Project Summary: Designing Photonic Nanobeams with High Quality Factors and High Optomechanical Coupling Factors using MATLAB/COMSOL LiveLink Scripting

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For the summer of 2017, I came to IST to design a photonic nanobeam with high quality and high optomechanical coupling factors. In this report, I will detail what I have done with my time here and what still needs to be done. I start with an introduction, why we care about designing nanobeams and will then briefly introduce the necessary theory for understanding the terms in the paper. I then describe codes I have written and progress made in designing the nanobeam. The results are consistent MATLAB scripted simulations, giving rise to quality factors over a million, mechanical frequencies over 2 MHz, and optomechanical coupling factors over 10 MHz.

INTRODUCTION

Light exists all around us. When we look at ourselves in the mirror, what we are actually seeing is light reflecting off of us onto the mirror and then into our eyes. Turn off the lights and we see nothing. Physicists have been exploiting this property of mirrors for centuries, in applications ranging from laser pointers to the detection of gravitational waves. Today, I want to focus on the trapping and containing of light. In the example of laser pointers, we place two mirrors a distance apart and bounce light back and forth between the mirrors, thus forming a cavity. Adding a lasing medium such as gas into this cavity, allows the photon to create more photons through a process called stimulated emission. Releasing this build-up of photons by slightly tilting one mirror, thereby making it leaky, creates a laser. A similar idea of the trapping and containing light can also be achieved through the use of photonic crystals.

Silicon is our photonic crystal of choice for our experiments. Altering the geometry of silicon can create devices that trap and contain light. Figure 1 is an example of such a device.

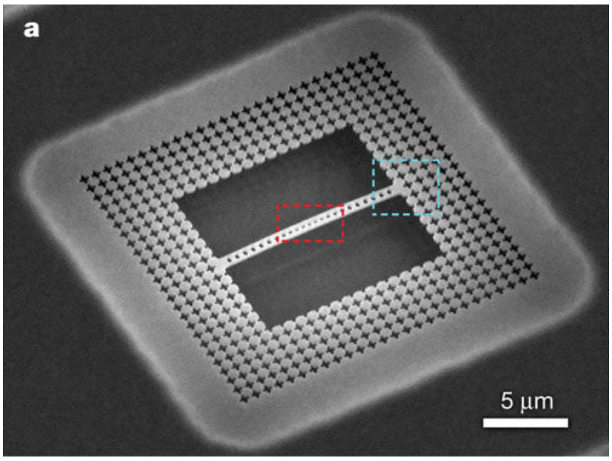

FIG. 1: Scanning electron microscope (SEM) image of a patterned photonic nanobeam slab (red) with a phononic shield starting on the outer boundaries (blue). [1]

In Figure 1, there is index guiding in the y and z directions, and Bragg scattering in the x-directions, allowing for a tight confinement of light inside the nanobeam structure. The nanobeam structure acts as a cavity for a specific range of frequencies depending on the geometry. For example, in my experience so far, it seems smaller hole sizes lead to higher frequencies. The phononic shield (in blue) acts to dampen acoustic radiation or noise. For our purposes, we will ignore this and focus on the nanobeam.

By cooling the nanobeam down to a few mK temperatures, you achieve what is known as the zero-point fluctuation, the lowest energy state of the device itself. In quantum mechanics, nothing is completely still meaning objects are always moving, albeit very little. Think of shaking a piece of rope. Shaking it faster and faster at certain frequencies causes more nodes to appear, and also more energy as your arms tire out. Of course, you can shake it diagonally, left and right, and all over, creating interesting patterns, which we call mechanical modes.

These silicon slabs are also called optomechanical crystals because of the strong confinement of both light and mechanics in the center of the beam (See Figure 2). As the mechanics fluctuate, the optical frequency also changes. This is due to physical distortions in the material itself as it moves. There are two types: the photoelastic effect and the moving dielectric boundary. As physicists, we find such physical interactions intriguing.

These nanobeams have applications in quantum communication networks [2]. Current communication networks process information using microwave light (gigahertz frequency) in their microprocessors and distribute information over long distances through optical fibers using terahertz frequencies (THz frequency). Recent advancements has also allowed for superconducting qubits

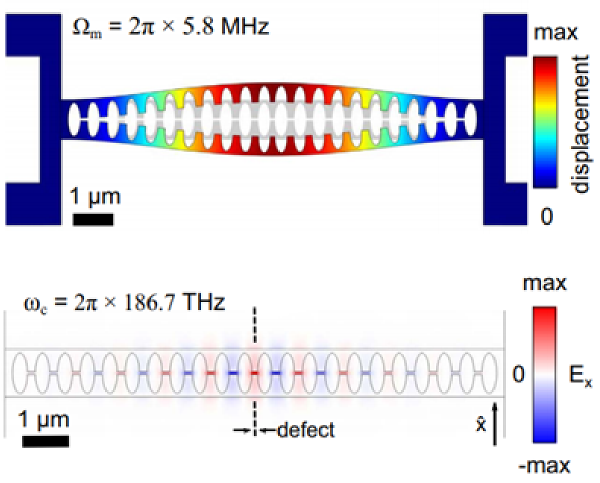

FIG. 2: An example of a nanobeam with a mechanical frequency of 5.8 MHz and optical frequency of 186.7 THz. The top image displays the mechanical displacement while the bottom displays the optical behaviour. Behaviour is maximized in the center of the beam. Figures taken from [6].

to operate at microwave frequencies. The parallel would be to distribute information also through optical fibers using terahertz frequencies, allowing for the creation of a quantum network. However, no such transducer currently exists. If we were to use microwave frequencies to distribute information with low loss, superconducting transmission lines would be required [3]. These optomechanical nanobeams offer a promising solution to convert between microwave and optical frequencies.

To understand how this conversion works, suppose we bring a light field close to the nanobeam. Experimentally, this is done by bringing a tapered optical fiber close to the nanobeam. The fields from the fiber then decay evanescently into the nanobeam, thus allowing light to be trapped in it. (For more on evanescent fields, look into a phenomenon called Frustrated Total Internal Reflection.) We use 1550nm light from a laser source. We then cool down the sample to its quantum ground state in a dilution refrigerator and use radiation pressure via lasers. By varying the radiation pressure, we can either dampen the resonator (nanobeam) via a detuning (using a lower frequency light as it is less energy) or excite it using a higher frequency light as it is more energy. As the mechanical displacement of the resonator changes, so does the optical frequency of the light inside the cavity. You can think of the silicon being stretched and shrunk at different points, which changes the intrinsic index of refraction. We measure this optical change.

Our motivation is to create a device with higher quality factors and optomechanical coupling factors. It's important that the light is contained, the interaction between mechanics and optics is strong, and we are operating in the sideband resolved regime.

THEORY

The first term to know is the optical quality factor. The optical quality factor is a measure of how well the cavity holds energy. Physically, we can describe this with

$$Q = \frac{\omega_0}{\gamma} \tag{1}$$

where ω_0 is the mode frequency and γ is the loss rate. ω_0 is used to ensure the scale invariance of Maxwell's Equations, making Q a dimensionless quantity. The quality factor can also be described as

$$Q = \frac{\omega_0 U}{P} \tag{2}$$

where U is the electromagnetic energy in the cavity and P is the outgoing power. Taking the reciprocal of (2), we obtain

$$\frac{1}{Q} = \frac{P}{\omega_0 U} \tag{3}$$

where $\frac{1}{Q}$ can be understood as the decay rate from the cavity. More specifically, $\frac{1}{Q}$ is the sum of two decay rates: $\frac{1}{Q} = \frac{1}{Q_w} + \frac{1}{Q_r}$ where $\frac{1}{Q_w}$ is the waveguide decay rate and $\frac{1}{Q_r}$ is the radiative decay rate. Because we are bringing in a tapered fiber to input light into the cavity, Q_w is very large. Thus we need to optimize our structure such that the radiative decay rate is minimized. This can be done by increasing the number of mirror cells to the nanobeam, making the band gap larger, or gently tapering to the defect versus an abrupt point defect, as abrupt defects result in significant radiation loss.

The optomechanical coupling factor describes how well the mechanics couple with the optics. Physically, the optmechanical coupling factor is described by

$$g = \frac{d\omega_0}{d\alpha} x_{zpf} = \frac{d\omega_0}{d\alpha} \sqrt{\frac{h}{2 m_{eff} \omega_m}} \tag{4}$$

Where α is a generalized coordinate, m_{eff} is the effective motional mass, and x_{zpf} is the zero point fluctuation of the resonator. As the displacement of the nanobeam changes, g describes the effect on the optical frequency ω_0. A higher value of g means better coupling between optics and mechanics, the interaction we are interested in utilizing for our quantum systems [4].

Lastly, we need a high mechanical frequency (ideally 200 MHz or more given 10^6 quality factor) to be sideband resolved. For now, we will try to achieve 2 MHz. See Figure 3 for a visual depiction of sideband resolution.

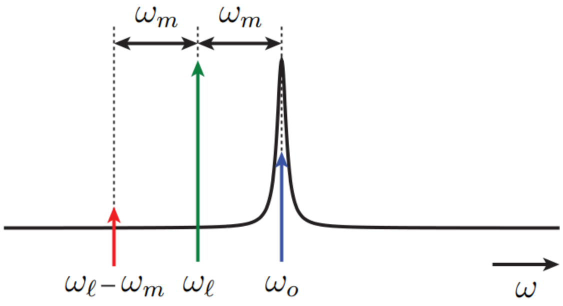

FIG. 3: See [5] for an explanation of sideband resolution.

METHODOLOGY

For our project, we will be using the COMSOL/MATLAB LiveLink interface which allows the user to run COMSOL from MATLAB. This functionality allows one to script simulations, make sweeps in changing parameters, and create optimization searches. Georg has built up a library of MATLAB functions for scripting purposes. Geometries can be drawn, meshing can be changed, all in a single main file that defines such parameters.

The goal is to have fully automated and scripted simulations that give stable and consistent quality and optomechanical coupling factors. Optimization algorithims can then be written to automatically find the best design. To get to this goal, we first had to develop a toolbox for understanding these simulations.

WHAT I'VE DONE

Learning COMSOL and Optimizing Computation time for Unit Cells

For the first two weeks, my project was optimizing the computation time for slotted unit cells. Pradyumna, last years intern, had computation times of 1 minute and 41 seconds per unit cell. (Pradyumna Unit Cell) My simulations take 22 seconds for the same geometry. The difference lies in geometry and meshing. For geometry, the idea is to think about how you can make the desired geometry with the least amount of steps. Pradyumna has 13 steps to draw the geometry, whereas I have only 7 steps. He draws many boxes in which he uses to make Boolean cuts to define his regions of Silicon and Air. I simply use less Boolean cuts. For meshing, he uses physics controlled meshing and sets it to $ExtremelyFine$. It should be noted that setting to $Finer$ makes the computation time just over a minute. What occurs is a bunching of elements near the vertex of the curve. I apply a Distribution to the curve, making the computation more efficient. The mesh is coarser but replicates the correct modes. Furthermore, faster computation times speeds up the band diagram generation process. See Figure 4 for meshing differences.

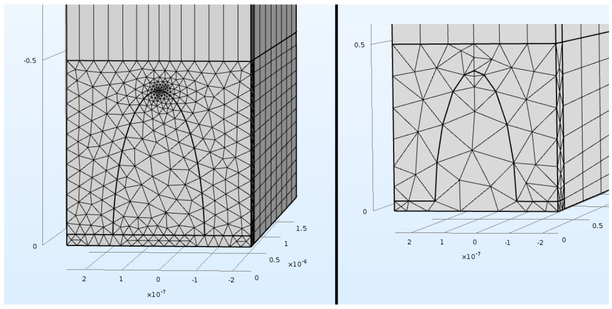

FIG. 4: Meshing for a unit cell. Pradyumna on the left and mine on the right. Both give the same optical modes.

What should be noted is that Pradyumna separates the domain of the air slot and air hole whereas I have it as one. This difference may become significant in the calculation of quality factors because of the number of elements in which you are solving. Generally the more elements, the more accurate the solution. See the folder named *Optimized Computation Time for Unit Cells* for files.

Band Diagram Generator — Unit Cell

The next step was to generate a band diagram of the unit cell. A program was already written by Matthias. My project was implementing my unit cell with a faster computation time. Additional features were added such as implementing the light cone (done by Georg), the region where there exists an infinite amount of modes (see pg 32 of Photonic Crystals), generating both antisymmetric and symmetric modes, and exporting the image of each mode. These images allow one to view the propagation of the mode as the value of k, the wavenumber, changes. This imaging is useful when we start changing the dimensions of these unit cells, (for example shrinking the lattice constant) and seeing how the mode changes. It also serves as a quick diagnostic in case your band plots has jumps or inconsistencies.

See the folder named *Band Diagram Generator — Unit Cell.* There are three geometries for which the band diagram codes have been written and optimized for: Verhagen slotted, Jaspar Chan mirror cell, and Georgs Zipper Beam. Each subfolder contains a simulated run for reference.

Band Gap Optimizer

The next idea was that a large band gap would result in higher quality factors due to less scattering or radiative losses. We implement fminsearch, MATLAB built-in function, to search for large band gaps given initial parameters. fminsearch itself is not a constrained optimization search algorithm, thus it is necessary that one downloads a modified version called fminsearchbnd. This modified function allows you to set bounds based on inequalities. For example, the width of the nanobeam may never be smaller than the vertical diameter of the air hole. Design parameters of what is feasible can then be specified.

We use two search functions. The first search function optimizes the bandgap to be as large as possible. The second function tightly centers the band gap around the desired central frequency. All data is written to a .dat file and a text file.

It should be noted that sometimes during optimization, the modes may bunch together. For example say our desired central frequency is 1.934×10^{14}. Our first mode is 1.7×10^{14} and our second mode is 2.1×10^{14}. Sometimes, it may occur that the second mode minimizes to the first mode, meaning the second mode becomes 1.701×10^{14}. To the function, these both mean the same. To avoid this, I have tried various functions involving absolute values and setting the optimization factor to Infinity (which resets fminsearch and generates a new search parameter). The ones in the file are what seems to work best. A better function could be utilized that possibly uses a absolute reference frame. All of this is documented in the MATLAB code.

Lastly, it should be noted that I do not know if larger band gaps are better than a tightly centered frequency, and by how much. In *Photonic Crystals: Molding the Flow of Light*, it is stated that the decay rate is strongest at the center of the band gap [4].

Another thought is whether all large band gaps would give the same performance. What I mean by same is suppose we have two band gaps that are the same size, but have different geometries. When we taper the beam, which depends on the geometry of the optimized mirror cell with large band gaps, would we obtain different values of opto-mechanical coupling and quality factors? My answer is I think yes for both because of what is being changed, for example the width of the beam would affect the mechanical frequency and the index of refraction. These would all be a point of investigation. All files are located in the folder named *Band Gap Optimizer*.

Fully Scripted Simulations of Nanobeams

What follows naturally is scripting our simulations such that an optimization over the whole beam can be carried out and sweeps can be done to find trends for intuition. Georg has built up a library of MATLAB functions in which you can call these functions, draw geometries, define meshing, and run simulations from MATLAB via the LiveLink interface. Using his functions, I drew a slotted beam. The geometry is automatically generated given initial parameters such as how many cells to taper over (in the function named *geometry_generator*). The tapering function is currently a quadratic function. The other function I tested is a cubic function, which led to lower quality factors. The reason behind these lower quality factors lies in where the strength of the taper is in regards to the location of the defect. In Figure 5, the slope is relatively flat, becomes stronger, and then weak. In the quadratic function, the slope is slow at the center and strong outwards. The tapering function is a parameter that can be optimized.

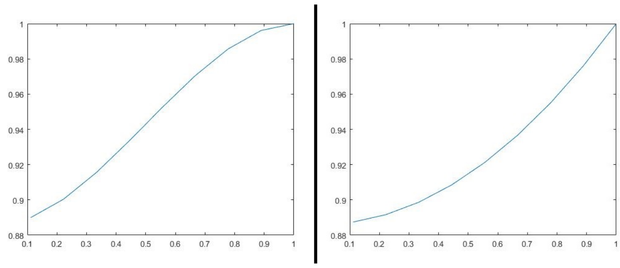

FIG. 5: On the left is the cubic tapering function, $y = (1 + d(2x^3 - 3x^2 + 1))$ and on the right is the quadratic tapering function, $y = x^2$.

Symmetry cuts were implemented to speed up simulation times. Everything is run from a central file named *d_beam*, in which geometry parameters can be designed, and for loops can be written for sweeps. Post-processing in the calculation of quality factors and optomechanical coupling factors is completely automated.

The initial sweeps however revealed instability in the quality factor. See Figure 6 for an example of this instability. As one increased the number of mirror cells, the quality factor begins to oscillate sinusodially instead of increasing exponentially or saturating (See pg 133 in Photonic Crystals) On the other hand, we do obtain the correct optical and mechanical modes and optomechanical coupling factors. See *Learning COMSOL and Optimizing Computation time for Unit Cells* for why this is.

The solution lies in the mesh. I need to emphasize: ***meshing is extremely important in the calculation of quality factors***. It took me a week to find appropriate meshing that gave an exponential increase that we ex-

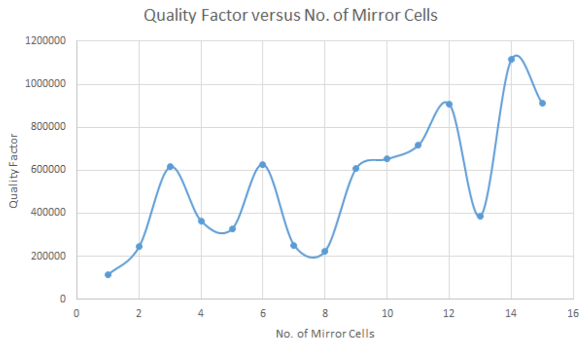

FIG. 6: As the number of mirror cells in the nanobeam are increased, the quality factor varies sinusodially. All other parameters are kept constant.

pect as we increase the number of mirror cells. Originally we had used physics-controlled meshing which automatically generates meshing based on the physics. For example, in materials such as air, COMSOL sets the maximum element to the $\frac{Wavelength}{5}$. For the nanobeam, where it is silicon, the mesh is much finer. However, physics controlled mesh does not account for inconsistencies in the regions you want more elements. For example, I use a distribution mesh on the curve, so that each curve is identical, meaning we solve at the same points each time. I also add a distribution mesh on the air slot edges. These changes gave me the desired exponential growth I was looking for. See Figure 7 for the meshing change. However, it was revealed that the quality factors decreased by half an order of magnitude compared to previous simulations of over a million Q. The lower quality factor is however, more accurate but concerning as after optimizing our band gap and tapering, we only have quality factors of 300,000. Nevertheless, 300,000 is already an improvement over Verhagens slotted beam design which had a quality factor of 800-1200 [6].

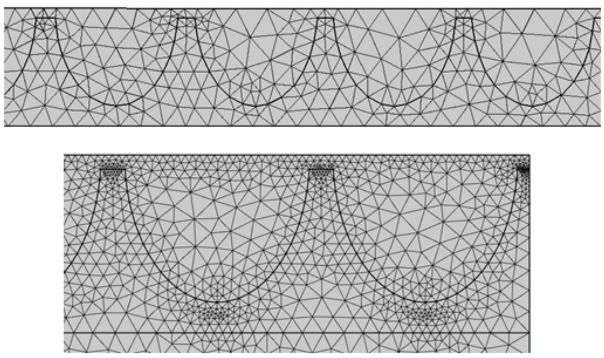

FIG. 7: Top is physics controlled mesh where at some regions are well defined and in others, not. A finer, more defined mesh is shown in the bottom image. Distributions have been applied at every edge to ensure consistency.

Simulation times can be reduced by making the mesh coarser. However, as geometry varies and changes, more consistent quality factors can be obtained by using high density meshing in the air slot. An idea would be to split the air slot and air hole into two domains instead of the one it is now. Distribution can then be applied on these edges. With a stable quality factor, we can now begin optimizing the computation time and then run accurate COMSOL sweeps and optimization searches for high quality and optomechanical coupling factor beams.

It should be noted that the converse of increasing the number of mirror cells was also swept. The number of mirror cells was kept constant and the size of the airbox was increased starting from just above the minima of zero, just above having no airbox. Simulations show that the size of the airbox does not matter much after a certain size. To double check if the airbox is large enough, it is advised to run this airbox sweep script. See Figure 8 for the graph of this sweep.

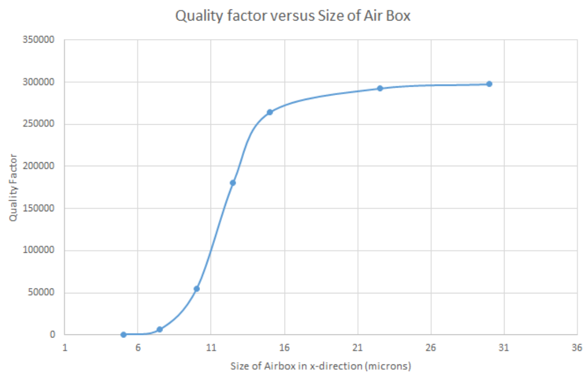

FIG. 8: The airbox in the x, y, and the z direction is increased and the quality factor is measured. Only the x-direction is shown in the figure.

Files are located in the Folder named Scripted Simulations. Scratch work can be found in drive D of the Simulations Computer.

Band Diagram Generator — Full Beam

In addition to having scripts, I have also expanded the band diagram generator for unit cells to generate band diagrams of the entire beam. We can see how the mode is pulled up or down based on what parameters are changed. Both anti-symmetric and symmetric modes can be selected. Figure 9 is an example of pulling a mode up to the desired central frequency. For all points after wavenumber $kx = 1$, we are solving at the X point, where wavenumber $kx = 1$ on the graph. All that is being changed is the lattice constant of the beam because of tapering. Please refer to the comments in each file.

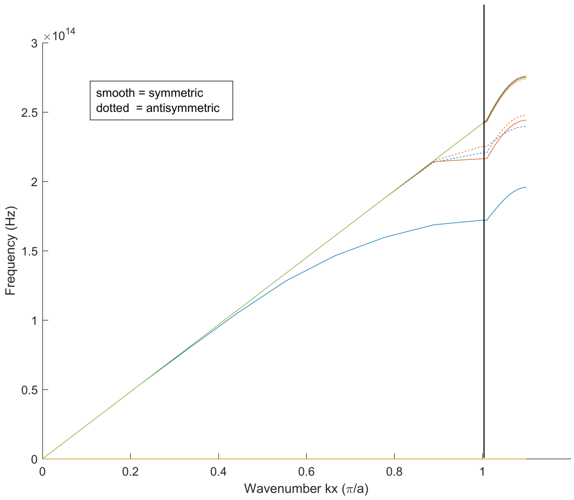

FIG. 9: Photonic band diagram of full tapered beam. The black line separates the unit mirror cell from the tapering or pulling up of the mode towards the desired central frequency. Dotted lines represent antisymmetric modes and solid lines represent symmetric modes.

Files are located in the folder *Band Diagram Generator — Full Beam*.

PROJECT: HIGH QUALITY FACTOR AND HIGH OPTOMECHANICAL COUPLING FACTORS

With the scripted simulations stable and working and a toolbox for finding band diagrams and imaging of modes, we now focus our attention on developing intuition for designing optomechanical nanobeams.

We conduct three sweeps: increasing the number of mirror cells, varying the defect depth, and varying the number of cells to taper over. For these sweeps, our mirror cell has an optimized band gap of 0.44×10^{14} and is centered around 1.934×10^{14}. The geometry parameters are $a = 619.98$, $a_0 = 549.30$, $w = 936.65$, $hy = 776.63$, $hx = 488.63$, and $airslot = 75.00$ where a is the lattice constant, a_0 is the defect cell, w is the width of the beam, hy is the vertical diameter of the airhole, hx is the horizontal diameter of the airhole, and $airslot$ is the width of the air slot. If not stated otherwise, there are eight cells which are tapered over and three mirror cells. We start with increasing the number of mirror cells.

In Figure 10, we see that increasing the number of mirror cells from 1 to 15 results in an exponential increase in the quality factor that saturates at 300,000. The parameters except for meshing have been identical to those in Figure 6. This graph suggests that only four mirror cells are needed, which tells us where to cut off

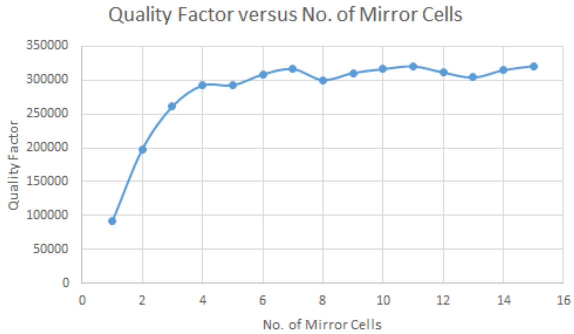

FIG. 10: This sweep is to serve as a stark contrast to Figure 6. All parameters have been kept with only the mesh having been changed. The quality factor saturates at 300,000 after the fourth mirror cell.

the number of mirror cells. The shorter the beam is, the higher the mechanical frequency can be.

Next, we vary the defect depth and record the quality and optomechanical coupling factor. The defect depth is defined on how deep you pull the mode into the band gap. All other parameters are recalculated (the tapering) based on this new defect cell. For example, our band gap has a central frequency of 1.934×10^{14} using a defect lattice constant of 549 nm. Instead of using 549 nm, we study what happens if we lessen or increase the defect lattice constant. The results are displayed in Figure 11.

As shown, the optical frequency in gray decreases linearly as the defect lattice constant is changed. This makes sense because for each defect cell, a certain mode exists, thus reinforcing the stability of the simulations. The quality factor peaks near 560 nm. This maxima deviates from what we expect. We expect frequencies from the center of the band gap to decay more strongly than those not centered. This slight shift could be incorporated in the subsequent designs, by tapering less. At little tapering, around 600 nm as the defect lattice constant, the quality factor decreases dramatically. This decrease makes sense because the optical mode goes nearly out of the band gap.

The optomechanical coupling factor versus defect depth reveals that the highest factors come when the tapering is less than our design defect cell lattice constant. The maxima is near 580 nm. This means the contribution from the moving boundary effect is greater when the tapering is less, although at 600 nm, g then starts to decrease. There are two data points which deviate. I did not have enough time to look deeper, but perhaps it could be due to a meshing problem.

Next, we increase the number of cells tapered over which results in an exponential increase in the quality factor and a linear increase for the optomechanical cou-

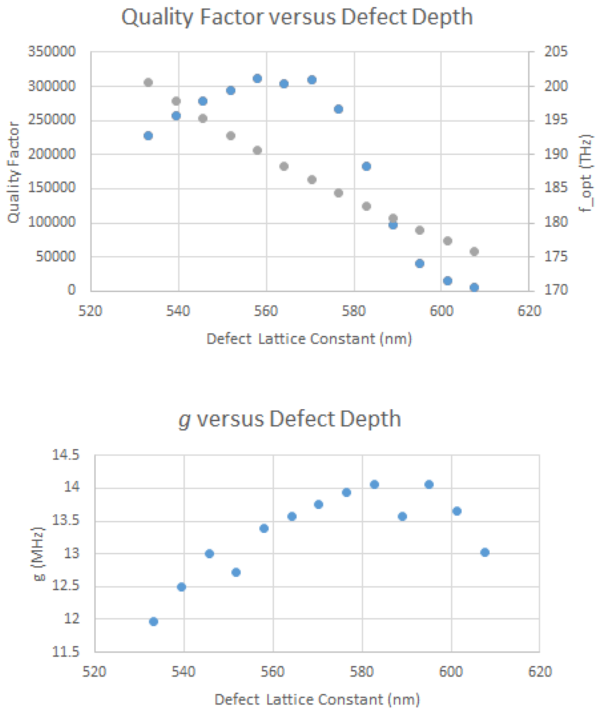

FIG. 11: In the top graph, the defect lattice constant is varied and the quality factor is recorded in blue with the corresponding optical frequency in gray. In the bottom graph, g is varied as a function of defect lattice constant. The tapering constants for the full length of the beam is recalculated for each new defect lattice constant. All other parameters remain the same. We taper over 8 cells.

pling factor. We see that the highest quality factors exist near our central frequency and at higher values of cells tapered over. The former makes sense and the latter also because there would be less radiative loss due to less lattice constant change between each cell. The optical frequency saturates at the designed defect lattice constant optical mode. See Figure 12.

Lastly, we vary the air slot gap size and measure g. As expected, g increases for smaller gap sizes due to a stronger confinement of energy (Figure 13).

To confirm whether these trends are universal, further work is needed to generate an optimized band gap for a mirror cell with different geometry parameters. Everything would be kept the same, and the same sweeps run.

After analysis of these graphs, a design was chosen which had four mirror cells and 13 tapered cells. The parameters are the same as before (rounded here): $a_0 =$ 549 nm, $a_M = 620$ nm, $w = 937$ nm, $hx = 489$ nm, $hy =$ 777 nm, $airslot = 75$ nm. However, the mechanical frequency was less than 2 MHz. To improve the mechanical frequency, the air slot was shortened length wise, stopping just after the tapering (shown in Figure 14). This

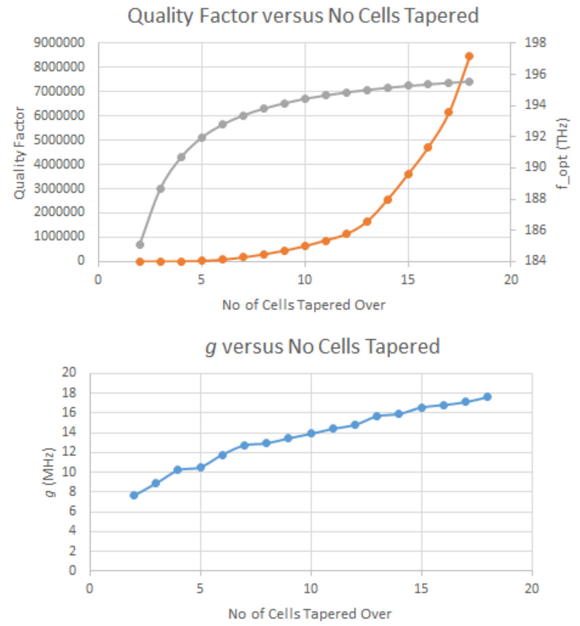

FIG. 12: In the top graph, the number of cells is varied and the quality factor is recorded in orange with the corresponding optical frequency in gray. In the bottom graph, g is varied as a function of the number of cells tapered over.

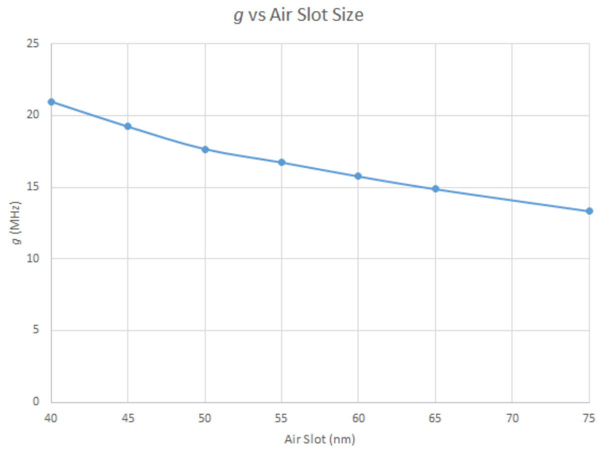

FIG. 13: The gap size or air slot is varied. The optomechanical coupling factor is recorded. All other parameters are kept constant.

shortening induces higher mechanical frequencies. The final design has a mechanical frequency of 2.6 MHz, 1.3 million quality factor, and 13 MHz as the optomechanical coupling factor. It should be noted g decreased from 16 MHz to 13 MHz as a tradeoff of the mechanical frequency increasing by a factor of 1.7.

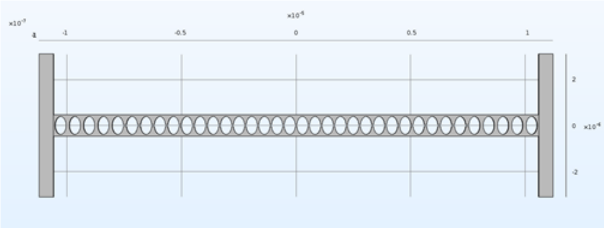

FIG. 14: This is the final nanobeam design. The parameters are: $a_0 = 549$ nm, $a_M = 620$ nm, $w = 937$ nm, $hx = 489$ nm, $hy = 777$ nm, $airslot = 75$ nm. There are 13 tapered cells and four mirror cells. The air slot stops after the tapering.

FURTHER WORK

In Jaspar Chan's thesis, Chan tapers both the lattice constant and hole size in designing high quality factor nanobeams [5]. In a paper by Marko Loncar, the size of the air holes were also tapered which resulted in high quality factors [7]. In a future sweep, the hole size can be tapered using a quadratic function. Another idea would be tapering both the hole and lattice constant at the same time.

So far we have been utilizing sweeps to gain intuition. The last step would be to write an optimization script such that running the script once would ensue in a long optimization search for the best design. A preliminary version was written but not completed. Please contact me for this.

CONCLUSION

The beginning of the internship consisted of developing a toolbox for designing photonic nanobeams Tools include the optimization of band gaps, band diagram generators of unit cells and full beams, image export of mode propagation, and new functions for tapering and geometry generation. Subsequently, a band gap was optimized, band diagrams were generated, and a full beam was written entirely using MATLAB-Comsol scripting.

Scripted simulations became fully automated with unrealistic behaviour fixed due to the meshing being fixed. The simulations are now stable, consistent, and reliable. With this stability, sweeps were run, resulting in many different studies including the number of mirror cels, the number of cells tapered over, and varying the defect depth. For each the quality and optomechanical coupling factor was calculated. The sweeps confirmed intuitions such as weaker tapering resulting in higher quality factors, the exponential increase and saturation of quality factors with the increase of mirror cells, and also gave rise to new intuitions such as subtle shifts in Q and g maximas than where we expect them to be. Other intuitions we confirmed include decreasing the air slot size, increases g as expected and designs where the defect optical frequency is near the edge of the band gap results in extremely low quality factors.

A design with high g, Q, and f_{mech} was chosen, its air slot length was chosen to increase its f_{mech} and one design was found that can be readily fabricated.

Due to duration of my stay and stable simulations taking long times, further work must be done in writing an optimization script and running it.

If there any questions about any of the programs, feel free to send me an email at ds3628@columbia.edu. I will promptly reply within two business days.

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I would like to thank Dr. Johannes Fink for giving me this opportunity. There was a lot of free reign in how I would achieve the goal you proposed for this project. It was challenging and a new experience for me. A deep thank you to Dr. Matthias Wulf for showing me how to think systematically and being there to help me think through next steps and debugging road blocks. And lastly thank you to Georg Arnold for showing me the way, helping me immensely with COMSOL/MATLAB simulations. You have all become my teacher, mentor, and friend.

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