

Supporting Information

## **Ultrasensitive Fano Resonance Biosensor Using Two Dimensional Hexagonal Boron Nitride Nanosheets: Theoretical Analysis**

Yongping Li,<sup>a,b</sup> Yufeng Yuan,<sup>a,\*</sup> Xiao Peng,<sup>a,\*</sup> Jun Song,<sup>a</sup> Junxian Liu,<sup>b</sup> and Junle Qu<sup>a</sup>

<sup>a</sup> Key Laboratory of Optoelectronic Devices and Systems of Ministry of Education and Guangdong Province, College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, 518060, People's Republic of China

<sup>b</sup> College of Physical Science and Technology, Guangxi Normal University, Guilin, 541004, People's Republic of China

\*Email: yfyuan@szu.edu.cn, pengxiao\_px@szu.edu.cn

## Determination of Reflectance and Sensitivity

In this study, we proposed a sensitive FR biosensor designed by phase modulation. The differential phase between p-polarized and s-polarized light can be given as,

$$\phi_d = |\phi_p - \phi_s| \quad (1)$$

In addition, the phase ( $\phi_p$ ) of p-polarized light can be obtained as,

$$\phi_p = \arg(r_p) \quad (2)$$

Where  $r_p$  is the reflection coefficient, and it can be determined by Fresnel's equation and Snell's law,

$$r_p = \frac{E_{rp}}{E_{ip}} = \frac{n_t \cos \theta_i - n_i \cos \theta_t}{n_t \cos \theta_i + n_i \cos \theta_t}, n_i \sin \theta_i = n_t \sin \theta_t \quad (3)$$

where  $n_i$  and  $n_t$  are the refractive index of different mediums at the interface.

Next, we employed the transfer matrix method to study the phase and reflectivity changes in our proposed configuration. All the layers are assumed to stack alone in the z-direction, and each layer is considered to be optically isotropic and non-magnetic. The first boundary of tangential electromagnetic fields was set as  $Z = Z_1 = 0$ , and the relation of tangential field between the first boundary and the final boundary  $Z = Z_{N-1}$  can be given as,[1-3]

$$\begin{bmatrix} U_1 \\ V_1 \end{bmatrix} = M \begin{bmatrix} U_{N-1} \\ V_{N-1} \end{bmatrix} \quad (4)$$

where U and V are the tangential components of the electric and magnetic fields respectively.

To calculate the total coefficient  $r_p$ , the matrix M was defined in equation (5), and k denotes the k-th layer in a Nth layered structure.

$$M = \prod_{k=2}^{N-1} M_k = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \quad (5)$$

with

$$M_k = \begin{bmatrix} \cos \beta_k & -i \sin \beta_k / q_k \\ -iq_k \sin \beta_k & \cos \beta_k \end{bmatrix} \quad (6)$$

where

$$q_k = \frac{(\epsilon_k - n_{SF11}^2 \sin^2 \theta_1)^{1/2}}{\epsilon_k} \quad (7)$$

and

$$\beta_k = \frac{2\pi d_k}{\lambda} \left( \varepsilon_k - n_{SF11}^2 \sin^2 \theta_1 \right)^{1/2} \quad (8)$$

Here,  $\theta_1$  is the incident angle in the first layer, and the  $\lambda$  is the incident wavelength.  $d_k$  and  $\varepsilon_k$  are the thickness of the k-th layer and the dielectric constant, respectively.

Then, the total complex reflection coefficient of the N layer for p-polarized light can be described as follows:

$$r_p = \frac{(M_{11} + M_{12}q_N)q_1 - (M_{21} + M_{22}q_N)}{(M_{11} + M_{12}q_N)q_1 + (M_{21} + M_{22}q_N)} \quad (9)$$

where  $q_1$  and  $q_N$  denote the corresponding relations for the first layer (SF11 prism) and N-th layer. Finally, the reflectivity of the p-polarized light at incident angle  $\theta$  can be expressed as:

$$R_p = |r_p|^2 \quad (10)$$

Here, all the above equations are applicable except

$$q_k = \left( \frac{\varepsilon_k}{\mu_k} \right)^{1/2} \cos \theta_k = \left( \varepsilon_k - n_1^2 \sin^2 \theta_1 \right)^{1/2}$$

For our proposed configuration, the intensity sensitivity can be described as,

$$S_I = \frac{\Delta R_p}{\Delta n} \quad (11)$$

where  $\Delta n$  is the variation in refractive index of sensing interface due to the molecular adsorption behavior

Also, the phase sensitivity is defined as:

$$S_p = \frac{\Delta \phi_d}{\Delta n} \quad (12)$$

Similarly, EF of phase detection sensitivity with h-BN-SiO<sub>2</sub>-Ag hybrid structure versus that of the SiO<sub>2</sub>-Ag hybrid structure can be expressed as,

$$EF = \frac{S_{h-BN-SiO_2-Ag}}{S_{SiO_2-Ag}} \quad (13)$$

## References

- [1] Wu L, Chu HS, Koh WS, Li EP. Highly sensitive graphene biosensors based on surface plasmon resonance. Opt Express. 2010;18:14395-400.
- [2] Zeng SW, Sreekanth KV, Shang JZ, Yu T, Chen CK, Yin F, et al. Graphene-Gold Metasurface Architectures for Ultrasensitive Plasmonic Biosensing. Adv Mater. 2015;27:6163-9.
- [3] Zeng S, Hu S, Xia J, Anderson T, Dinh X-Q, Meng X-M, et al. Graphene-MoS<sub>2</sub> hybrid nanostructures enhanced surface

plasmon resonance biosensors. *Sensors and Actuators B: Chemical*. 2015;207:801-10.