High-$Q$ resonant modes in a photonic crystal heterostructure nanocavity and applicability to a Raman silicon laser

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When a heterostructure is created at the center of a photonic crystal line-defect cavity to form a nanocavity, the photonic band gap contains several high-quality ($Q$) factor resonant modes. We have studied the optical properties of these modes to examine their applicability to Raman silicon lasers, which require two high-$Q$ resonant modes with a frequency spacing of 15.6 THz. Our experimental and numerical analyses reveal four types of resonant modes. We demonstrate that pairing the resonant mode originating from the first-order propagation mode with that arising from the second-order propagation mode is the most promising approach toward the realization of Raman silicon lasers.

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I. INTRODUCTION

Because silicon (Si) has an indirect band gap, with radiative electron-hole recombination of very low efficiency, the realization of Si-based lasers has proved to be difficult.1 Instead of utilizing the interband transition, stimulated Raman scattering (SRS) in Si rib waveguides has been proposed as a route to achieve optical gain.2 The Raman gain coefficient of crystalline Si is as high as that of commonly used Raman laser materials.3 Furthermore, Si rib waveguides fabricated on Si-on-insulator (SOI) substrates exhibit tight confinement of light that enhances the SRS.4 Therefore, this method has succeeded in achieving net optical gain5–13 and has resulted in the continuous-wave (cw) operation of Raman Si lasers.14 However, these lasers need the assistance of reverse-biased p-i-n diodes in order to remove the free carriers generated by two-photon absorption15 and they have thresholds as high as 20 mW, even when a high-quality ($Q$) ring-cavity structure on the cm scale is used.16

We have recently reported on the realization of a μm-scale Raman Si laser with an ultralow threshold of 1 μW, using a photonic crystal (PC) heterostructure nanocavity without any p-i-n diode.17 A key aspect was the exploitation of an unusual pair of high-$Q$ resonant modes to confine the pump light and Stokes Raman scattered light inside the cavity. We utilized the ground-state heterostructure nanocavity modes that originate from the first-order and second-order propagation modes associated with the line defect forming the cavity (Fig. 1). However, the optical properties of the nanocavity mode created by the second-order mode have not been studied in detail. Furthermore, many higher-order resonant modes with high $Q$ factors can be formed in a heterostructure cavity. Therefore, all these resonant modes should be investigated and their suitability for Raman Si lasers should be analyzed in detail.

In this article, we report on the whole set of high-$Q$ resonant modes that are formed within the photonic band gap (PBG) for a two-step heterostructure cavity. By examining various properties of these modes ($Q$ value, frequency, electric field distribution, and modal symmetry), we show that the ground-state heterostructure nanocavity modes originating from the two propagation modes are the most suitable pair for utilization in Raman Si lasers.

II. SAMPLE STRUCTURE

Nanocavities in two-dimensional (2D) PC slabs are exceptional optical resonators possessing both high $Q$ factors and small volumes.18–25 Figure 1(a) shows the structure of the samples studied here. A 2D PC consisting of a triangular lattice of circular air holes with radii of 110 nm was formed in a 220-nm-thick Si slab. The fundamental lattice constant $a_1$ was 410 nm. The upper line defect formed by a missing row of air holes is the excitation waveguide used to inject light into the cavity. The lower line defect formed by 39 missing air holes is the cavity that gives rise to the resonant modes for the Raman laser. The width ($w$) of the excitation waveguide and the distance from the cavity ($l$) were varied in different samples, as explained later. The width of the cavity was $\sqrt{3}a_1 = 710$ nm (W1). Figure 1(b) presents the band diagram of the cavity in the $x$ direction, which is divided into five frequency regions. These regions were identified from the photonic band structure [Fig. 1(c)] for the line defect forming the cavity, which was calculated by the three-dimensional (3D) finite-difference time domain (FDTD) method. The PBG corresponds to the range between the two slab modes. The line defect supports two propagation modes inside the PBG, whose dispersion relations are denoted by dashed and solid curves. We classify them as the odd-propagation mode and even-propagation mode, respectively, based on the symmetry of their electric fields $E_x$ with respect to the $xz$ plane of the line defect (see Fig. 4). Total internal reflection at the slab-air interface results in low-loss propagation for both modes below the light line (dotted line), and the corresponding frequency ranges for each mode are shaded the same color as their dispersion relation curves. The mode gap is the band that does not contain any propagation mode.

A two-step heterostructure nanocavity was created at the center of the structure as shown in Fig. 1(a). The lattice
constant in the \( x \) direction was increased by 5 nm every two periods upon approaching the center (the lattice constant in the \( y \) direction was not changed). As a result, optical confinement regions are generated at the lower-frequency edge of the even-propagation band due to changes in the confinement for the odd-propagation band is achieved in a similar manner.26–29 It should be emphasized that, in general, only the resonant modes associated with the even-propagation mode have been examined in studies on Raman Si lasers.30,31 Here we additionally focus on the resonant modes that arise from the odd-propagation mode.

### III. EXPERIMENTAL METHOD

Figure 2 shows the setup used for spectroscopic measurements. The light from a tunable cw laser was split into two beams. One beam was sent to a high-resolution wavelength meter. The other was modulated by a mechanical chopper at a frequency of \( \sim 1 \) kHz with a 50% duty ratio and was focused by a 0.42-numerical-aperture (NA) objective lens on the facet of the excitation waveguide. The transmitted light from the opposite facet and the dropped light from the cavity in the direction vertical to the slab were collected by 0.40-NA lenses. The sample was placed on a high-precision 5-axis stage and the positions of the optical components were adjusted using near-infrared (NIR) cameras such that only the dropped and transmitted light passed through pinhole apertures, analogous to the situation in confocal microscopy. The intensities of the dropped and transmitted light were measured by lock-in amplifier systems as a function of the laser wavelength. Because the PBG for 2D-PCs is inactive for transverse magnetic (TM) polarization, incident and transmitted light with transverse electric (TE) polarization were used.

All resonant modes were excited by utilizing the even-propagation mode of the excitation waveguide because incident light on the waveguide facet easily couples to this mode (coupling to the odd-propagation mode is more difficult). We constructed several samples with different values of \( w \) and \( l \) in order to control the frequency of the even-propagation band and the magnitude of the evanescent mode coupling between the propagation mode and the resonant modes: one pair of samples had \( w = 1.07 \) W1 (W1 = 710 nm) and \( l = 5, 6 \), which were used for measuring the resonant modes near as a FP cavity.26–29

![FIG. 1. (Color) (a) Schematic of a measured nanocavity sample. (b) Band diagram for the cavity in the \( x \) direction. (c) Calculated photonic band structure for a line defect with parameters \( a_1 \) and W1.](image)

![FIG. 2. (Color online) Setup for spectroscopic measurements.](image)
the lower edge of the even-propagation band. A second pair of samples with \( w = 0.95 \) W1 and \( l = 4, 5 \) covered the middle frequency region. A third pair with \( w = 0.91 \) W1 and \( l = 3, 4 \) were used to investigate the higher-frequency region, including the odd-propagation band. All samples had the same cavity structure and were fabricated on the same chip.

IV. EXPERIMENTAL RESULTS

Figure 3(a) presents the frequencies \( f \) and \( Q \) values of all the resonant modes that were experimentally observed between 1450 nm \( (f = 0.282) \) and 1590 nm \( (f = 0.258) \). This range almost covers the odd- and even-propagation bands denoted in Fig. 1(c) where high-\( Q \) modes are formed (the \( Q \) factors are much lower above the light line). In Fig. 3(b) the dropped and transmitted spectra for the lowest-frequency mode at \( f = 0.259 \) are shown. Similar spectra were obtained for the other resonant modes. The \( Q \) values in Fig. 3(a) do not include the load of the excitation waveguide and were estimated from the wavelength \( (\lambda_0) \), linewidth \( (\Delta \lambda) \), and transmittance \( (T_0) \) at the resonant peak using the following relation:

\[
Q = \frac{\lambda_0}{\Delta \lambda \sqrt{T_0}}.
\]  

(1)

The open (blue) and solid (red) circles in Fig. 3(a) indicate resonant modes originating from the odd- and even-propagation modes, respectively. We were able to determine the origin of each mode using the polarization properties of the dropped light. Dropped light originating from the odd-propagation mode was polarized in the \( x \) direction whereas that from the even-propagation mode was polarized in the \( y \) direction, as shown in the insets. These properties can be explained by the far-field cancellation effect in \( E_x \) (\( E_y \)) for the even- (odd-) propagation mode. The nanocavity modes were distinguished from the FP modes using their emission images. Emission from the nanocavity modes is located at the center of the heterostructure, whereas emission from the FP modes occurs at the cavity edges, as shown in Figs. 3(c) and 3(d). The lowest-frequency resonant modes in both the odd and even sets are the heterostructure nanocavity modes (solid lines). The higher-frequency modes are all FP modes (dashed lines). In summary, four types of resonant modes were observed, as expected: an even nanocavity mode, even FP modes, an odd nanocavity mode, and odd FP modes. The FP modes follow the FP resonance condition of \( k_l = (\pi/L) m \) for each propagation mode, where \( k_l \) is the wave vector, \( L \) is the cavity length, and \( m \) is the modal integer number. The dispersion curves presented in Fig. 1(c) determine the relation between \( k \) and \( f \). Therefore, for most of the range, the modal number of the FP modes increases with frequency. We note that fewer odd FP modes were observed than even FP modes because several of the odd FP modes were not spectrally resolved due to their small \( Q \).

V. DISCUSSION

We will now evaluate the applicability of the observed resonant modes to Raman Si lasers from the viewpoint of \( Q \) and \( f \). A Raman Si laser requires two high-\( Q \) resonant modes to confine the pump light and the Stokes Raman-scattered light. We refer to these as the pump mode and Stokes mode, respectively, and we define the \( Q \) and \( f \) for the pump (Stokes) mode as \( Q_p \) and \( f_p \) (\( Q_S \) and \( f_S \)). To achieve lasing, the frequency spacing between the modes should be matched to the Si Raman shift of 15.6 THz. High \( Q \) factors are also important; \( Q_S \) is particularly significant in order to overcome the free carrier absorption loss associated with two-photon absorption (TPA). Because the Raman gain depends linearly on the pump power whereas the TPA-induced loss has a superlinear dependence, the Raman gain can be made to exceed the losses in the low pump region by increasing \( Q_S \). Although the value of \( Q_S \) depends on a number of parameters (for example the free carrier lifetime, Raman gain coefficient, TPA coefficient, and modal overlap), we have experimentally confirmed that a \( Q_S \) of \( \sim 1 \times 10^6 \) is required for cw operation (details will be reported elsewhere). Although such a high value is not required for \( Q_p \), values larger than a few tens of thousands are advantageous for practical operation with a threshold less than several tens of \( \mu \)W.

In the lower-frequency range of Fig. 3(a), \( Q \) values of more than \( 1 \times 10^6 \) were obtained for the even nanocavity mode and several of the even FP modes, which might also be candidates for the Stokes mode. In the higher-frequency range from which the pump mode should be selected, the odd nanocavity mode, odd FP modes, and even FP modes were all observed. We note that a separation of 15.6 THz from \( f_S \equiv 0.260 \) is impossible
for pump modes with \( f < 0.275 \), even if \( a_1 \) is decreased to its lower limit for the operation wavelength of \( \sim 1.2 \) \( \mu \)m which is determined by the band gap of Si. Because the \( Q \) factors of the even FP modes with \( f > 0.275 \) are less than 10 000, the odd nanocavity mode and odd FP modes at \( f \approx 0.277 \) emerge as candidates for the pump mode. Table I summarizes the possible Stokes and pump modes and indicates that the resonant mode originating from the even-propagation mode should be paired with that arising from the odd-propagation mode. The frequency spacing between these modes can be tuned to 15.6 THz by varying the air hole radius.\(^{17} \)

Next, we consider the applicability of all four types of modes for SRS by examining the modal overlap of their electric fields. Figures 4(a)–4(f) show the calculated \( E_y \) for a line-defect cavity consisting of 39 missing air holes with a two-step heterostructure. The photonic parameters used in this FDTD calculation are the same as in Fig. 1. Figures 4(a)–4(c) show \( E_y \) for the first, second, and third resonant modes created by the even-propagation mode. The modal numbers \( m \) for these modes are defined as \( m = 1, 2, \) and 3. Figures 4(d)–4(f) show \( E_y \) for the resonant modes arising from the odd-propagation mode. The distributions in Figs. 4(a) and 4(d) imply that the ground-state modes with \( m = 1 \) are the heterostructure nanocavity modes, in agreement with the experimental results.

A pair of pump and Stokes modes should have large modal overlap for efficient SRS. Here the modal symmetries of \( E_x \) and \( E_y \), modal number \( m \), Raman tensor of Si, and crystallographic direction in which the cavity is formed are important factors. As shown in Fig. 4, even-odd mode pairs with the same \( m \) have similar distributions in the \( x \) direction whereas mode pairs with different \( m \) have different distributions. Therefore, the former situation is favorable for large overlap. However, even-odd mode pairs have the opposite symmetries in \( E_x \), with respect to the \( xz \) plane (\( \sigma_{xz} \)) and \( yz \) plane (\( \sigma_{yz} \)) at the center of the defect. Although not shown here, this is also the case in \( E_x \). These properties are favorable if we would fabricate the nanocavity along the [100] crystal direction on a (001) SOI substrate. This is because the SRS gain via the Raman tensor of Si is proportional to the following integral in such a cavity:\(^{17} \)

\[
\int_{Si} |E_{x,S}^* E_{y,p} + E_{y,S}^* E_{x,p}|^2 dxdydz. \tag{2}
\]

Here the subscripts \( S \) and \( p \) indicate the Stokes and pump modes, and the label Si refers to the integral excluding the air holes. The overlap integrals between the cross components are important in Eq. (2) and the cross components for even-odd mode pairs with the same \( m \) have the same symmetry. In contrast, the SRS gain is proportional to the overlap integrals between the same components for a cavity fabricated along the [110] direction:

\[
\int_{Si} |E_{x,S}^* E_{x,p} - E_{y,S}^* E_{y,p}|^2 dxdydz. \tag{3}
\]

In this situation the combination of even-odd mode pairs is unfavorable. In addition, the negative terms are disadvantageous for any pair of modes. The relative magnitudes of the \( Q \) factors displayed in Table I are insensitive to the direction of fabrication ([100] or [110]) because both the periodic refractive

<table>
<thead>
<tr>
<th>For Stokes mode</th>
<th>( Q_S )</th>
<th>For pump mode</th>
<th>( Q_p )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Even nanocavity mode ( f = 0.259 )</td>
<td>Highest ( \gg 10^6 )</td>
<td>Odd nanocavity mode ( f = 0.275 )</td>
<td>High ( \gg 10^5 )</td>
</tr>
<tr>
<td>Even FP mode ( f = 0.260 \sim 0.261 )</td>
<td>High ( \gg 10^6 )</td>
<td>Odd FP mode ( f = 0.277 \sim 0.278 )</td>
<td>Medium ( 10^4 \sim 10^5 )</td>
</tr>
</tbody>
</table>

**TABLE II.** Magnitudes of Eq. (2) for even-odd resonant mode pairs with \( m = 1 \) to 3. These values are normalized by the value for a pair of ground-state nanocavity modes.

<table>
<thead>
<tr>
<th>Resonant mode</th>
<th>( m = 1 )</th>
<th>( m = 2 )</th>
<th>( m = 3 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Even ( m = 1 )</td>
<td>1</td>
<td>0.07</td>
<td>0.06</td>
</tr>
<tr>
<td>Even ( m = 2 )</td>
<td>0.47</td>
<td>0.20</td>
<td>0.05</td>
</tr>
<tr>
<td>Even ( m = 3 )</td>
<td>0.05</td>
<td>0.28</td>
<td>0.30</td>
</tr>
</tbody>
</table>
magnitudes of the integral in Eq. (2) for this pair are 10 to 20 times smaller than the two ground-state nanocavity modes by decreasing the length of the FP cavity; however, the calculated $Q$ factors are as high as $2 \times 10^7$ and $6 \times 10^5$, respectively. By applying techniques to increase the $Q$ factors by shifting the air hole positions, sufficiently high $Q$ values for lasing will be obtained even in FP cavities with shorter lengths. Raman lasing with high output power will be expected for this design due to the large volume.

VI. SUMMARY

We have studied the optical properties of high-$Q$ resonant modes in a PC heterostructure cavity in order to investigate their applicability to Raman Si lasers. Four types of resonant modes were observed, which have highest $Q$ factors near the lower edges of the original propagation bands. After consideration of all the relevant factors, the pair of ground-state heterostructure nanocavity modes that originate from the first-order (even) and second-order (odd) propagation modes is the most suitable combination for Raman Si lasers. A pair of higher-order modes might also have some potential. The optical properties reported in this paper will be helpful in studies of Raman Si lasers or amplifiers in other types of PC devices.

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