Rigorous coupled-wave analysis of absorption enhancement in vertically illuminated silicon photodiodes with photon-trapping hole arrays

Supplementary material

Jun Gou[1,2], Hilal Cansizoglu[1], Cesar Bartolo-Perez[1], Soroush Ghandiparsi[1], Ahmed S. Mayet[1], Hossein Rabiee-Golgir[1], Yang Gao[1], Jun Wang[2], Toshishige Yamada[3,4], Ekaterina Ponizovskaya Devine[3], Aly F. Elrefaie[1,3], Shih-Yuan Wang[3], and M. Saif Islam[1,*]

[1]Electrical and Computer Engineering, University of California - Davis, Davis, CA 95618, USA

[2]State Key Laboratory of Electronic Thin Films and Integrated Devices, University of Electronic Science and Technology of China, Chengdu 610054, China

[3]W&WSens Devices, Inc., 4546 El Camino, Suite 215, Los Altos, CA 94022, USA

[4]Electrical Engineering, Baskin School of Engineering, University of California, Santa Cruz, Santa Cruz, CA 95064, USA

[*]sislam@ucdavis.edu

S1. Formulation of rigorous coupled-wave analysis (RCWA)

Fig. S1 shows a schematic representation of a crossed grating with hole array in hexagonal lattice. In the attached rectangular Cartesian coordinate system, the x and y axes are parallel to periodic directions, and the z axis is perpendicular to the grating plane. The device is divided into three layers along the z direction: the incident layer (I: air, $z < 0$), the grating layer (II: silicon with hole array, $0 \le z \le h$), and the substrate layer (III: Si for bulk wafer or Si on SiO_2 film for the SOI wafer, $z > h$). The propagation direction of the incident plane wave is given by polar angle θ, azimuthal angle φ, and polarization angle ψ.

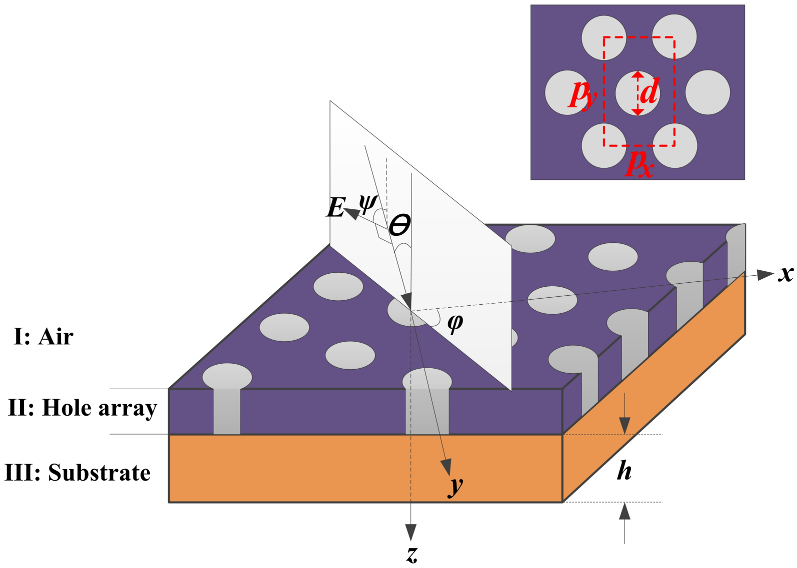

Fig. S1 Periodic hole array in hexagonal lattice illuminated by a plane wave with a rectangular Cartesian coordinate system added for clarity.

The unit electric field of the incident plane wave in layer I is expressed as

$$E_{inc}(x,y,z) = u\exp[-ik_0 n_i(\sin\theta\cos\varphi x + \sin\theta\sin\varphi y + \cos\theta z)] \tag{1}$$

where u is the unit electric-field vector,

$$\begin{aligned} u &= (\cos\psi\cos\theta\cos\varphi - \sin\psi\sin\varphi)e_x \\ &+(\cos\psi\cos\theta\sin\varphi + \sin\psi\cos\varphi)e_y + (-\cos\psi\sin\theta)e_z \end{aligned} \tag{2}$$

where e_x, e_y, and e_z are the unit basis vectors along x, y and z axis, respectively.

The electric fields in layer I and layer III can be written as, respectively,

$$E_{\mathrm{I}}(x,y,z) = E_{inc}(x,y,z) + \sum_m\sum_n R_{mn}\exp[-i(k_{xm}x + k_{yn}y - k_{\mathrm{I},zmn}z)] \tag{3}$$

$$E_{\mathrm{III}}(x,y,z) = \sum_m\sum_n T_{mn}\exp\{-i[k_{xm}x + k_{yn}y + k_{\mathrm{III},zmn}(z-h)]\} \tag{4}$$

where R_{mn} and T_{mn} are the normalized electric field of the [m n] order reflected wave in layer I and transmitted wave in layer III, respectively. The wave vectors k_{xm}, k_{yn}, $k_{\mathrm{I},zmn}$, $k_{\mathrm{III},zmn}$ are, respectively,

$$k_{xm} = k_0 n_i \sin\theta\cos\varphi - \frac{2\pi m}{p_x} \tag{5a}$$

$$k_{yn} = k_0 n_i \sin\theta \sin\varphi - \frac{2\pi n}{p_y} \tag{5b}$$

$$k_{l,zmn} = \begin{cases} \sqrt{k_0^2 n_l^2 - k_{xm}^2 - k_{yn}^2} & k_{xm}^2 + k_{yn}^2 \le k_0^2 n_l^2 \\ -i\sqrt{k_{xm}^2 + k_{yn}^2 - k_0^2 n_l^2} & k_{xm}^2 + k_{yn}^2 > k_0^2 n_l^2 \end{cases} \qquad l = \mathrm{I}, \mathrm{III} \tag{5c}$$

In layer I, $n_{\mathrm{I}}=n_i=n_{air}$, in layer III, $n_{\mathrm{III}}= n_{\mathrm{Si}}$.

The electric field and magnetic field in layer II (grating layer) can be expressed in terms of spatial harmonics by Fourier series expansion, respectively,

$$E_{\mathrm{II}}(x,y,z) = \sum_m \sum_n [S_{xmn}(z)e_x + S_{ymn}(z)e_y + S_{zmn}(z)e_z]\exp[-i(k_{xm}x + k_{yn}y)] \tag{6}$$

$$H_{\mathrm{II}}(x,y,z) = -i\sqrt{\frac{\varepsilon_0}{\mu_0}} \sum_m \sum_n [U_{xmn}(z)e_x + U_{ymn}(z)e_y + U_{zmn}(z)e_z]\exp[-i(k_{xm}x + k_{yn}y)] \tag{7}$$

where $S_{mn(z)}$, $U_{mn(z)}$ are the amplitudes of normalized electric field vector and magnetic field vector of [m n] order spatial harmonic.

The time dependence of exp($i\omega t$) is assumed. In layer II,

$$\nabla \times E_{\mathrm{II}} = -i\omega\mu_0 H_{\mathrm{II}} \tag{8}$$

$$\nabla \times H_{\mathrm{II}} = i\omega\varepsilon(x,y)E_{\mathrm{II}} \tag{9}$$

where $\varepsilon(x,y)$ is the permittivity of the grating layer which is represented by means of Fourier expansion. The electric field can be decomposed into normal component (E_N) and tangential component (E_T). The electric displacement (D) can be written as $D=[\varepsilon(x,y)]E_T+[1/\varepsilon(x,y)]^{-1}E_N$, where the brackets denote the formation of a Toeplitz-matrix out of a vector of Fourier components. At the boundaries (z=0 and $z=h$), E_T is continuous and can be treated with Laurent's rule. E_N is discontinuous, but the normal component of the electric displacement ($D_N=[1/\varepsilon(x,y)]^{-1}E_N$) is continuous and can be treated by the inverse rule [1,2]. Utilizing the boundary conditions of electromagnetic field at z=0 and $z=h$, the quantities $S_{xmn(z)}$, $S_{ymn(z)}$,$U_{xmn(z)}$, $U_{ymn(z)}$ can be obtained by solving the Maxwell curl equations in Cartesian coordinates and represented by the eigenmodes, respectively,

$$S_{xmn}(z) = \sum_j g_j w_{1mn,j} \exp(\lambda_j z) \tag{10}$$

$$S_{ymn}(z) = \sum_j g_j w_{2mn,j} \exp(\lambda_j z) \tag{11}$$

$$U_{xmn}(z) = \sum_j g_j w_{3mn,j} \exp(\lambda_j z) \tag{12}$$

$$U_{ymn}(z) = \sum_j g_j w_{4mn,j} \exp(\lambda_j z) \tag{13}$$

where λ_j and $w_{lmn,j}$ (l=1, 2, 3, 4) are eigenvalues and eigenvectors, g_j are coefficients determined from the boundary conditions. λ_j and $w_{lmn,j}$ can be obtained by solution of matrix eigenvalue problem with a size of $4n\times 4n$ using eig function in Matlab programs [3], where n is the number of spatial harmonics (orders) retained. Then, R_{mn} and T_{mn} can be solved by using the field equations to match the boundary conditions at grating interfaces (z=0 and z=h). Reflection diffraction efficiency (η_{Rmn}) and transmission diffraction efficiency (η_{Tmn}), defined as the power of reflected and transmitted light diffracted into a particular order [m n] to the incident power, can be calculated by, respectively,

$$\eta_{Rmn} = \mathrm{Re}(\frac{k_{\mathrm{I},zmn}}{k_0 n_i \cos\theta})(|R_{xmn}|^2 + |R_{ymn}|^2 + |R_{zmn}|^2) \tag{14}$$

$$\eta_{Tmn} = \mathrm{Re}(\frac{k_{\mathrm{III},zmn}}{k_0 n_i \cos\theta})(|T_{xmn}|^2 + |T_{ymn}|^2 + |T_{zmn}|^2) \tag{15}$$

where the subscripts x, y, and z represent the components of R_{mn} and T_{mn} along the x, y, and z directions, respectively. The absorption can be obtained by,

$$A = 1 - \sum_m \sum_n (\eta_{Rmn} + \eta_{Tmn}) \tag{16}$$

S2. Reflection calculation at Si/SiO$_2$ interface

When a beam of light illuminates from the SOI device layer (p-Si) into SiO_2 film with a refractive index of n_{SiO2}=1.4721 at the wavelength of 850 nm [4], the critical angle of total reflection (θ_c) can be calculated as 23.79° using equation (17).

$$sin\theta_c = \frac{n_{SiO_2}}{n_{Si}} \tag{17}$$

Therefore, the reflection ($R_N^{'}$) of transmitted wave (T_N) in the SOI device layer at Si/SiO$_2$ interface can be calculated by equation (18), depending on the deflection angle (θ_N) of the transmitted wave. In equation (18), $\theta_{RN} = \arcsin(\frac{n_{Si} sin\theta_N}{n_{SiO_2}})$ is the refraction angle of light in SiO$_2$ film. If $\theta_N \geq \theta_c$, all the transmitted waves in the SOI device layer will be reflected by the SiO$_2$ film ($R_N^{'} = 1$).

$$R_N^{'} = \begin{cases} \dfrac{(n_{Si} - n_{SiO_2})^2}{(n_{Si} + n_{SiO_2})^2} & \theta_N = 0 \\ \dfrac{sin^2(\theta_N - \theta_{RN})\left(1 + \dfrac{cos^2(\theta_N + \theta_{RN})}{cos^2(\theta_N - \theta_{RN})}\right)}{2sin^2(\theta_N + \theta_{RN})} & 0 < \theta_N < \theta_c \\ 1 & \theta_N \geq \theta_c \end{cases} \tag{18}$$

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