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Abstract

Theoretical Analysis of Low-Threshold Avalanche Effect in WSe_2 Stepwise van-der-Waals Homojunction Photodiodes †

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Abstract

In this work, we report simulation-assisted analysis of a room-temperature (300 K) low-threshold avalanche photodiode (APD) based on a WSe_2 homojunction. Device simulations were conducted using a two-band model and the Chynoweth formalism for impact ionization, with material parameters extracted for few-layer and multi-layer homojunction WSe_2 structures. The simulated results accurately reproduce experimental dark and photocurrent characteristics, with an avalanche threshold voltage of approximately ~1.6 V-over 26 times lower than that of conventional InGaAs APDs. The structure exhibits ultra-low dark current (10–100 fA) and high sensitivity, enabling detection of optical signals as low as 7.7×10^4 photons. The analyzed low voltage avalanche photodetector enables utilization in a wide range of applications.

Keywords: avalanche photodetector; 2D single-photon avalanche detector; WSe_2 homojunction

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1. Introduction

Avalanche multiplication is an effect in which the carriers gain energy by high-electric field acceleration to produce secondary electron–hole pairs [1]. That mechanism requires the minimum threshold energy (E_t) comparable to the material bandgap (E_g) [1–3] to improve the device performance. Typically, photovoltaic efficiency could overcome the Shockley–Queisser limit, increasing from 34% to 46% [4–6]; however, in practical applications, it is difficult to achieve a threshold energy close to its minimum limit, resulting in low energy conversion efficiency during the carrier multiplication process. Typically, to activate impact ionization, the electric-field energy must be 22 times higher than the bandgap energy [2–7]. This is related to intense electron–phonon (e-p) interactions in typical bulk materials, resulting in significant energy waste during the carrier acceleration process what delays impact ionization mechanism. For bulk InGaAs APD, the room-temperature electron mean free path is approximately 140 nm [8,9], while the multiplication region is usually 1 µm thick [10], which indicates that the carriers exhibit 7× times more chances of scattering during acceleration process in which energy is transferred to the lattice and dissipated by phonon emissions.

In this work, we report on numerical simulations of the room-temperature low-threshold avalanche effect in a WSe_2 homojunction. The avalanche threshold voltage

is significantly reduced to approximately ~1.6 V, which is at least 26 times lower than that of the traditional InGaAs (42 V) avalanche diode [10]. The device architecture demonstrates a low background dark current (10–100 fA) within analyzed voltage [11]. The gain within the range 100–1000 was reached for −2 V depending on the light power conditions.

2. Device Design

The stepwise van-der-Waals (vdW) junction is characterized by the weak e-p interaction, which generates fewer phonons in WSe_2 as the thickness approaches the monolayer limit. This is the most important feature for understanding the intrinsic weak e-p interaction properties of Transition Metal Dichalcogenide (TMD) materials and the enhanced electric field, both of which should benefit the charge carrier avalanche process. In this work, we numerically simulated the stepped WSe_2 avalanche devices. The stepwise n-WSe_2 flake was mechanically exfoliated onto a SiO_2/Si substrate, and the electrical contacts were established by depositing Pt/Au electrodes on both sides. The morphological transition between few-layer and multi-layer WSe_2 is atomically abrupt, with thicknesses of 8 monolayers (ML)/5.6 nm (energy bandgap, E_g ~ 1.6 eV) and 29 ML/20.3 nm (E_g ~ 1.2 eV), respectively [11]. Figure 1 shows a visualization of the device.

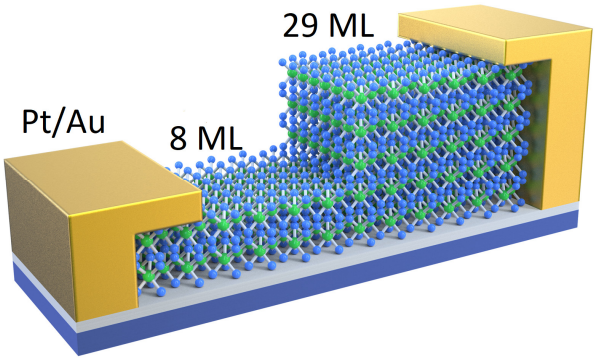

Figure 1. Schematic visualization of the device structure comprising a few-layer (8 ML) and multi-layer (29 ML) with Pt/Au contacts deposited on a SiO_2/Si substrate [11].

3. Simulation Results

All simulations were conducted for the device at a temperature of 300 K, with a fixed series resistance of 50 GΩ (reverse voltage). The material parameters included an electron affinity of 4.21 eV, corresponding to a 29 ML WSe_2 structure (8 ML-3.7 eV), and an assumed carrier concentration of 1×10^{15} cm^{-3}. The WSe_2 ML were assumed to be unintentionally n-type doped. Figure 2 presents the results of numerical fitting for dark current.

The photocurrent in comparison with experimental data for low-threshold APDs based on the 2D WSe_2 material system calculated for illumination at 520 nm with light powers of 2.52 nW, 9.97 nW and 25.78 nW is presented in Figure 3a. The corresponding gain characteristics, derived from the simulation and experimental results, are also shown. The proper fitting to the experimental results was reached. The gain within the range 100–1000 was reached for −2 V depending on the light power conditions. The simulations employed a two-band model implemented in the APSYS device solver. Impact ionization was simulated using Chynoweth's model, with ionization coefficients adapted from the data depicted in Figure 2a. The dynamic resistance as a function of bias voltage is illustrated in Figure 2c and was also implemented to fit to the dark/photocurrent experimental curves.

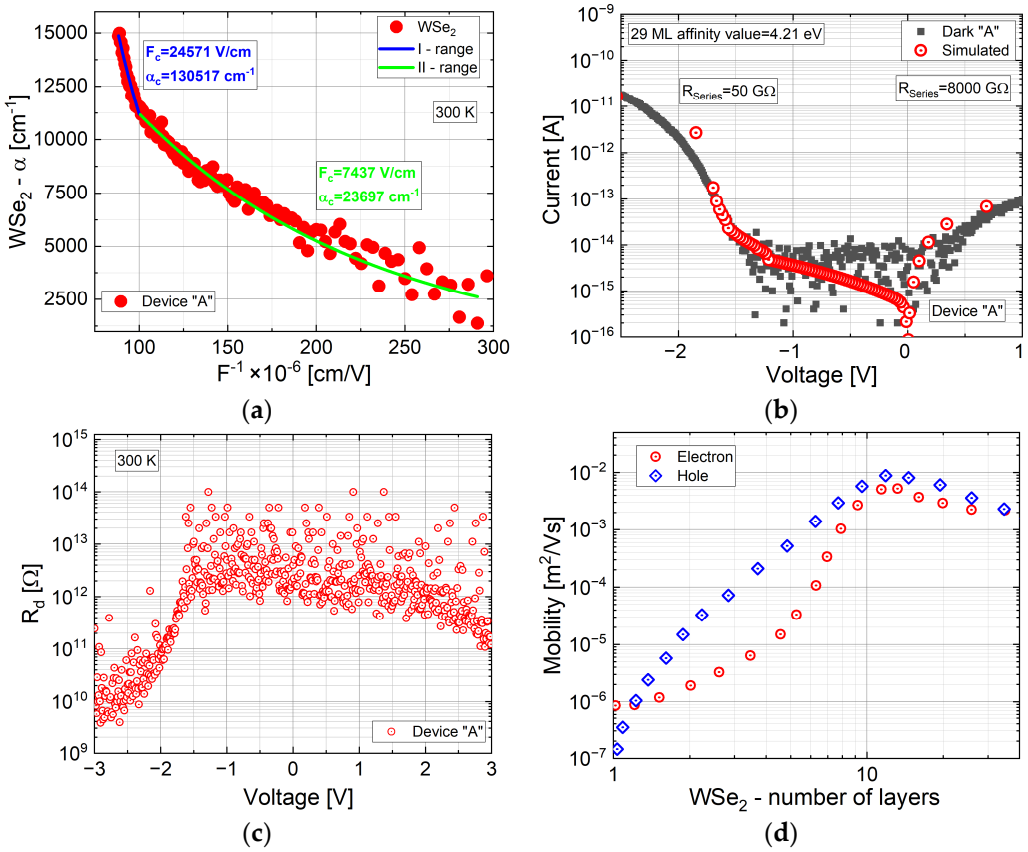

Figure 2. Impact ionization coefficient for the WSe_2 material system (**a**), dark current fitting for a low-threshold WSe_2-based avalanche photodiode (**b**) device resistance versus voltage (**c**), and assumed carrier mobilities versus ML number (**d**).

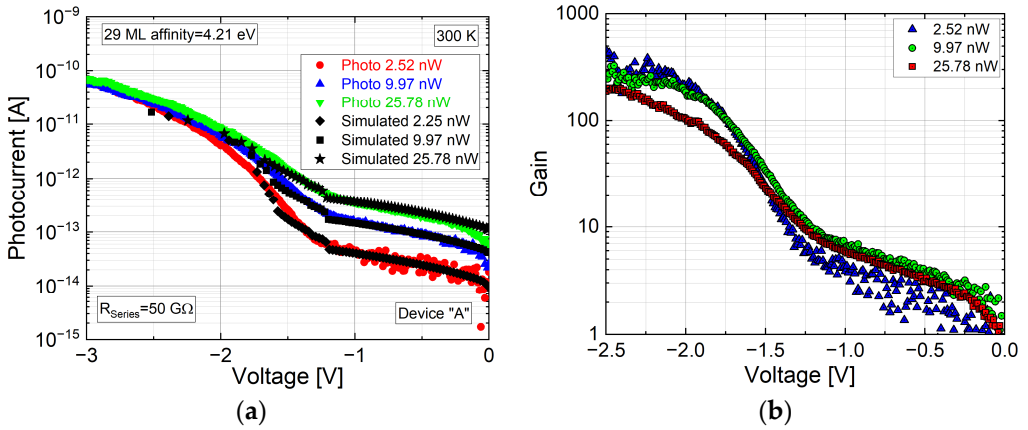

Figure 3. Photocurrent fitting under illumination at 520 nm with optical powers of 2.52 nW, 9.97 nW and 25.78 nW (**a**) and corresponding gain (**b**).

4. Conclusions

The simulation results of the APD with reduced avalanche threshold voltage to the level of ~1.6 V was presented. The proper fitting to the experimental results to include dark and photocurrent was reached. Large series resistance ~50 GW was extracted. The gain within the range 100–1000 was reached for −2 V depending on the light power conditions. The simple two band model proved to be correct to simulate the 2D material based device performance.

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