Numerical Modeling of Photodetectors Made from Two-Dimensional Materials

Ergun Simsek, Raonaqul Islam, and Curtis R. Menyuk
University of Maryland Baltimore County, Baltimore, MD, USA (simsek@umbc.edu)

***Abstract*—A concise numerical model, based on drift-diffusion equations and wave propagation in a multilayered medium, has been developed to investigate photodetectors composed of two-dimensional materials. Comparisons between the numerical results and experiments validate the precision of the proposed approach in calculating the quantum efficiency as a function of incident wavelength. The formulation also enables the calculation of advanced photodetector parameters such as phase noise and bandwidth.**

I. Introduction

Two-dimensional (2D) materials, particularly monolayers and a few layers of transition metal dichalcogenides (TMDs), have recently emerged as promising candidates for diverse optoelectronic applications [1]–[4]. Monolayer MoS_2, for instance, exhibits unique properties, including a direct bandgap transformation upon transitioning from its bulk form, making it advantageous for applications such as transistors and optoelectronics [5], [6]. In contrast to graphene, MoS_2's direct bandgap allows for direct photon absorption and emission, enhancing its suitability for spintronics exploration. Various synthesis methods, such as chemical vapor deposition and liquid exfoliation, enable practical device fabrication [3].

Despite experimental advancements in photodetectors based on 2D materials such as monolayer of MoS_2, there is a notable scarcity of numerical investigations characterizing the performance metrics of these devices; see [7] as an example. In this work, we introduce a compact yet accurate one-dimensional drift-diffusion framework [8] that takes wave propagation in multilayered media account to evaluate single-layer MoS_2 photodetectors, employing precise models to determine material properties [5], [6]. This approach, encompassing low-temperature photocarrier dynamics and layered media analysis, represents a unique contribution to the assessment of 2D material-based photodetectors.

II. Numerical Model

Figure 1 illustrates the design under consideration: a monolayer of MoS_2 is placed on top of a silicon-oxide-coated silicon substrate. The gates on the top function as source and drain contacts. The third contact is formed at the bottom for gating. The device is illuminated from the top, perpendicularly.

To calculate the carrier transport behavior, we solve for the drift-diffusion equations [8] that include the current continuity equations for both electrons and holes and the Poisson's equation, that are given by

$$\frac{\delta(n - N_{\rm D}^{+})}{\delta t} = G_{\rm L} - R(n,p) + \frac{\nabla \cdot \mathbf{J}_{\rm n}}{q}, \tag{1}$$

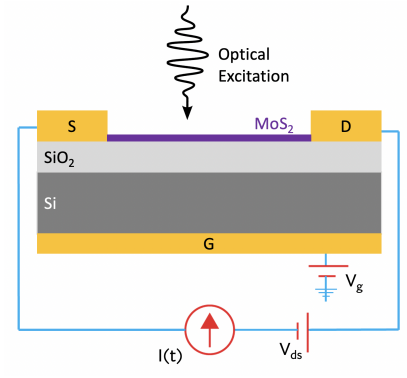

Fig. 1. Schematic illustration of the 2D material-based photodetector.

$$\frac{\delta(p - N_{\rm A}^{-})}{\delta t} = G_{\rm L} - R(n,p) + \frac{\nabla \cdot \mathbf{J}_{\rm p}}{q}, \tag{2}$$

$$\nabla \cdot \mathbf{E} = \frac{q}{\varepsilon}(N_{\rm D}^{+} + p - n - N_{\rm A}^{-}), \tag{3}$$

where, q is the charge of electron, $G_{\rm L}$ is generation rate of the MoS_2 layer, R is the recombination rate, ε is the permittivity of MoS_2, and $N_{\rm D}^{+}$ and $N_{\rm A}^{-}$ are the ionized donor and acceptor impurity concentrations. $\mathbf{J}_{\rm n}$ and $\mathbf{J}_{\rm p}$ are current densities for electrons and holes, which are determined with the drift-diffusion equations:

$$\mathbf{J}_{\rm n} = qn\mathbf{v}_{\rm n}(\mathbf{E}) + qD_{\rm n}\nabla n, \tag{4}$$

$$\mathbf{J}_{\rm p} = qp\mathbf{v}_{\rm p}(\mathbf{E}) - qD_{\rm p}\nabla p, \tag{5}$$

where, $D_{\rm n}$ and $D_{\rm p}$ are the electron and hole's diffusion coefficients, $\mathbf{v}_{\rm n}(\mathbf{E})$ and $\mathbf{v}_{\rm p}(\mathbf{E})$ are electric-field dependent electron and hole drift velocities, respectively.

To calculate the complex electrical permittivity of MoS_2 as a function of wavelength, temperature, and gating, we used the model described in [5]. The bandgap of monolayer MoS_2 is calculated using the Varshni equation, $E_{\rm g}(T) = E_{\rm g}(0) - \alpha T^2/((T+\beta))$ [9], where, $E_{\rm g}(0) = 1.95$ eV, $\alpha = 5.9 \times 10^{-4}$ eV/K, and $\beta = 430$ K considered for our simulations. The other material parameters for monolayer MoS_2 are provided in Table I.

To evaluate the load resistance ($R_{\rm Load}$) of the device, we first calculate the sheet resistance, $R_{\rm sh} = 1/qn\mu(T)$, of the MoS_2 monolayer, then use the obtained value to find $R_{\rm Load} = \sqrt{\rho_i \times R_{\rm sh}}$ assuming $\rho_i = 1/[(T-100)/107]^3$ is the interfacial resistance between the contact and MoS_2, with T being the temperature.

TABLE I
MATERIAL PARAMETERS OF MoS_2 AT $T = 300K$ USED IN OUR SIMULATIONS.

Parameter Name	**Symbol**	**Value**
Energy bandgap at 300 K	E_{g}	1.87 eV
Electron's effective mass	m_{e}^{*}	0.35
Hole's effective mass	m_{h}^{*}	0.50
Electron affinity	χi	4.27 eV
Radiative recombination coefficient	B_{r}	10^{-7} cm^3/s
Auger coefficient	$C_{\mathrm{n}}, C_{\mathrm{p}}$	10^{-24} cm^6/s
Density of states in conduction band	N_{C}	3.76×10^{11} cm^{-2}
Density of states in valence band	N_{V}	5.76×10^{11} cm^{-2}
Hole saturation velocity	$v_{\mathrm{p,sat}}$	4.2×10^{6} cm/s
Electron saturation velocity	$v_{\mathrm{n,sat}}$	1×10^{7} cm/s
Electron lifetime	τ_{n}	1×10^{-9} s
Hole lifetime	τ_{p}	10×10^{-9} s

The density of the induced carriers depends on the thickness and property of the oxide layer in between, i.e., $n_{\mathrm{s}} = \varepsilon_{\mathrm{ox}}(V_{\mathrm{g}} - V_{\mathrm{th}})/t_{\mathrm{ox}}$, where $\varepsilon_{\mathrm{ox}}$ is the permittivity of the oxide layer, t_{ox} is the thickness of the oxide layer, V_{th} is the threshold voltage, and V_{g} is the applied gate voltage.

III. NUMERICAL RESULTS AND CONCLUSION

We assume that the monolayer MoS_2 is 0.65 nm thick and 1 μm wide. The oxide and silicon layers have thicknesses of 270 nm and 2 μm, respectively. To calculate the local electric field inside the MoS_2, we exclude the source and drain contacts, and we treat the bottom (gate) contact as a thin film of perfectly conducting material. Figure 2 shows the output current (I_{ds}) calculated at different drain voltages (V_d) when gate voltage $V_g = 0$.

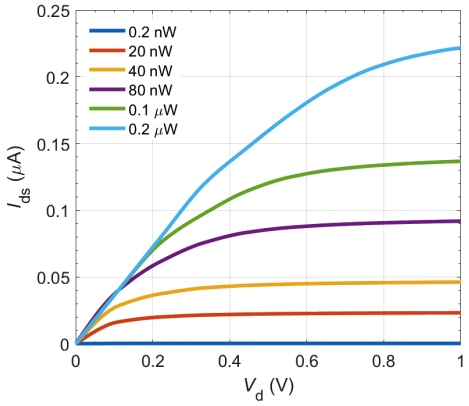

Fig. 2. Output current (I_{ds}) at different drain voltages (V_d) when gate voltage $V_g = 0$.

For quantum efficiency, we assume that the applied voltages are $V_{\mathrm{ds}} = -0.5$ V and $V_{\mathrm{g}} = 10$ V. The results for varying illumination wavelengths is shown in Fig. 3 with the black curve which reaches a peak at approximately 561 nm. This pattern closely mirrors the internal quantum efficiency derived from experimental simulations, denoted by the red circles [2],

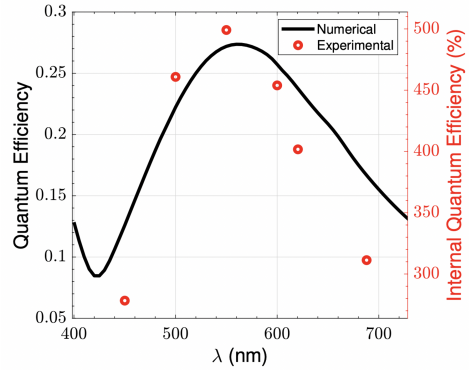

Fig. 3. Numerically obtained total quantum efficiency (left y-axis) and internal quantum efficiency (right y-axis) experimentally obtained [2].

corresponding to the right y-axis. Generally, the quantum efficiency is expected to reflect the absorption characteristics of the monolayer MoS_2. However, the influence of the SiO_2 and Si layers, incorporated through the plane-wave propagation in-layered-media, introduces modifications. This observation not only validates the precision of the drift-diffusion model in characterizing the MoS_2 photodetector but also underscores the importance of including the background in overall calculations.

The computation for each wavelength takes less than two minutes on a desktop computer. A more detailed analysis of the device, such as its bandwidth and how its phase noise changes with modulation frequency, will be discussed at the conference.

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