Effective Heat Dissipation From Plasmon Enhanced Monolayer WSe_2 Phototransistors

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***Abstract*—We numerically demonstrate that monolayer WSe_2 phototransistors exhibit significantly reduced heating when plasmonic nanoparticles are positioned beneath the WSe_2 layer and on top of silicon nanopillars.**

***Index Terms*—2D materials, phototransistors, plasmonic resonance, quantum efficiency, heat dissipation.**

I. Introduction

Over the past two decades, the transition metal dichalcogenide (TMD) monolayers have attracted significant attention for both photonic and optoelectronic applications, such as phototransistors [1], lasers [2], and solar cells [3] due to their remarkable optical and electronic properties [1]–[8]. However, weak absorbance and low quantum yield in TMD monolayers due to their being atomically thin limit the efficiency of TMD-based optoelectronic devices. Many researchers have attempted to remedy this issue by placing metal nanoparticles (MNPs) on top of the TMD monolayers [5]–[8] as shown in Fig. 1(a). MNPs indeed enhance the local electric field via plasmonic resonances and increase the absorption. However, they also lead to a serious temperature rise under strong optical excitation. As a result, the mobility of the electrons decreases and hence the quantum efficiency drops. To mitigate this heating issue while still capitalizing on plasmonic field enhancement, we propose placing the MNPs beneath the WSe_2 layer but atop silicon nanopillars (SNPs), as depicted in Fig. 1(b). The proximity of the metal nanoparticles is expected to offer robust plasmonic enhancement, while the SNPs facilitate efficient heat dissipation from the MNPs to the silicon substrate, thereby preventing overheating.

II. Modeling

To investigate and compare the performances of the conventional and proposed phototransistors, we conduct a series of numerical simulations and calculations as follows. First, heat flow simulations are conducted using Ansys Lumerical's HEAT module to determine the temperature distribution assuming different optical incident powers. Second, we use Ansys Lumerical's FDTD module to calculate the electric field inside the WSe_2 layer by using the temperature distribution obtained in the first step. Third, we solve the drift-diffusion equations that take into account the temperature and electric field distributions that we obtained in the first two steps, and we calculate the quantum efficiency (Q_{eff}) of the device along with other parameters such as phase noise and bandwidth. The material parameters of monolayer WSe_2 are listed in Table I.

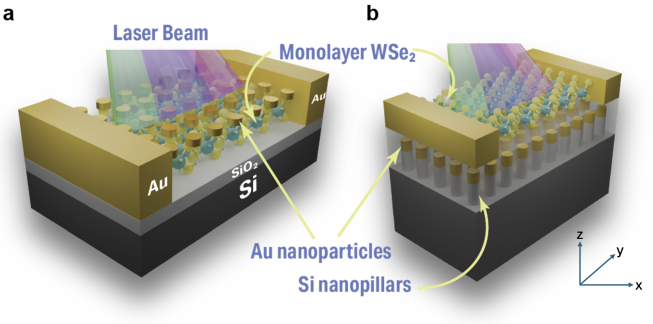

Fig. 1. Schematic illustrations of (a) a conventional plasmon-enhanced WSe_2 phototransistor with MNPs on top and (b) the proposed design with MNPs-SNPs beneath the WSe_2 layer. For both designs, the height and diameter of gold nanoparticles are 65 nm and 75 nm, respectively; the inter-particle spacing is 200 nm along the x- and y-axes; the SiO_2 layer is 270 nm thick. SNPs are 200 nm tall; hence there is a 5 nm gap between the WSe_2 film and MPNs in the proposed design.

TABLE I
Material parameters of WSe_2 at $T = 300K$ used in our simulations. m_0 is the electron mass.

Parameter Name	Symbol	Value
Energy bandgap	E_g	1.65 eV
Electron's effective mass	m_e^*	$0.33m_0$
Hole's effective mass	m_h^*	$0.46m_0$
Electron affinity	χ_i	3.70 eV
Radiative recombination coefficient	B_r	10^{-13} cm^3/s
Electron's Auger coefficient	C_n	5.26×10^{-27} cm^6/s
Hole's Auger coefficient	C_p	6.67×10^{-25} cm^6/s
Density of states in conduction band	N_C	3.08×10^{11} cm^{-2}
Density of states in valence band	N_V	5.08×10^{11} cm^{-2}
Hole saturation velocity	$v_{p,sat}$	6.48×10^5 cm/s
Electron saturation velocity	$v_{n,sat}$	7.65×10^5 cm/s
Electron lifetime	τ_n	40×10^{-9} s
Hole lifetime	τ_p	40×10^{-8} s

III. Numerical Results

For all our numerical results, we assume a broadband optical excitation, i.e. 400 nm $\leq \lambda \leq$ 750 nm, where λ is the wavelength. The device is illuminated from the top normally. The gate and drain-to-soure voltages are set to 10 V and 0.5 V, respectively. Figure 2 summarizes the results of the first step of our numerical investigation. Figure 2(a) shows that when MNPs are positioned on top and in contact with the WSe_2 film, the temperature rises to 420 K for an incident optical power of 25 mW. However, for the same optical excitation,

the temperature does not even reach 330 K for the proposed design, as shown in Fig. 2(b). We plot the maximum temperature ($T_{\max}$) experienced inside the WSe_2 film as a function of incident optical power for WSe_2-coated SiO_2/Si substrates without any MNPs, with MNPs atop, and with MNPs-SNPs underneath. As expected, the conventional design experiences a rapid temperature increase with increasing optical power, while the SNPs in the proposed design dramatically slow down this increase.

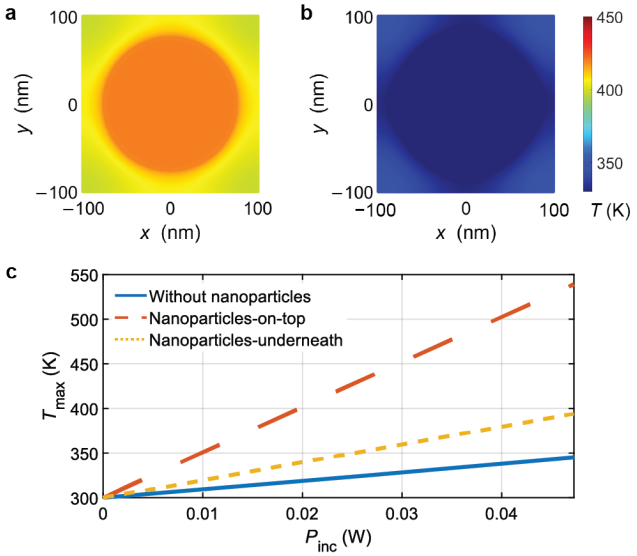

Fig. 2. Temperature profile along the WSe_2 film for the phototransistors with (a) MNPs atop and (b) MNPs-SNPs underneath. (c) Maximum temperature inside the WSe_2 film as a function of incident optical power.

In our electromagnetic simulations, we observe that MNPs cause an average enhancement of 5.5 times in the electric field inside the WSe_2 film compared to the structure without any MNPs. However, for the proposed design, the average field enhancement is 4.5 times.

The proposed design has a smaller temperature rise than the original design, but it also has a slightly lower field enhancement. To calculate the overall effect of these competing mechanisms on the quantum efficiency, we solve the drift-diffusion equations [9] taking into account that several material properties (mobilities, bandgaps, diffusion coefficients, etc.) are functions of the local temperature and electric field that we previously obtained. Figures 3(a) and (b) show how Q_{eff} changes as a function of wavelength for five incident powers ranging from 0.5 mW to 50 mW. Clearly, the conventional design offers a slightly higher Q_{eff} (10% at 610 nm) than the proposed design (9% at 620 nm) at a low incident power. However, when the incident power is increased to 50 mW, the maximum achievable Q_{eff} is 5% for the conventional design, whereas it is 6.6% for the proposed design.

IV. Conclusion

We numerically show that the absorption of the monolayer WSe_2 can be enhanced by strategically positioning metal

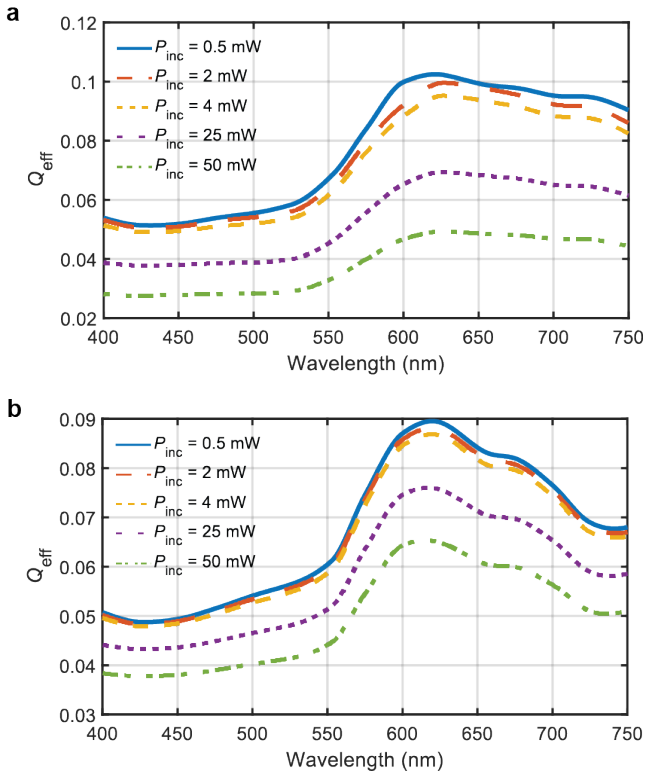

Fig. 3. Calculated Q_{eff} of the phototransistors with (a) MNPs atop and (b) MNPs-SNPs beneath the WSe_2 film as a function of incident wavelength.

nanoparticles beneath the WSe_2 film. The silicon nanopillars supporting the metal nanoparticles provide efficient heat dissipation due to silicon's high thermal conductivity. Under strong optical excitations, the proposed phototransistor exhibits higher quantum efficiency than conventional designs in which nanoparticles are placed on top.

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