A new method for second harmonic generation

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We report a new method for second harmonic generation (SHG) by using centro-symmetric dielectric, of which $\chi^{(2)}$ is zero, rather than common nonlinear material. By designing the unique structure of centro-symmetric dielectric, which consists of two photonic crystals and several air waveguides, the efficient second-harmonic (SH) has obtained for the sharp enhancement of the electric quadrupole polarization. Based on finite difference time domain (FDTD) algorithm, the electromagnetic field distribution in the structure and the intensity of SH along the waveguide are analyzed. When the beam intensity of the pumping wave is 1.3 MW/mm², the conversion efficiency of power is 0.307% for a photonic crystal waveguide with a length of 40 μ m.

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The mechanisms of second harmonic generation (SHG) were developed in the 1960s^[1], which include electric dipole (ED) polarization, magnetic dipole (MD) polarization, electric quadrupole (EQ) polarization, and magnetic quadrupole (MQ) polarization etc. Because ED polarization is the largest in conventional nonlinear bulk material, ED approximation is adopted to analyze SHG usually. However, as the second-order susceptibilities $\chi^{(2)}$ are zeros in materials with inversion symmetry, EQ becomes the major origin of nonlinearity. Since susceptibilities Q of EQ polarization is 3-4 magnitudes less than $\chi^{(2)}$, it is hard to observe the SHG in this kind of materials. But the EQ polarization can be enlarged if we increase the spatial gradient of the E-field within the dielectric with special measures. In fact, through applying dc E-field, Terhune has observed the SHG from the crystal calcite possessing a center of inversion in 1960s^[2]. However, for high voltage over 10 kV and lower conversion efficiency there are no good prospects for Terhune's technology. In recent years the photonic band edge effects (PBEE) of photonic crystals (PCs) have been discussed in several papers[3-5], which can increase the density of modes (DOM) violently and decrease sharply the group velocity of electro-magnetic waves. So it is possible by using PBEEs to increase spatial gradient of the E-field even in low pumping power, it is mean that only if some suited micro structures had been designed the second harmonic will be generated in the centro-symmetric dielectric of which $\chi^{(2)}$ is zero by harnessing the EQ polarization properties and waveguide modes.

The configuration described in the paper is shown in

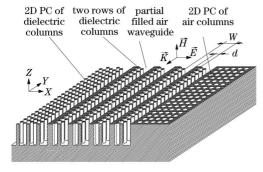


Fig. 1. Configuration of the PCs and waveguides.

Fig. 1. It consists of PC of air columns (PC1), PC of dielectric columns (PC2) and several air waveguides. The unit of the PC1 is triangular lattice and the unit of PC2 is rectangular lattice. The waveguides, which are filled partly by a layer of the same dielectric with a fill factor of f = W/D, are spaced by dielectric columns. All of them are two-dimensional (2D) structure formed by the same material with inversion symmetry. In PCs for the localization of the light field the E-field can be partly enlarged $^{[6,7]}$, but this is insufficient to excite obvious SHG. It is necessary to enhance the gradient of Efield greatly through some special means accordingly. We choose the PBEEs. Therefore we have designed a special PC (Fig. 1) with the band edge just near the pumping frequency, which can enlarge the E-field gradient to the utmost. In addition, the asymmetrical structure itself will also enlarge light field gradient. That is why the two PCs are different and the waveguides are partly filled in the structure. The parameters aiming at CO_2 laser with a wavelength of 10.6 μ m (the pumping source) are as follow, material is Si, the dielectric constant ε is 11.9, the lattice constant a is 3.1 μm , the radius of air columns r_1 of PC1 is 0.4a, the radius of dielectric columns r_2 of PC2 is 0.2a, the width of the waveguides is 1.6a, the fill factor f is 0.6, the length of waveguide is 40 μ m.

For the lossless materials case and referred to the slowly varying envelope approximation in time (SVEAT), the excited second-harmonic (SH) fulfills the following equation [8-10]

$$\nabla \times \nabla \times E^{2\omega}(x, y, z, t) + \mu_0 \varepsilon(x, y, z) \frac{\partial^2 E^{2\omega}(x, y, z, t)}{\partial^2 t}$$
$$= -\mu_0 \frac{\partial^{2\text{NL}, Q}(x, y, z, t)}{\partial^2 t}, \tag{1}$$

$$P_i^{\text{NL},Q} = \sum Q_{ijkl} E_j \nabla_k E_l, \qquad (2)$$

where $\vec{P}^{\text{NL},Q}$ is the source term of nonlinear coming from the EQ interact, and Q_{ijkl} is the EQ susceptibilities. E_j , E_l are the found frequency field in the waveguide which can be solved from Maxwell equations.

We solved the Eq. (1) by finite difference time domain (FDTD) algorithm to find the intensity of SH. The spatial sampling step is $\Delta x = \Delta y = 0.11 \ \mu \text{m}$, and the time

sampling step is $\Delta t = 0.2$ fs. The exciting source, regarded as a plane wave, is applied at the position of x=35 μ m. The incident angle is 15° to the direction x and lasting time is 300 fs. The distribution of electromagnetic field in this configuration is shown in Fig. 2 where Fig. 2(a) is amplitude distributions in xy plane of E_x . From Fig. 2 we can see that the electromagnetic fields are mostly localized in the area between PC1 and PC2 for the effect of photonic band gap (PBG). The two lines of dielectric columns are insufficient to form PBG, and it can only modulate electromagnetic fields and make the energy couple or transfer among waveguides. All modes of electromagnetic field are forbidden in PBG of PCs and thus there is almost no energy entering PC1. However it is not the same in PC2. Since the SH frequency is near the edge of the PBG of PC2, the electromagnetic wave can be transmitted back and forth in PC2 and the area of waveguides and dielectric columns, just like a resonant cavity. In order to see the huge variation of E-field more obviously, the gradient of the cross section distribution at $x=5 \mu \text{m}$ along y direction is plotted in Fig. 2(b). We calculated the SH intensity when the effective susceptibility of electric quadrupole polarization is 10^{-16} esu. The variation curve of SH along direction x is shown in Fig. 3. Since the exciting source is applied at $x=35 \mu m$ position, the SH intensity increases with the decrease of coordinate values. The variation trend is identical with the SHG in typical nonlinear bulk materials as showing with dotted line in Fig. 3. When the corresponding beam intensity is $S_{in} = 1.3 \text{ MW/mm}^2$, the SH intensity is 0.4 MW/mm², that is the conversion efficiency is 0.307%, Compared with the conversion efficiency of a typical nonlinear material under the case of perfect phase matching, this efficiency is a bit lower, but it

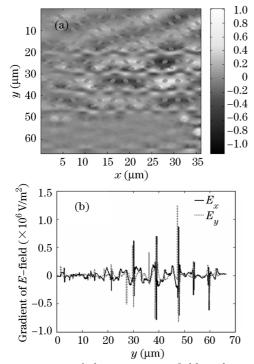


Fig. 2. Distribution of electromagnetic field in the configuration. (a) Amplitude distributions of E_x , (b) gradient of the cross-section distribution of E_x and E_y at $x=5~\mu{\rm m}$ along ydirection.

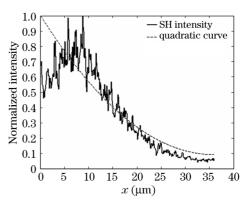


Fig. 3. SH intensity along the waveguide.

is comparable to the conversion efficiency of the photonic crystal slabs in Ref. [11].

In conclusion, we have discussed a new method for SHG which increase EQ polarization rather than ED polarization. A special configuration structure of Silicon with inversion symmetry has been presented. Light field distribution and SH intensity in this configuration are calculated. The SH intensity increases with the decrease of coordinate values, and the trend of increase of SH is consistent with quadratic curve as same as the proceeding in nonlinear bulk materials. Combined with nanolithography technologies, SHG originated from quadrupole effect can be optimized for applications by designing the PCs with centrosymmetric materials.

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