Simulation of the phonon-limited electron mobility in multi-layer MoS_2 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 MoS_2 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 MoS_2, provide interesting properties, including the capability of ultra-thin (up to atomic layer thin) body devices. Some works deal with the modeling of monolayer MoS_2 phonon-limited mobility [1]. However, its behavior for multilayer MoS_2 devices is not so well explored. Kim et al. [2] have examined the mobility of thick MoS_2 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 MoS_2 FETs considering the confinement quantization, in an approach that can be useful for multilayer MoS_2 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 MoS_2 band structure resembles that of bulk MoS_2 [3]. The conduction band is characterized by six equivalent valleys, distributed along the Γ-K symmetry lines (Λ 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 MoS_2. 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}=10nm and T_{sc}=2nm, 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 MoS_2 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 MoS_2 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 $N_i=5x10^{12}cm^{-2}$, and a maximum is observed around T_{sc}=5nm. 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 MoS_2 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 MoS_2 thickness, having a maximum around 5nm of MoS_2 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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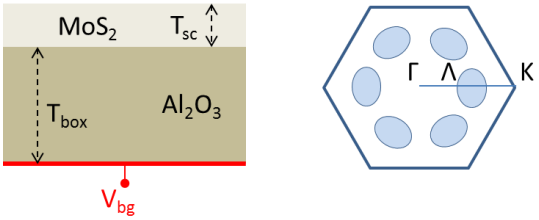

Fig.1. Geometry of the back-gate MoS_2 FET device (left) and schematic representation of the six degenerated Λ valleys (right).

MoS_2	
Dielectric constant	ε_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_2O_3	
Dielectric constant	ε_r=9
Potential barrier	ΔE_c=2.6eV
Effective mass	$m^*=0.2\ m_0$

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

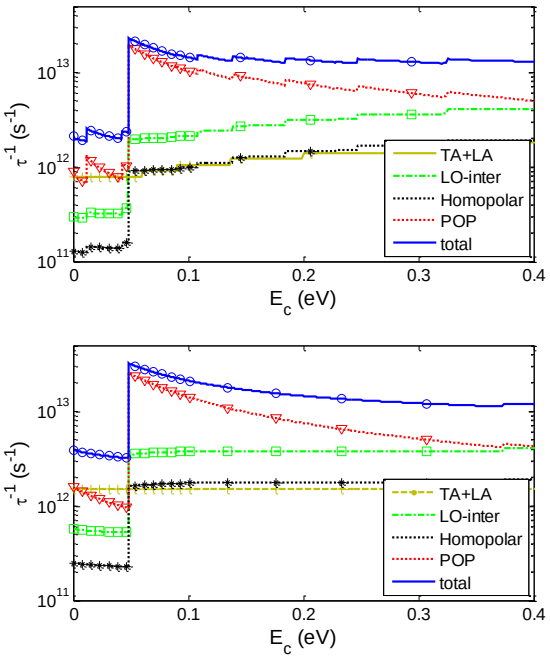

Fig.2. Inverse momentum relaxation time of the first subband as a function of E_c, for T_{sc}=10nm (top) and 2nm (bottom), and N_i=5x10^{12}cm^{-2}. The contribution of each scattering mechanism is also depicted.

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Parameter	**Value**
MoS_2 density	ρ=7.03x10^{-3} kg/cm^3
LA deformation potential	D_{LA}=2.8eV
Longit. sound velocity	v_l=6.7x10^5 cm/s
TA deformation potential	D_{TA}=1.6eV
Transversal sound velocity	v_t=6.7x10^5 cm/s
HO deformation potential	D_{HO}=4.1x10^8 eV/cm
HO phonon energy	E_{HO}=50 meV
LO deformation potential	D_{LO}=2.6x10^8 eV/cm
LO phonon energy	E_{LO}=48 meV
LO intervalley degeneration	d_v=5
POP phonon energy	E_{POP}=48 meV
HF dielectric constant	$\varepsilon_\infty=7\varepsilon_0$

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

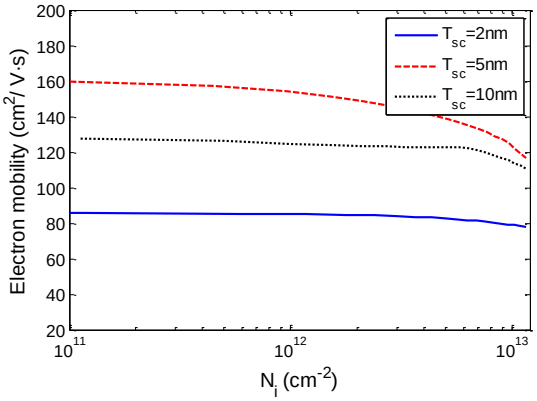

Fig.3. Phonon-limited electron mobility as a function of the inversion charge, for device thickness T_{sc}=2nm (solid), 5nm (dashed) and 10nm (dotted).

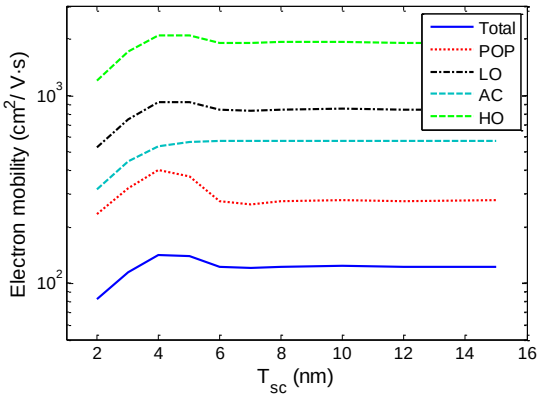

Fig.4. Phonon-limited electron mobility as a function of the device thickness, for N_i=5x10^{12} cm^{-2}. The mobility associated to each scattering mechanism is also shown.