Supplemental Material

A Second Harmonic-mode Filter For Multiple Physical Quantities Detection Based On 1-D Layered Hyperstructure

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1. Fabrication of layered structures and realisation of the experimental set-up for second harmonic generation and monitoring

The layered structure proposed in this paper is a theoretical design that pursues theoretical effects and focuses less on fabrication. Then, if specific manufacturing is required, it can be done as follows [1]:

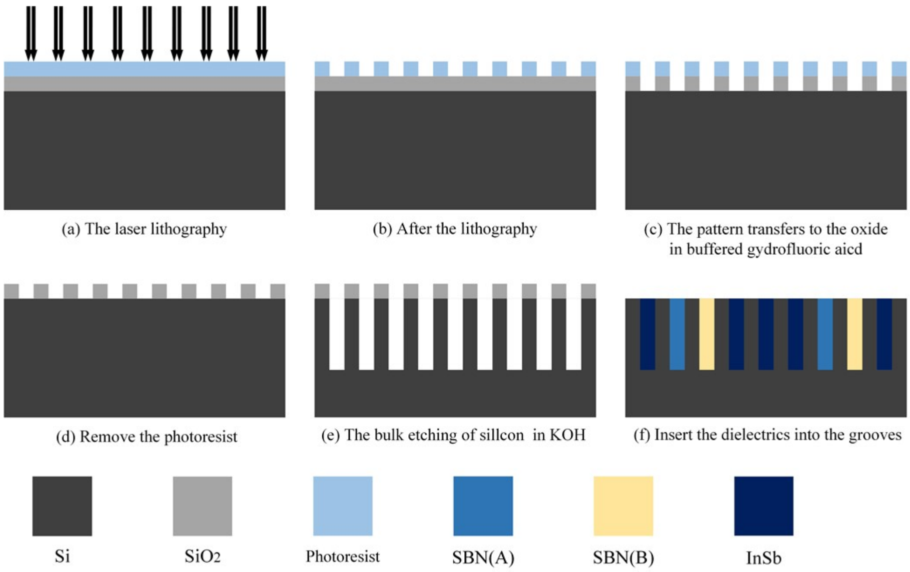

Fig.S1. The diagrams of the fabrication process flow of the proposed layered structure. Specific materials are indicated on the lower side of the process flow.

During the fabrication process, we use the etching method to realize the layered structure. A silicon wafer is selected as the substrate, and then wet anisotropic etching techniques are used to etch vertical grooves of different thicknesses according to the corresponding ratios of the two materials in the proposed structure of the wafer. More specifically, the wet anisotropic etching method can be accomplished by utilizing 44 wt% potassium hydroxide (KOH) aqueous solution at 85 °C, and the thermally grown SiO_2 layer can be used as the hard mask during the process of etching. When there are grooves that conform to the designed conditions of our theoretical research on the silicon substrate, we can add the corresponding material into the corresponding position. From a theoretical point of view, when the height and width of the substrate extend freely, it can be considered an ideal structure, and its characteristics are consistent with our theoretical analysis. The specific fabrication process flow of the proposed layered structure be found in Figs.S1(a)-(f).

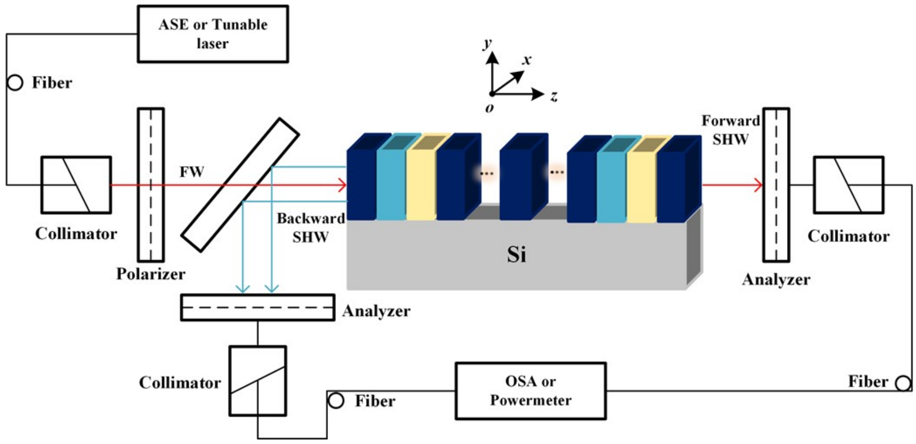

Fig. S2. Experimental setup for the generation and collection of SHW signals [2].

Fig. S2 illustrates the experimental setup for the generation and collection of second harmonic wave (SHW) signals. The SHW signal collection includes both forward and backward signals. The laser, generating a fundamental wave (FW) at frequency ω, is adjusted by a collimator before being directed into the sample, allowing for the optimal coupling of the fundamental wave into the sample. [2] An amplified Ti: sapphire laser (operating in the 0 THz - 150 THz range, reaching a maximum value near 18.5 THz) is chosen for the laser source, known for its high peak power and low single-pulse energy, making it an ideal light source for the second harmonic generation effect. In this study, the laser can be continuously tuned within the range of 17 THz - 20 THz, inducing frequency or amplitude shifts in the SHW signal. The analysis layer serves to filter out excitation light, fluorescence, and potential background light, ensuring the precise collection of SHW signals. Polarizers are employed to selectively filter TE and TM light. The SHW signal, after passing through the analysis layer, is detected using a photomultiplier tube [3]. Finally, signal collection, storage, and analysis are carried out using a computer and a power meter.

2. Detailed derivation of FW amplitude formula

For the SHW, where the intense light interacts with a nonlinear medium, the relationship between P and E is nonlinear and can be expressed as [4]:

$$P = \varepsilon_0 \chi^{(1)} \cdot E + P_{NL}. \tag{S1}$$

where, P is the polarization strength, E is the electric field strength, P_{NL} is the nonlinear component, and ε_0 is the vacuum dielectric constant. Maxwell's equations for anisotropic, nonlinear, nonmagnetic media can be derived by bringing Maxwell's equations and material equations into Eq.(S2a)-(S2c):

$$\nabla \times \boldsymbol{E} = -\mu_0 \frac{\partial \boldsymbol{H}}{\partial t}, \tag{S2a}$$

$$\nabla \times \boldsymbol{H} = \frac{\partial \boldsymbol{D}}{\partial t} + \sigma \boldsymbol{E}, \tag{S2b}$$

$$\boldsymbol{D} = \varepsilon \cdot \boldsymbol{E} + P_{NL}, \tag{S2c}$$

where μ_0 and σ denote the vacuum magnetic and electric conductivity, respectively, and $\varepsilon = \varepsilon_0 [1 + \chi^{(1)}]$. The propagation equation of EW in nonlinear dielectrics is given as follows:

$$\nabla \times \nabla \times \boldsymbol{E} + \mu_0 \sigma \frac{\partial \boldsymbol{E}}{\partial t} + \mu_0 \frac{\partial^2 \varepsilon \cdot \boldsymbol{E}}{\partial t^2} = -\mu_0 \frac{\partial^2 P_{NL}}{\partial t^2}. \tag{S3}$$

The nonlinear fluctuation Eq.(S3) is then simplified using $n = (\varepsilon/\varepsilon_0)^{1/2}$ to obtain Eq. (S11):

$$\nabla^2 \boldsymbol{E} - \frac{n^2}{c^2} \frac{\partial^2}{\partial t^2} \boldsymbol{E} = \mu_0 \frac{\partial^2}{\partial t^2} P_{NL}. \tag{S4}$$

Therefore, the corresponding nonlinear fluctuation equations in the fundamental and SHW forms can be written as:

$$\nabla^2 (E^{(f)}) - \frac{\varepsilon^{(f)}}{\varepsilon_0 c^2} E^{(f)} = \mu_0 \frac{\partial^2}{\partial t^2} P_{NL}^{f}, \tag{S5a}$$

$$\nabla^2 (E^{(s)}) - \frac{\varepsilon^{(s)}}{\varepsilon_0 c^2} E^{(s)} = \mu_0 \frac{\partial^2}{\partial t^2} P_{NL}^{s}, \tag{S5b}$$

where $\varepsilon^{(f,s)}$ and $P_{NL}^{(f,s)}$ denote the dielectric constant and nonlinear polarizability for FW and SHW, respectively. Next, the transmission matrices for the FW and SHW are derived using the transfer matrix method. In each homogeneous medium, the amplitude of the FW can be expressed as Eq.(S6):

$$E_\lambda^{(f)}(z) = E_\lambda^{(f)+} e^{i[k_{z\xi}(f)(z - z_{\lambda-1}) - \omega t]} + E_\lambda^{(f)-} e^{-i[k_{z\xi}(f)(z - z_{\lambda-1}) - \omega t]}, \tag{S6}$$

where $E_\lambda^{(f)+}$and $E_\lambda^{(f)-}$ represent the amplitude of the compound electric field in the positive and negative FW, respectively. $z_0 = 0$, $z_\lambda = z_{\lambda+1} - d_\lambda$, $k_{z\xi}^{(f)}$represents the component of the FW wavevector propagating along the z-direction within the medium. And $k_{z\xi}^{(f)} = n_\xi^{(f)} k_f \cos(X_\xi^{(f)})$, $X_\xi^{(f)} = \arcsin(n_0 \sin\theta / n_\xi^{(f)})$, $k_f = \omega/c$, ($\xi = a, b, p, 0$). c is the magnitude of the propagation speed of EWs in a vacuum.

3. Detailed derivation of FW transfer matrix

In any layer, the magnetic field consists of the combination of transmission and reflection waves, and it can be represented using Eq.(S7) [5]:

$$H(x,z) = H_0^+ e^{i(k_x x + k_{z\xi} z)} + H_0^- e^{i(k_x x - k_{z\xi} z)} = H^+ + H^-, \tag{S7}$$

where $k_{x\xi}^{(f)}$ represents the component of the FW wavevector propagating along the x-axis within the ξ-layer. It remains unchanged during the transmission in the layered structure. Furthermore, the relationship between $k_{x\xi}^{(f)}$ and $k_{z\xi}^{(f)}$ can be represented using Eq.(S8):

$$k_{x\xi}^2 = \frac{\omega^2}{c^2} \frac{\varepsilon_x^2 - \varepsilon_{xz}^2}{\varepsilon_x} - k_{z\xi}^2. \tag{S8}$$

According to Maxwell's curl equation for the magnetic field, Eq.(S9) can be derived:

$$\frac{\partial}{\partial z}H_y = i\omega\varepsilon_x\varepsilon_0 E_x + \omega\varepsilon_0\varepsilon_x E_z. \tag{S9}$$

Therefore, by combining Eq.(S7) and Eq.(S9), the expression for the tangential component of the electric field can be calculated as follows:

$$E_x(x,z) = \left(\frac{ik_x\varepsilon_{xz}}{\varepsilon_0\varepsilon_x\varepsilon_{TM}} + \frac{k_z}{\varepsilon_0\varepsilon_{TM}}\right)H_y^+ + \left(\frac{ik_x\varepsilon_{xz}}{\varepsilon_0\varepsilon_x\varepsilon_{TM}} - \frac{k_z}{\varepsilon_0\varepsilon_{TM}}\right)H_y^-. \tag{S10}$$

To simplify, define:

$$N_\xi^{(f,s)} = \frac{k_{z\xi}^{(f,s)}}{n_\xi^{(f,s)2}}, \tag{S11a}$$

$$M_\xi^{(f,s)} = -\frac{ik_{x\xi}^{(f,s)}\varepsilon_{xz}}{n_\xi^{(f,s)2}\varepsilon_x}. \tag{S11b}$$

From the boundary continuity conditions of the electromagnetic field in consecutive layers (i and j), obtain:

$$\begin{bmatrix} H_j^+ \\ H_j^- \end{bmatrix} = \boldsymbol{T}_j^{-1}\boldsymbol{T}_i \begin{bmatrix} H_i^+ \\ H_i^- \end{bmatrix}, \tag{S12}$$

where

$$\begin{aligned} \boldsymbol{T}_j^{-1}\boldsymbol{T}_i &= \frac{1}{2N_j}\begin{bmatrix} N_j - M_j + (N_i + M_i) & N_j - M_j - (N_i - M_i) \\ N_j + M_j - (N_i + M_i) & N_j + M_j + (N_i - M_i) \end{bmatrix} \\ &= \begin{pmatrix} \frac{N_i - M_i}{2N_i} & \frac{1}{2N_i} \\ \frac{N_i + M_i}{2N_i} & -\frac{1}{2N_i} \end{pmatrix}\begin{pmatrix} 1 & 1 \\ M_j + N_j & M_j - N_j \end{pmatrix}. \end{aligned} \tag{S13}$$

To simplify the equations, set:

$$\boldsymbol{D}_\xi = \begin{pmatrix} 1 & 1 \\ M_\xi^{(f)} + N_\xi^{(f)} & M_\xi^{(f)} - N_\xi^{(f)} \end{pmatrix}. \tag{S14}$$

For ordinary media, as they are not influenced by the magnetic field, $M_\xi^{(f)} = 0$. Additionally, the phase change of the transmitted and reflected waves within the ξ-layer can be expressed as follows :

$$\boldsymbol{P}_\xi = \begin{pmatrix} e^{ik_\xi^{(f)}d_\xi} & 0 \\ 0 & e^{-ik_\xi^{(f)}d_\xi} \end{pmatrix}. \tag{S15}$$

The transmission matrix for the FW of this proposed LHS can be represented using Eq.(S16):

$$\begin{aligned} \boldsymbol{T} = \boldsymbol{D}_0^{-1}(\mathbf{D}_p\mathbf{P}_p\mathbf{D}_p^{-1}\mathbf{D}_b\mathbf{P}_b\mathbf{D}_b^{-1}\mathbf{D}_a\mathbf{P}_a\mathbf{D}_a^{-1}\mathbf{D}_p\mathbf{P}_p\mathbf{D}_p^{-1})^N \\ \mathbf{D}_p\mathbf{P}_p\mathbf{D}_p^{-1}(\mathbf{D}_p\mathbf{P}_p\mathbf{D}_p^{-1}\mathbf{D}_b\mathbf{P}_b\mathbf{D}_b^{-1}\mathbf{D}_a\mathbf{P}_a\mathbf{D}_a^{-1}\mathbf{D}_p\mathbf{P}_p\mathbf{D}_p^{-1})^N\boldsymbol{D}_0. \end{aligned} \tag{S16}$$

So, the changes to the field of FW in this structure along z-axis can be expressed by Eq. (S17):

$$\begin{pmatrix} E_\lambda^{(f)+} \\ E_\lambda^{(f)-} \end{pmatrix} = \boldsymbol{T}^{(f)}\begin{pmatrix} E_0^{(f)+} \\ E_0^{(f)-} \end{pmatrix}. \tag{S17}$$

4. Solution of SHW Output Amplitude

According to Maxwell's equations, the electric and magnetic fields in each layer within nonlinear structures are represented using the following equations [6]:

$$\begin{pmatrix} E_\lambda^{(s)}(z) \\ H_\lambda^{(s)}(z) \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ N_\xi^{(s)} & -N_\xi^{(s)} \end{pmatrix} \begin{pmatrix} E_\lambda^{(s)+}(z) \\ E_\lambda^{(s)-}(z) \end{pmatrix} + \begin{pmatrix} 1 & 1 \\ \dfrac{2N_\xi^{(f)}k_f}{k_s} & -\dfrac{2N_\xi^{(f)}k_f}{k_s} \end{pmatrix} \begin{pmatrix} A_\xi (E_\lambda^{(f)+})^2(z) \\ A_\xi (E_\lambda^{(f)-})^2(z) \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \end{pmatrix} C_\xi E_\lambda^{(f)+} E_\lambda^{(f)-}, \tag{S18}$$

where $E_\lambda^{(s)+}$and $E_\lambda^{(s)-}$ represent the amplitude of the compound electric field in the positive and negative SHW, respectively. $k_{z\xi}^{(s)}$ represents the component of the SHW wavevector propagating along the +*z*-direction and -*z*-direction within the medium. And $k_{z\xi}^{(s)} = n_\xi^{(s)} k_s \cos X_\xi^{(s)}$, $X_\xi^{(s)} = \arcsin(n_0 \sin\theta / n_\xi^{(s)})$, $k_s = 2\omega/c$, ($\xi = a, b, p, 0$). Furthermore, the variables A_ξ and C_ξ in the equations can be expressed as:

$$A_\xi = \frac{-4\mu\varepsilon_0 \chi_\xi^{(2)} \omega^2}{k_\xi^{(s)2} - 4k_\xi^{(f)2}}, \tag{S19a}$$

$$C_\xi = \frac{-4\mu\varepsilon_0 \chi_\xi^{(2)} \omega^2}{k_\xi^{(s)2}}. \tag{S19b}$$

The first part of Eq.(S18) represents the free wave amplitude of the SHW field, the second part represents the constrained wave amplitude of the SHW field, and the third part represents the interference of the FW at the frequency of forward and backward with the SHW. For convenience, several matrices are defined as follows:

$$\boldsymbol{G}_\xi = \begin{pmatrix} 1 & 1 \\ M_\xi^{(s)} + N_\xi^{(s)} & M_\xi^{(s)} - N_\xi^{(s)} \end{pmatrix}, \quad \boldsymbol{B}_\xi = \begin{pmatrix} 1 & 1 \\ \dfrac{2N_\xi^{(f)}k_f}{k_s} & -\dfrac{2N_\xi^{(f)}k_f}{k_s} \end{pmatrix},$$

$$\boldsymbol{Q}_\xi = \begin{pmatrix} e^{ik_\xi^{(s)}d_\xi} & 0 \\ 0 & e^{-ik_\xi^{(s)}d_\xi} \end{pmatrix}, \quad \boldsymbol{F}_\xi = \begin{pmatrix} e^{i2k_\xi^{(f)}d_\xi} & 0 \\ 0 & e^{-i2k_\xi^{(f)}d_\xi} \end{pmatrix},$$

where the range of ξ is defined as $\xi = a, b, p, 0$. Considering the periodicity of the structure, the transfer matrix for the entire one-dimensional LHS containing *N* cells can be obtained through recursion, where *N* is the period of LHS. Using Eq.(S20), the reflected SHW field can be obtained by right-sided incidence and left-sided reflection:

$$\begin{pmatrix} E_t^{(s)+}(z) \\ 0 \end{pmatrix} = \boldsymbol{T}^{(s)} \begin{pmatrix} 0 \\ E_0^{(s)-} \end{pmatrix} + (\boldsymbol{GG}_1 + \boldsymbol{GG}_2 + \boldsymbol{GG}_3) \tag{S20a}$$

$$GG_1=\sum_{s=1}^{N}G_0^{(-1)}S^{N-s}$$
$$\left[(N_3B_pF_p-SB_p)\begin{pmatrix}A_p(E_{4s-3}^{(f)+})^2\\A_p(E_{4s-3}^{(f)-})^2\end{pmatrix}+(N_3-S)\begin{pmatrix}C_p\\0\end{pmatrix}E_{4s-3}^{(f)+}E_{4s-3}^{(f)-}\right.$$
$$+(N_2B_aF_a-N_3B_a)\begin{pmatrix}A_a(E_{4s-2}^{(f)+})^2\\A_a(E_{4s-2}^{(f)-})^2\end{pmatrix}+(N_2-N_3)\begin{pmatrix}C_a\\0\end{pmatrix}E_{4s-2}^{(f)+}E_{4s-2}^{(f)-}$$
$$+(N_1B_bF_b-N_2B_b)\begin{pmatrix}A_b(E_{4s-1}^{(f)+})^2\\A_b(E_{4s-1}^{(f)-})^2\end{pmatrix}+(N_1-N_2)\begin{pmatrix}C_b\\0\end{pmatrix}E_{4s-1}^{(f)+}E_{4s-1}^{(f)-}$$
$$\left.+(B_pF_p-N_1B_p)\begin{pmatrix}A_p(E_{4s}^{(f)+})^2\\A_p(E_{4s}^{(f)-})^2\end{pmatrix}+(1-N_2)\begin{pmatrix}C_p\\0\end{pmatrix}E_{4s}^{(f)+}E_{4s}^{(f)-}\right] \tag{S20b}$$

$$GG_2=G_0^{(-1)}S^N\left[(B_pF_p-G_\mathrm{p}Q_\mathrm{p}G_\mathrm{p}^{(-1)}B_p)\begin{pmatrix}A_p(E_{4N+1}^{(f)+})^2\\A_p(E_{4N+1}^{(f)-})^2\end{pmatrix}\right.$$
$$\left.+(1-G_\mathrm{p}Q_\mathrm{p}G_\mathrm{p}^{(-1)})\begin{pmatrix}C_p\\0\end{pmatrix}E_{4N+1}^{(f)+}E_{4N+1}^{(f)-}\right] \tag{S20c}$$

$$GG_3=\sum_{s=1}^{N}G_0^{(-1)}S^NG_\mathrm{p}Q_\mathrm{p}G_\mathrm{p}^{(-1)}S^{N-s}$$
$$\left[(N_3B_pF_p-SB_p)\begin{pmatrix}A_p(E_{4N+4s-2}^{(f)+})^2\\A_p(E_{4N+4s-2}^{(f)-})^2\end{pmatrix}+(N_3-S)\begin{pmatrix}C_p\\0\end{pmatrix}E_{4N+4s-2}^{(f)+}E_{4N+4s-2}^{(f)-}\right.$$
$$+(N_2B_aF_a-N_3B_a)\begin{pmatrix}A_a(E_{4N+4s-1}^{(f)+})^2\\A_a(E_{4N+4s-1}^{(f)-})^2\end{pmatrix}+(N_2-N_3)\begin{pmatrix}C_a\\0\end{pmatrix}E_{4N+4s-1}^{(f)+}E_{4N+4s-1}^{(f)-}$$
$$+(N_1B_bF_b-N_2B_b)\begin{pmatrix}A_b(E_{4N+4s}^{(f)+})^2\\A_b(E_{4N+4s}^{(f)-})^2\end{pmatrix}+(N_1-N_2)\begin{pmatrix}C_b\\0\end{pmatrix}E_{4N+4s}^{(f)+}E_{4N+4s}^{(f)-}$$
$$\left.+(B_pF_p-N_1B_p)\begin{pmatrix}A_p(E_{4N+4s+1}^{(f)+})^2\\A_p(E_{4N+4s+1}^{(f)-})^2\end{pmatrix}+(1-N_2)\begin{pmatrix}C_p\\0\end{pmatrix}E_{4N+4s+1}^{(f)+}E_{4N+4s+1}^{(f)-}\right] \tag{S20c}$$

Where:

$$S=G_\mathrm{p}Q_\mathrm{p}G_\mathrm{p}^{(-1)}G_bQ_bG_b^{(-1)}G_\mathrm{a}Q_\mathrm{a}G_\mathrm{a}^{(-1)}G_\mathrm{p}Q_\mathrm{p}G_\mathrm{p}^{(-1)}, \tag{S21a}$$

$$N_3=G_\mathrm{p}Q_\mathrm{p}G_\mathrm{p}^{(-1)}G_bQ_bG_b^{(-1)}G_\mathrm{a}Q_\mathrm{a}G_\mathrm{a}^{(-1)}, \tag{S21b}$$

$$N_2=G_\mathrm{p}Q_\mathrm{p}G_\mathrm{p}^{(-1)}G_bQ_bG_b^{(-1)}, \tag{S21c}$$

$$N_1=G_\mathrm{p}Q_\mathrm{p}G_\mathrm{p}^{(-1)}. \tag{S21d}$$

where $\boldsymbol{T}^{(s)}=\boldsymbol{G}_0^{-1}(\boldsymbol{S})^N\boldsymbol{N}_1(\boldsymbol{S})^N\boldsymbol{G}_0$. Based on Eq.(S20), $E_0^{(s)-}$ (the SHW field reflected from the -z-axis) and $E_\mathrm{t}^{(s)+}$ (the SHW field transmitted from the +z-axis) can be calculated. The SHW field distribution within this LHS can also be obtained in the same way.

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