

Resonator Simulator

v1.01 (8/28/16)

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Summary

Simulates the temperature dependence of the resonant frequency for doped silicon resonators. The quality factor due to thermoelastic dissipation and gas damping (drag and squeeze-film) in rarified air can also be simulated.

The screenshot shows the Resonator Simulator software interface. The window title is "ResonatorSim" and the version is "v1.01 (Aug 28, 2016)" with the URL "http://micromachine.stanford.edu/".

Silicon Parameters

- Wafer Orientation: 100
- Flat/Notch: <110>
- Doping Type: n
- Concentration: 5e19 /cm³
- Temperature Points: -40 25 85 °C

COMSOL Model

- Geometry File: [Select File]
- Filename to Save: []
- Model Orientation: 0 ° from flat
- Simulate TED:
- # Modes to Search: 6
- Frequency: 1.00e6 Hz
- Mode Select: Manual

Boundary Conditions

- Fixed: []
- Drive: []
- Link Adjacent?:
- Symmetry: []
- Sense: []

Gas Damping

- Calculate Qgas: (Squeeze Film & Drag Force only)
- Surface #s: []
- Use Drive/Sense: []
- Pressure: 1 Pa
- Gas Mass: 29 g/mol
- Gap: 1.5 μm

Buttons

- Save COMSOL Files:
- Go! []
- Stop []

Results

- Frequency vs. Temperature []
- Plot []
- Force Q: Q: 10e3
- Vbias: 15 V
- Planes of Symmetry: 0
- Cfeed: 30 fF
- Gap: 1.5 μm

Config

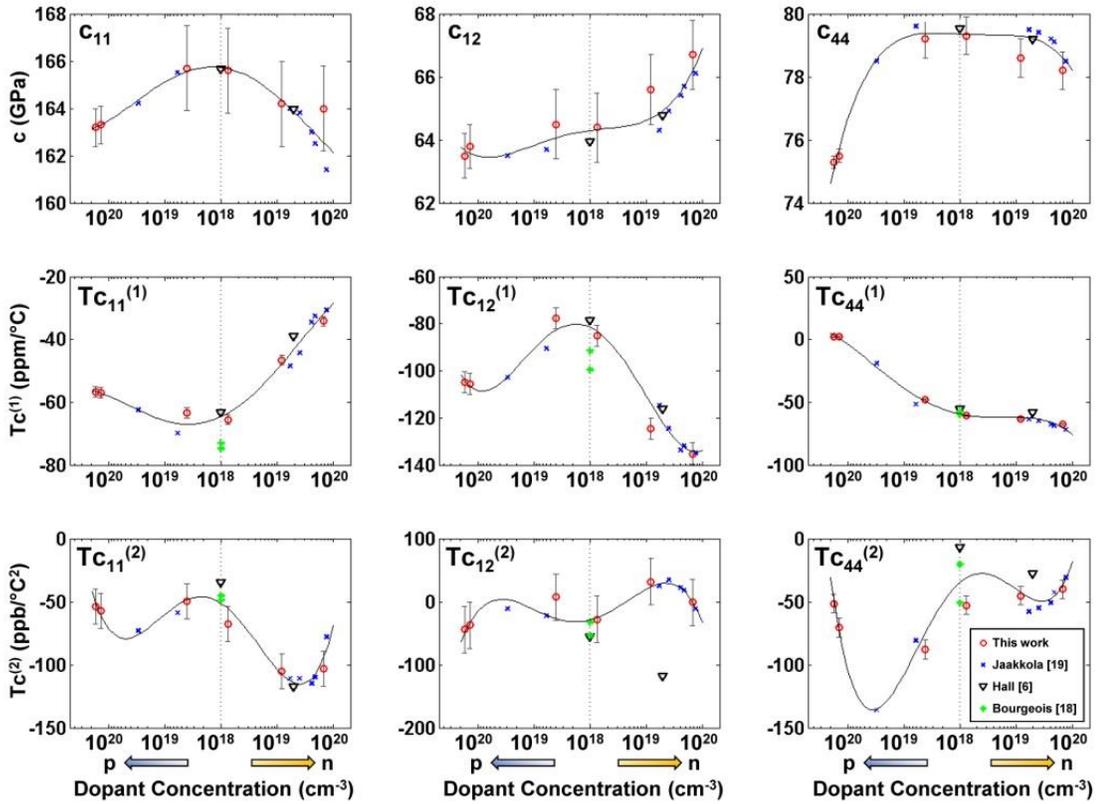
- Load []
- Save []

Required Software

- MATLAB 2015b (May work on other versions but only tested with this)
- COMSOL 5.0 with MATLAB LiveLink (May work on other versions but only tested with this)

1] Introduction

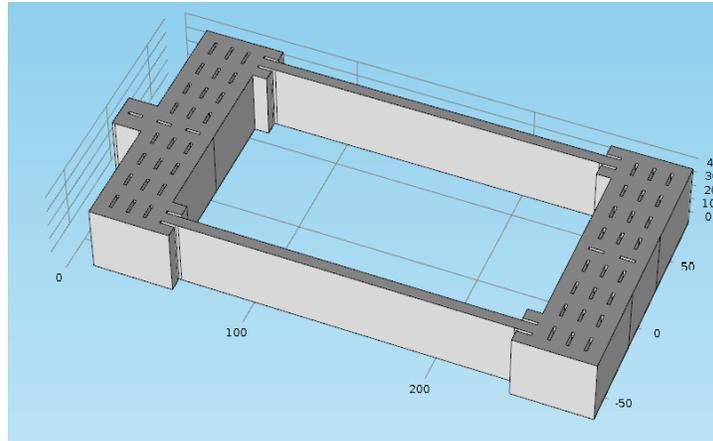
- This MATLAB code for COMSOL allows for the simulation of the frequency-temperature dependence of an arbitrary linear resonant mode shape in heavily doped silicon. From work done in this group [9] and other groups (VTT [10], CSEM [3], and IBM [11]), the temperature dependence of the elastic constants of heavily doped silicon have been extracted: p-type up to 1.75e20cm⁻³, and n-type up to 7.5e19cm⁻³. These extracted values (up to 2nd order, as shown below, with least squares fits to a 4th order polynomial) can be used in conjunction with finite element analysis to simulate frequency-temperature dependences of doped silicon resonators.



- This user guide assumes the reader is familiar with COMSOL Multiphysics finite element software, and will assume COMSOL models already exist for the device of interest, and the eigenfrequency and mode shape are known.
- Other useful literature on the effect of doping on the elastic constants are [12-17].
- The quality factor due to thermoelastic dissipation and gas damping (drag and squeeze-film perpendicular to surface) is also calculated. The quality factor simulated here should be used for order-of-magnitude estimates.

2] Usage

- 2.1 First, create a model and build the geometry of the silicon resonator in COMSOL. A solid mechanics model can be used here.



- 2.2 For the material, if only silicon will be used in the simulation, this step can be skipped.

For composite resonators, assign the materials silicon (poly, single-crystal, etc. doesn't matter as it will be overridden), and silicon oxide to the local model (i.e. not a global material). SiO₂ is supported with only a linear TCE, and no . (Warning: these composite resonator results have not been verified!)

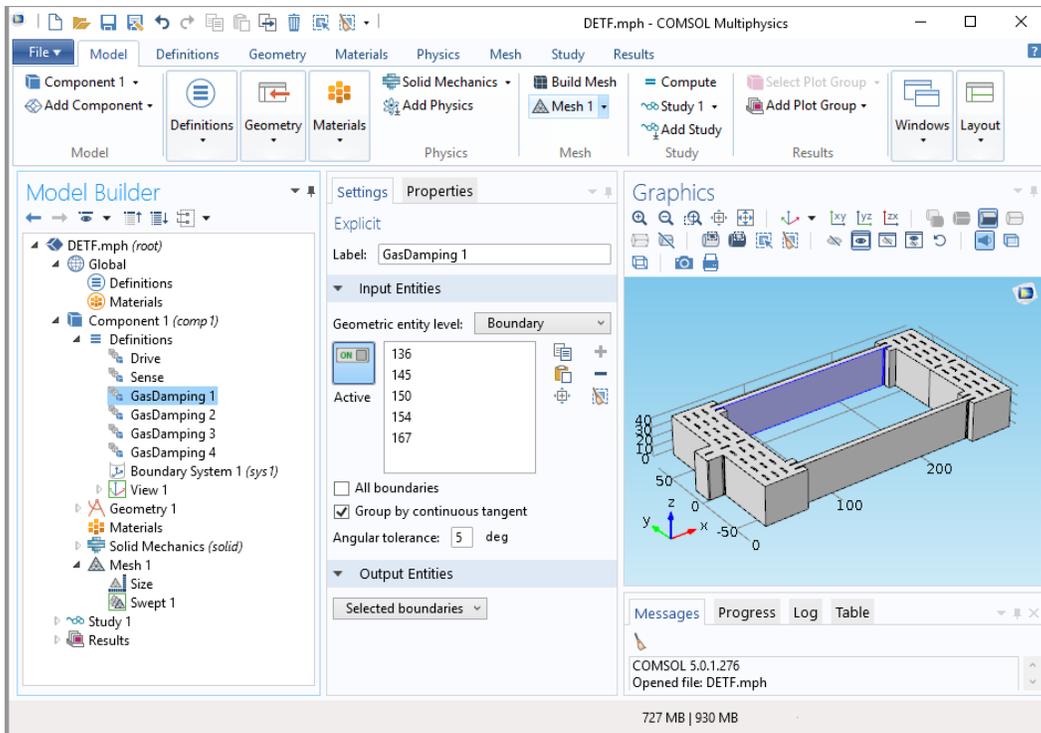
- 2.3 For modeling of the electrical response of voltage-biased capacitive resonators, it is useful to define the excitation (drive/sense), and gas damping regions. Under the model definitions, add Selections->Explicit and rename the labels for the following cases

- Drive: Ac voltage applied across a gap to this surface to drive the resonator into motion

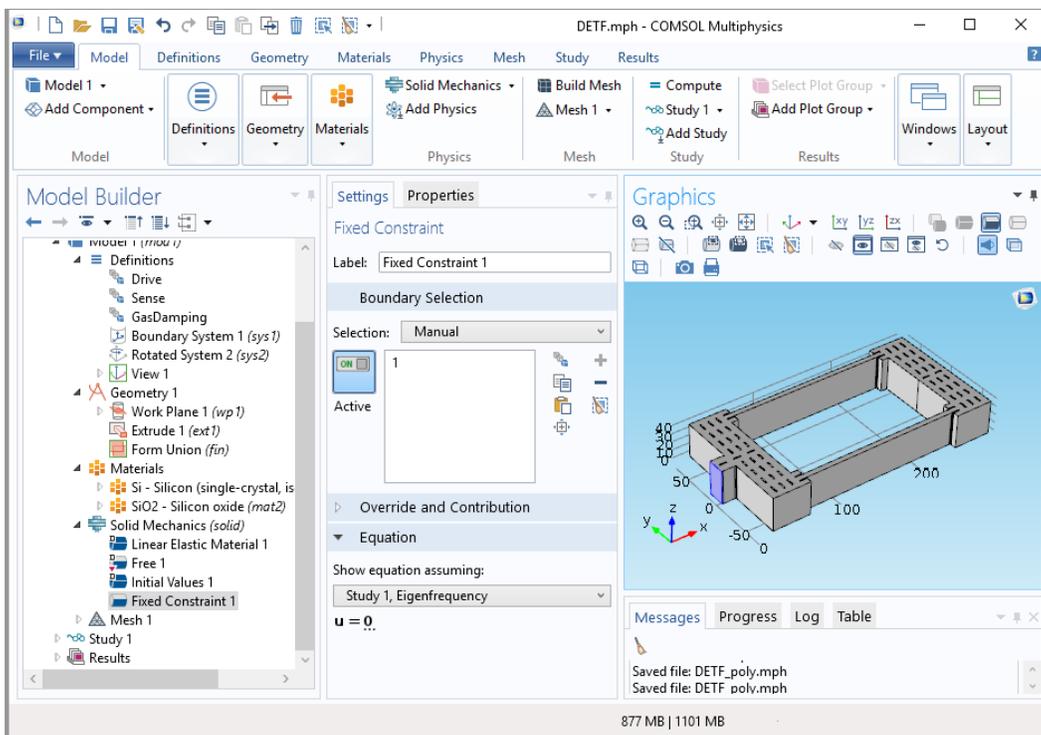
- Sense: Motion sensed across this gap

- GasDamping: The gas surrounding the resonator can be a source of damping. The quality factor estimation due to gas damping is implemented on the drive/sense surfaces using models for rarified air (valid for low pressures). Note that only motion perpendicular to the surfaces are accounted for. Q_s for drag (Christian [6]), squeeze-film (Bao [7]), and a frequency-dependent combination model [8] are calculated at the temperature range mid-point. Q_{gas} scales inversely with pressure and to the inverse square-root of temperature (in K). Note that the gas damping surfaces should be defined separately for each discontinuous surface, and the labels should start with "GasDamping": e.g. "GasDamping 1", "GasDamping 2". Surfaces with opposite modal displacement normals (as when the part of a surface's displacement is outward and another part inward) should be divided accordingly so that the effective perimeters for squeeze-film damping can be calculated accurately.

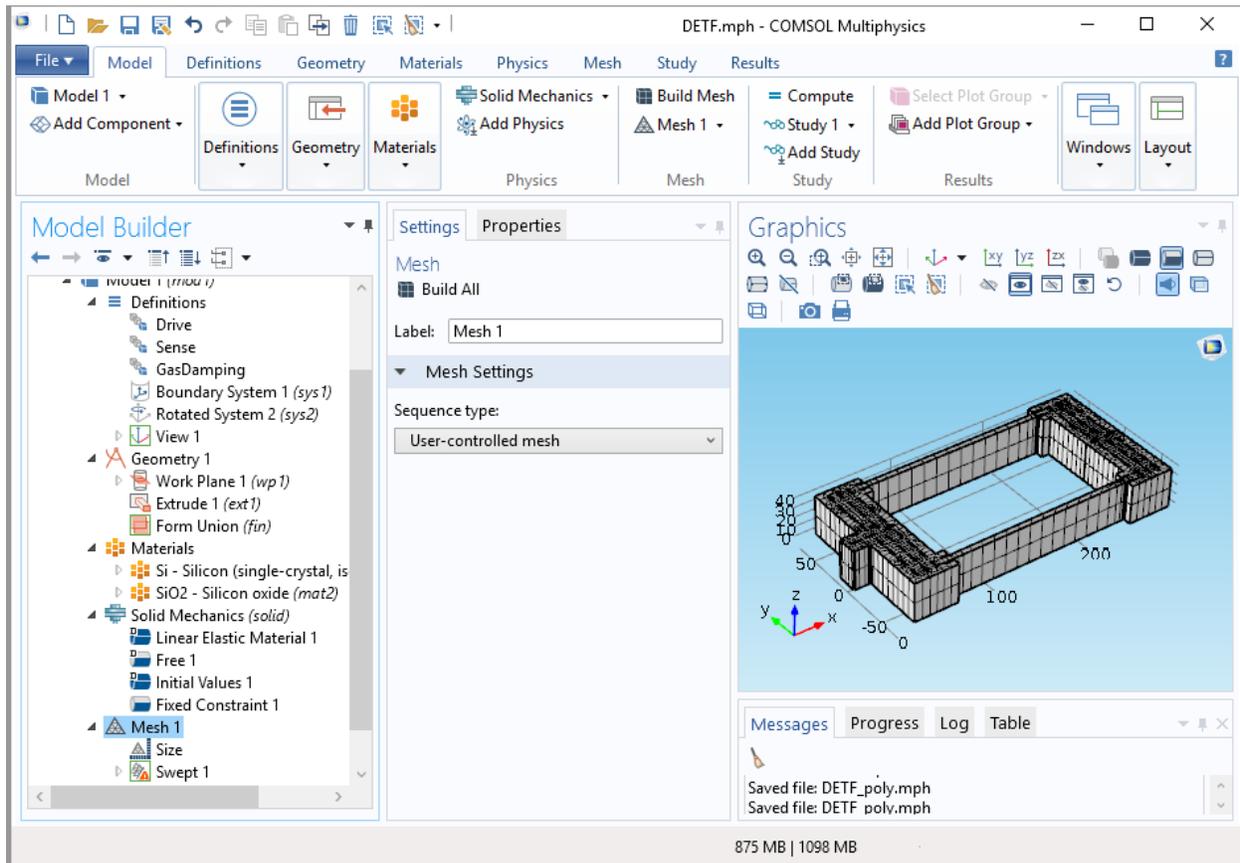
Also change the Geometric Entity level to *Boundary* and select the surfaces for the above cases. The option "Group by continuous tangent" may be helpful to help multiple linked surfaces.



2.4 Next, add the boundary conditions. Only two conditions are supported here: “Fixed” and “Symmetry”. Select the surfaces as desired.



- 2.5 Last, define the mesh. This step is recommended as the default mesh may not always be ideal. Save the model as an .mph file.



- 2.6 Launch COMSOL with Matlab Livelink. Run the script Resonator Simulator.m and change paths if necessary. Select the various options as follows:

- Wafer type: (100), (110), (111), or Poly. In-plane orientation on wafer (in degrees)
- Doping type (p or n), and concentration (in cm^{-3})
- Temperature points: Specify in Matlab array format, e.g. -40:20:80
- Geometry file: Select the .mph file saved previously.
- Filename to save: additional files with this base name will be generated during the solution in the \savedfiles\ directory (comsol .mph files, matlab data .mat files)
- Approximate resonant frequency of mode. This will be passed to COMSOL to search for the eigenfrequency.
- Model orientation: Rotation of device on the wafer from the flat/notch.
- Modes to search: # of eigenfrequency modes that COMSOL returns that will be displayed for selection.
- Mode selection: How the appropriate mode should be selected. Manual allows you to pick the first mode, auto picks the most likely mode (maximum response).

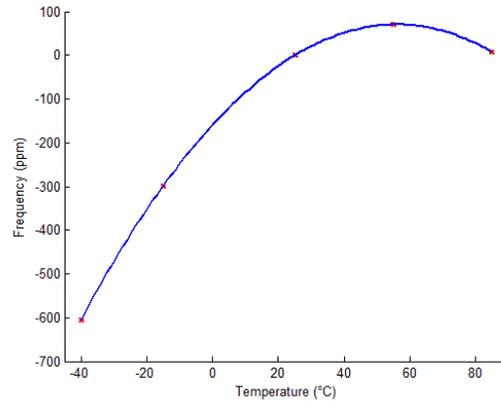
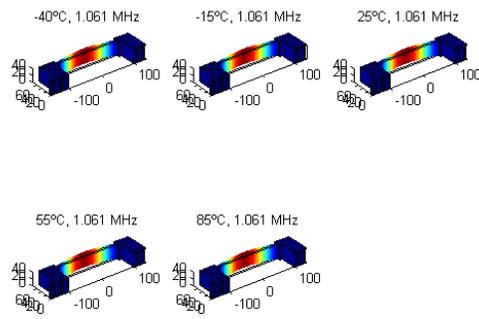
- Simulate Qted?: Quality factor due to thermoelastic dissipation, as implemented by COMSOL. Qted simulations take a little longer. Note: material properties for doped silicon in the simulation of Qted are not available as of this time. Properties for undoped silicon have been used from literature [1-5], but some inaccuracy should thus be expected. These material properties are located in “functions\getTherm.m” and should be adjusted accordingly if material properties are known.
- Boundary Conditions: Index # of surfaces for boundary conditions (fixed and symmetry conditions) and drive/sense surfaces. This should be auto-populated when loading in a .mph file and should only be available for input only when input is a mesh or script. These numbers can be obtained from the main COMSOL program.

Gas damping, surface index #s should be separated by a semi-colon if the specified surfaces are to be treated separately for modal displacements in opposite directions - separating the surfaces with a comma will link the surfaces without accounting for the inner perimeters – use this when adjacent surfaces are displacing in the same direction.

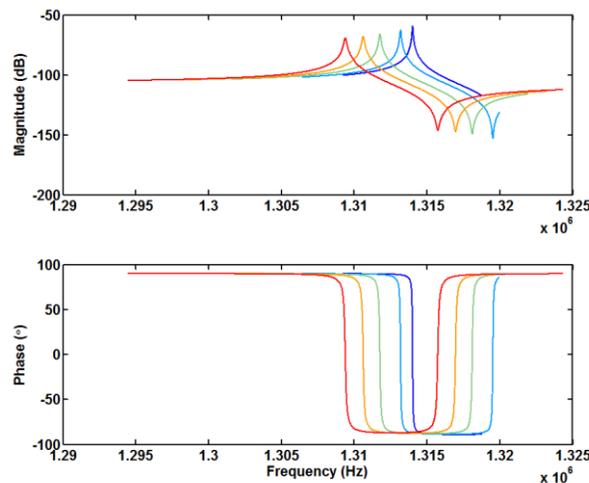
- Link Adjacent: For curved structures with many surface segments, instead of listing every surface, checking this box will select all adjacent surfaces to the selected surface, within a tolerance of “modelfile.linktol” (defaults to 10°).
- Simulate Qgas? Calculates theoretical values of gas damping as limited by motion perpendicular to surface. Models: Bao (drag), Christian (squeeze-film), and frequency dependent (combination).
- Gas damping - pressure, gas mass, and gap: used for simulating Qgas.
- Save COMSOL Files: Saves the raw .mph files at each temperature step. These can be opened directly in COMSOL for verification.
- Upon running, settings for the last simulation run will be stored in the \savedfiles\ directory under the specified save filename.
- Notes:
 - Electrostatic actuation perpendicular to the selected surfaces is assumed here for Qted and Qgas simulations.
 - Qted and Qgas are typically seen to limit the experimentally observed Q for lower frequency flexural resonators. Akhieser, surface losses, anchor losses or other damping mechanisms are not simulated here, and could play a large role for certain resonators.
 - This code only simulates first order effects (resonances within the linear regime)!

2.7 After the code has completed, you should be presented with a plot of the *Selected Modes*, as well as a plot indicating the frequency-temperature dependence in ppm/°C. It is important to ensure that the *Selected Modes* window displays the same mode for each temperature point. This ensures that the frequency is tracked for that particular mode shape. The frequency-temperature plots should be more-or-less quadratic in nature, due to only the quadratic temperature dependences of the elastic constants used in the simulation.

Selected Modes:



2.8 Other plots: after running the simulation, frequency sweeps can be plotted using a simple parallel plate capacitive model (without fringe fields). This assumes electrostatic transduction perpendicular to the surfaces. This frequency response also accounts for electrostatic softening and feedthrough capacitance, though values of the feedthrough capacitor and other things such as bias voltage needs to be pre-defined as in the options in the GUI. The gap size here pertains to the electrostatic gap size, which should be the same as the gas damping gap size above, but is put as an option here to allow the user to quickly see the effect of changing the gap size. The Q used is as calculated in the simulation, or if not available, a Q of 10 k is assumed. The limiting mechanism (TED, gas, AKE - akhieser) is also displayed in parentheses. An option is also available to force a Q on the frequency sweep response if the Q value is known. The plot on below shows the simulated frequency response for a DETF resonator at various temperatures from -40°C



(blue) to 80°C (red). First order electrostatic softening effects are accounted for, as is the quality factor due to thermoelastic dissipation.

The data is also output directly to Matlab base workspace:

- fout: Structure with fields

- fraw: Simulated mechanical eigenfrequency due to elastic constant change with temperature
 - fadj: As above, but accounting for thermal expansion
 - fc: Frequency at midpoint of temperature range
 - fppm: Frequency change in ppm, centered at fc
 - coeff: Coefficients of a second order polynomial fit, in [ppm/(°C)², ppm/(°C), ppm]
- Qout: Structure with fields
 - ted: Quality factor due to thermoelastic dissipation
 - gas: Quality factor due to gas damping
 - chr: Christian's model
 - bao: Bao's model
 - fd: Frequency dependent model
- dataout: Other useful data
 - modeshape: Selected modal displacement
 - meff: Effective mass calculated at fout.fc
 - f: Center frequency
 - k: Effective stiffness
 - drarea: Total drive electrode area
 - nd: Scaling factor for drarea due to mode shape
 - snarea: Total sense electrode area
 - ns: Scaling factor for drarea due to mode shape
 - nel1-3: Scaling factors for electrostatic spring softening (nel1 is for the linear term, and nel2 nel3 are for higher order terms)

3] Changelog

v1.01 (8/28/16)

Fixed bug in gas damping quality factor prediction

v1.0 (2/15/16), unreleased test

Read directly from .mph files

GUI and stability improvements

Bug fixes with mode detection

Frequency Response plotting in GUI

Qgas calculation fixes

v0.3 (7/19/15)

Polysilicon option added using Voigt averaging of crystalline properties.

v0.2 (4/26/15)

1. Autodetect mode implementation changed.
2. Quality factor due to thermoelastic dissipation as implemented using the thermoelasticity module in COMSOL.
3. Added gas damping quality factor calculation for resonators in rarified air.
4. Note: configuration files from the previous version cannot be used, and it is necessary to re-setup the model.

v0.1 (5/14/14)

Initial release

4] Disclaimer

The authors in no way guarantee the accuracy of these results. The elastic constants have been extracted by several research groups independent of each other, and have been verified to hold true of several different modes. However, many other effects could limit the accuracy of this method. Nonlinearities, for one, are known to significantly affect the results, and software bugs may well be present. This code is offered free-of-charge on a no-guarantee basis. Best efforts will be made to maintain the software – please email the author with any bug reports. Updates can be found on <http://micromachine.stanford.edu/projects/doping/>.

5] References

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