Accurate modeling and characterization of photothermal forces in optomechanics

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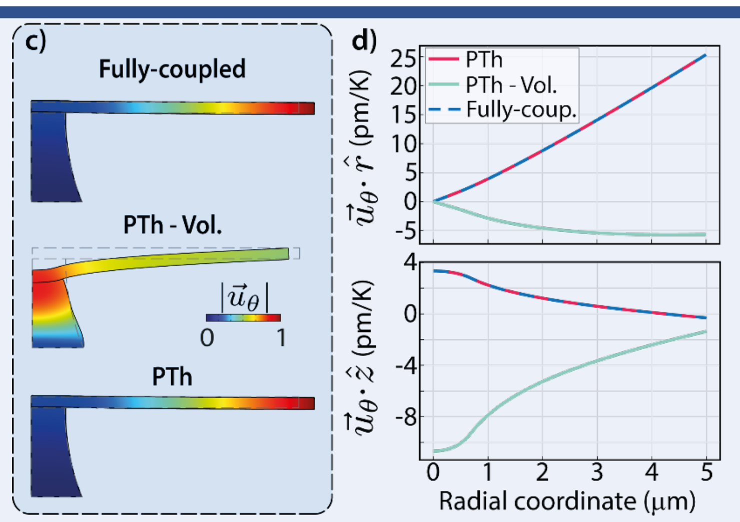
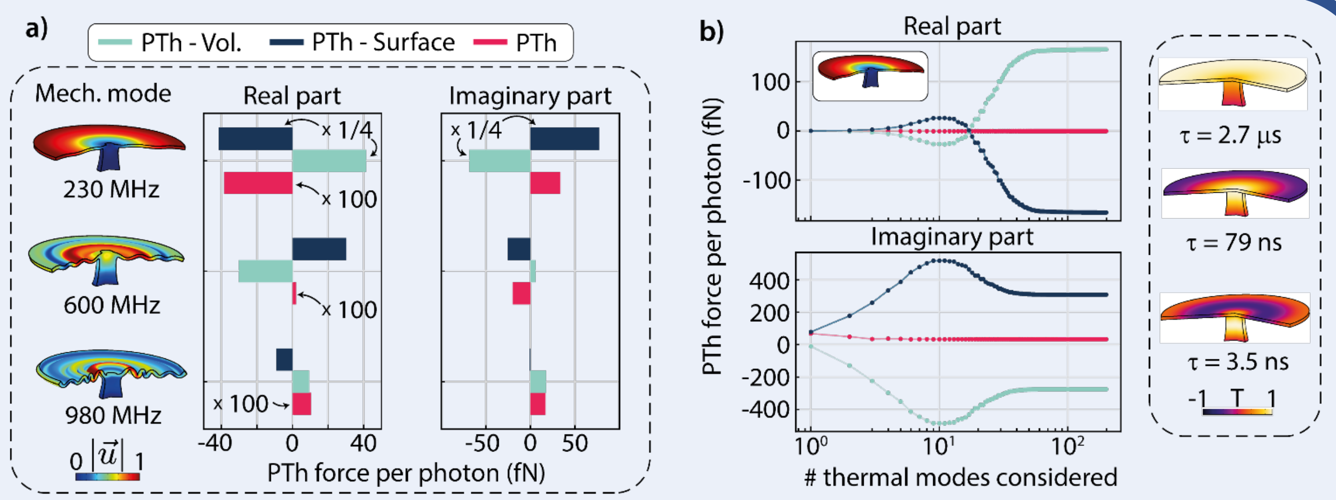
Available files – Main text

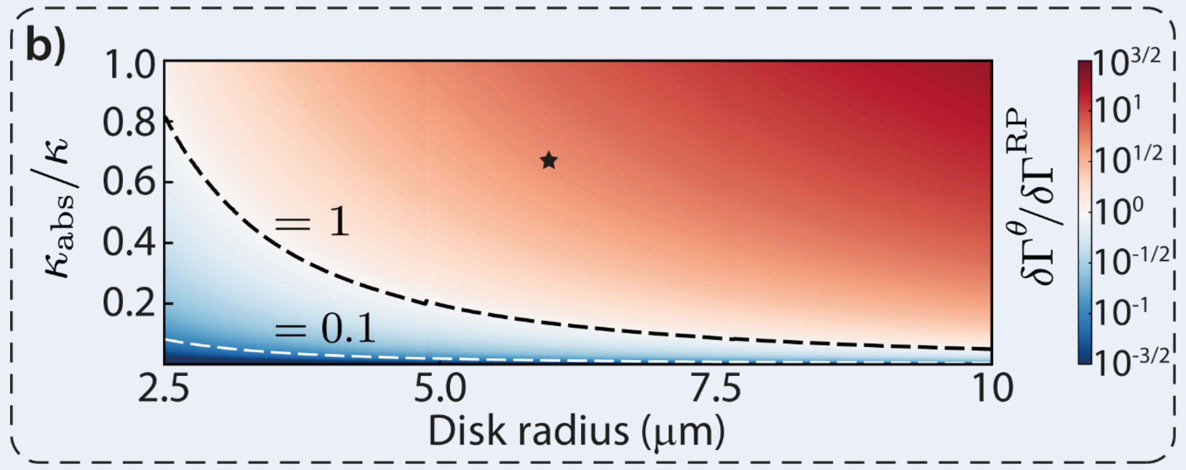
- Fig. 1: Fully-coupled vs PTh forces (Comsol 5.3a, Python)



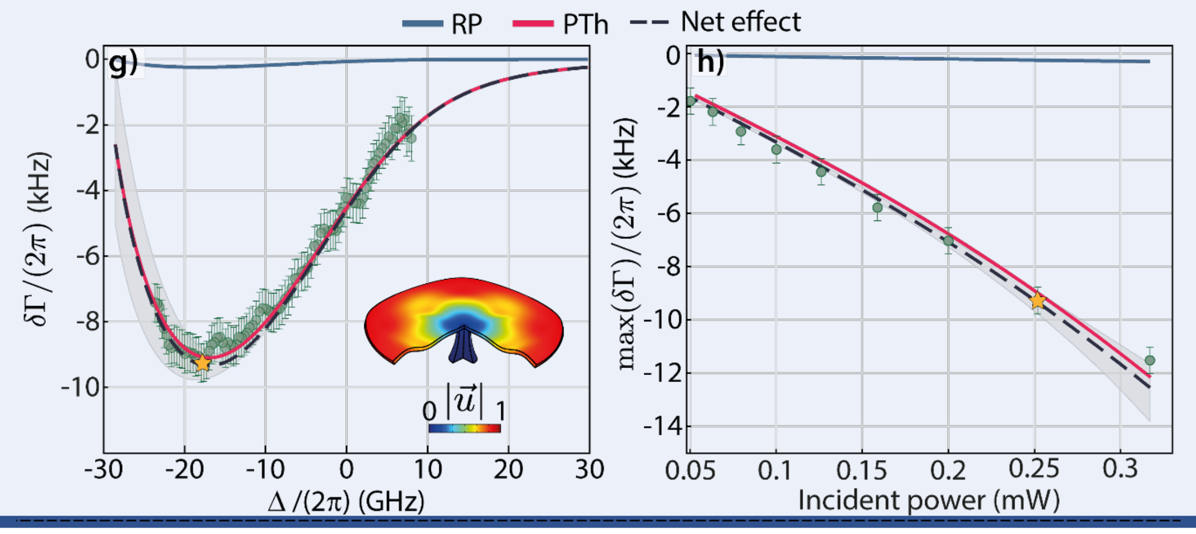
- Fig. 2: Surface vs Boundary loads (Comsol 5.3a, Python)



- Fig. 3: Optomechanical backaction (Comsol 5.3a, Python)



- Fig. 4 - Experimental data analysis and simulations (Python, Comsol 5.4)



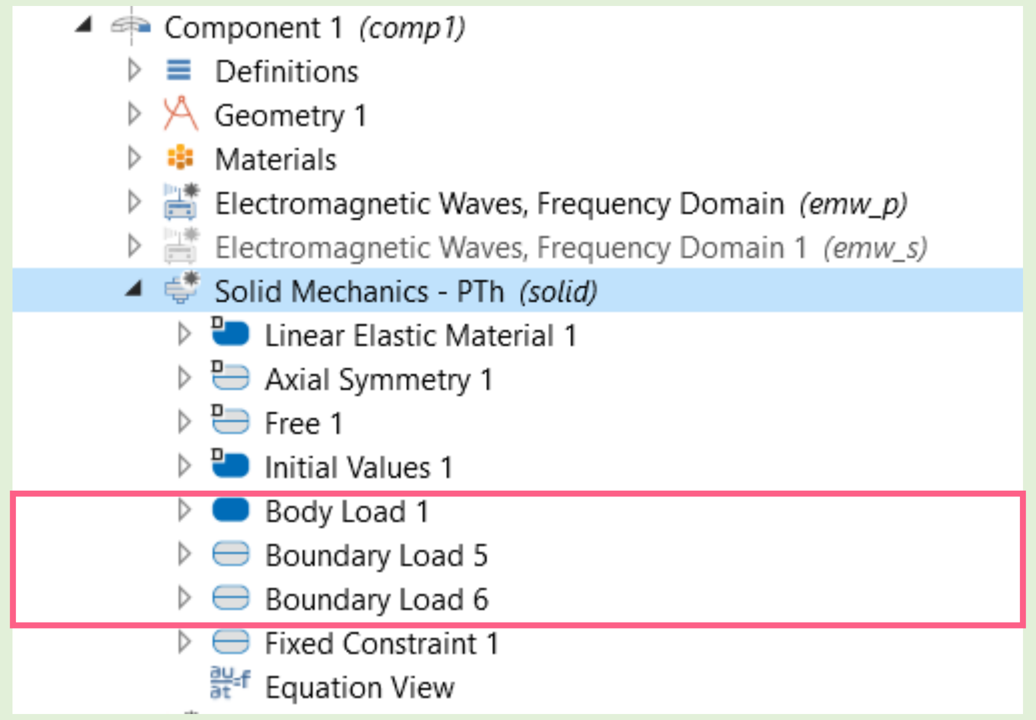
Details in the structure of the simulations can be found in the repository for: "Brillouin Optomechanics in Nanophotonic Structures" - DOI: 10.1063/1.5088169.

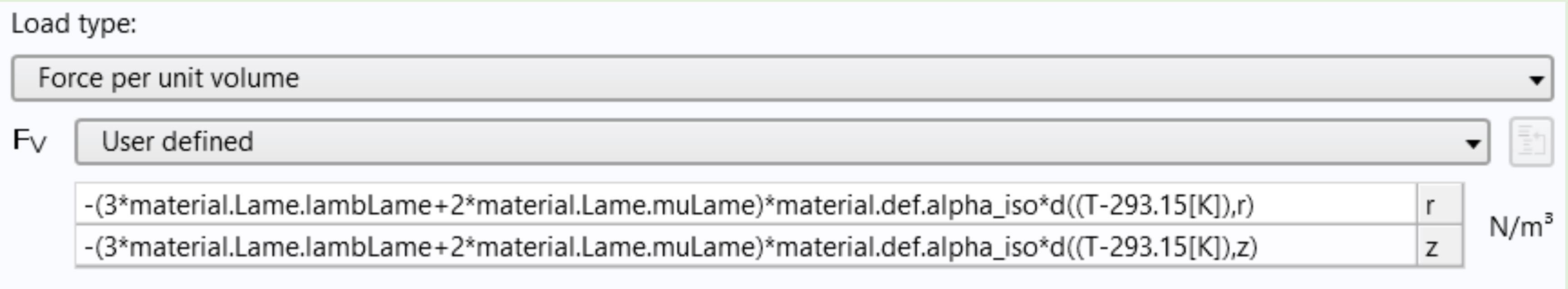
Fig. 1: Fully-coupled vs PTh forces

In file “Comsol_simulation_fig1.mph” we calculate thermal displacements imposed on a GaAs microdisk. The first order TE optical mode is computed and used as a heat source. Thermal displacements are then calculated through two different methods: a fully-coupled thermoelastic model and body/boundary loads calculated directly from the model presented in the main text. Results are then compared in the .ipynb file available.

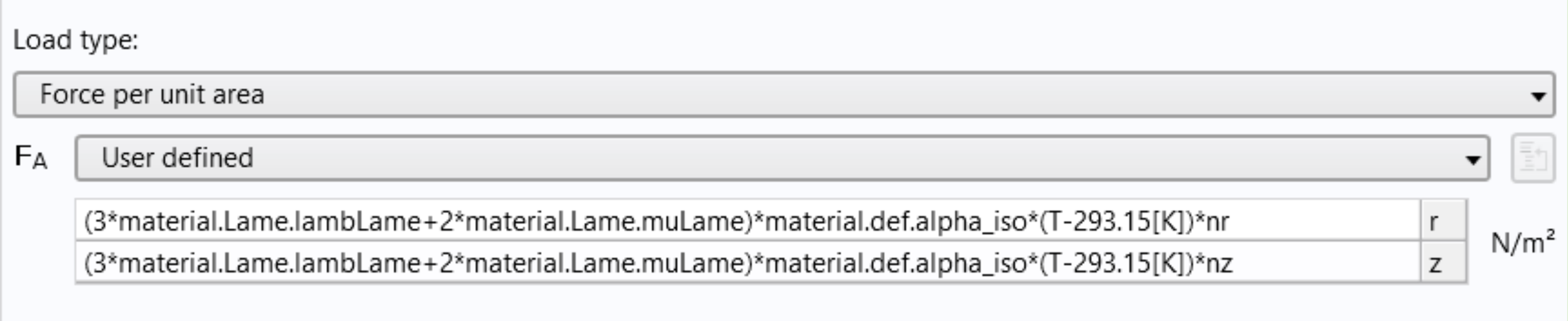
In Comsol:

- Run Study 1 - Optics. This will compute the optical mode which will be used in the rest of the simulations.
- Run Study 2 - Fully Coupled, which calculates the fully coupled model for the thermoelastic solid. Note that this will run the “Solid Mechanics – Fully Coupled” module, defined under Component 1, where the mechanical response is calculated in the absence of any loads. Furthermore, in the Study 2 - Fully Coupled node, we enabled the following Multiphysics Couplings: Thermal expansion and Temperature Coupling. Those are needed for computing the fully coupled solution.
- Run Study 3 - PTh model, which returns the thermal displacement generated through the body/boundary loads defined in “Solid Mechanics – PTh” and shown here for clarity. Note that the definitions of the loads match those given in the main text.





Body Load



Boundary Load

- Run Study 4 – PTh - Vol. This will compute the thermal deformations in the absence of the boundary loads, as defined in “Solid Mechanics – PTh – Volume”.
- Data is plotted in the 1D graphs named “Deformation – Cut – [...]” and can be exported in the Export node under results, after choosing an appropriate path.
- Output files are named: “**Fully_coupled_u.txt**”, “**Fully_coupled_w.txt**”, “**PTh_u.txt**”, “**PTh_w.txt**”, “**PTh_vol_u.txt**”, “**PTh_vol_w.txt**”, where u and w stand for the radial and z direction displacements, respectively.

Fig. 1: Fully-coupled vs PTh forces

In file "Comsol_simulation_fig1.mph" we calculate thermal displacements imposed on a GaAs microdisk. The first order TE optical mode is computed and used as a heat source. Thermal displacements are then calculated through two different methods: a fully-coupled thermoelastic model and body/boundary loads calculated directly from the model presented in the main text. Results are then compared in the .ipynb file available.

In Python:

- Data is loaded and plots are generated directly on. Please, keep in mind that all data files generated in Comsol have to be on the same folder as the .ipynb file, unless a different path is specified. In case the names of the data files are modified, remember to appropriately set them in the .ipynb file.

Fig. 2: Surface vs Boundary loads

In file “Comsol_simulation_fig2.mph” we obtain the surface and volume contributions to the photothermal forces, again for a GaAs microdisk. The PTh response is easily obtained for the three mechanical modes in Fig. 2 through appropriate choice of the frequency guess for the mechanical mode solution. In file “Comsol_simulation_fig2_RP.mph” the radiation pressure coupling for the breathing mode of microdisks of different radii is calculated.

In Comsol: Comsol_simulation_fig2

- Open file **“Comsol_simulation_fig2.mph”.** Under Study 1 – PTh -> Eigenfrequency 1, set the Search for frequencies around to one of the following: 230e6, or 604e6 or 981e6, depending on the mechanical mode of interest. In order to generate Fig. 2, the three computations are necessary.
- Run Study 1 – PTh. The first order TE optical mode is computed, along with the mechanical mode chosen. Furthermore, 380 thermal modes are obtained for evaluating the PTh response.
- In Results -> Derived Values, compute Global Evaluation 1 and export the data obtained. This procedure is repeated for each of the mechanical modes considered. The output data is found in files “**thermal_mode_analysis_1st.txt**” (230e6 mode), “**thermal_mode_analysis_2nd.txt**” (604e6) and “**thermal_mode_analysis_3rd.txt**” (981e6). After each computation, make sure you clear the results in the output table.

In Comsol: Comsol_simulation_fig2_RP

- Open file **“Comsol_simulation_fig2_RP.mph”.** This file is built for calculating the radiation pressure coupling for a disk with a radius of 6 μm. The mechanical breathing modes (1st order) and the first order TE optical modes are considered in this calculation. For this purpose, appropriate guesses are set for the mechanical and optical frequencies.
- Run Study – RP.
- In Results -> Derived Values, compute Global Evaluation 1 and export the data obtained. The output is found in file “**RP_1st.txt**”

Fig. 2: Surface vs Boundary loads

In file “Comsol_simulation_fig2.mph” we obtain the surface and volume contributions to the photothermal forces, again for a GaAs microdisk. The PTh response is easily obtained for the three mechanical modes in Fig. 2 through appropriate choice of the frequency guess for the mechanical mode solution. In file “Comsol_simulation_fig2_RP.mph” the radiation pressure coupling for the breathing mode of microdisks of different radii is calculated.

In Python:

- Data generated in Comsol is loaded directly into the Python file. The effective thermal response functions h1 and h2 (defined in the supplemental material) are computed from the photothermal contributions of each of the thermal modes. All relevant plots are then generated. Please, keep in mind that all data files generated in Comsol have to be on the same folder as the .ipynb file, unless a different path is specified. In case the names of the data files are modified, remember to appropriately set them in the .ipynb file.

Fig. 3: Optomechanical backaction

In file "Comsol_simulation_fig3.mph" we evaluate the photothermal forces, acting on GaAs microdisk. The PTh response is obtained by considering the first 200 thermal modes of the structure and is evaluated for microdisks of several radii. For this purpose, the first order mechanical breathing and TE optical modes are considered. In file "Comsol_simulation_fig3_RP.mph" the radiation pressure coupling for the breathing mode of microdisks of different radii is calculated.

In Comsol: Comsol_simulation_fig3

- Open file **"Comsol_simulation_fig3.mph"**. This file is built for calculating the photothermal coupling for disks of several different radii. The mechanical breathing modes (1st order), the first order TE optical modes, and the first 200 thermal modes are considered in this calculation. For this purpose, we prepared input files with appropriate guesses for the mechanical frequencies for a given disk radius (between 2.5 and 10 μm). Those were obtained in a previous, large scale, simulation. The input files are named "**freq_guessX_zenodo.txt**" and "**rDiskX_zenodo.txt**", where X ranges from 1 to 6, according to the range of disk radii considered e.g. files "**rDisk1_zenodo.txt**" and "**freq_guess1_zenodo.txt**" encompass radii of 2.5e-6 to 3.3e-6 m, while "**rDisk5_zenodo.txt**" and "**freq_guess5_zenodo.txt**" encompass radii of 7.5e-6 to 8.86e-6 m.
- Under Study – PTh-> Parametric Sweep, click "Load from file" (yellow folder icon) and choose "freq_guessX_zenodo.txt". Repeat this procedure for "rDiskX_zenodo.txt".
- Run Study – RP. A table with the required data is automatically generated (make sure you choose an appropriate path and file name under Results->Tables->table_pcolor), based on the probes defined in Component 1-> Definitions. These tables are found in files: "**table_pcolor_vX.txt**".
- Repeat this procedure for X = 1,2,3,4,5,6.

In Comsol: Comsol_simulation_fig3_RP

- Open file **"Comsol_simulation_fig3_RP.mph"**. This file is built for calculating the radiation pressure coupling for disks of several different radii. The mechanical breathing modes (1st order) and the first order TE optical modes are considered in this calculation. For this purpose, we prepared input files with appropriate guesses for the mechanical frequencies for a given disk radius (between 2.5 and 10 μm). Those were obtained in a previous, large scale, simulation. The input files are named "**freq_guessX_zenodo.txt**" and "**rDiskX_zenodo.txt**", where X ranges from 1 to 6, according to the range of disk radii considered e.g. files "**rDisk1_zenodo.txt**" and "**freq_guess1_zenodo.txt**" encompass radii of 2.5e-6 to 3.3e-6 m, while "**rDisk5_zenodo.txt**" and "**freq_guess5_zenodo.txt**" encompass radii of 7.5e-6 to 8.86e-6 m.
- Under Study – RP-> Parametric Sweep, click "Load from file" (yellow folder icon) and choose "freq_guessX_zenodo.txt". Repeat this procedure for "rDiskX_zenodo.txt".
- Run Study – RP. A table with the required data is automatically generated (make sure you choose an appropriate path and file name under Results->Tables->table_pcolor_RP), based on the probes defined in Component 1-> Definitions. These tables are found in files: "**table_pcolor_vX_RP.txt**".
- Repeat this procedure for X = 1,2,3,4,5,6.

Fig. 3: Optomechanical backaction

In file “Comsol_simulation_fig3.mph” we evaluate the photothermal forces, acting on GaAs microdisk. The PTh response is obtained by considering the first 200 thermal modes of the structure and is evaluated for microdisks of several radii. For this purpose, the first order mechanical breathing and TE optical modes are considered. In file “Comsol_simulation_fig3_RP.mph” the radiation pressure coupling for the breathing mode of microdisks of different radii is calculated.

In Python:

- Data generated in Comsol is loaded directly into the Python file. The effective thermal response functions h1 and h2 (defined in the supplemental material) are computed from the photothermal contributions of each of the thermal modes. All relevant plots are then generated. Please, keep in mind that all data files generated in Comsol have to be on the same folder as the .ipynb file, unless a different path is specified. In case the names of the data files are modified, remember to appropriately set them in the .ipynb file.

Fig. 4: Experimental data analysis

In the folder "Fig4", experimental data concerning both the non-linear optical and mechanical linewidth characterization is analysed. This analysis was broken into three .ipynb files:

- 1-Analysis_optical_non-linear_characterization.ipynb -> Optical data is fitted according to a simple model for the optical non-linearities, which is then shown to reproduce the transmission data. Generates figures: Fig.4 b), c) and d).
- 2-Analysis_mechanical_linewidth_characterization.ipynb -> The mechanical power spectral density is fitted according to a single Lorentzian resonance model, allowing the determination of the mechanical linewidth and frequency as a function of both the laser detuning and the incident power on the cavity. Generates figures: Fig.4 e) and f).
- 3-Comparison_non-linear_optical_model_vs_experimental_mechanical_data.ipynb -> Our theory for the photothermal force is applied along with the model for the optical non-linearities. This allowed us to make predictions about the amplitudes of both photothermal and radiation pressure effects on the mechanical linewidth variation. Finally those predictions are compared with the experimental data. Generates figures: Fig.4 g) and h).

The folders "1-Optical_non-linear_characterization" and "2-Mechanical_linewidth_characterization", contain the experimental data, whereas the folder "1-Simulation_data" contains multiple Comsol simulation results, which are explored in the next pages.

In Python: For all notebook files in the folder "Fig4"

- The notebooks are meant to be run in order, because the first two notebooks generate .par used in the third notebook.
- For safety, always restart your Python Kernel after significant parameter changes.
- Be careful with the order in which the cells are run. After changing a parameter on a given cell, it is recommended to re-run all the cells after it.
- The paths used in the importing of experimental and simulation data where only tested for Windows 10. We have used a Windows Anaconda distribution of Python 3.8.3. A reduced number of extra packages such as "mpmath" and "pyLPD" is also necessary for running our scripts.

Fig. 4: - Isotropic simulations

In file “Comsol_simulation_fig4_iso.mph” of the folder “1-Simulation_data”, we evaluate the photothermal response of a mechanically isotropic GaAs microdisk, with dimensions similar to the fabricated device reported in the main text. The PTh response is obtained for the first 200 thermal modes of the structure and considering its coupling with the 6th order TE optical mode. The goal of this simulation is obtaining parameters that only depend on approximately isotropic properties of GaAs, i.e. the thermal resistance, thermal lifetimes, and thermo-optical frequency pulling. Those are used in the computations for Fig. 4.

In Comsol: Comsol_simulation_fig4_iso

- Open file “Comsol_simulation_fig4_iso.mph”. Study 1 – PTh -> Eigenfrequency 1 is set for computing the first order mechanical breathing mode of the structure, the 6th order TE optical mode and 200 thermal modes of the cavity. The mechanical calculation is only performed for completeness, but is unnecessary for the following analysis.
- Run Study 1 – PTh.
- In Results -> Derived Values, compute Global Evaluation 1 and export the data obtained. Data is displayed in “photothermal_analysis_fab_iso.txt”.

Fig. 4: - Anisotropic simulations

In file “Comsol_simulation_fig4_aniso.mph” of the folder “1-Simulation_data” folder, we evaluate the photothermal response of a mechanically anisotropic GaAs microdisk, with dimensions similar to the fabricated device reported in the main text. The PTh response is obtained for the first 200 thermal modes of the structure and considering their coupling to the 6th order TE optical mode and the mechanical breathing mode. The goal of this simulation is obtaining parameters that only depend on anisotropic properties of GaAs, i.e. the photothermal force per temperature, called Λ in the main text, and the single-photon radiation pressure coupling, g0.

In Comsol: Comsol_simulation_fig4_aniso

- Open file **“Comsol_simulation_fig4_aniso.mph”**. The node “study_optics_2D” is set for computing the 6th order TE optical mode of the microdisk in a reduced 2D axisymmetric geometry. “study_mech_vs_aniso” computes the anisotropic mechanical breathing mode. Exploring symmetries of the system, the simulation domain may be taken as only ¼ of the disk+pedestal structure. “study_thermal_modes” computes 200 thermal modes of the microdisk, also in an axisymmetric geometry.
- Run “study_optics_2D”.
- Run “study_mech_vs_aniso”.
- Run “study_thermal_modes”.
- In Results -> Derived Values, compute Global Evaluation 1 and export the data obtained. Data is displayed in “**RP _analysis_fab_aniso.txt**”.
- In Results -> Derived Values, compute Global Evaluation 2 and export the data obtained. Data is displayed in “**photothermal_analysis_fab_aniso.txt**”.

Notes:

- Anisotropy is implemented by prescribing the stiffness tensor of GaAs into the simulation files. This is seen in Component 1 -> Solid Mechanics -> Linear elastic material :

D User defined

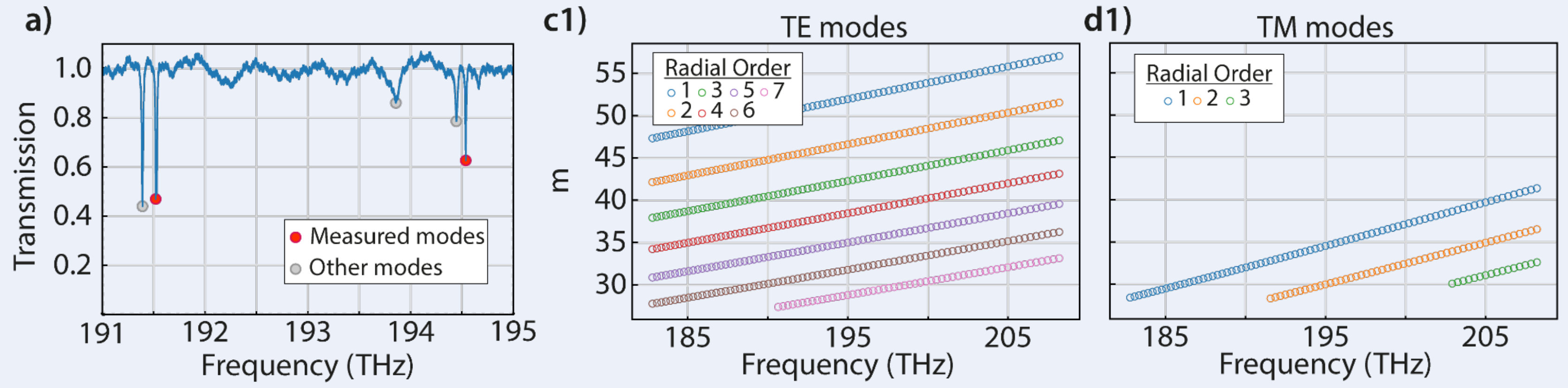
C11	C12	C12	0	0	0
C12	C11	C12	0	0	0
C12	C12	C11	0	0	0
0	0	0	C44_neta	0	0
0	0	0	0	C44_neta	0
0	0	0	0	0	C44_neta

Pa

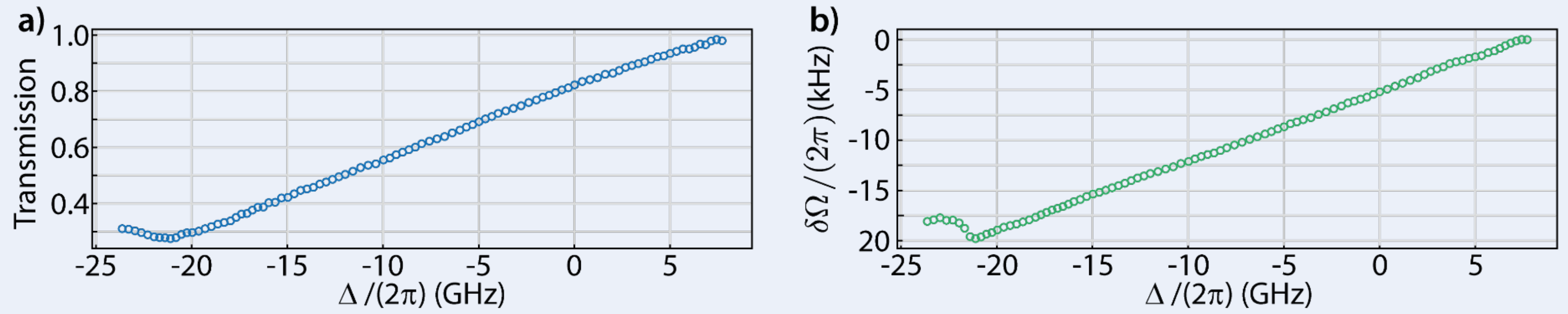
- C44_neta depends on the variable neta, which can be set between 0 and 1 for varying the degree of mechanical anisotropy.
- 2D solutions like the optical and thermal responses are made compatible with 3D solutions (mechanical modes) by extruding the 2D solutions into the 3D geometry. This is accomplished using Comsol’s built-in operator “genext1”.

Available files – Supplemental material

- Fig. S1: Optical mode identification (Comsol 5.4, Python)



- Fig. S2: Mechanical frequency static thermal shift (Python)



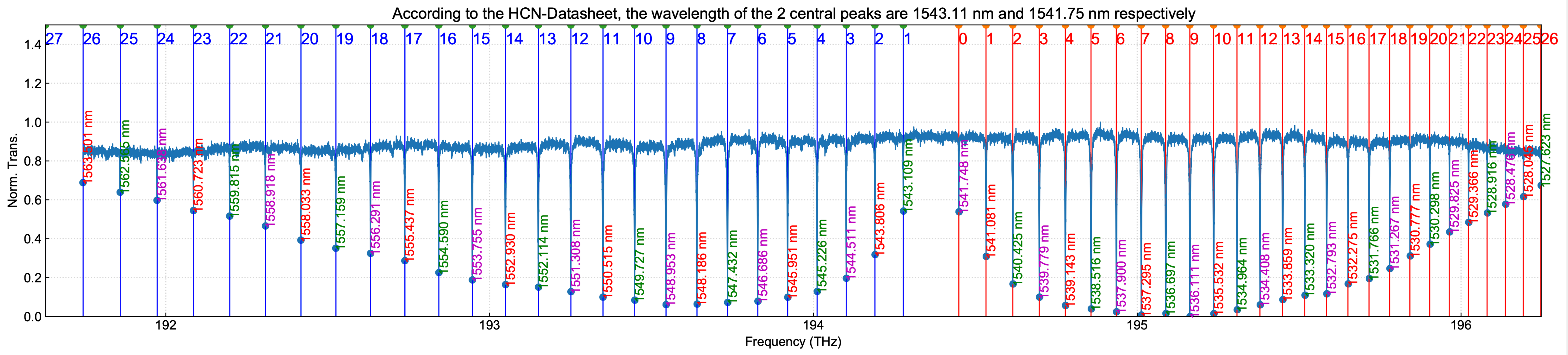
Details in the structure of the simulations can be found in the repository for: "**Brillouin Optomechanics in Nanophotonic Structures**" - DOI: 10.1063/1.5088169.

Fig. S1: Optical mode identification

For identifying the optical mode we compare the measured optical free-spectral-range (FSR) with a FEM simulation of our device. To precisely measure the FSR of our device we calibrate our transmission spectra using a Mach-Zhender interferometer (MZI) and a Hydrogen Cyanide (HCN) gas cell.

In Python: Measurement folder

- For safety, always restart your Python Kernel after significant parameter changes.
- Be careful with the order in which the cells are run. After changing a parameter on a given cell, it is recommended to re-run all the cells after it.
- Keep all files in the same folder since the notebook uses the raw data, NIST calibration for the HCN cell and cprint.py file.
- The first few cells are for gathering data, normalizing its DC background and displaying it.
- After finding the MZI and HCN peaks an interpolation for all horizontal (originally time) data is performed to create the laser frequency axis. In order to verify the accuracy of such procedure, we compare the modified data with all NIST's HCN optical absorption data base (“frequency_calibration_validation.pdf”– see bellow).
- Finally, the frequency distance between consecutive optical modes is measured, which results in the cavity's FSR.



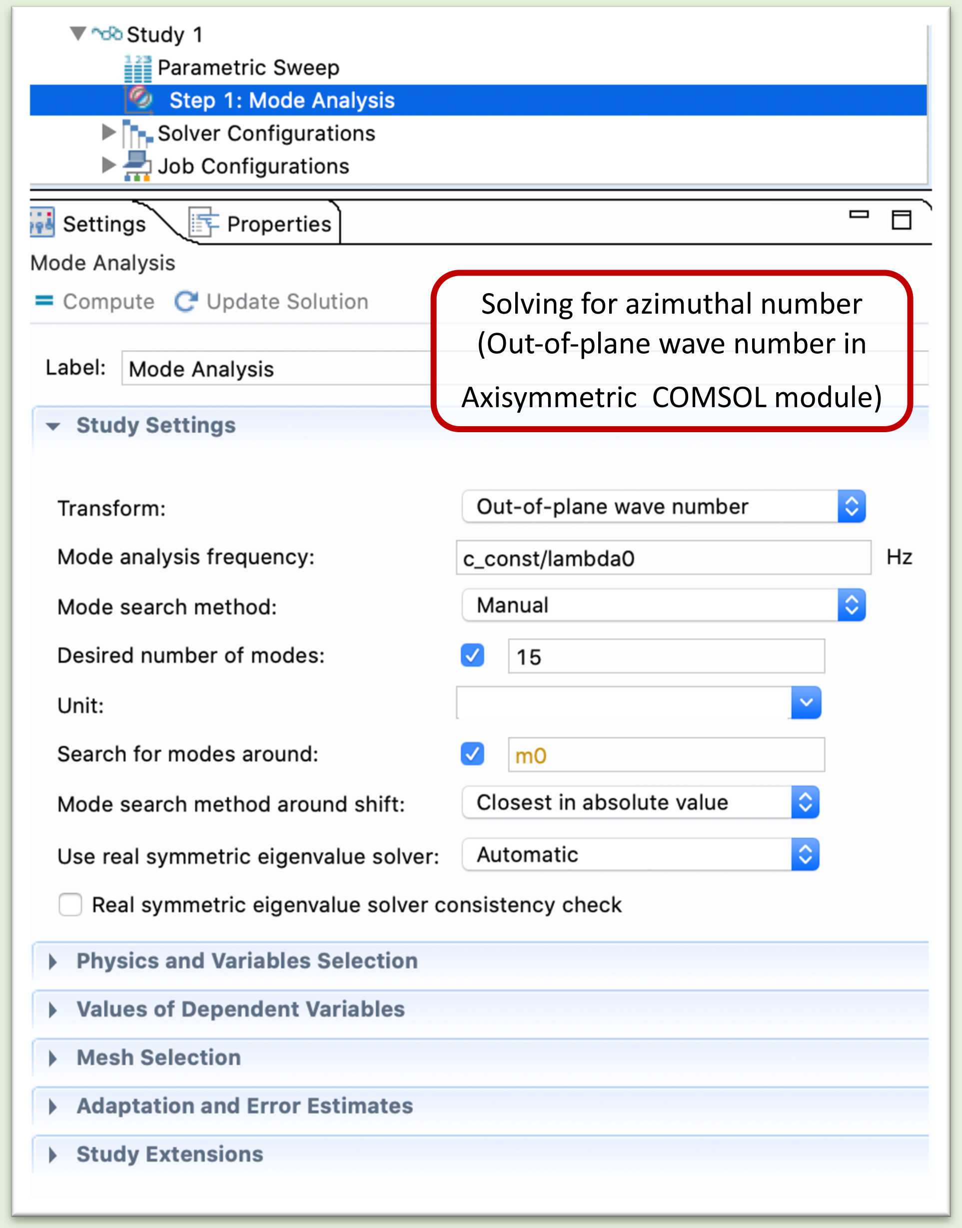
HCN data and NIST standard superimposed after laser frequency calibration

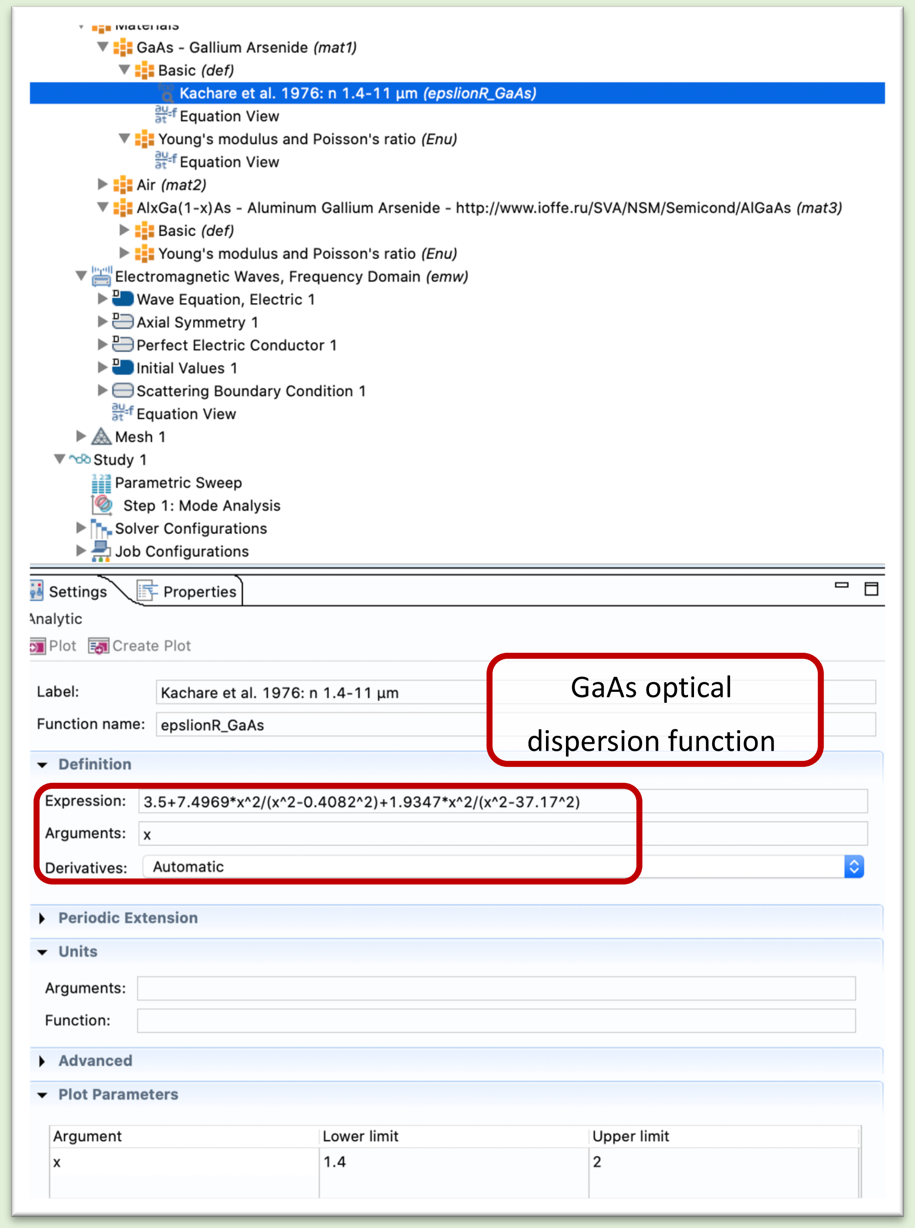
Fig. S1: Optical mode identification

For identifying the optical mode we compare the measured optical free-spectral-range (FSR) with a FEM simulation of our device. In the "/simulation" folder the COMSOL file "GaAs_Disk_Dispersion_figS1.mph" is used to produce a "GaAs_Disk_Dispersion_figS1.csv" table that is plotted using the "plot_optical_dispersion_GaAs_Disk .ipynb" Python notebook. The fitted values for the FSR and

In Comsol: GaAs_Disk_Dispersion_figS1.mph

- For simulating the dispersion of the disk we solve for the azimuthal mode number (m_0) as a function of the input frequency (Study – Mode Analysis). This is necessary since we need to include the GaAs layer material's dispersion[a].
- The results from the simulations are output in a table exported in .csv format (GaAs_Disk_Dispersion_figS1.csv) in order to be plotted in python.

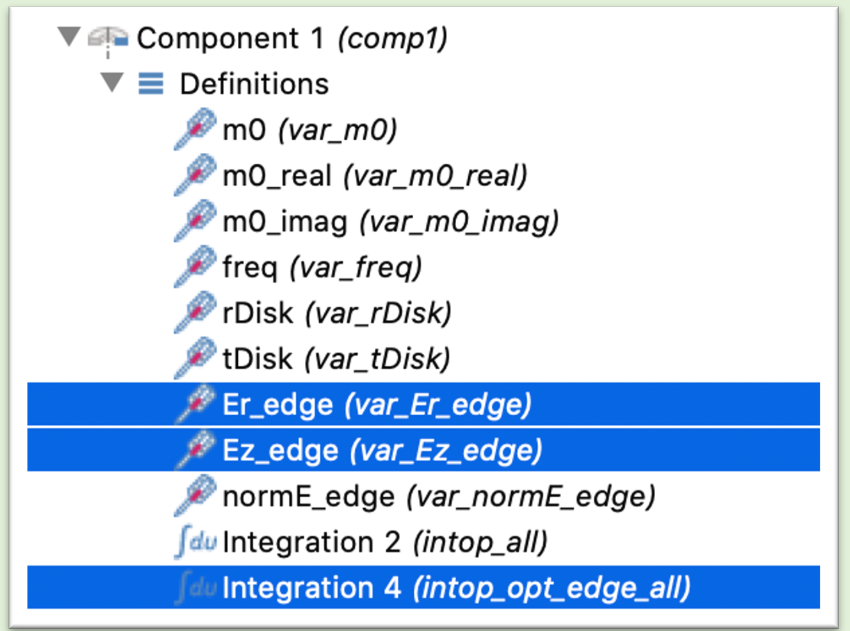




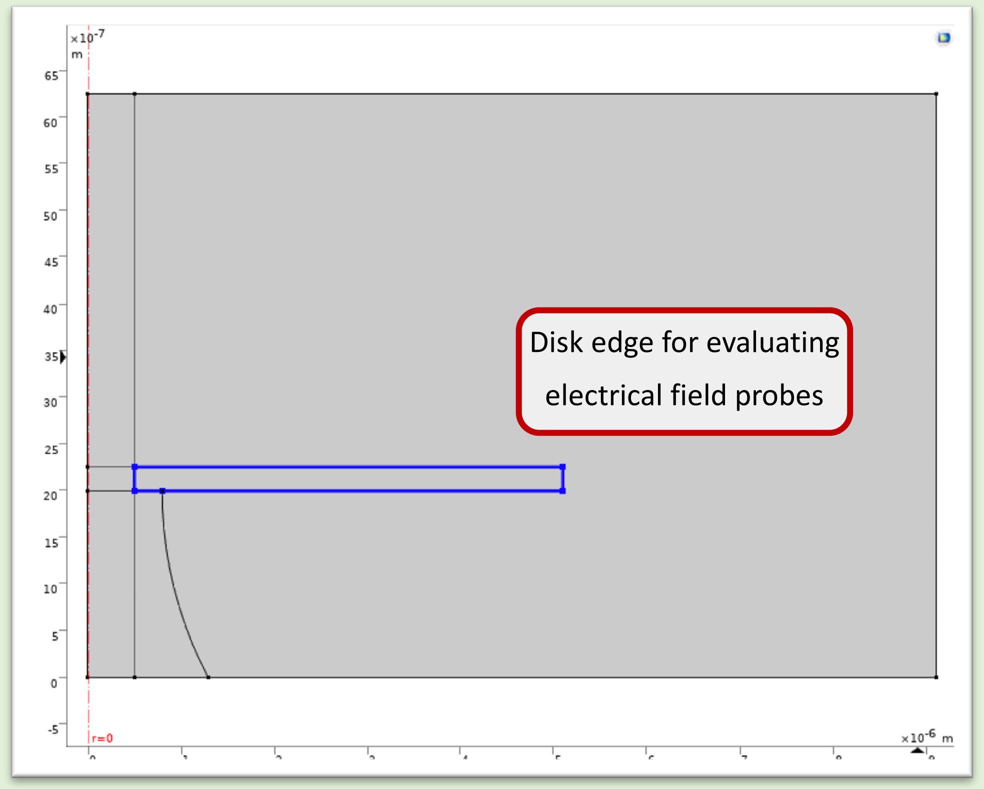
[a] A. H. Kachare, *et al.* "Refractive index of ion-implanted GaAs", *J. Appl. Phys.*, **47**, 4209-4212 (1976).

Notes:

- In order to identify each optical mode polarization we also export optical probes for the integrated electrical field r- and z-component at the disk's edge.
- Also to ease the identification of the confined optical modes, Scattering boundary conditions are placed far from the disk, which enabled to retrieves the optical mode quality factor.



"Er_edge" and "Ez_edge" probes used for defining the mode polarization



In Python:

- Data generated in Comsol is loaded directly into the Pandas dataframe (Python). Er_{edge} and Ez_{edge} probes are used to defines mode polarization and subsequentely determine the radial order number by simply ordering m_0 for each frequency. The final step is to fit the dispersion curve to obtain the FSR.

Fig. S2: Static thermal mechanical frequency shift

The plots are generated along with those of Fig. 4 of the main text. The data treatment is found in: “Analysis_mechanical_linewidth_characterization.ipynb”.