Supplemental Document

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Optimization of diamond optomechanical crystal cavities: supplement

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1. OPTIMIZATION PROCESS

The optimization process is fully described by the flowchart in Fig S1. It starts with a set of randomly generated geometries that are treated before serving as the initial generation of the genetic algorithm (GA). The geometries are built based on the parameters described in this material in subsection A. The data treatment consists of filtering and adjusting the data in a way all the initial geometries have optical modes in the desired frequency range. This process is described in subsection C.

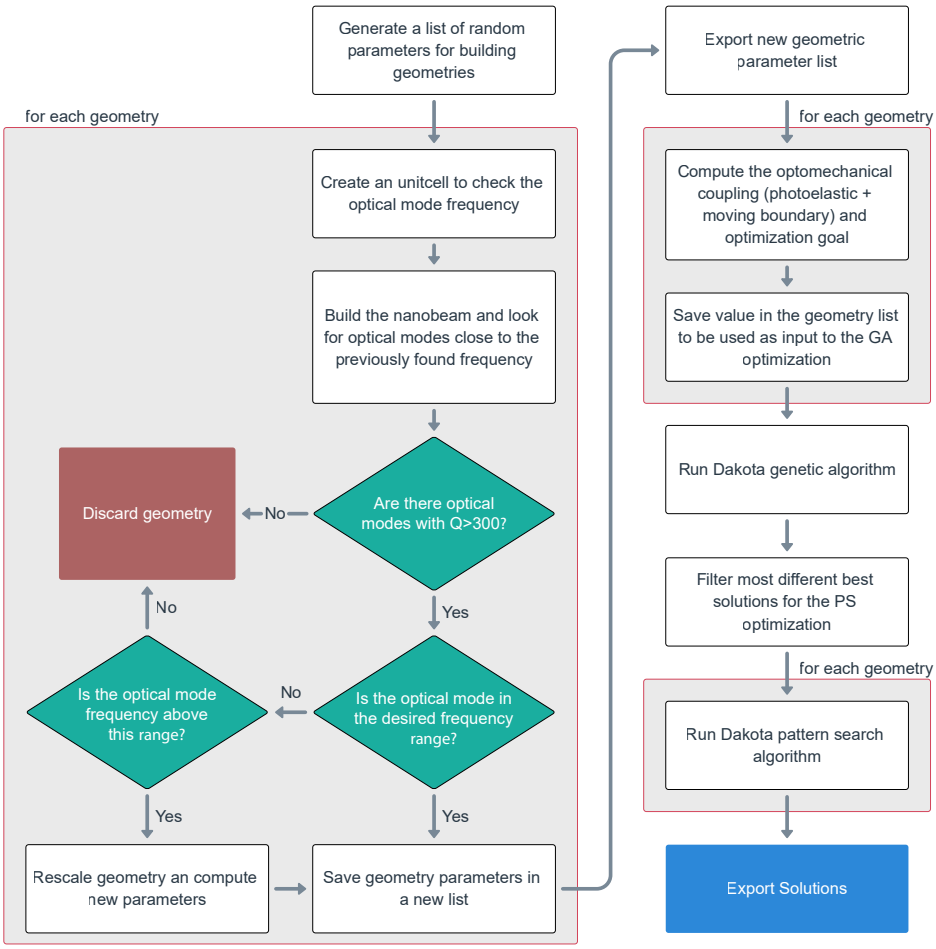

Fig. S1. Flowchart of the optimization process.

Comsol is then used to simulate each of the reparameterized geometry and compute the optimization parameter q. The geometries and their associated q-values are given to Dakota as the initial population necessary to start the GA, which performs a global optimization. After running the GA some of the tested geometries are selected to be locally optimized by a pattern search (PS) algorithm. The selection criteria are described in subsection D. Dakota then runs some

steps of the PS algorithm using the selected solutions as the initial parameter. In the end, we have one locally optimized solution for each selected solution of the GA.

A. Nanobeam parameterization

The geometric parameters of the nanobeam are:

- w the nanobeam width,
- t the nanobeam thickness,
- N the number of defects from the central defect to the mirrors,
- M the number of holes (defects + mirrors),
- a_j the j-th cell's lattice parameter,
- h_{xj} the j-th cell's x-component of the hole diameter,
- h_{yj} the j-th cell's y-component of the hole diameter.

The four first parameters from the list were used as they are and the nanobeam width was the only one from them used as an optimization variable. The last three parameters were parameterized in function of:

- a_N the mirrors lattice parameter,
- d_0 to define the central defect's lattice parameter,
- γ_N to define the x-component of the hole diameter at the mirror,
- γ_0 to define the x-component of the hole diameter at the central defect,
- η_N to define the y-component of the hole diameter at the mirror,
- η_0 to define the y-component of the hole diameter at the central defect,
- $\delta = 50\,\text{nm}$ the fabrication precision limit.

To define the geometry of a unit cell between the mirrors and the central defect we define $x_j \equiv j/N$ where j is the cell index counting from the central defect ($j = 0$), to the first mirror ($j = 8$) and a function $f(x_j) = 2x_j^3 - 3x_j^2 + 1$, which is limited between 1 and 0 for our domain and has a null derivative at 0 and 1. The j-th lattice parameter is defined as:

$$a_j = (1 - d_j)a_N \tag{S1}$$

$$d_j = d_0 f(x_j) \tag{S2}$$

The equations to parameterize h_{xj} and h_{yj} are:

$$h_{xj} = (a_j - 2\delta)\eta_j + \delta \tag{S3}$$

$$h_{yj} = (w - 3\delta)\gamma_j + \delta \tag{S4}$$

$$\eta_j = \eta_N - (\eta_N - \eta_0)f(x_j) \tag{S5}$$

$$\gamma_j = \gamma_N - (\gamma_N - \gamma_0)f(x_j) \tag{S6}$$

They ensure $\delta \leq h_{xj} \leq a_j$ and $\delta \leq h_{yj} \leq w - 2\delta$, which means no hole or wall is smaller than δ. This parameterization requires γ_N, γ_0, η_N, η_0 and d_0 to be bounded between 0 and 1.

B. Simulation

All simulations were performed in Comsol® using built-in diamond (100) and air as materials. Diamond has refractive index $n = 2.417$ and Young's modulus given by $E = (C_{11} - C_{12})(C_{11} + 2 * C_{12})/(C_{11} + C_{12}) = 1050\,\text{GPa}$. The elasticity matrix is defined as:

$$D = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$

with $C_{11} = 1076\,\text{GPa}$, $C_{12} = 125\,\text{GPa}$ and $C_{44} = 578\,\text{GPa}$. We also used the diamond photoelastic coefficients $(\rho_{11}, \rho_{12}, \rho_{44}) = (-0.25, 0.043, -0.172)$ to compute the photoelastic component of the optomechanical coupling.

The unit cell simulations account for a quarter of the cell using proper symmetry conditions at the internal boundaries, Floquet periodicity at the cell limits, and scattering boundary conditions (SBC) at the external boundaries as a filter for optical modes. The nanobeam simulations account for one eight of the nanobeam and were performed using perfectly matched layers (PML) instead of SBC at the external boundaries to improve accuracy on losses evaluation.

The geometries were created using the previously described parameterization through Comsol® methods. Optical and mechanical studies are computed independently by another Comsol® method, and the value of the integrals of optical fields are stored so they don't need to be recalculated during the evaluation of the optomechanical coupling for each mechanical mode, which strongly reduces each simulation's computational time. The simulation files are available at Zenodo® through the DOI: 10.5281/zenodo.6560537.

C. Initial parameters generation

The optimization method has two steps: a global optimization with a genetic algorithm (GA) and a multi-start local optimization using a pattern search (PS) method. To improve the efficiency of the GA we fed it with an initial population containing geometries capable of confining optical modes between 183.9 THz and 198.4 THz. To generate such an initial population we first create a file with randomly generated geometries using Dakota LHS sampling with restricted conditions as described in Table S1. Each generated geometry was tested by simulating first the central defect unit cell with periodic conditions at the transversal plane (yz) and scattering bound conditions at the other planes to identify the expected frequency for the nanobeam confined mode. After this we simulate the whole nanobeam and ran the optical study, looking for modes close to the expected value. At this point, the program discards all geometries that don't have optical modes with $Q_o > 300$ and the geometries with low-frequency modes ($\nu_o < 183.9$). The geometries with $\nu_o > 198.4$ are then rescaled and reparameterized. Geometries with low frequency are not rescaled because they could make walls or holes to be thinner than the fabrication resolution limit.

To scale the geometry to find a confined optical mode in the expected frequency range we estimate an expected scaling factor by dividing the frequency of the mode with the highest quality factor by the maximum allowed frequency and start to test scaling factors S_f in a range between the expected factor more or less 10%. We multiply all geometric parameters, except the nanobeam thickness and the number of holes, by the scaling factor and if a mode is found with an allowed frequency we reparameterize the geometry in a way the mirrors and the central defect cells are kept the same but the geometry can again be written by equations S1-S6. The reparameterization equations are:

$$w' = wS_f \tag{S7}$$

$$a' = aS_f \tag{S8}$$

$$\eta'_m = \frac{(a_N - 2\delta)\eta_m S_f + \delta(S_f - 1)}{a_N S_f - 2\delta} \tag{S9}$$

$$\eta'_0 = \frac{[a_N * (1 - d_0) - 2\delta]\eta_0 S_f + \delta(S_f - 1)}{a_N * (1 - d_0) S_f - 2\delta} \tag{S10}$$

$$\gamma'_m = \frac{(w - 3\delta)\gamma_m S_f + \delta(S_f - 1)}{wS_f - 3\delta} \tag{S11}$$

$$\gamma'_0 = \frac{(w - 3\delta)\gamma_0 S_f + \delta(S_f - 1)}{wS_f - 3\delta} \tag{S12}$$

After this, the new list containing the scaled geometries is used as input parameters for the GA.

D. GA output selection

The GA randomly mutates geometries looking for solutions with a higher value of the optimization goal q. Solutions with a low q-value are discarded and the remaining ones mutate again to generate new solutions. After a while, it is common though to reach a branch of solutions with high q derived from the same solution and very similar to each other. Performing local optimizations in many solutions of the same branch is therefore an overkill process. Hence, to find solutions with different optimization strategies, we define clusters of solutions in the parameters space and select only the ones with the highest q. Two solutions are considered to belong to the same cluster if the normalized distance between then $D \equiv \sum_i [(p_{1i} - p_{2i})/(p_{1i} + p_{2i})]^2$, where p_{1i} and p_{2i} refers to each one of the geometry parameters of the solutions, is smaller than a minimum distance D_{min}. To define D_{min} we initially discard all solutions with $q < 0.3(q_{max} - q_{min}) + q_{min}$, then we start the selection with $D_{min} = 0$ and we increase D_{min} by 0.03 until reach less than 20 selected solutions. At least we start to slowly decrease D_{min} again by 0.001 until reach at least 20 selected solutions.

2. OUTPUT GEOMETRIES

The parameter values for the geometries presented in the paper are listed in Table S2

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parameter	lower bound	upper bound
w	400 nm	800 nm
a_N	500 nm	950 nm
d_0	0.05	0.6
η_N	0.1	1
γ_N	0.1	1
η_0	0	1
γ_0	0	1

Table S1. Bounds restriction for GA initial population generation.

parameter	geometry 1	geometry 2
N	8	8
M	13	13
t	450 nm	450 nm
w	633.9 nm	584.3 nm
a_N	610.8 nm	569.2 nm
d_0	0.184	0.178
η_N	0.513	0.557
γ_N	0.839	0.677
η_0	0.733	0.357
γ_0	0.561	0.773

Table S2. Parameters of the optimized solutions presented in the paper.