

Resonant Frequency-Temperature Dependence Simulation

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The screenshot shows a control panel titled "Resonant Frequency-Temperature Dependence". It contains several input fields and buttons:

- Wafer Type: 100 (dropdown)
- Flat Orientation: <110>
- In Plane Orientation: 0 (degrees from flat)
- Doping Type / Conc.: n (dropdown), 5.00e+19 cm-3
- Model Geometry or Mesh: models\bar_mesh.mphbin (text field), Select File (button)
- Frequency: 7.0000e+06 Hz
- Fixed Surfaces: (empty text field)
- Symmetry Surfaces: (empty text field)
- Autotrack Surfaces: 1
- Mode Type: In Plane (dropdown)
- Config: Load (button), Save (button), Go! (button), Stop (button)

Things you need:

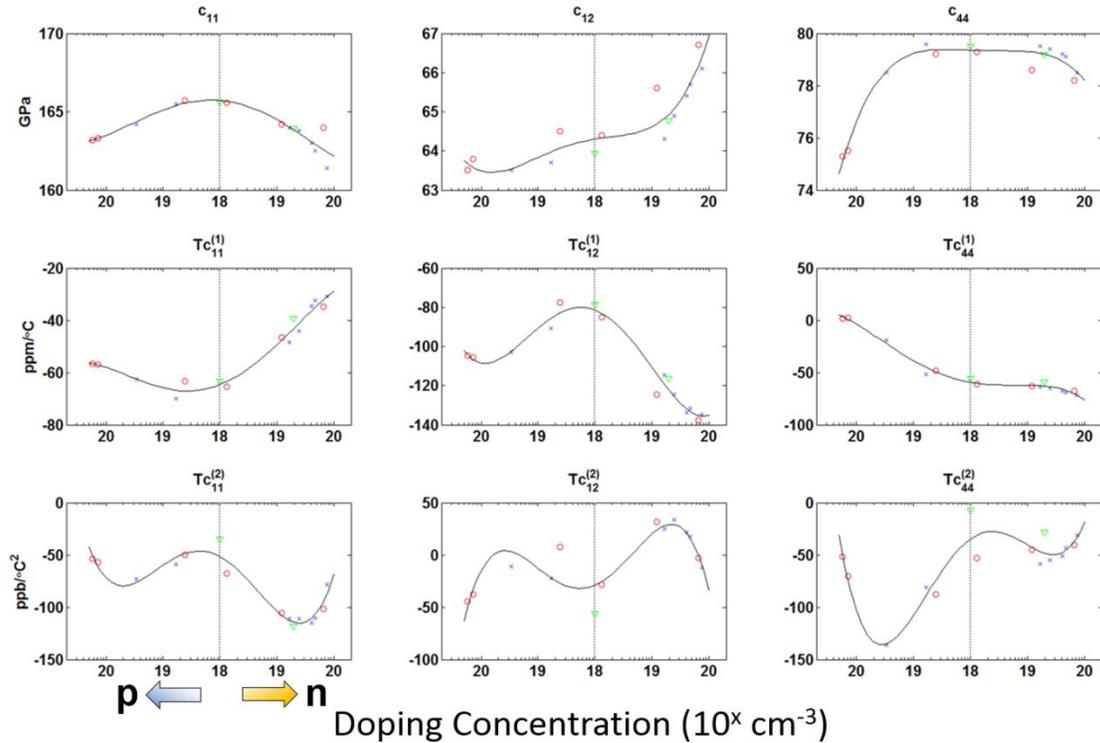
- MATLAB 2012 or 2013 (May work on other versions but only tested with these)
- COMSOL 4.3 or 4.4 with MATLAB LiveLink (May work on other versions but only tested with these)
- COMSOL model of resonant device. Can be a geometry, a mesh (.mphbin), or a Matlab code (.m) for creating the geometry. See [Exporting COMSOL Geometry](#).

Options:

- Wafer type: (100), (110), (111). In-plane orientation on wafer (in degrees)
- Doping type (p or n), and concentration (in cm^{-3})
- Resonant frequency of mode
- Index # of surfaces for boundary conditions (fixed and symmetry conditions). Obtain from COMSOL, see [Picking Surfaces for Applying Boundary Conditions](#).
- Index # of surfaces for [tracking mode shapes](#), and if the mode is in-plane or out-of-plane.

1] Introduction

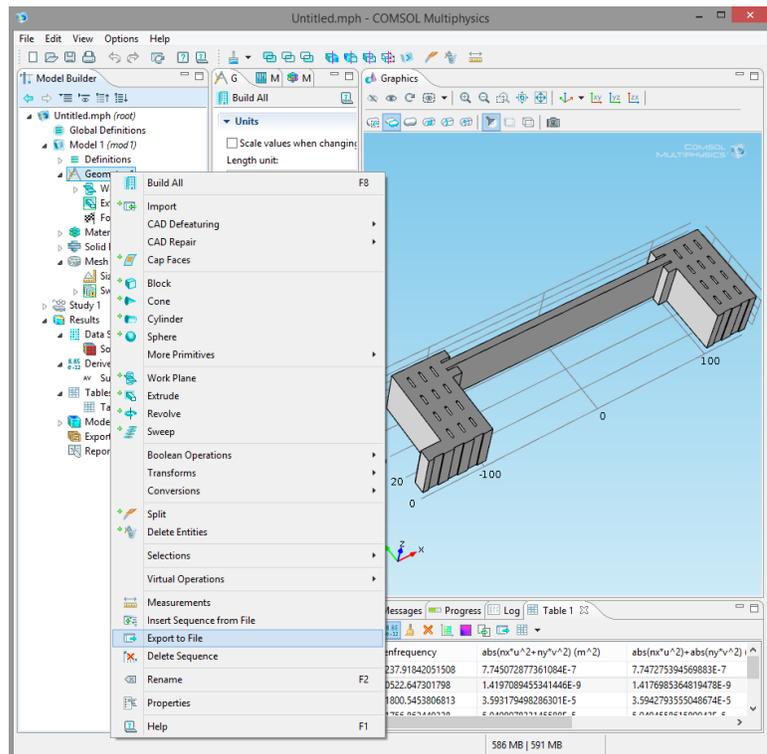
This MATLAB code for COMSOL allows for the simulation of the frequency-temperature dependence of an arbitrary linear resonant mode shape in heavily doped silicon. From work done in this group [1] and other groups (VTT [2], CSEM [3], and IBM [4]), the temperature dependence of the elastic constants of heavily doped silicon have been extracted: p-type up to $1.75 \times 10^{20} \text{cm}^{-3}$, and n-type up to $7.5 \times 10^{19} \text{cm}^{-3}$. 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.

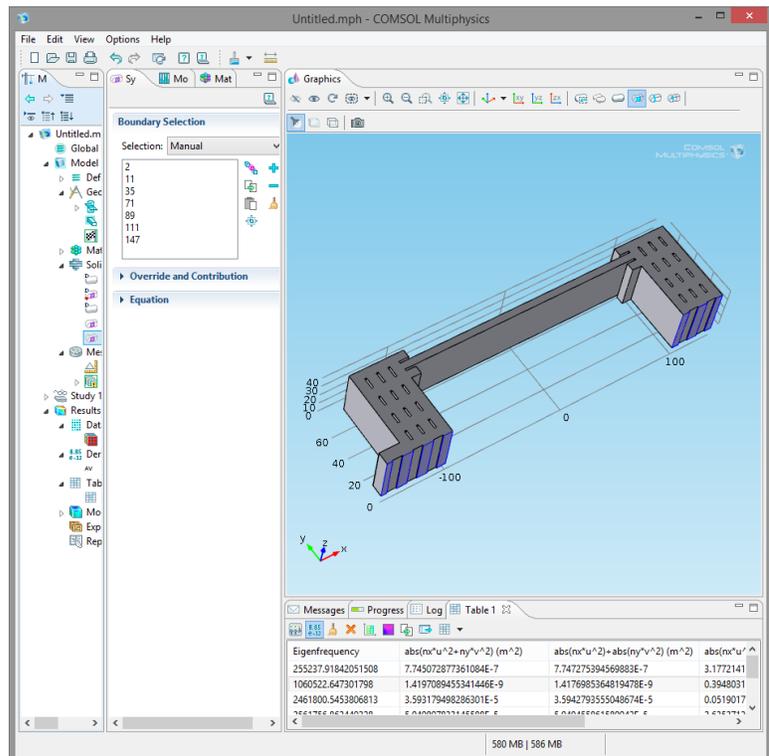
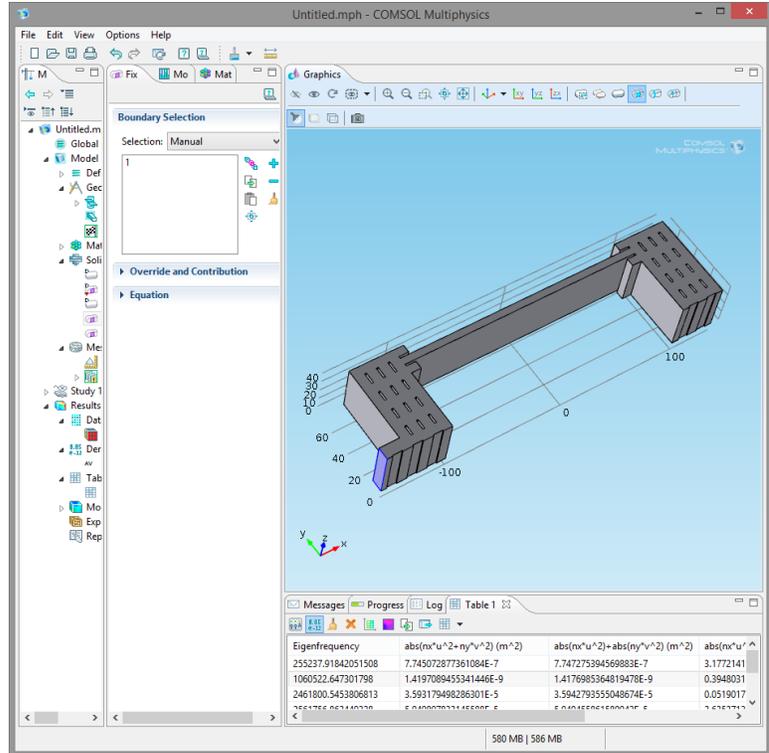
2] Exporting COMSOL Geometry

COMSOL models can be exported either as a geometry, or a mesh. Right-click on the geometry, or mesh, and click *Export to File*. Save the file with an *.mphbin* extension, preferably in the *models* folder of the script.



3] Picking Surfaces for Applying Boundary Conditions

As performed routinely for modeling in COMSOL, boundary conditions need to be applied. For fixed conditions, we graphically select the surface, and **note down the selection #**. This will be used later in the MATLAB script to define the fixed points. Similarly, symmetry surfaces can also be defined. Exploiting symmetry helps to reduce the computation time as well as eliminate other modes that are not of interest that might interfere with the simulation.



4] The Code

Frequency-temperature simulation is performed using the best fits for the elastic constants at the requested doping level. These elastic constants are calculated at various temperature points, and then substituted into the finite element model to obtain the eigenfrequency for the desired mode. By tracking the variation of the eigenfrequency across the various temperature points, the frequency-temperature dependence can be extracted.

The GUI is launched by running the *fTpred.m* script. From here, the wafer type, device orientation, doping can be specified, and the geometry file selected. The device in-plane orientation is specified as counter-clockwise from the flat (i.e. rotating the device on the wafer by that specified angle counter-clockwise from the flat should result in the simulations) - this matters mostly for (110) wafers. 6 modes will be generated by default (can be increased up to 12 by changing *fmodes* in the script), around the frequency specified. Also enter in the fixed and symmetry surface #s. You can also save/load the specified configuration (saved as a *.mat* file with the specified variables).

5] Selecting the Desired Resonant Mode

One important question is: how can the desired modes be selected for various temperatures? One way is to ask the user to pick the mode. If the *Autotrack Surfaces* field is left blank, the code defaults to prompting the user to select the desired mode amongst several possible mode shapes around the specified frequency. When prompted, simply click on the desired frequency. The code will prompt the user about 2 or 3 times, and will automatically search for the desired mode for subsequent temperature points (based on quadratic extrapolation).



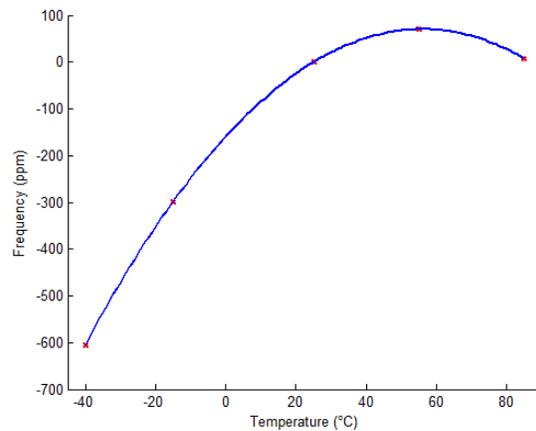
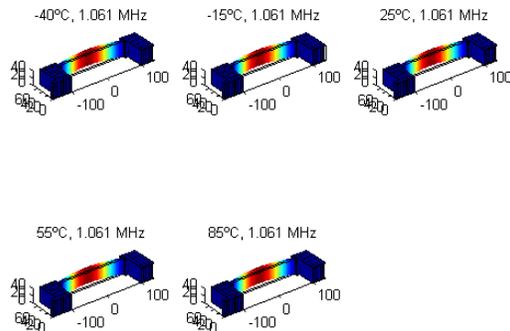
Another method of recognizing the mode shape is to pick a surface (or surfaces) that experiences a large normal displacement. Two options are available for this: in-plane and out-of-plane. The code then selects the mode with the maximum squared relative displacement on that surface. For this, the *Autotrack Surfaces* field must be filled, and the *Mode Type* field must be specified as *In Plane* or *Out of Plane*. The desired mode should be within $\pm 20\%$ of the specified frequency.

6] Interpreting the Results

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/ $^{\circ}\text{C}$. It is important to ensure that the *Selected Modes* window displays the same mode for each temperature point. The temperature points can be changed by editing the values of the array *T_C* in *fTpred.m*. 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:



7] 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 [1]. 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 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/>.

8] References

- [1] E. J. Ng, V. A. Hong, Y. Yang, C. H. Ahn, C. L. M. Everhart, T. W. Kenny, "Temperature Dependence of the Elastic Constants of Doped Silicon", to be published, JMEMS '14.
- [2] A. Jaakkola, M. Prunnila, T. Pensala, J. Dekker, and P. Pekko, "Determination of Doping and Temperature Dependent Elastic Constants of Degenerately Doped Silicon from MEMS Resonators," *arXiv: 1401.1363 [cond-mat.mtrl-sci]*, 2014.
- [3] C. Bourgeois, E. Steinsland, N. Blanc, and N. F. deRooij, "Design of Resonators for the Determination of the Temperature Coefficients of Elastic Constants of Monocrystalline Silicon," *IEEE International Frequency Control Symposium 1997*, pp. 791-799, 1997.
- [4] J. J. Hall, "Electronic Effects in Elastic Constants of N-Type Silicon," *Physical Review*, vol. 161, pp. 756-761, 1967.