Effective Mass Calculations Using COMSOL Multiphysics® for Thermomechanical Calibration

Nano/Micro-Mechanical Sensors

Yoctogram ($10^{-24}$ g) mass resolution

Attonewton ($10^{-18}$ N) force transduction

Sub-attometer ($10^{-19}$ m) displacement sensitivity

J. Chaste et al., Nature Nanotech. 7 (2012) 301

E. Gavartin et al., Nature Nanotech. 7 (2012) 509

O. Arcizet et al., PRL 97 (2006) 133601
Proper calibration of a resonator is crucial to ensure accurate measurements. Thermomechanical calibrations provide a powerful, noninvasive calibration by which the thermal motion of any resonator structure can be calibrated.

**Equipartition Theorem:**

\[
\langle U \rangle = \frac{1}{2} m \omega^2 \langle z^2 \rangle = \frac{1}{2} k_B T
\]
Extended Resonator Structure

General Displacement

\[ R(x, t) = \sum_{n} a_n(t) r_n(x) \]

\[ |r_n(x_0)| = 1 \]

\( x_0 \) is the position of the measurement

\( a_n(t) \) is the true physical displacement
Extended Resonator Structure

General Displacement

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$$a_n(t)$$ is the true physical displacement

Potential Energy

$$dU = \frac{1}{2} \omega^2 |a_n(t) r_n(x)|^2 \rho(x) dV$$

$$\Rightarrow U = \frac{1}{2} m_{eff} \omega^2 |a_n(t)|^2$$
Effective Mass Integral (EMI)

\[ m_{eff} = \int \rho(x) |r_n(x)|^2 dV \]

<table>
<thead>
<tr>
<th>Device Geometry</th>
<th>Effective Mass Ratio ((m_{eff} / m))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cantilever</td>
<td>1/4</td>
</tr>
<tr>
<td>Doubly Clamped Beam</td>
<td>Mode Dependent</td>
</tr>
<tr>
<td>String</td>
<td>1/2</td>
</tr>
<tr>
<td>Simple Torsional Resonator</td>
<td>1/3</td>
</tr>
<tr>
<td>Circular Membrane</td>
<td>Mode Dependent</td>
</tr>
<tr>
<td>Rectangular Membrane</td>
<td>1/4</td>
</tr>
</tbody>
</table>
Effective Mass Integral (EMI)

\[ m_{eff} = \int \rho(x)|r_n(x)|^2 dV \]

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</thead>
<tbody>
<tr>
<td>Cantilever</td>
<td>1/4</td>
</tr>
<tr>
<td>Doubly Clamped Beam</td>
<td>0.3965 0.4390 0.4371</td>
</tr>
<tr>
<td>String</td>
<td>1/2</td>
</tr>
<tr>
<td>Simple Torsional Resonator</td>
<td>1/3</td>
</tr>
<tr>
<td>Circular Membrane</td>
<td>0.2695 0.2396 0.2437</td>
</tr>
<tr>
<td>Rectangular Membrane</td>
<td>1/4</td>
</tr>
</tbody>
</table>
Complex Devices

Bottle Resonator

\[ f_0 = 96.3 \text{ MHz} \]
\[ f_0 = 99.7 \text{ MHz} \]
\[ f_0 = 102.4 \text{ MHz} \]
Recipe:

1. Simulate the mechanical deformation of the device for the mode of interest using the Eigenfrequency Study in the Structural Mechanics Module.

2. Determine the relative displacement at the point of measurement using Point Evaluation in Derived Values.

3. Perform a Volume Integration of the structure’s density multiplied by the normalized displacement
   \[ \text{solid.rho} \times \left( \frac{\text{solid.disp}}{\text{pointdisplacement}} \right)^2 \]
   over the entire geometry of the resonator.
## Results – Benchmark Calculations

<table>
<thead>
<tr>
<th>Device Geometry</th>
<th>Effective Mass Ratio (Analytical)</th>
<th>Effective Mass Ratio (COMSOL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cantilever</td>
<td>0.2500</td>
<td>0.2498 (0.08%)</td>
</tr>
<tr>
<td>String</td>
<td>0.5000</td>
<td>0.4969 (0.62%)</td>
</tr>
<tr>
<td>Torsional Resonator</td>
<td>0.3333</td>
<td>0.3314 (0.58%)</td>
</tr>
<tr>
<td>Doubly Clamped Beam (First Mode)</td>
<td>0.3965</td>
<td>0.3959 (0.15%)</td>
</tr>
<tr>
<td>Circular Membrane</td>
<td>0.2696</td>
<td>0.2693 (0.11%)</td>
</tr>
<tr>
<td>Rectangular Membrane (First Mode)</td>
<td>0.2500</td>
<td>0.2498 (0.08%)</td>
</tr>
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Complex Devices

Bottle Resonator

\[ f_0 = 96.3 \text{ MHz} \]

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\[ f_0 = 102.4 \text{ MHz} \]
Complex Devices

**Bottle Resonator**

\[
f_0 = 96.3 \text{ MHz} \\
m_{\text{eff}}/m = 0.1890
\]

\[
f_0 = 99.7 \text{ MHz} \\
m_{\text{eff}}/m = 0.1928
\]

\[
f_0 = 102.4 \text{ MHz} \\
m_{\text{eff}}/m = 0.1506
\]
Thermomechanical calibration provides a powerful, non-invasive method by which nano/micro-mechanical resonators can be calibrated.

In order to ensure accurate calibration, the effective mass of a device must be precisely known.

COMSOL Multiphysics® simulation can be used to determine the effective mass of any resonator, regardless of material or geometry, providing a straightforward method by which any nano/micromechanical resonator can be calibrated.

Thank you