with the charge density and a non-monotonic behavior with the MoS₂ thickness, having a maximum around 5nm of MoS₂ thickness and decreasing for thinner devices. We would like to highlight that these results are for phonon-limited mobility only, and a different behavior could be found if other scattering mechanisms were considered.

References

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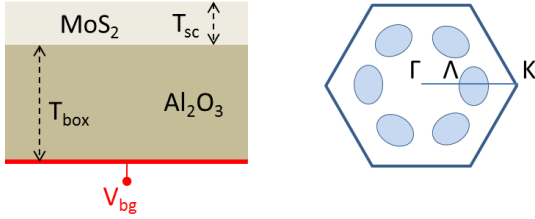


Fig. 1. Geometry of the back-gate MoS₂ FET device (left) and schematic representation of the six degenerated Λ valleys (right).

MoS ₂	
Dielectric constant	$\epsilon_r=7$
Λ valleys degeneration	$d_v=6$
Confinement effective mass	$m^*=0.49m_0$
Density-of-states effective mass	$m_{DOS}=0.62m_0$
Al ₂ O ₃	
Dielectric constant	$\epsilon_r=9$
Potential barrier	$\Delta E_c=2.6eV$
Effective mass	$m^*=0.2 m_0$

Table 1. Simulation parameters for electrostatic calculation. Extracted from [2,4].

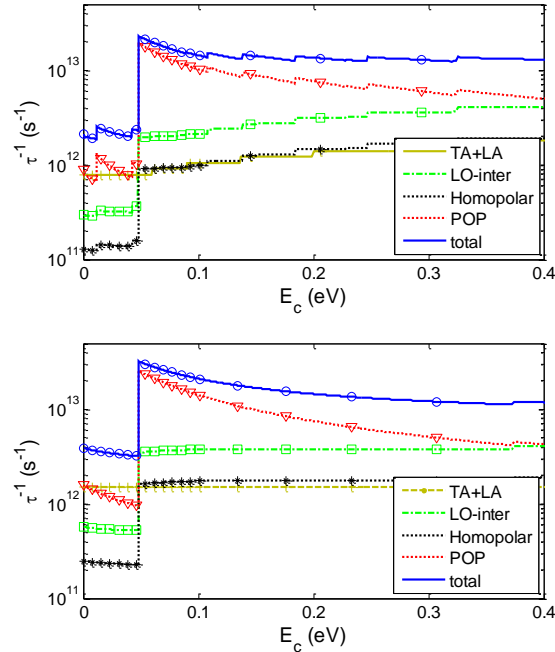


Fig. 2. Inverse momentum relaxation time of the first subband as a function of E_c , for $T_{sc}=10$ nm (top) and 2nm (bottom), and $N_i=5 \times 10^{12} \text{cm}^{-2}$. The contribution of each scattering mechanism is also depicted.

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Parameter	Value
MoS ₂ density	$\rho=7.03 \times 10^{-3} \text{ kg/cm}^3$
LA deformation potential	$D_{LA}=2.8eV$
Longit. sound velocity	$v_l=6.7 \times 10^5 \text{ cm/s}$
TA deformation potential	$D_{TA}=1.6eV$
Transversal sound velocity	$v_t=6.7 \times 10^5 \text{ cm/s}$
HO deformation potential	$D_{HO}=4.1 \times 10^8 \text{ eV/cm}$
HO phonon energy	$E_{HO}=50 \text{ meV}$
LO deformation potential	$D_{LO}=2.6 \times 10^8 \text{ eV/cm}$
LO phonon energy	$E_{LO}=48 \text{ meV}$
LO intervalley degeneration	$d_v=5$
POP phonon energy	$E_{POP}=48 \text{ meV}$
HF dielectric constant	$\epsilon_r=7\epsilon_0$

Table 2. Scattering parameters employed for mobility calculation (after [1]).

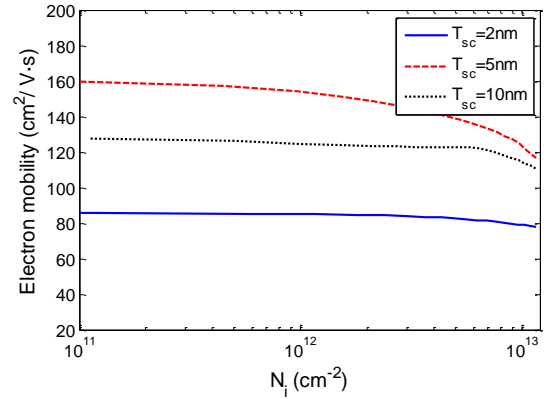


Fig. 3. Phonon-limited electron mobility as a function of the inversion charge, for device thickness $T_{sc}=2$ nm (solid), 5nm (dashed) and 10nm (dotted).

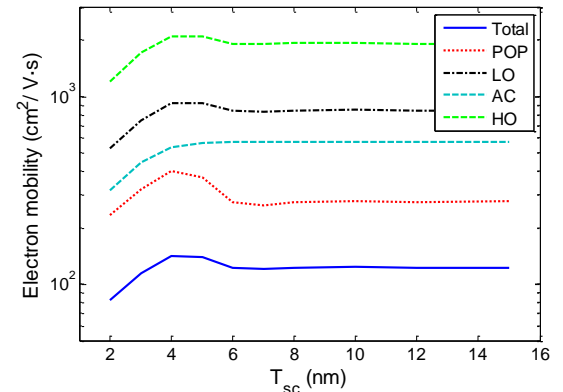


Fig. 4. Phonon-limited electron mobility as a function of the device thickness, for $N_i=5 \times 10^{12} \text{cm}^{-2}$. The mobility associated to each scattering mechanism is also shown.