

# Enhanced Second Harmonic Generation in Doubly Resonant Photonic Crystal Cavities Made of Silicon

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#### Abstract

We investigate numerically the formation of non-linear cavity modes in photonic crystal cavities made of silicon. We employ a numerical method based on the multiple scattering matrix algorithm to show that silicon based photonic crystal cavities exhibit doubly resonant defect modes, which can be generated via surface second harmonic generation. We show that by carefully designing the geometric parameters of the optical cavity the non-linear effects can be strongly enhanced leading to increased efficiency of light generation at the second harmonic.

### **1. Introduction**

In this paper we demonstrate that by using a doubly resonant photonic crystal (PhC) cavity made of silicon one can achieve a significant enhancement of the second harmonic generation (SHG). Due to its inversion symmetry, silicon has only third-order bulk optical nonlinearities. Quadratically non-linear optical interactions can be achieved, however, in Si by employing surface SHG. Since this second-order nonlinear optical interaction is usually weak, it is desirable to provide means to enhance it so it can be employed to chip-level active devices made of silicon. To this end, it is well known that resonant cavities based on dielectric media exhibit very high quality factors, Q, and as such have several major applications in micro- and nano-scale photonics [1]. In particular, significant efforts have been directed towards the enhancement of non-linear optical effects in such structures [2]. In this connection, we will show in what follows how, by careful tailoring of the geometrical parameters of PhC cavities made of silicon, one can induce strong second-order non-linear interactions induced by surface and bulk polarization sources.

### 2. Theoretical and Computational Approach

We employ in what follows a numerical method based on the multiple scattering method (MSM) formalism [3]. In order to simplify our analysis, we consider a two-dimensional PhC consisting of a hexagonal lattice of air cylinders in a silicon background. In order to create a defect mode (cavity), one cylinder in the PhC is filled with Si (see a schematic of the geometry of the PhC cavity in Fig. 1a). The PhC cavity is designed so as it has a localized cavity mode at the frequency  $\omega_0$ , located in a low-frequency bandgap and another cavity mode with frequency  $2\omega_0$ , which is inside a high-frequency bandgap (see also Fig. 1b). In the presence of non-linear optical interactions the two modes at the fundamental frequency (FF) and second harmonic (SH) are coupled *via* two distinct non-linear polarization sources, a dipole-allowed surface polarization generated at the Si-air interface,  $\mathbf{P}_s = \chi_S : \mathbf{EE}$ , and a bulk, non-local polarization



in Si,  $\mathbf{P}_b = \boldsymbol{\chi}_b : \mathbf{E} \nabla \mathbf{E}$  [4]. Here  $\boldsymbol{\chi}_s$  and  $\boldsymbol{\chi}_b$  are the non-linear surface and bulk susceptibilities, respectively, and  $\mathbf{E}$  is the electric field. We assume in what follows that the undepleted pump approximation holds, thus, there is no energy transfer from the SH back to the FF.



Fig. 1: a) Schematic of the photonic crystal cavity. b) Band structure of the photonic crystal obtained by using a  $5 \times 5$  supercell; bandgaps are denoted by using blue shaded colouring. Horizontal green lines indicate cavity modes.

In the MSM formalism, the incident field is expanded into a Fourier-Bessel series as  $U_z^{inc}(r,\varphi) = \sum_{\infty}^{\infty} a_m J_m(kr)e^{im\varphi}$ , where  $J_m$  are Bessel functions of the first kind and  $a_m$  are the expansion coefficients. As excitations fields we used multipole sources, which are represented as  $U_z^{inc} = a_{m_0} J_{m_0}(kr)e^{im\varphi}$ . The coefficients  $a_m$  are the only quantities needed to calculate the fields at the FF and SH (see Ref. [3] for details). In what follows, due to the symmetry properties of the hexagonal lattice, we set  $m_0 = 3$ .

### **3. Results and Discussions**

Defect modes in PhCs are formed inside photonic bandgaps so that we have designed the PhC such that, for the TE polarization, it has two bandgaps, the frequency of one of them being at about twice the frequency of the other one. As a result, this doubly resonant PhC cavity provides an enhanced non-linear interaction between the two cavity modes and, consequently, a dramatic increase in the SHG. Specifically, the modes at the FF and SH provide strongly localized field distributions and thus there is a strong non-linear coupling between them. We have calculated the band structure of our PhC, for a design with r/a = 0.449 using a commercially available photonic band solver. The results, shown in Fig. 1b, reveal that two defect modes can be identified at  $a/\lambda = 0.817$  and  $a/\lambda = 0.415$ , each within the corresponding bandgap. Note also that the low frequency bandgap contains two additional localized modes. By exciting the cavity at the lower frequency, the strong non-linear coupling between the two modes leads to significant SHG at the higher-frequency mode.

To verify this conclusion, we have calculated the field distributions at both the FF and SH using the MSM algorithm, for the case in which the two cavity modes are nonlinearly coupled *via* the non-linear surface and bulk polarizations. We considered a PhC cavity with r = 466 nm and a = 1038 nm. With these values for the geometrical parameters the frequencies of the interacting modes correspond to  $\lambda_{FF} = 2500$  nm and  $\lambda_{SH} = 1250$  nm. It is worth mentioning here that other spectral regimes could be easily accessed by simply changing the geometrical parameters of the design.

The resulting field profiles of the cavity modes, shown in Fig. 2, indicate that the two cavity modes are indeed coupled in the non-linear regime, with the field components at the FF and SH being the linear cavity modes. As expected, for the SH case, the mode order is twice as large as that of the mode at the FF, respectively,  $n_{FF} = 6$  and  $n_{SH} = 12$ . We can also conclude from the field profiles in Fig. 2 that the fields at the FF and SH are strongly confined at the centre of the PhC cavity with leakage only occurring up to the second row of holes. This is again to be expected as the frequency of these modes lies in the





Fig. 2: Field profile  $|E(\mathbf{r})|^2$  at the FF (left panel) and SH (right panel) for r/a = 0.449.

bandgap of the photonic crystal. The resulting strong field localization coupled with low radiative losses, are strong indicators of a very high Q factor, especially at the SH, and consequently a high efficiency of the SHG interaction.

### 4. Conclusion

In conclusion, we have demonstrated that the non-linear effects associated with surface second harmonic generation in silicon based photonic crystals can be greatly enhanced by a careful design of the PhC cavities. Thus, doubly resonant PhC cavities can be used to enhance significantly the SHG interaction by inducing a strong non-linear coupling between cavity modes with high Q. The efficiency of the SHG interaction can be further increased by using PhC cavities made of silicon strained by a silicon nitride layer [5]. In this approach the non-linear interaction is determined by a bulk, local non-linear polarization, which is much larger than the two non-linear polarization sources considered here. Consequently, these structures show significant potential for developing new on-chip devices that will allow for active non-linear photonic systems with new or advanced functionality.

### Acknowledgments

This research is partially supported by the grant FP7-REGPOT-2011-1-284595 (HOST). The authors acknowledge the use of the UCL Legion High Performance Computing Facility, and associated support services, in the completion of this work.

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