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Cavity-enhanced second-harmonic generation via nonlinear-overlap optimization: supplementary material

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This document provides supplementary information to "Cavity-enhanced second-harmonic generation via nonlinear-overlap optimization," http://dx.doi.org/10.1364/optica.3.000233. We review the temporal-coupled mode equations describing second harmonic generation in doubly resonant cavities and motivate the dimensionless nonlinear coupling $\bar{\beta}$ described in Eq. 3 of the main text. We provide further details on the topology optimization formulation for second harmonic gen-eration and describe generalizations to other nonlinear processes. Finally, we present more detailed descriptions of the optimized micropost and gratings cavities.

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1. COUPLED-MODE THEORY FOR SECOND HARMONIC GENERATION

The temporal coupled mode equations describing second harmonic generation (SHG) in a doubly-resonant cavity coupled to a channel are [1]:

$$\frac{da_1}{dt} = i\omega_1\left(1+\frac{i}{2Q_1}\right)a_1 - i\omega_1\beta_1 a_1^* a_2 + \sqrt{\omega_1\left(\frac{1}{Q_1}-\frac{1}{Q_1^{\text{rad}}}\right)}s_{1+}, \quad \textbf{(S1)}$$

$$\frac{da_2}{dt} = i\omega_2\left(1+\frac{i}{2Q_2}\right)a_1 - i\omega_2\beta_2 a_1^2, \quad \textbf{(S2)}$$

$$s_{1-} = \sqrt{\omega_1\left(\frac{1}{Q_1}-\frac{1}{Q_1^{\text{rad}}}\right)}a_1 - s_{1+}, \quad \textbf{(S3)}$$

$$s_{2-} = \sqrt{\omega_2\left(\frac{1}{Q_2}-\frac{1}{Q_2^{\text{rad}}}\right)}a_2 \quad \textbf{(S4)}$$

such that $|a_k|^2$ is the modal energy in the cavity and $|s_{k\pm}|^2$ is the input/output power in the waveguide, and where Q_k and Q_k^{rad} denote the total and radiative quality factors corresponding to mode k. The nonlinear coupling coefficient β_1, obtained from perturbation theory [1], is given by:

$$\beta_1 = \frac{1}{4}\frac{\int d\mathbf{r}\,\epsilon_0\sum_{ijk}\chi_{ijk}^{(2)}(\mathbf{r})\left(E_{1i}^* E_{2j} E_{1k}^* + E_{1i}^* E_{1j}^* E_{2k}\right)}{\left(\int d\mathbf{r}\,\epsilon_0\epsilon_1(\mathbf{r})|\mathbf{E}_1|^2\right)\left(\sqrt{\int d\mathbf{r}\,\epsilon_0\epsilon_2(\mathbf{r})|\mathbf{E}_2|^2}\right)}.$$

with $\beta_2 = \beta_1^*/2$ far off from material resonances where Kleinman symmetry is valid [2], as required by conservation of energy [1]. In general, the overlap integral in the numerator is a sum of products between different E-field polarizations weighted by off-diagonal components of the nonlinear $\chi^{(2)}$ tensor. For simplicity, however, in the main text we only consider the simple case of diagonal $\chi^{(2)}$ involving same–polarization interactions described by an effective $\chi^{(2)}_{\text{eff}}$, resulting from an appropriate orientation of the crystal axes of the nonlinear material. All of these considerations suggest a simple dimensionless normalization of β, given by:

$$\bar{\beta} = \frac{\int d\mathbf{r}\,\bar{\epsilon}(\mathbf{r})E_2^* E_1^2}{\left(\int d\mathbf{r}\,\epsilon_1|\mathbf{E}_1|^2\right)\left(\sqrt{\int d\mathbf{r}\,\epsilon_2|\mathbf{E}_2|^2}\right)}\sqrt{\lambda_1^3}, \quad \textbf{(S5)}$$

such that $\beta_2 = 4\bar{\beta}\chi^{(2)}_{\text{eff}}/\sqrt{\epsilon_0\lambda_1^3}$. As defined in the text, $\bar{\epsilon}(\mathbf{r}) = 1$ for nonlinear dielectric and $\bar{\epsilon}(\mathbf{r}) = 0$ for the surrounding linear medium.

Most SHG experiments operate in the small-signal regime of small input powers, leading to negligible down-conversion and pump depletion. Ignoring the down-conversion or β_1 term in Eq. S1, one obtain the following simple expression for the second harmonic output power:

$$\frac{P_2^{\text{out}}}{\left(P_1^{\text{in}}\right)^2} = \frac{8}{\omega_1}\left(\frac{\chi_{\text{eff}}^{(2)}}{\sqrt{\epsilon_0\lambda_1^3}}\right)^2 Q_1^2 Q_2 |\bar{\beta}|^2 \left(1-\frac{Q_1}{Q_1^{\text{rad}}}\right)^2\left(1-\frac{Q_2}{Q_2^{\text{rad}}}\right). \tag{S6}$$

In the limit of large up-conversion and non-negligible down-conversion, solution of the coupled-mode equations yields the maximum efficiency (defined as $\eta = P_2^{\text{out}}/P_1^{\text{in}}$) and corresponding critical power [1]:

$$\eta^{\max} = \left(1-\frac{Q_1}{Q_1^{\text{rad}}}\right)\left(1-\frac{Q_2}{Q_2^{\text{rad}}}\right), \tag{S7}$$

$$P_1^{\text{crit}} = \frac{2\omega_1\epsilon_0\lambda_1^3}{\left(\chi_{\text{eff}}^{(2)}\right)^2}\frac{1}{|\bar{\beta}|^2 Q_1^2 Q_2}\left(1-\frac{Q_1}{Q_1^{\text{rad}}}\right)^{-1}. \tag{S8}$$

2. FORMULATION FOR TOPOLOGY OPTIMIZATION OF ARBITRARY NONLINEAR FREQUENCY CONVERSION PROCESS

Nonlinear frequency conversion processes can be viewed as frequency mixing schemes in which two or more *constituent* photons at a set of frequencies $\{\omega_n\}$ interact to produce an output photon at frequency Ω such that $\Omega = \sum_n c_n\omega_n$, where the photon number coefficients $\{c_n\}$ can be either negative or positive, depending on whether the corresponding photons are created or destroyed in the process. In general, because the optical nonlinear response of materials is a tensor and hence the frequency conversion process mixes different polarizations [2]. However, for notational simplicity, we will describe our optimization problem only for a single component of the susceptibility tensor. If one wishes to consider the full tensorial properties, one can easily add extra optimization terms (weighted by the tensor components) by following the same approach described below.

Given a specific nonlinear tensor component $\chi_{ijk\ldots}$, where $i,j,k,\ldots \in \{x,y,z\}$, mediating an interaction between the polarization components $E_i(\Omega)$ and E_{1j}, $E_{2k},\ldots$, we begin with a collection of point dipole currents, each at the *constituent* frequency ω_n, $n \in \{1,2,\ldots\}$ and positioned at the center of the computational cell $\mathbf{r}'$, such that $\mathbf{J}_n = \hat{\mathbf{e}}_{n\nu}\delta(\mathbf{r}-\mathbf{r}')$, where $\hat{\mathbf{e}}_{n\nu} \in \{\hat{\mathbf{e}}_{1j},\ \hat{\mathbf{e}}_{2k},\ldots\}$ is a polarization vector chosen so as to excite the desired E-field polarization components of the corresponding mode. Given the choice of incident currents $\mathbf{J}_n$, we solve Maxwell's equations to obtain the corresponding *constituent* electric-field response $\mathbf{E}_n$, from which one can construct a nonlinear polarization current $\mathbf{J}(\Omega) = \bar{\epsilon}(\mathbf{r})\prod_n E_{n\nu}^{|c_n|(*)}\hat{\mathbf{e}}_i$, where $E_{n\nu} = \mathbf{E}_n\cdot\hat{\mathbf{e}}_{n\nu}$ and $\mathbf{J}(\Omega)$ has polarization $\hat{\mathbf{e}}_i$ generally different from the constituent polarizations $\hat{\mathbf{e}}_{n\nu}$. Here, (*) denotes complex conjugation for negative c_n and no conjugation otherwise. Finally, we maximize the radiated power $-\text{Re}\left[\int \mathbf{J}(\Omega)^*\cdot\mathbf{E}(\Omega)\,d\mathbf{r}\right]$ from $\mathbf{J}(\Omega)$.

The formulation is now given by:

$$\begin{aligned}
&\max_{\bar{\epsilon}}\ f(\bar{\epsilon};\omega_n) = -\text{Re}\left[\int \mathbf{J}(\Omega)^*\cdot\mathbf{E}(\Omega)\,d\mathbf{r}\right], \qquad \text{(S9)}\\
&\mathcal{M}(\bar{\epsilon},\omega_n)\mathbf{E}_n = i\omega_n\mathbf{J}_n,\ \mathbf{J}_n = \hat{\mathbf{e}}_{n\nu}\delta(\mathbf{r}-\mathbf{r}'),\\
&\mathcal{M}(\bar{\epsilon},\Omega)\mathbf{E}(\Omega) = i\Omega\mathbf{J}(\Omega),\ \mathbf{J}(\Omega) = \bar{\epsilon}\prod_n E_{n\nu}^{|c_n|(*)}\hat{\mathbf{e}}_i,\\
&\mathcal{M}(\bar{\epsilon},\omega) = \nabla\times\frac{1}{\mu}\nabla\times-\epsilon(\mathbf{r})\omega^2,\\
&\epsilon(\mathbf{r}) = \epsilon_{\text{m}} + \bar{\epsilon}\ (\epsilon_{\text{d}}-\epsilon_{\text{m}}),\ \bar{\epsilon}\in[0,1].
\end{aligned}$$

In practice, we maximize a frequency-averaged version of the power output $\langle f(\omega)\rangle$ rather than $f(\omega)$ itself since the latter has poor convergence [3], i.e., we maximize $\langle f\rangle = \int d\omega'\,\mathcal{W}(\omega';\omega,\Gamma)f(\omega')$, where we simply choose the weighting function $\mathcal{W}$ to be a simple lorentzian with the desired resonance ω and a certain linewidth Γ,

$$\mathcal{W}(\omega') = \frac{\Gamma/\pi}{(\omega'-\omega)^2+\Gamma^2} \tag{S10}$$

(Note that this linewidth is not necessarily the same as the intrinsic radiative linewidth of the cavity in that Γ is a computational artifice introduced to aid rapid convergence [3].) In Ref. [3], it is shown by means of contour integration that this averaging is equivalent to evaluating f at a complex frequency $f(\omega+i\Gamma)$, also equivalent to adding a uniform loss $i\Gamma/\omega$ to $\mu(\mathbf{r})$ and $\epsilon(\mathbf{r})$. In our implementation of the optimization process, we typically begin with a large Γ which affords rapid convergence to a stable geometry in a few hundred iterations. Γ is then decreased by an order of magnitude every time the optimization converges until $\Gamma \sim 10^{-5}$ at which point the structure settles to within a linewidth Γ of the desired frequencies (perfect frequency matching).

Application of this formulation to the problem of second harmonic generation is straightforward and described in the main text, in which case $\Omega = \omega_2 = 2\omega_1$ and $\mathbf{J}(\Omega) = \mathbf{J}_2 = \bar{\epsilon}(\mathbf{r})\ (\hat{\mathbf{e}}_{1j}\cdot\mathbf{E}_1)^2\hat{\mathbf{e}}_{2i}$. Note that for the structures described in the text, we chose $\hat{\mathbf{e}}_{1j} = \hat{\mathbf{e}}_{2i} = \hat{\mathbf{e}}_y$. In addition to the problem statement of Eq. S9, the optimization algorithm also benefits from gradient information of the objective function, which exploits the adjoint variable method [3–5]. Here, we simply quote the result for the gradient of our SHG objective function (dropping the polarization index y for simplicity), $\langle f(\bar{\epsilon};\omega_1)\rangle = -\text{Re}\left[\left\langle \int \mathbf{J}_2^*\cdot\mathbf{E}_2\,d\mathbf{r}\right\rangle\right]$,

$$\begin{aligned}
\frac{\partial\langle f\rangle}{\partial\bar{\epsilon}} = &-\text{Re}\Big[E_2\,(E_1^*)^2 + (\epsilon_{\text{d1}}-\epsilon_{\text{m}})\omega_1^2 u_1^* E_1^*\\
&+(\epsilon_{\text{d2}}-\epsilon_{\text{m}})\omega_2^2 u_2 E_2 + i\omega_2 u_2 E_1^2\\
&+i\omega_2\omega_1^2(\epsilon_{\text{d1}}-\epsilon_{\text{m}})u_3 E_1\Big],
\end{aligned}$$

where the functions u_k are solutions of the following scattering problems:

$$\begin{aligned}
\mathcal{M}_1 u_1 &= \bar{\epsilon}E_1^* E_2,\\
\mathcal{M}_2 u_2 &= \bar{\epsilon}E_1^2,\\
\mathcal{M}_1 u_3 &= 2\bar{\epsilon}E_1^* u_2.
\end{aligned}$$

3. OPTIMIZED 1D CAVITY DESIGNS

Figure S1 shows the dielectric and E_y field profiles of the three optimized structures, including (a) AlGaAs/Al_2O_3 micropost, (b) GaAs gratings in SiO_2, and (3) LN gratings in air. Along the x cross-section, each computational pixel of thickness Δ represents *either* a high dielectric (nonlinear) or low dielectric (linear) material. For example, in the AlGaAs/Al_2O_3 micropost cavity (assuming $n_1(\text{AlGaAs}) = 3.02$ and $n_2(\text{AlGaAs}) = 3.18$ for AlGaAs with 70% Al [6], and $n(Al_2O_3) = 1.7$), we took $\Delta = 0.015\,\lambda_1$.

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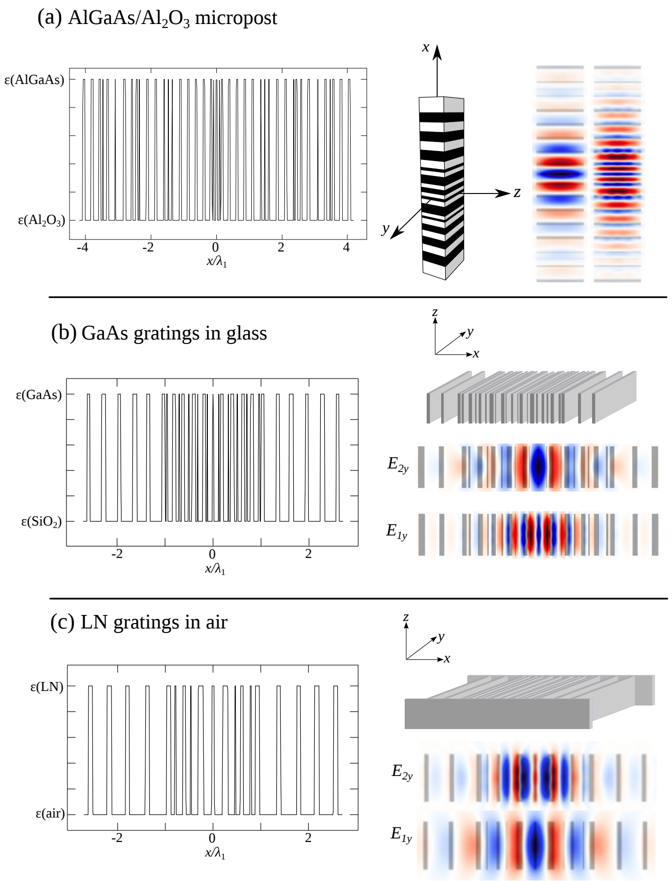

Fig. S1. Cross-sectional dielectric profiles and electric field distributions for AlGaAs/Al_2O_3 micropost (a), GaAs gratings in SiO_2 (b) and LN gratings in air (c).

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