Design and modeling of optomechanical cavities

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We have designed a silicon optomechanical crystal (OMC) nanobeam with a cavity in the center that enables to confine the light through an optical trap. The OMC is constructed on the basis of a unitary cell that is repeated several times to create a mirror region that is placed on the sides and a defect region in between. The latter consists of a set of cells whose dimensions have been reduced towards the center so that in varying the sizes of the cell through a one-dimensional chain of these cells using the gaps in the optical bands it is possible to achieve optical modes confined to the center of the chain. Regarding the mechanical modes, we have focused our study on string-type mechanical modes oscillating outside the plane of the sample, that are well coupled to photonic cavity modes. Our work has consisted of optimizing the optomechanical (OM) coupling by introducing an angle (α) in the walls of the cell so that we have been able to break its vertical symmetry and achieve modes with large OM coupling coefficient g. We have concluded that, following this strategy, g increases significantly as we increase the angle, going from $\frac{g}{2\pi} = 0.0045\,MHz$ for the chain with α=0º to obtaining $\frac{g}{2\pi} = 1.2413\,MHz$ and $\frac{g}{2\pi} = 1.7298\,MHz$ for α=30º and α=40º, respectively, when considering the mechanical mode with one antinode that appears at around 4 MHz.

I. INTRODUCTION

In recent years, interest has grown in studying optomechanical crystals, which are periodic structures that allow us to control light waves and phonons. Exploiting the band energy gaps that are generated both in the optical and in the phononic parts, traps can be created to guide or confine the light and motion. These gaps allow us to couple the two modes of vibration (OM coupling), forming what are called photonic crystal OM cavities (Aspelmeyer et al. [5]).

Different studies such as the one from Chan et al. [1] have shown a good coupling of these modes through the design of cavities in the periodic structure.

The strong interaction between phonons and photons, quantified by the OM coupling rate (g), has been well demonstrated theoretically and experimentally in many works. In the Oudich et al. [2] work a silicon piece such as the one shown in Figure 1a was studied. By varying the radius of the cavity (r), the size of the wings (hx) and the pitch (a), it is possible to confine the light in the center of a one-dimensional chain of said cells and obtain a sizeable coupling between cavity optical modes and mechanical modes. The results of that study were positive but focused on in-plane cavity mechanical modes. Given that the unit cell is symmetrical regarding the xy plane, the optical modes are also symmetric to it and, as we will show later on, the coupling with out-of-plane mechanical modes becomes practically null.

Our objective in this work has been to explore strategies to increase the OM coupling with out-of-plane mechanical modes while keeping the optical cavity modes in the range of the tunable lasers that are present in the lab. Thus, we have dedicated ourselves to studying this type of unit cell by adding a certain angle to its height (Figure 1b). This allows us to break the symmetry on the z axis so that we get more mass at the bottom than at the top. With this change, we expect to shift the electromagnetic field spatial distribution towards the bottom of the unit cells and thus enhance the contribution to g of the bottom surface deformation at the expense of the contribution of the top one.

A. Methods

For the entire process of modeling and OM study we have used the multiphysics COMSOL program [8].

The sizes for a, hx, hy, r, and t are the same ones for the original unit cell (Figure 1a). For construction reasons regarding the unit cell, we have it with these sizes at half its height. The building material is Silicon because of its good optical and mechanical properties and its cheap price.

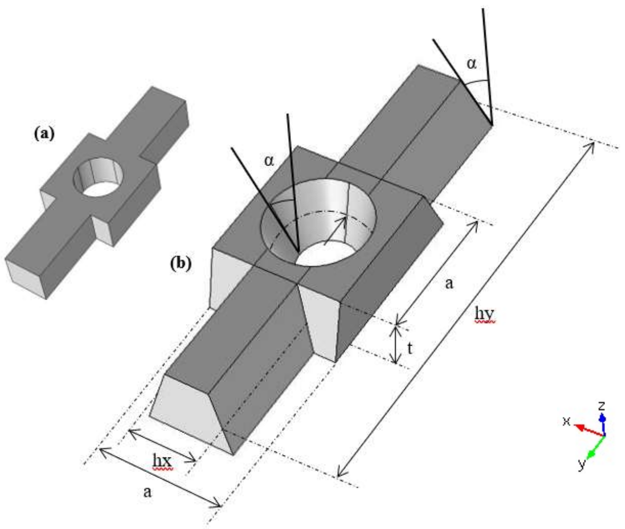

Fig.1. *(a) Unit cell corresponding to the Oudich et al. [2] work. (b) Unit cell designed by us with the parameters a = 500nm, hx = 0.5a, hy = 3a, r = 0.3a nm, t = 220nm, α = 30º.*

II. EQUATIONS

To understand where this whole study is framed, perhaps it is interesting to propose the following device: the paradigmatic example of an optomechanical cavity is a Fabry-Perot optical cavity in which one of the mirrors is attached to a spring. The photons that remain between the walls make pressure and cause the oscillation of the moving wall. When the mirror moves, there is a shift of the wavelength of the photons

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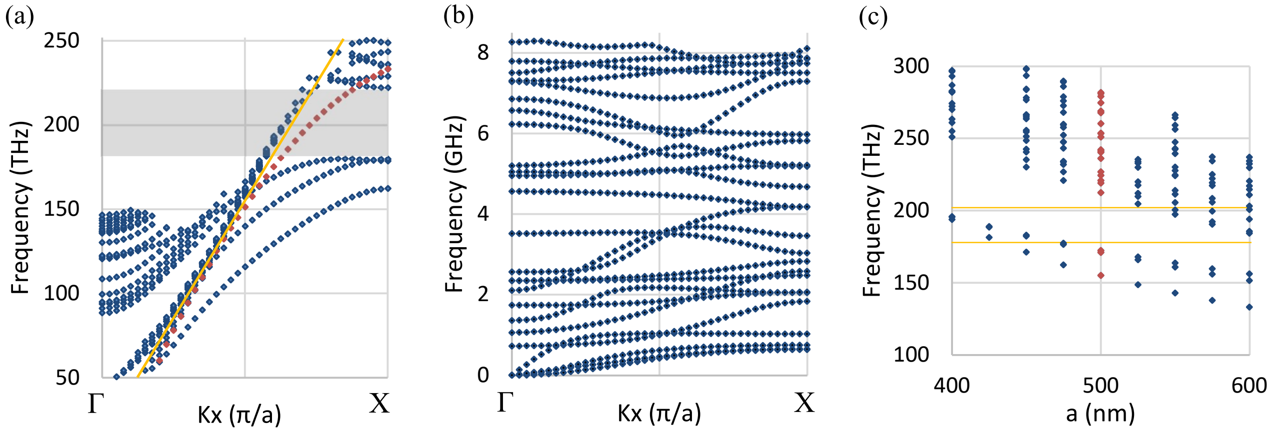

Fig.2. *(a) Band diagram for optical modes. In yellow, the light line; in red, de TM modes. (b) Band diagram for mechanical modes. (c) Parametric study of the optical modes as a function of pitch a for point X in the band diagram of (a). In yellow, our laser range; in red, the modes for the dimension a = 500 nm.*

supported by the cavity. The figure of merit that quantifies the strength of this interaction is the OM coupling rate (g), which reflects the optical shift of an optical resonance (in Hz) as a consequence of the motion of a mechanical mode in its quantum ground state (Aspelmeyer et al. [5]).

Thus, our study is described according to quantum, although it goes hand in hand with classical theories. That is why we can use all the band theory typical of "Solid State Physics" [4].

As we can see in Aspelmeyer et al. [5] expression 22 and 23, the Hamiltonian of the system and the restoring force are given by the following expressions:

$$\hat{H} = \hbar\omega_0 a^\dagger a + \hbar\Omega_m b^\dagger b - \hbar g a^\dagger a(b^\dagger + b) + \cdots \quad (1)$$

$$F = -\frac{d\hat{H}_{int}}{dx} = \hbar\frac{g}{x_{zpf}} a^\dagger a \quad (2)$$

where ω_0 is the confined light frequency, Ω_m is the mechanical oscillation frequency, $a^\dagger a$ and $b^\dagger b$ are the creation and annihilation operators of single photon and phonons respectively, $\hat{H}_{int}$ corresponds to the third addend of the Hamiltonian, $x_{zpf} = \sqrt{\frac{\hbar}{2m_{eff}\Omega_m}}$ is the mechanical amplitude around the equilibrium point when the mode is in the ground state, $g = Gx_{zpf}$ is the coupling coefficient and G comes from the variation of the frequency in the cavity as a function of the distance between mirrors $G = -\frac{\partial\omega_0}{\partial x}$.

The goal is to achieve a design with a larger OM coupling g. To evaluate it, we follow the expressions introduced by Chan et al. [1]:

$$g_{MI} = -\frac{\omega_0}{2}\frac{\oint_{\partial V}(\boldsymbol{U}\cdot\boldsymbol{n})\left(\Delta\varepsilon\left|E_\parallel\right|^2 - \Delta\varepsilon|D_\perp|^2\right)dS}{\int_V \boldsymbol{E}\cdot\boldsymbol{D}dV} \quad (3)$$

$$g_{PE} = -\frac{\omega_0}{2}\frac{\left\langle E\left|\frac{\partial\varepsilon}{\partial x_i}\right|E\right\rangle}{\int_V \boldsymbol{E}\cdot\boldsymbol{D}dV} \quad (4)$$

where **U** is the normalized displacement field ($max\{|\boldsymbol{U}|\}$, **n** is the outward facing surface normal, **E** is the electric field, **D** is the displacement field, ε is the material permittivity, $\Delta\varepsilon \equiv \varepsilon_{silicon} - \varepsilon_{air}$, and $\Delta\varepsilon^{-1} \equiv \varepsilon_{silicon}^{-1} - \varepsilon_{air}^{-1}$. As our medium is isotropic of refractive index n, $\frac{\partial\varepsilon_{ij}}{\partial x} = -\varepsilon_0 n^4 p_{ijkl}S_{kl}$ where p is a tensor of rank 4 and S is strain tensor.

Using the symmetries of our crystal, the calculation can be simplified as follows:

$$\begin{aligned}\left\langle E\left|\frac{\partial\varepsilon}{\partial x_i}\right|E\right\rangle = -\varepsilon_0 n^4 \int dV \Big[&2Re\{E_x^*E_y\}p_{44}S_{xy} \\ &+ 2Re\{E_x^*E_z\}p_{44}S_{xz} + 2Re\{E_y^*E_z\}p_{44}S_{yz} \\ &+ |E_x|^2\left(p_{11}S_{xx} + p_{12}(S_{yy}+S_{zz})\right) \\ &+ \left|E_y\right|^2\left(p_{11}S_{yy} + p_{12}(S_{xx}+S_{zz})\right) \\ &+ |E_z|^2\left(p_{11}S_{zz} + p_{12}(S_{xx}+S_{yy})\right)\Big]\end{aligned} \quad (5)$$

where $(p_{11}, p_{12}, p_{44}) = (-0.094, 0.017, -0.051)$ for a Silicon crystal.

As in Oudich et al. [2], the OM coupling coefficient is obtained by calculating the photonic shift caused by the structure motion introduced by the phonon. If we take the photoelastic effect (PE) and the moving interfaces effect (MI) into account, we obtain the two contributions of the coupling coefficient g_{PE} and g_{MI}. To obtain g/2π, we have the sum of g_{PE}/2π and g_{MI}/2π multiplied by the mechanical amplitude x_{zpf}.

III. DEVELOPING SECTIONS

Next, we will develop everything that we have been announcing, starting with the unit cell modeling, followed by the study of the optical and mechanical modes and, finally, the OM coupling.

A. Modeling of the unit cell

As it can be seen in Figure 2a, the optical gap is practically identical to the gap found for the OMC without an angle [2]. Instead, in Figure 2b, we can see that there is not a complete gap. This is not worrisome as the bands seen in the diagram can be distinguished by different symmetries. In the end,

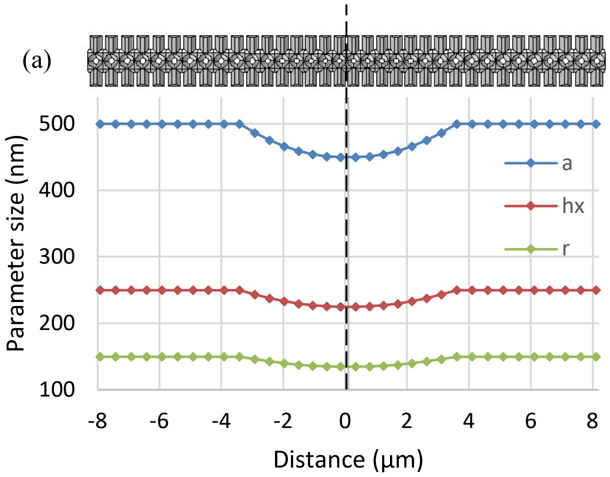

Fig.3. *Variation of the parameters a (blue), hx (red) and r (green) as a function of the position in the one-dimensional chain tied at both ends and formed by the studied cells.*

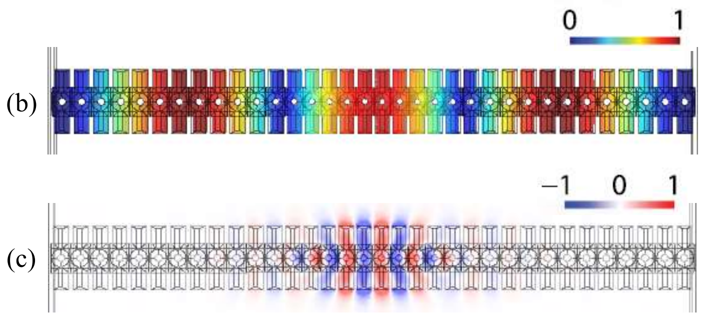

Fig.4. *(a) Deformation profile of a mechanical mode having three antinodes corresponding to the frequency 2.5395·10^{7} Hz. (b) Ey of an optical mode corresponding to the frequency 1.8453·10^{14} Hz. Both modes for an angle of 30º.*

finding a range in which there is a gap between the bands of the chosen symmetry is enough for the coupling we want to make. These types of gaps are called "pseudo-gaps". However, we are mostly interested in modes close to the gamma point at frequencies in the order of tens/hundreds of MHz, and what matters is that our chain is tied at both ends, so getting total gaps or pseudo-gaps is not relevant.

As our laser emits with a wavelength between 1480 nm and 1680 nm, which corresponds to a frequency range between 178 THz and 202 THz, the optical gap must be in such figures, as well as the mode we choose for the OM coupling. Then, looking at Figure 2a, we can conclude that the gap is located in the correct place. It is worth noting that, in Figure 2a, the yellow line corresponds to the light line.

The band that appears in the gap around 200 THz (red dots) corresponds to the TM polarization in the figure, which is not relevant to our study since, in the experiment we excite the OMC with TE polarization. Despite setting perfect conductor conditions in the direction of the chain length (y-axis), it somehow sneaks in the perpendicular direction.

We have varied the parameters a, r and hx (see Figure 1b) to design the defects in the one-dimensional chain of cells. We want to make an optical trap in the center so that the light does not propagate at the ends and gets confined to the center. This means that at the chain's ends we need the parameters to be those corresponding to the gap of the optical bands (Figure 2a).

As it can be seen in Figure 2c, for a frequency around 180 THz we have a gap. If we vary the cell parameter a making it smaller, it can be seen that the bands go up in energy, so that it would be possible to create confined optical modes by introducing smaller cells in between two mirror regions constructed by the repetition of larger cells. Therefore, we have built the OMC with a = 500 nm at the ends (mirror regions), and we have varied a, together with r and hx, as shown in Figure 3.

Those parameters have been reduced in a hyperbolic way towards the center down to a factor Γ=0.9 of the values on the mirror region with the same factor Γ for all the geometrical parameters. In this way, the center cells have these parameters 10% lower.

B. Optical and mechanical modes

We look for mechanical modes vibrating outside the x-y plane, that is, string-like modes that vibrate in the z direction. These are like the harmonics that arise from vibrating a string tied at both ends, where the string is clamped to the silicon layer at both sides. As the optical modes will be centered in the chain and we are looking for a good OM coupling, we must look for the phononic modes that are centered, those with odd numbers of antinodes.

With this symmetry in our structure, we can achieve a good coupling between the mechanical modes of interest and the optical modes. Comparing the results of the chosen modes (Figure 4a with 4b), to see that the position of the most intense part in the case of the mechanical mode coincides with that of the optical mode.

The frequency at which we find the chosen mechanical mode is 2.5395·10^{7} Hz in the case of the unit cell with an angle of 30º. Modes that oscillate outside the x-y plane are in the low frequency range (tens of MHz). We have chosen this mode before the fundamental one because its frequency is more interesting for nonlinear dynamics applications (D. Navarro-Urrios et al. [6]). Also, we have looked for the most energetic optical mode that has a frequency of 1.8453·10^{14} Hz, which falls within the laser range defined above. This fundamental mode does not significantly vary as a function of the chosen angle because, in the way our OMC is designed, the average hole radius always varies in the same way regardless of the chosen angle.

Next, we will discuss whether our design has been the correct one to break the vertical symmetry and thus achieve a

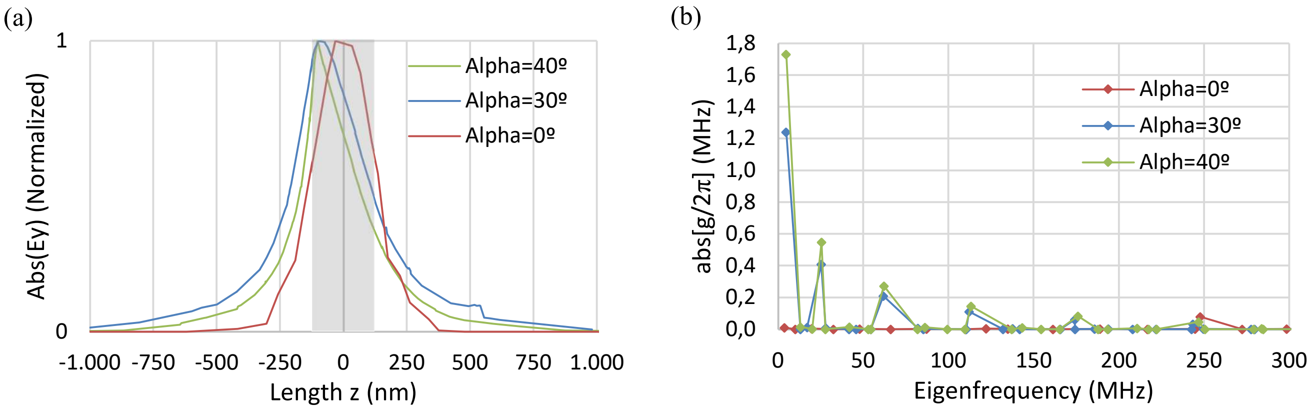

Fig.5. *(a) Energy in the y-axis direction as a function of the height of the cell in the z-axis direction having the center of the unit cell at z = 0, for the angle values 0º (red), 30º (blue) and 40º (green). (b) OM coupling coefficient as a function of frequency for each angle. (c) Table with the OM coupling coefficient values for the one anti-node (g1/2π) and the three-antinodes (g2/2π) mechanical modes.*

(c)

Alpha (º)	$g_1/2\pi$ (MHz)	$g_2/2\pi$ (MHz)
0	0,0111	0,0045
30	1,2413	0,4093
40	1,7298	0,5487

higher OM slice along the z direction, in the center of the OMC, we have plotted Figure 5a. We trace the electric field in the y-axis direction through the z-axis in the center of the unit cell. This plot verifies that the mode is shifted towards the negative values of the z-axis, which corresponds to the lower part of the cell.

In this same study, we do not see an important difference between the one-dimensional chain with the angle of 40º compared to that of 30º, but we do see a difference regarding the cell with the vertical walls, 0º.

C. Optomechanical Coupling

From equations (3) and (4), we obtain the value of the OM coupling for the moving dielectric boundary and the photoelastic effect.

$$\frac{g}{2\pi} = \frac{1}{2\pi}(g_{PE} + g_{MI})x_{zpf} \tag{6}$$

We will look at the total sum of the two coefficients of the OM coupling although, at low frequencies, g_{PE} can be neglected regarding g_{MB} so that the values we have represented are practically the values of g_{MB} in absolute value.

In Figure 5b we can see that, by adding an angle to the initial cell, the OM coupling increases by an order of magnitude giving very large coupling values. As we have said, the values of the OM coupling are located in a low frequency range of 4 MHz for the one-antinode mechanical mode, and 25 MHz for the three-antinode mechanical mode.

We have calculated this value for 3 different angles: 0º (corresponding to the unit cell by Oudich et al. [2]), 30º and 40º and we have registered the maximum values for each angle. The values of g/2π obtained are 0.0045 MHz, 1.2413 MHz and 1.7298 MHz respectively (see Table 4c). The relatively large g/2π value for de cell with 0º that we can find at 247 MHz corresponds to an in-plane mechanical mode that is not affected by the presence of the wall angle.

We have not been able to study higher angles because the width of the unit's cell wings overlapped with those of the neighbors, losing the sense of the proposed design.

A good improvement to do could be to make a program with Matlab or another language with which we would be able to optimize all the parameters, especially the Alpha angle.

IV. CONCLUSIONS

In this work we have looked for a cavity design in a nanobeam with a certain angle to be able to break the vertical symmetry of the initial unit cell and achieve a greater OM coupling.

The band structure fits well into the range we need for later fabrication and allows us to create the desired photonic crystal to create an optical trap. The optical mode that we have chosen is the fundamental one and appears at around $1.85 \cdot 10^{14}$ Hz regardless of the angle. This mode is created from the lower band in the optical gap.

First, we conclude that designing the unit cell in a non-symmetrical way, displaces the optical modes confined in our cell towards the lower part of the beam, taking more advantage of the mechanical oscillation in what concerns the OM coupling.

With that design we have demonstrated that optical modes couple nicely with mechanical modes that oscillate outside the x-y plane. In our case, we have a large OM coupling with mechanical oscillations with an odd number of antinodes. These types of modes are found in the low frequency, near the point Γ, in our case at frequencies around few/tens of MHz.

The results obtained with our design optimize the coupling at least an order of magnitude more than the design of the unit cell without an angle. We have explicitly obtained values for the coefficient $g/2\pi$ of 1.27 MHz for an angle of 30º and 1.73 MHz for an angle of 40º for the mode with one antinode. Compared with 0.09 MHz for a one-dimensional chain without angle (α = 0º), we conclude that the greater the angle, the greater the coupling we get.

The fabrication of this kind of structures seems feasible as it would only require modifications on the Reactive Ion Etching recipe to pass from vertical to tilted walls (Henri Jansen et al. [7]).

V. APPENDIX

We add other parametric studies corresponding to Figures 5a and 5b that we have done in the same way as Figure 2c. The radius does not influence as much as the length hy of our unit cell. In our study we have not varied hy, which could be interesting if with this variation we manage to further optimize the part.

On the other hand, we also made a study of the bands in position X as a function of the angle to see how it varied from an angle of 0º to 30º. It can be seen in Figure 6c, that as we increase the angle, the gap becomes larger by the lower band, but it is reduced by the upper band.

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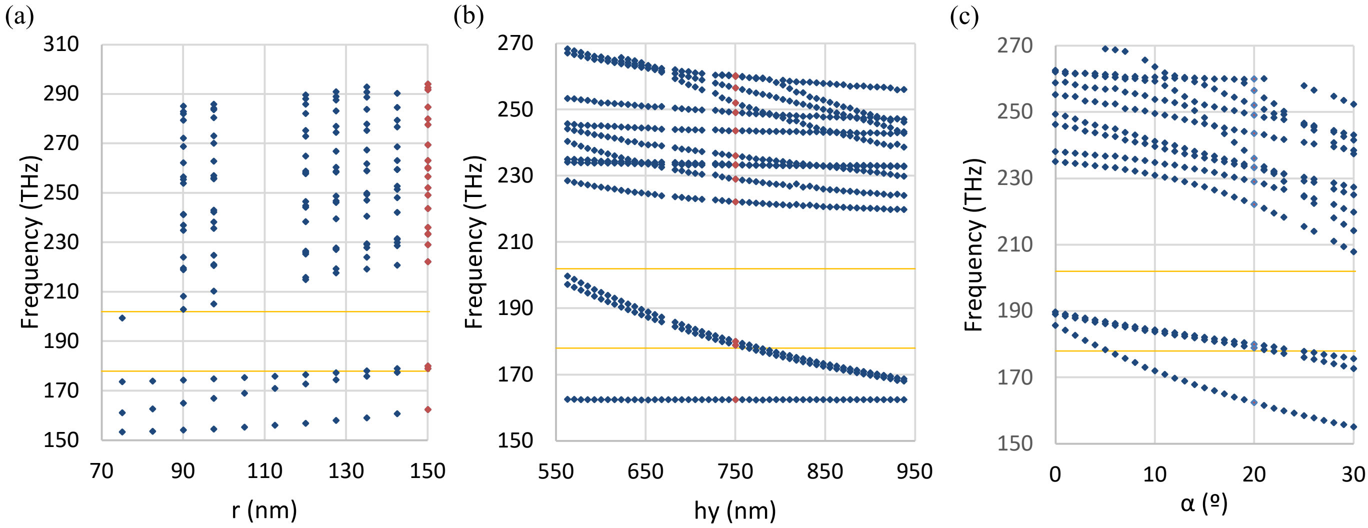

Fig.6. *In yellow, our laser range. (a) Parametric study of the optical modes as a function of the radius r for point X in the band diagram of Figure 2c. In red, the modes for the dimension r = 150 nm. (b) Same study for the length of the unit cell hy. In red, the modes for the dimension hy = 750 nm. (c) Same study for angle α.*

[1] J. Chan, A. H. Safavi-Naeini, J. T. Hill, S. Meenehan, and O. Painter, Appl. Phys. Lett. 101, 081115 (2012).

[2] Mourad Oudich, Said El-Jallal, Yan Pennec, Bahram Djafari-Rouhani, Jordi Gomis-Bresco, Daniel Navarro-Urrios, Clivia M. Sotomayor Torres, Alejandro Martínez and Abdelkader Makhoute, PHYSICAL REVIEW B 89, 245122 (2014).

[3] J. Gomis-Bresco, D. Navarro-Urrios, M. Oudich, S. El-Jallal, A. Griol, D. Puerto, E. Chavez, Y. Pennec. Djafari-Rouhani. Alzina, A. Martínez & C.M. Sotomayor Torres. 10.1038/ncomms5452

[4] Solid State Physics - Neil W. Ashcroft & N.David Mermim. Cornell University.

[5] M. Aspelmeyer, T. J. Kippenberg, and F. Marquardt, "Cavity optomechanics," Rev. Mod. Phys., vol. 86, p. 1391, 2014, https://doi.org/10.1103/revmodphys.86.1391.

[6] D. Navarro-Urrios, N. Capuj, M. Colombano, P. D. Garcia, M. Sledzinska, F. Alzina, A. Griol, A. Martinez, C. Sotomayor-Torres, Nature Communications, 8, 14965 (2017)

[7] Henri Jansen, Han Gardeniers, Meint de Boer, Miko Elwenspoek and Jan Fluitman. J. Micromech. Microeng. 6 14 (1996).

[8] COMSOL simulations were launched using a CSIC licence associated to ICN2.