Quasi-phase-matching with Spontaneous Domain Inversion in an Integrated Lithium Niobate Micro-racetrack Resonator

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(Dated: June 28, 2021)

Quasi-phase-matching (QPM) technology is the most popular and significant method to achieve efficient nonlinear frequency conversion. The realization of periodically poling to achieve QPM in photonic integrated circuits (PICs) is a challenging issue for the requirement of CMOS compatible and large-scale fabrication. Here we realize a spontaneous periodical domain inversion without poling but by dispersion engineering and designing the orientation of the crystal due to the circular propagation of light waves in an integrated lithium niobate micro-racetrack resonator (MRR). The QPM second harmonic generation (SHG) with a normalized conversion efficiency of 2.25%/W (160th-order QPM) has been achieved in the high-quality factor resonator of ∼10⁶ with the straight waveguide (TE₀₀ mode) of ultra-low propagation loss of 0.0022dB/cm. The efficiency can be further enhanced by using a first-order QPM, and the bandwidth can be made broader by employing a shorter interaction length for photonics and quantum optics. The configurable spontaneous quasi-phase-matching lithium niobate MRR on X-cut thin-film lithium niobate on insulator (LNOI) provides a significant on-chip integrated platform for other optical parametric processes.

Lithium niobate (LN) is a superior platform for optics and microwave photonics, benefited from its electro-optic, acousto-optic, and nonlinear optic properties. After the commercialization of thin-film lithium niobate on insulator (LNOI), many integrated optical devices are designed and fabricated [1–4], such as micro-laser[5–8], modulator [9–12], waveguide amplifier [13] and nonlinear frequency conversion structure [14–17]. As for integrated optical frequency conversion devices, high-quality factor microcavity is an outstanding platform [18–21], which has a long photon lifetime and small mode volume and can enhance the interaction of light and matter. The key point of high-efficiency frequency conversion is phase matching. To date, excellent works of frequency conversion based on modal phase matching (MPM) [22], cyclic phase matching (CPM) [23, 24] and quasi-phase-matching (QPM) [15, 25–27] in microcavities on LNOI have been reported. For high conversion efficiency, QPM would be a better choice because of the fundamental modes involved. And the frequency conversion could work in the different bands due to the variable artificial periodic structure that QPM requires.

In reports of recent decades, the periodically reversed domains in LN can be obtained by the electric field [28–30], femtosecond laser [31] and atomic force microscope-induced domain inversion [32]. But domain inversion requires extra steps for fabrication, increasing the cost and complexity. Meanwhile, as the period decreases, the difficulty increases, mainly resulting from the domain wall crosslinking.

Based on our previous works about frequency conversion on PPLN and LN cavity [33–36], here we propose and demonstrate spontaneous quasi-phase-matching (SQPM) second harmonic generation (SHG) in a micro-racetrack resonator (MRR) on X-cut LNOI, using dispersion engineering and CMOS compatible fabrication process. The periodically inverted domains appear spontaneously for the circular propagation of light in the MRR, after the fabrication without domain inversion. The SHG of the fundamental modes of two transverse electric waves (TE₀₀) in the MRR on X-cut LNOI has the largest modal overlap and the biggest nonlinear coefficient (d₃₃). Besides, the high-quality factor of the MRR enables the light to propagate a long distance in an equivalent periodically poled lithium niobate (PPLN) waveguides, and provides high SHG conversion efficiency.

Electric field poling is a traditional and mature method to obtain PPLN. The periodic structure usually consists of two parts, one of which has inverted domain and negative effective nonlinear efficiency dₑₑ, shown in Fig. 1(a). Different from the Sinc function squared oscillation, the intensity of the second harmonic wave (SH) will continue to increase in the periodically inverted domains, that is the reason QPM has very high SHG efficiency. Rotating the inverted part along the dashed arrow path and assuming that light also propagates along the path, shown in Fig. 1(b), the light equivalently passes through a periodic structure. It should be noted that the crystal orientation of the two parts is now in the same direction. The length of the half-period of PPLN is called coherence length (Lₑₑ) and the intensity of SH will increase after propagating an odd number of Lₑₑ. For bending the
FIG. 1. (a) Light propagates through a PPLN with a uniform period. (b) Light propagates through a single period in the PPLN. The equivalent single period appears when the inversed domain and the direction of light propagation could both rotate 180°. (c) Light circulates in an MRR on X-cut LNOI, with crystal orientation perpendicular to the straight waveguides. (d) The schematic diagram of azimuth angle θ in the MRR. Since the directions of k and Z at the straight waveguide remain constant, θ remains 0.5π or 1.5π. (e) The relationship between effective nonlinear coefficient and SHG intensity with θ.

FIG. 2. (a) The conformal transformation for the half-ring waveguide in the MRR. Light to dark green indicates a gradual increase in the index of refraction from n_{eff}/n_0 to n_0. (b) Phase delay in a quarter-circle waveguide varies with the radius of half-ring for both FW and SH, with waveguide parameters W, h, t and α determinate.

propagation path of the light, half-ring waveguides can be adopted. Designing the geometric parameters of the half-ring waveguides and choosing the proper amount of L_e, an MRR is combined, where fundamental wave (FW) and SH are resonant and QPM is achieved, depicted in Fig. 1(c). We can define the azimuth angle θ as the angle between the wave vector k and the crystal orientation +Z, which is shown in Fig. 1(d). The relationship between d_{eff} and SHG intensity with θ is shown in the Fig. 1(e). The crystal orientation +Z of LN means the MRR can be fabricated on X-cut LNOI. And the most fascinating thing is that the QPM occurs spontaneously in the MRR, without any extra poling technology.

The half-ring waveguides connecting the two straight parts should be well designed so that the phase delay of FW and SH in it equals the integer multiple of 2π (i.e., 2Nπ). The refractive index of transverse electric (TE) waves in the circular waveguide on X-cut LNOI can be described by

\[ n_e(\theta) = \left( \frac{\sin^2 \theta}{n_0} + \frac{\cos^2 \theta}{n_e} \right)^{-1/2}, \]

where n_0 and n_e are the ordinary and extraordinary refractive indexes of LN respectively. Due to the refractive index varies with θ, the mode analysis method of microring employing axisymmetric condition [37] on Z-cut LNOI is inappropriate. Instead, we can employ a method called conformal transformation [38] to calculate the effective refractive index of TE waves in the half-ring waveguide. Fig. 2(a) shows the conformal transformation from a curved waveguide with a uniform refractive index to a straight waveguide with a gradual refractive index, and the cross-section of the half-ring waveguide in the MRR and its transformed cross-section. The half-ring waveguide can be dissolved into tiny bent curved waveguides and transformed into straight ones, so the phase delay of FW and SH can be calculated exactly. Because of the periodicity of Eq. (1), we can sum the phase delays of FW and SH in the quarter-circle waveguide related to θ in range of (0, π/2) for simplicity. Fig. 2(b) shows the phase delay of FW and SH in the quarter-circle waveguide varies with its outside radius, and the inserted modal distributions of TE_{00} modes of FW and SH are simulated by finite element method (FEM). The outside radius R_2, top width W, sidewall angle α, and thickness t of the half-ring waveguide have a difference to the phase delay. We optimize these parameters based on the single-mode condition in the rib waveguide and the integer condition for phase delay. When R_2 = 126.625 μm, W = 1 μm, t = 0.38 μm and α = 60°, the phase delays of both FW and SH in the quarter-circle waveguide are Nπ. Therefore, the total phase delay in the half-ring waveguide equals 2Nπ.

Once we determine W and t, and α, the effective refractive index of the straight waveguide of the MRR can
be calculated under the same geometric parameters. In the straight waveguide, the phase mismatch between FW and SH is \( \Delta k = 4 \pi (n_{\text{eff,SH}} - n_{\text{eff,FW}}) / \lambda \). \( n_{\text{eff,FW}} \) and \( n_{\text{eff,SH}} \) are the effective refractive indexes of FW and SH respectively, shown in Fig. 2(d). And \( \lambda \) is the vacuum wavelength of FW. According to the QPM condition, the reciprocal vector introduced by periodic structure is \( G = 2 \pi m / \Lambda = \Delta k \), with \( \Lambda = 2L_0 \). \( L_0 \) corresponds to the length of the straight waveguide, and \( m \) is a positive odd, representing the order of QPM. The length of the straight waveguide should be

\[
L_0 = mL_c = \frac{m \lambda}{4(n_{\text{eff,SH}} - n_{\text{eff,FW}})}.
\]

Meanwhile, the resonance of FW and SH in the MRR requires

\[
2L_0n_{\text{eff,FW}} = M_{\text{FW}} \lambda
\]
\[
2L_0n_{\text{eff,SH}} = M_{\text{SH}} \lambda / 2,
\]

where \( M_{\text{FW}} \) and \( M_{\text{SH}} \) are positive integers. Therefore, combining Eqs. (2) and (3), the calculation results are \( m = 169 \) and \( L_0 = 231.978 \mu \text{m} \).

So far, we have completed the design of the MRR. Since we study the TE\(_{00}\) modes in the MRR, we need to design the coupling waveguide specially to achieve the critical coupling of the fundamental mode and suppress the coupling of higher-order modes. Pulley coupling waveguide [39] is employed for the TE\(_{00}\) modes of FW, shown in Fig. 3(a). The critical coupling condition can be described as

\[
n_{\text{ring}} R_{\text{ring}} = n_{\text{wg}} R_{\text{wg}}, \quad n_{\text{ring}}, \quad n_{\text{wg}} \quad \text{are the effective refractive indexes of the TE}_{00} \text{modes in the half-ring and coupling waveguide respectively, and} \quad R_{\text{ring}}, \quad R_{\text{wg}} \quad \text{are the related mode radiiuses. We can choose appropriate width of the pulley coupling waveguide and the gap between the ring and the coupling waveguide to meet the critical coupling condition. For FW critical coupling, the width of the coupling waveguide \( W_{\text{wg}} \) is 0.8 \( \mu \text{m} \), the gap \( g \) is 0.61 \( \mu \text{m} \) and the central angle \( \theta_0 \) is 30°.}

The MRR is fabricated on a 600 nm thick X-cut LNOI (by NanoLN). Amorphous silicon thin film is deposited on LNOI as a hard mask, by plasma-enhanced chemical vapor deposition (PECVD). The MRR patterns are defined in ZEP520A resist using standard electron beam lithography. The patterns are first transferred into the hard mask by reactive ion etching (RIE) with sulfur hexafluoride (SF\(_6\)). Subsequently, the patterns are transferred into the LN film, using inductively coupled plasma reactive ion etching (ICP-RIE) with Argon (Ar). Finally, RCA cleaning is performed to remove the hard mask and small particles. The LN film is etched at a total of 380 nm, leaving a slab of 220 nm. Fig. 3(b)-(d) shows the scanning electron microscope images of the MRR. And the experimental setup is shown in Fig. 3(e). An infrared tunable laser (New Focus TLB-6728) is amplified by an erbium-doped optical fiber amplifier (EDFA) and selected TE polarization with a polarization controller (PC). The FW and SH are separated by a wavelength division multiplexing (WDM). A photodetector (PD) and an oscilloscope (OSC) are used for measuring the transmission spectrum of FW. And SH is detected by an optical spectrum analyzer (OSA).
The measured transmission spectrum of FW is shown in Fig. 4(a) and the Lorentz fitting for TE_{00} is shown in Fig. 4(b). The ratio of the circumference of the MRR to the wavelength of FW is calculated as $m_{axi} + M_{FW} = 1539$, where $m_{axi}$ denoting the wavenumber of FW in the half-ring waveguides, is determined from Fig. 2(b), and $M_{FW}$ denoting the wavenumber of FW in the straight waveguides, is determined by Eq. (3). The loaded quality factor is $Q_{in,FW} = 9.82 \times 10^7$ and the intrinsic quality factor is $Q_{in,FW} = 1.47 \times 10^8$. The propagation loss of the rib waveguide is estimated as 0.0022 dB/cm at the 1550 nm band. Fig. 4(c) shows the spectrum of the SH.

For TE modes of both FW and SH, $d_{eff}$ of SHG is the largest nonlinear coefficient $d_{33}$. According to the coupled-mode theory in the undepleted regime, the conversion efficiency can be derivated as (See Supplemental Material)

$$
\eta = \eta_0 \frac{\sigma_{SH} \times \iint |A_{FW}|^4 d\sigma_{SH}}{(\iint |A_{FW}|^2 d\sigma_{FW})^2}, \quad (4)
$$

with

$$
\eta_0 = \frac{8Q_{in,FW}^4 d_{eff}^2 \varepsilon_0 n_{eff,SH} n_{eff,FW}^2}{(m_{axi} + M_{FW})^4 \pi^2 \varepsilon_0 n_{eff,FW}^2}, \quad (5)
$$

where $A_{FW}$ is the in-coupled amplitude of FW, $\sigma$ is the cross sectional area of the mode in the straight waveguide ($\sigma_{FW}$ for FW and $\sigma_{SH}$ for SH) and the integral items can be calculated using FEM. From Eq. (4) and (5), the theoretical conversion efficiency in this work is around 18.8%/W.

The measured intensity of the SH and FW are plotted in Fig. 4(d). The intracavity power means the power in the resonator and the on-chip power means the power export from the resonator. The extracted conversion efficiency of SHG is 2.25%/W. As the FW power increases, the measured data begin to deviate from linearity, mainly resulting from the thermal detuning of FW. The reason that the experimental conversion efficiency is lower than the theoretical calculation is the coupling loss of SH at the pulley waveguide, which could be optimized by an add-drop waveguides structure.

Limited by the fabrication accuracy, the designed FW wavelength for SQPM SHG may deviate from the resonant mode of the MRR, as shown in the resonant modes drawn with a dotted line in Fig. 5(a). In our designed MRR, the top width of the waveguide is the main error, which results on the change of the width of the electron beam resist after development. It is calculated that an error of 10 nm in the top width of the waveguide will result in a deviation of 0.66 nm in the resonant mode at the 1550 nm band. At this level or greater error, the resonant mode and SHG wavelength deviation can easily occur. Fortunately, MRRs with large radius half-ring waveguides and long straight waveguides bring small FSRs, which help to solve the deviation. When the FSR of the MRR is close to (or less than) the SHG bandwidth, shown in Fig. 5(a), the resonant modes will be dense enough and there is at least one resonant mode that matches the SHG wavelength. Fig. 5(b) shows the SHG bandwidth is 0.82 nm for our designed and fabricated MRR, with the radius of the half-ring waveguide ($r$) at 126.625 $\mu$m and the length of the straight waveguide ($L_0$) at 231.978 $\mu$m. From Fig. 4(a) we know that the FSR of the MRR is 0.812 nm. Thus, there is always one resonant mode in the SHG bandwidth and we can obtain SHG with considerable efficiency by selecting resonant modes in the experiment. However, the method of matching the resonant mode with the SHG wavelength has a certain cost. Eq. (5) could be approximately deduced as

$$
(\eta_0) \propto \left( \frac{Q_{in,FW}}{\pi R + L_0} \right)^4, \quad (6)
$$

which shows that MRRs with larger $R$ and $L_0$ bring lower SHG efficiency. Therefore, with accurate fabrication or precision modulation (e.g., thermo-optic or electro-optic modulation) of the refractive index of the straight waveguide, the resonant modes with larger FSR in a smaller MRR can well match the SHG wavelength, and higher SHG efficiency will be obtained.

In summary, without periodically electric field poling, we demonstrate SQPM SHG in an integrated MRR on X-cut LNOI by dispersion engineering and design of the orientation of crystal. The periodically inversed domains arise spontaneously due to the circular propagation of light in the MRR, and the QPM mechanism is realized by periodically switching the sign of the maximum nonlinear coefficient. We can also design the radius of the half-ring waveguide, which could be optimized by an add-drop waveguides structure.
and the length of the straight waveguide in the MRR to achieve different optical parametric processes. This method is beneficial to reducing the fabrication complexity of nonlinear frequency conversion and quantum source devices in LN photonic integrated circuits.

This work was supported by the National Natural Science Foundation of China (Grant Nos. 91950107, 11734011), the National Key R & D Program of China (Grant Nos. 2019YFB2203501 and 2017YFA0303701), Shanghai Municipal Science and Technology Major Project (2019SHZDZX01-ZX06), and SJTU No. 21X010200828. And we wish to acknowledge Prof. Qiang Lin for the helpful discussion.

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