Particle Swarm Optimization for Robust Nanobeam Photonic Crystal Cavities

Jaden Hou[1,2], Neelesh Kumar Vij[1], Abhijit Biswas[1], Jasvith Raj Basani[1], Edo Waks[1]

[1]Quantum Photonics Group, University of Maryland, College Park, Maryland 20742, USA

[2]Poolesville High School, Maryland 20837, USA

Abstract

Strong light-matter interactions are important for applications in quantum computing, communication, and sensing. Photonic crystal cavities have emerged as promising candidates for realizing strong interactions among photons and quantum emitters. In particular, nanobeam cavities (Deotare & Loncar, 2012) have attracted interest due to their low mode volumes, high quality factors, and highly directional emission. However, fabrication imperfections that result in sidewall roughness introduce losses, which results in reduced quality factors. To address this challenge, we apply particle swarm optimization (PSO) (Vasco et al., 2020) to designs proposed by Biswas et al. (2024) to make the nanobeam cavities more robust to loss caused by fabrication imperfections. By optimizing the geometric parameters of the cavity, we achieve a maximum quality factor of approximately 2500, which indicates that there is a fundamental limitation imposed on the quality factor caused by the scattering of the optical mode from the sidewalls. Varying the geometry of the nanobeam and its impact on the confinement of the optical mode remains to be investigated. Our work advances the understanding of fabrication tolerance on nanobeam cavities and paves the way for the design of robust photonic crystal cavities.

Introduction

Motivated by advancing progress in both classical and quantum computing, integrated photonic circuits have emerged as promising candidates for information processing in the optical domain. In particular, photonic crystal cavities have enabled the strong trapping of light, essential for classical communication and the construction of gates for quantum computation However, fabrication imperfections leading to scattering losses of the optical mode are a leading cause of degraded performance in PhCs. This research explores the possibilities of using particle swarm optimization (PSO) in an attempt to generate a design that can handle the sidewall roughness.

Nanobeam Photonic Crystal Cavities

Nanobeam cavities are high-Q, small-mode volume optical resonators used for the localization of light (Deotare & Loncar 2012). Generally, a photonic crystal cavity uses Distributed Bragg Reflection (DBR) in two dimensions and Total Internal Reflection (TIR) in the remaining dimension to confine light (Englund et al., 2005). Nanobeam cavities, however, use DBR in the longitudinal direction and TIR in the other two dimensions (Deotare & Loncar, 2012). As such, nanobeam cavities are waveguides with Bragg mirrors on either side of the cavity (Quan et al., 2010). Two parameters that can be used to characterize photonic crystal cavities are quality factor, a measure of how well a cavity confines light (Q) (Englund et al., 2005), and mode volume, a measure of how well a cavity spatially confines light (Zhou et al., 2019).

In the photonics community, strong light-matter interactions are difficult to achieve but are of interest (Vahala, 2003). However, when working with singular photons, strong light-matter interactions are extremely difficult to achieve. High-quality nanobeam cavities allow us to maximize these light-matter interactions (Deotare & Loncar, 2012), which are important for quantum computing, communication, and sensing. Yet, high-quality nanobeam cavities are difficult to achieve experimentally due to a common issue of nanobeam cavities, sidewall roughness.

Fabrication imperfections can result in rough surfaces during the production of nanobeam cavities. This surface roughness, which normally presents as sidewall roughness, leads to a loss as the electromagnetic mode of the light interacts with the imperfections on the edges of the nanobeam cavity (Roberts et al., 2022). As a result, experimental quality factors face large decreases in the quality factor of a nanobeam cavity. In one case, a simulated $2 * 10^6$ Q nanobeam cavity was found to have an experimental Q of around $2 * 10^3$, a decrease by an order of 10^3 (Biswas et al., 2024). One way to decrease the effect of sidewall roughness is to create a design where the electromagnetic mode of the nanobeam cavity is strongly confined, reducing interference and scattering from the sidewalls.

Evidence of sidewall roughness can be seen in Figure 1. The electromagnetic mode of the light interacts with the sidewalls on both sides of the nanobeam.

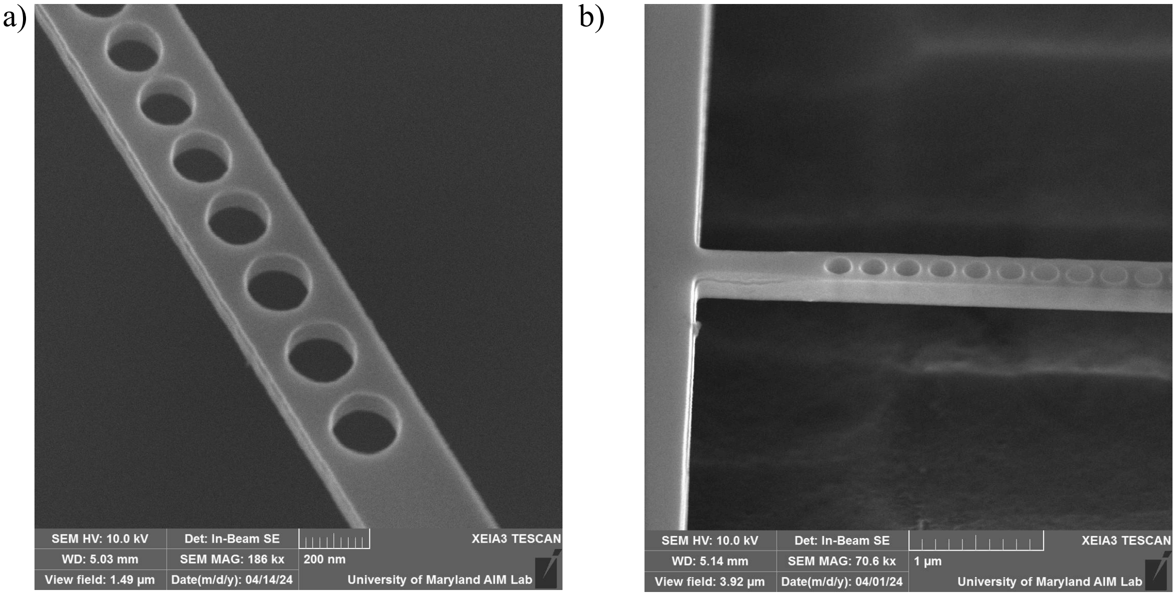

Figure 1. a) SEM image of fabricated nanobeam cavity with sidewall roughness on both sidewalls of the nanobeam (Biswas, 2024) b) SEM Image of fabricated nanobeam cavity where imperfections are apparent on the left edge of the sidewalls (Biswas, 2024)

Numerical Simulations

The finite-difference time-domain (FDTD) method, a computational method that uses Maxwell's equations for electromagnetic simulation, is commonly used to simulate nanophotonic devices. A feature of interest is its ability to run multiple simulations with varying parameters and analyze its characteristics in a process called parameter sweeping as well as measuring how light propagates through the device (Tidy3D, 2022); such would not be possible experimentally. Additionally, the simulation enables the measurement of electric field patterns that allow the classification of modes.

PSO is a non-gradient-based global optimization strategy that was modeled after the natural swarming theory (Kennedy & Eberhard, 1995). The algorithm first generates a number of particles, places them at randomly selected locations, and runs a recursive algorithm to find the optimal set of parameters that minimizes a cost function (Miranda, 2018). The number of particles determines how large the swarm is and the initial location of each particle can be randomly generated. It uses three parameters to determine each iteration of the algorithm: inertia (w), cognitive factor (c_1), and social factor (c_2) (Wang et al., 2017). The inertia indicates the particle's desire to continue moving in the direction it previously moved and is randomly determined at the start of the algorithm. The cognitive factor indicates the particle's desire to move toward its best position. The social factor indicates the particle's desire to move toward the swarm's best position. Additionally, the number of particles ($n_{particles}$) can be changed (Miranda, 2018).

Vasco and Savona (2021) used particle swarm optimization for an L3 cavity, a 2D design of a photonic crystal cavity with three central missing holes, and reached a quality factor of 4.33 * 10^7. However, the paper uses the guided mode expansion method instead of the FDTD method, which is not feasible for nanobeam cavities as they are one-dimensional.

Methodology

The quasi-experimental design included parameter sweeps and the use of an optimization algorithm to change various parameters of the design and observe its impact on the quality factor of the nanobeam iteratively. Initial particle placements are randomly generated and specific parameter values during the optimization are controlled by the algorithm.

The experiment was based on a Gallium Arsenide nanobeam photonic crystal cavity with linear taper design due to its high coupling efficiency when coupled with single-mode lensed fiber (Biswas et al., 2024). The nanobeam, shown in Figure 2, is 180 nm thick and 285 nm wide and experimentally has a Q-factor of around 1000 for the 900-940 nm. The nanobeam is also mirrored with 15 holes on either side. The central four (N_taper) holes of each side are linearly tapered. The radius of a tapered hole is determined by multiplying the lattice parameter of the hole by a ratio of 0.33. Using a lattice parameter (a) of 252 nm and a central lattice parameter (a_center) of 188 nm, we can taper the rest of the tapered holes by using a step of (a - a_center) / Ntaper.

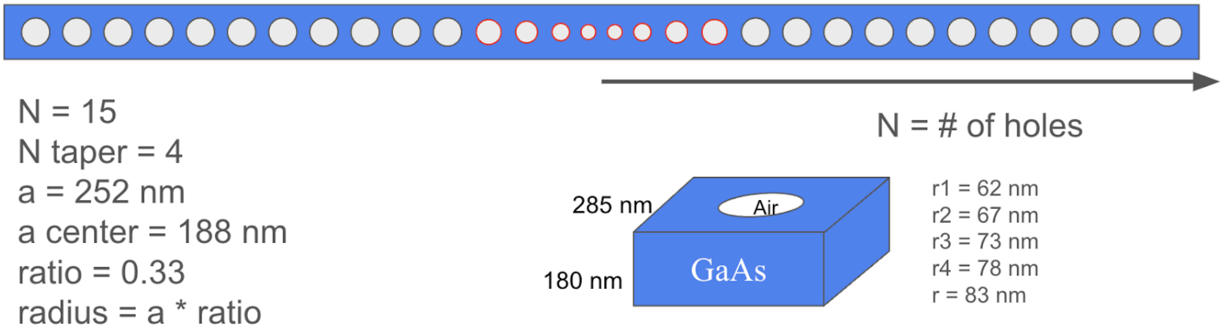

Figure 2. Dimensions of initial linear taper design

A Python-based FDTD solver (Tidy3D, 2022) was utilized for the simulation. The FDTD method is recognized as an accurate and efficient approach for simulating Maxwell's field equations across multiple parameters with varying values (Teixeira et al., 2023), a process known as a parameter sweep. To determine the simulation bounds—specifically, the optimal distance for absorbing boundaries or Perfectly Matched Layers (PML) to maximize accuracy—the simulation size was swept by multiplying a factor with the nanobeam width. This ensured that the PML did not interfere with the light simulation as it leaked from the nanobeam, yielding accurate results.

To model the loss due to sidewall roughness, the nanobeam was padded with an artificial medium with an imaginary refractive index. Two sets of simulations were conducted: one with an absorbing background medium, representative of general loss, and another with an absorbing sidewall medium, representative of loss specifically due to sidewall roughness, as it only simulated loss along the rough sides rather than in all dimensions. For both sets of simulations, the imaginary refractive index (k) was varied to identify a value that best represented the quality factor loss. It was observed that the thickness of the absorbing sidewall medium influenced the nanobeam's resonant wavelength. Therefore, a range of sidewall thicknesses was swept to find one that closely matched the original nanobeam's resonant wavelength of around 940 nm.

Particle swarm optimization was selected as the optimization method due to its non-gradient-based, global optimization capabilities. Given the experiment's complexity and the variety of parameters, specific parameter adjustments are challenging for gradient-based methods. Particle swarm optimization is also computationally efficient and requires fewer algorithm-specific parameter adjustments compared to other algorithms (Gad, 2022). A global optimization approach was necessary to determine the global maximum quality factor for a given parameter. A Python-based PSO library (Miranda, 2018) was employed with two key parameters, c_1 and c_2, to run multiple optimizations with varied parameter values and specific configurations. Number of holes in central radius taper, central lattice parameter, lattice parameter, and the ratio between the lattice parameter and radius (Ntaper, a_center, a_lattice, ratio) were the parameters being optimized. A w of 0.5, $n_{particles}$ of 5, and number of iterations between 7 and 20 were kept constant.

Parameter Sweeps

Parameter sweeps were performed to simulate general loss (Fig. 3) and sidewall roughness loss (Fig 4.) that best matched the experimentally observed quality factor. In Figure 3a, the quality factor appears to exponentially decay, meaning an increase in the refractive index of the background medium correlates to an exponential decrease in how well the cavity confines light. A k value between 0.01 and 0.03 provides a Q value between 1078.39 and 340.31, values which are in our area of interest. As shown in Figure 3b, the resonant wavelength remains constant at around 940 nm between 0.01 and 0.03 and linearly increases after this range. Thus, a k value between 0.01 and 0.03 would best simulate general loss.

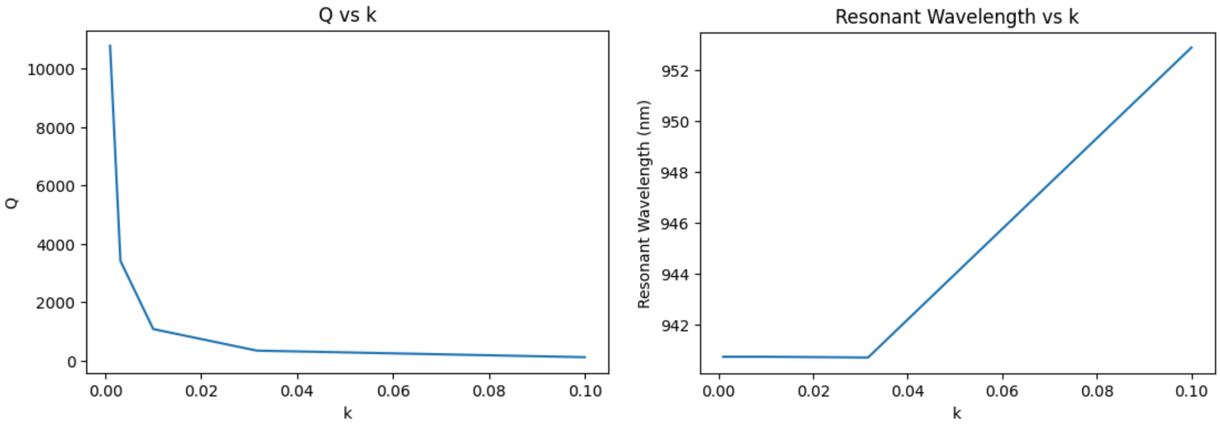
a) b)

Figure 3. Sweeping k with absorbing background medium. a) Quality factor for changing k value b) Resonant wavelength for changing k value

To find the optimal parameters for absorbing slab sweeps a sweep for slab width and a multi-parameter sweep for a slab width of 0.06 nm, 0.065 nm, and 0.07 nm was performed (Fig. 4). In Figure 4a, it is shown that sweeping k for absorbing slabs results in a similar exponential decay as an absorbing background medium. Changing the slab width results in a vertical offset of the decay. The same is true for Figure 4b.

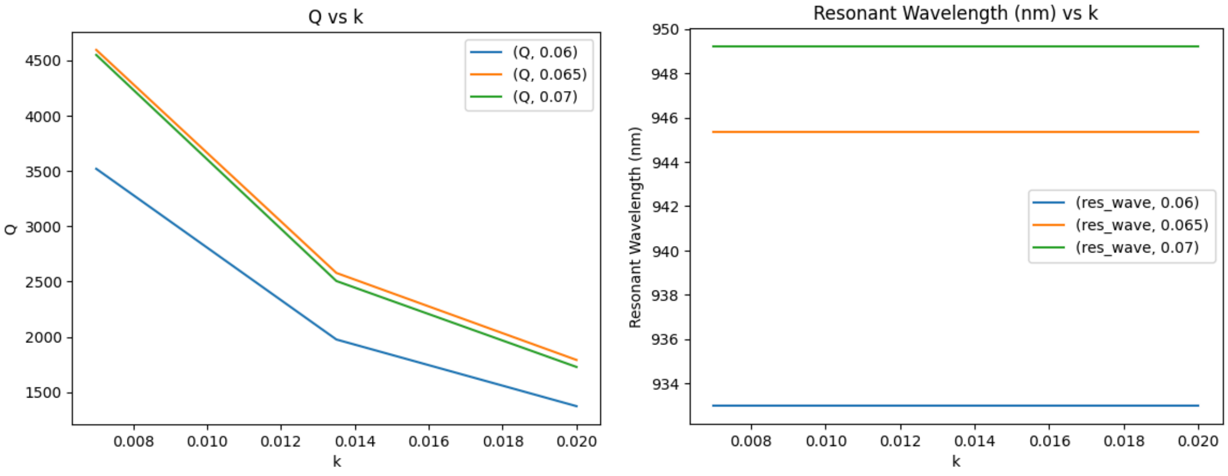
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Figure 4. Sweeping k and slab width with absorbing slab. a) Quality factor for changing k and differing slab widths in nm. b) Resonant wavelength for changing k and differing slab width in nm.

To get a Q and resonant wavelength near the target value, a slab width between 60 nm and 65 nm was selected. Performing the same sweep of k to the design with absorbing slabs (Fig 5) results in similar patterns as the design with absorbing background medium (Fig 3). A k value between 0.027 and 0.051 provides a Q value between 590.43 and 1372.61 and a resonant wavelength around 940 nm.

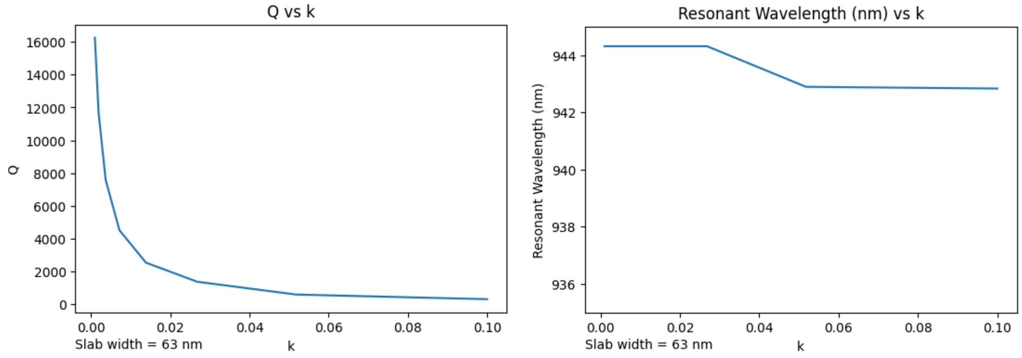
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Figure 5. Sweeping k with absorbing slabs. a) Quality factor for changing k value b) Resonant wavelength for changing k value

In Figure 6, it is shown that the Q value appears to exponentially decay and oscillate. However, between 60 and 65 nm, the Q value remains within 1000 to 2000. The resonant wavelength also remains near 940 nm.

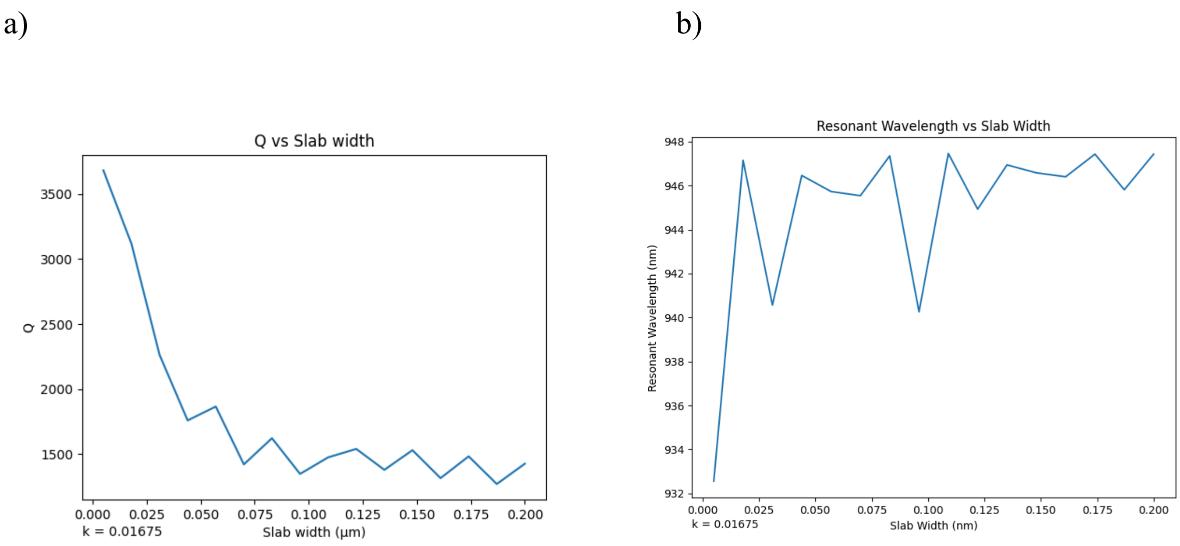

Figure 6. Sweeping slab width for resonant wavelength. a) Quality factor for changing slab width b) Resonant wavelength for changing slab width.

Selection of Parameters

A k of 0.1675 and 63 nm slab width design gives a quality factor of 1668, and is observed to be the best match to simulate the target experimental quality factor of around 1000 (Fig 6). A decrease of Q on the order of 10^4 was observed between the simulations without an absorbing slab and with the absorbing slab.

Mesh Size = 40	With Absorbing Background Medium	With Absorbing Slab	Without Absorbing Slab
Quality Factor	643	1668	11471504
Resonant Wavelength (nm)	940.71 nm	947.43 nm	940.58 nm

Figure 7. FDTD Simulation results with a mesh size of 40, k value of 0.1675, and 63 nm slab width.

Particle Swarm Optimization

With the absorbing slab design, PSO was done to find the optimal configuration of the parameters. Variation of the PSO-specific search parameters was used to attempt to navigate through local minimums as shown in Figure 8. The maximum quality factor found was 2.46 * 10^3, a value on the same order of magnitude as the unoptimized design with an absorbing slab. This indicates that the scattering of the optical mode from the sidewalls may cause a fundamental limitation on the quality factor.

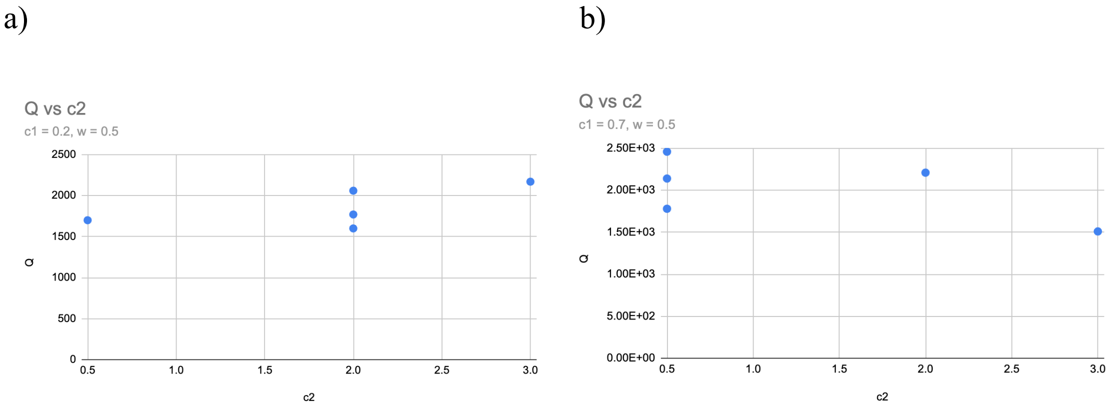
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Figure 8. a) PSO results for changing c_2 at a constant c_1 of 0.2. b) PSO results for changing c_2 at a constant c_1 of 0.7.

Conclusion

Preliminary results indicate that particle swarm optimization of robust nanobeam photonic crystal cavities is fundamentally limited by the scattering of the optical mode from side roughness. However, PSO is highly dependent on the location of initial parameters as well as the initial design. Using a different design would change the global maximum quality factor of the design. Using different PSO-specific search parameters would also change the outcome of the search. Compute time was a limiting factor for the number of iterations and particles of the optimization. Future research should include: including the nanobeam width into the PSO and using different geometries for the holes of the cavity to confine the electromagnetic mode of light.

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