Simulation study of the electron mobility in few-layer MoS$_2$ metal–insulator-semiconductor field-effect transistors

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A B S T R A C T

This work analyzes the electron mobility in few-layer MoS$_2$-based metal–insulator-semiconductor field-effect transistors. To do it, the Poisson and Schrödinger equations are self consistently solved using the effective mass approximation to model the six equivalent Λ valleys characteristic of multilayer MoS$_2$. The mobility is calculated using the Kubo-Greenwood approach under the momentum relaxation time approximation. The influence of the semiconductor thickness, the temperature and the bias conditions are analyzed. A good agreement with the experimental results presented in the literature is achieved, with electron mobilities ranging between 140 and 200 cm^2 V^{-1} s^{-1} at $T = 300$ K.

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1. Introduction

Bidimensional materials have driven the attention of the scientific community for the last years as one of the best alternatives to the traditional Si-based technology. As graphene, transition metal dichalcogenide (TMDC) semiconductors, and in particular MoS$_2$, have interesting properties to design and fabricate ultra-thin body devices. As an example, the band gap of MoS$_2$ can be modified by varying its thickness [1–3] or applying stress [4], to the point of changing its behavior from semiconductor to metal. Interesting optoelectronic properties of MoS$_2$ have also been demonstrated, due to the direct bandgap behavior of monolayer films [3] or the charge variation induced by circular light [5]. The dependence of the gap on the thickness could be useful to make more efficient solar panels [6]. In most of these potential applications, advantage is taken from the variations of the MoS$_2$ properties caused by the transition from multilayer to monolayer thicknesses.

In order to analyze the performance of MoS$_2$-based devices, both electrostatics and transport properties need to be studied. In this scenario, the carrier mobility (μ) has to be calculated, and several phonon-limited mobility models have been developed for monolayer MoS$_2$ films [7–10] and for thick MoS$_2$ field-effect transistor (FET) structures employing bulk expressions [11]. However, there is a lack of studies on the behavior of MoS$_2$ devices with thicknesses in the range of a few nanometers, from 2 nm to

10 nm, which we will denominate *few-layer* MoS$_2$. Here, the phonon-limited electron mobility of such devices is analyzed. The quantum confinement is taken into account under the effective mass approach, the value of which is extracted from *ab initio* simulations [4,12,13]. Then, the Schrödinger and Poisson equations are self-consistently solved in a one dimensional heterostructure, and their results are used to evaluate the mobility using the Kubo-Greenwood technique.

The outline of this paper is as follows. First, in Section 2, we present the numerical model and the simulation parameters we have employed. Next, Section 3 presents the main results obtained from the simulator, including the variation of the electron mobility with the temperature, thickness and gate bias. Finally, Section 4 summarizes the main conclusions of this work.

2. Model

Fig. 1 depicts the studied device, a back-gated metal–insulator-semiconductor transistor with MoS$_2$ as the channel material, with thickness T_{sc} ranging from 2 nm to 10 nm. Al$_2$O$_3$ is considered as the gate insulator, with thickness $T_{ox} = 10$ nm, and Ti is used for the metal gate. The electrostatic analysis is carried out along the confinement direction (y), and the transport is assumed along the x coordinate.

2.1. Numerical solver

In order to analyze the electrostatic behavior of the metal–insulator-semiconductor heterostructure, we have developed a

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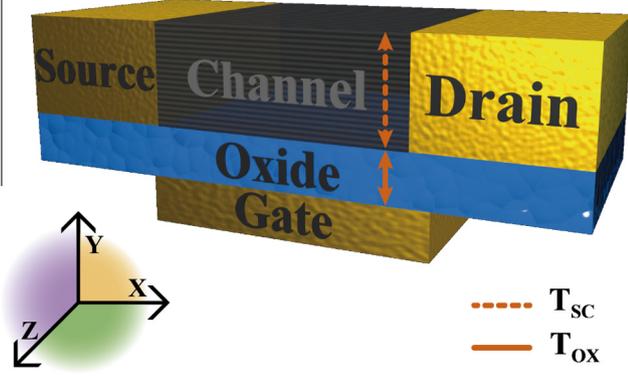*E-mail addresses:* jmgonzalme@correo.ugr.es (J.M. Gonzalez-Medina), franruiz@ugr.es (F.G. Ruiz).

Fig. 1. Back-gated transistor studied in the confinement direction y.

numerical simulator, which solves the one dimensional Schrödinger-Poisson equation system self-consistently, using the finite difference method. The Poisson equation is used to calculate the potential:

$$\frac{\partial}{\partial y}\varepsilon(y)\frac{\partial}{\partial y}\phi(y) = -\rho[\phi(y)], \tag{1}$$

where $\varepsilon(y)$ is the position dependent permitivity, $\phi(y)$ is the electric potential and $\rho[\phi(y)]$ is the charge density. A Dirichlet condition is used for the back-gate, where the gate bias is applied, while a Neumann condition is used for the top channel side, where no contact is considered. The charge density is calculated from the 2D electron gas density of states expression [14] and the wavefunctions and the energy subbands which result from the Schrödinger equation. Here, it is solved using the parabolic Effective Mass Aproximation (EMA) as

$$\left(-\frac{\hbar^2}{2}\frac{\partial}{\partial y}\frac{1}{m^*(y)}\frac{\partial}{\partial y} + V_{\mathrm{h}} - q\phi(y)\right)\xi_i(y) = E_i\xi_i(y), \tag{2}$$

where V_{h} corresponds with the heterostructure potential gap, $m^*(y)$ is the effective mass along the y direction, E_i are the energy levels and $\xi_i(y)$ their corresponding wavefunctions. The Schrödinger equation has to be solved for each considered conduction band valley, and the total charge is evaluated by adding up the contribution of all of them. In order to assure the convergence, the potential is over-relaxed in the self-consistent loop.

Once the electrostatic behavior of the device is calculated, we go on analyzing the electron mobility (μ) in the transport direction. Its value is limited by different scattering mechanisms such as longitudinal and transversal acoustic phonons (LA and TA), longitudinal optical phonons (LO), homopolar phonons (Ho) and polar optical phonons due to Frölich interaction (POP). Each mechanism has an associated scattering rate, which is calculated and applied to the explicit Momentum Relaxation Time (MRT) approach to solve the linearized Boltzmann Transport Equation. Assuming isotropic bands in the unconfined directions, the relation between the mobility of the i-th subband and its MRT, $\tau_i(E)$, is given by [14]

$$\mu_i = \frac{e}{n_i\pi\hbar^2}\int_0^\infty dE\,(E - E_i)\tau_i(E)\left|\frac{\partial f_0(E)}{\partial E}\right|, \tag{3}$$

where E_i and n_i are the energy minimum and the electron density of the i-th subband, and $f_0(E)$ is the Fermi–Dirac distribution function. Then, the total mobility can be evaluated as:

$$\mu = \frac{\sum_i n_i\mu_i}{\sum_i n_i}. \tag{4}$$

The expression for the MRT depends on the phonon scattering process considered. For intravalley isotropic, elastic, phonon scattering processes, such as LA and TA phonons, the MRT can be calculated as:

$$\frac{1}{\tau_i^{\mathrm{ac}}(E)} = \frac{2\pi k_{\mathrm{B}} T D_{\mathrm{ac}}^2}{\rho\hbar v_s^2}\sum_j F_{j,i}\,g_j(E), \tag{5}$$

where the summation runs over the subbands j corresponding to the same valley as the i-th subband. k_{B} denotes the Boltzmann constant, T is the temperature, ρ is the semiconductor volumetric density, v_s corresponds to the sound velocity in the material for a given phonon process, $g_j(E)$ is the density of states of the j-th subband and $F_{j,i}$ is the so-called form factor between the i-th and j-th subbands, calculated as:

$$F_{j,i} = \int\left|\xi_j^*(y)\xi_i(y)\right|^2 dy, \tag{6}$$

Ho, LO and POP phonons are modeled as inelastic processes. For intra-valley Ho phonons, the following expression is used:

$$\frac{1}{\tau_i^{\mathrm{Ho}}(E)} = \frac{\pi D_{\mathrm{Ho}}^2}{\omega_{\mathrm{Ho}}\rho}\sum_j F_{j,i}\left[n_{\mathrm{Ho}} + \frac{1}{2}\mp\frac{1}{2}\right]\left[\frac{1 - f_0(E\pm\hbar\omega_{\mathrm{Ho}})}{1 - f_0(E)}\right]g_j(E\pm\hbar\omega_{\mathrm{Ho}}), \tag{7}$$

where, $\hbar\omega_{\mathrm{Ho}}, n_{\mathrm{Ho}}$ and D_{Ho} are the homopolar phonon energy, number and optical deformation potential, respectively. The phonon number is calculated as:

$$n_{\mathrm{Ho}} = \frac{1}{e^{\frac{\hbar\omega_{\mathrm{Ho}}}{k_{\mathrm{B}}T}} - 1}. \tag{8}$$

A similar expression is used to calculate the LO intervalley MRT, but taking into account the valley degeneracy of the transition, and employing the corresponding values $\hbar\omega_{\mathrm{LO}}, n_{\mathrm{LO}}$ and D_{LO}.

For anisotropic processes, such as POP, a $Q = |\mathbf{k} - \mathbf{k}'|$ dependent expression must be evaluated, which is given by

$$\frac{1}{\tau_i^{\mathrm{POP}}(E)} = U\sum_j m^{\mathrm{tr}}\left[\frac{1 - f_0(E\pm\hbar\omega_0)}{1 - f_0(E)}\right]\int_0^{2\pi} d\theta I_{i,j}(Q)\frac{1}{Q}\left(1 - \frac{|\mathbf{k}'|}{|\mathbf{k}|}\cos(\theta)\right), \tag{9}$$

where m^{tr} is the transport effective mass, which is constant along the integral as we are assuming spherical bands; $I_{i,j}(Q)$ is the form factor, which is calculated as

$$I_{i,j}(Q) = \int dy\,\xi_j^*(y)\xi_i(y)\cdot\left(\int dy'\,\xi_j^*(y')\xi_i(y')e^{-Q|y-y'|}\right), \tag{10}$$

and U is given by

$$U = \frac{q^2\hbar\omega_{\mathrm{POP}}}{8\pi\hbar^3}\left(\frac{1}{\varepsilon(\infty)} - \frac{1}{\varepsilon(0)}\right)\left(n_{\mathrm{POP}} + \frac{1}{2}\pm\frac{1}{2}\right), \tag{11}$$

with $\varepsilon(\infty)$ and $\varepsilon(0)$ the high and low frequency semiconductor dielectric constants, respectively, $\hbar\omega_{\mathrm{POP}}$ the POP energy and n_{POP} the phonon number, which is evaluated as in Eq. (8). The calculation of Eq. (10) is quite time consuming and therefore we have tabulated it, using a lineal interpolation scheme to get the scattering matrix.

Once the MRT for each process is calculated, the total MRT can be determined as

$$\frac{1}{\tau_{i,\mathrm{total}}(E)} = \sum_s\frac{1}{\tau_i^s(E)}, \tag{12}$$

where the superscript s denotes the scattering mechanism. The resulting $\tau_{i,\mathrm{total}}(E)$ value is then used in Eq. (3) to determine the electron mobility of each subband, μ_i.