Simulation tools for Damping in High Frequency Resonators

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***Abstract*— This paper presents the development of HiQLab, a simulation tool to compute the effect of damping in high frequency resonators. Existing simulation tools allow designers to compute resonant frequencies but few tools provide estimates of damping, which is crucial in evaluating the performance of such devices. In the current code, two damping mechanisms: *thermoelastic damping* and *anchor loss* have been implemented. Thermoelastic damping results from irreversible heat flow due to mechanically-driven temperature gradients, while anchor loss occurs when high-frequency mechanical waves radiate away from the resonator and into the substrate. Our finite-element simulation tool discretizes PDE models of both phenomena, and evaluates the Quality Factor (Q), a measure of damping in the system, with specialized eigencomputations and model reduction techniques. The core functions of the tool are written in C++ for performance. Interfaces are in Lua and MATLAB, which give users access to powerful visualization and pre- and post-processing capabilities.**

I. Introduction

Electromechanical high-frequency resonators have important applications as physical and chemical sensors as well as signal processing. When changes in the external environment cause changes in the geometry or material properties of these sensors, changes in the resonance occur which can be electronically sensed. While existing commercial tools allow designers to compute resonant frequencies, few tools provide estimates of all aspects of damping (see e.g. ANSYS, ABAQUS, SUGAR), which is crucial in evaluating the performance of such devices.

II. Software Capabilities and Architecture

HiQLab [1] is an open source finite element simulation tool developed for simulating high frequency (HF) resonators, and is capable of 1D, 2D, 3D, and axisymmetric steady-state or static analysis. The element library includes elements for elasticity, scalar wave problems, and coupled electromechanical and thermomechanical problems. Efficient algorithms to compute eigenfrequencies of the system and Arnoldi-based model reduction methods are implemented for fast transfer function evaluation. By utilizing MATLAB [7]'s functions, resonant motion and energy fluxes can also be visualized.

The software consists of core modules and elements written in C++ combined with third-party numerical software written in Fortran or C. Two interfaces have been constructed, one through the scripting language Lua [6] and the other through the commercial software package MATLAB. Using the MATLAB interface, one has full access to MATLAB's rich array of visualization tools and numerical routines. The Lua interface has fewer features, but also has less memory overhead, and does not require a MATLAB license. We chose Lua as our mesh description and user interface language because of its simplicity and speed, the same attributes which make it a popular language in game design. A diagram of a sample session of HiQLab is shown in Figure 1. An input file written in Lua describing the mesh is read into the main program through either of the interfaces. This file is used to generate a *mesh object* which stores the problem geometry, global force and displacement vectors, and boundary conditions. This object is equipped with standard assembly loops to build global tangent stiffnesses and residuals from the element contributions. The matrices that are generated can be processed with standard numerical libraries [2]–[4] or passed on to MATLAB. Finally the results are displayed in either interface.

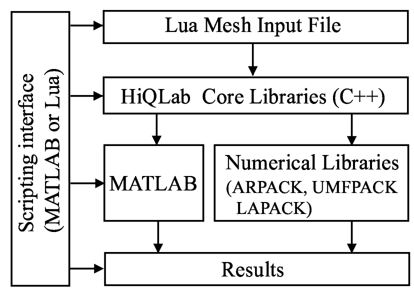

Fig. 1. HiQLab flow diagram

III. Damping Mechanism Modeling and Coupled Element Modeling

A. *Damping and the Quality Factor (Q)*

The Quality Factor (Q) is a measure of how much damping exists in the resonating device. This index is defined in terms of energy loss by the following equation:

$$Q^{-1} = \frac{\text{Energy Loss per radian}}{\text{Maximum Stored Energy}} = \sum_{i \in \{\text{Damping Mechanisms}\}} Q_i^{-1}. \quad (1)$$

The additive decomposition of Q into its separate mechanisms shown above is valid when damping is small.

In the case of HF resonators, damping mechanisms such as air damping, anchor loss and thermoelastic damping (TED) have been experimentally observed to be the dominant sources of damping [5]. Currently, HiQLab is capable of simulating anchor loss and TED.

We compute Q by one of two methods. The first method is through evaluation of the transfer function, where Q is computed by dividing the peak frequency by the band width at -3dB. The transfer function can be computed efficiently in HiQLab by reduced-order modeling techniques [10], which simultaneously reduces the degrees of freedom required resulting in an increase in speed, and retains accuracy. The second method is through evaluating the complex-valued eigenfrequency ω of the system corresponding to the mode of interest. This frequency is related to Q by

$$Q = \frac{\mathbf{Re}(\omega)}{2\mathbf{Im}(\omega)}. \tag{2}$$

In evaluating the damping, HiQLab can take advantage of underlying structure for efficient eigenfrequency computation.

B. Anchor loss

Anchor loss is the mechanism in which elastic energy is lost through radiation from the anchors. In the case of a MEMS resonator, the resonating device is much smaller than the silicon substrate on which it is situated, and waves radiating from the anchor are attenuated by the time they reach the far surfaces of the silicon wafer. For FEA, a finite domain must be selected for analysis and proper boundary conditions must be specified for accurate simulations; see Figure 2. For the MEMS resonator, the boundary condition must be able to simulate a semi-infinite domain. In HiQLab, this is modeled using *Perfectly Matched Layers* (PML) [9]–[11], which absorb waves from any angle of incidence on the boundaries with no impedance mismatch. Complex coordinate stretching is introduced in the region where PML is applied. Finite element discretization of the model results in complex symmetric mass and stiffness matrices. This complex symmetric structure is taken advantage of in HiQLab to produce an Arnoldi-based reduced-order model which can evaluate the transfer function with high-order accuracy.

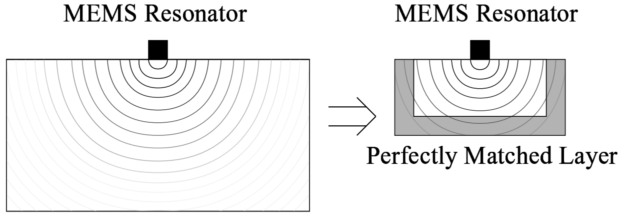

Fig. 2. Perfectly Matched Layers for Anchor Loss Simulations

C. Thermoelastic Damping

Thermoelastic damping (TED) is the mechanism in which vibrating energy in the resonator is lost through the coupling of the mechanical domain with the thermal domain [12]. Time varying stresses induce time varying strains, which create local temperature fluctuations. These variations in temperature inside the resonator cause heat flow, an irreversible process, resulting in energy loss. This source of damping can be accurately modeled by solving the coupled thermomechanical equations, which consist of the balance of linear momentum equation coupled with the energy balance equation. Since deformations in MEMS resonators are typically small, linear elasticity and small temperature fluctuations are assumed. Under these assumptions, spatial discretization by the finite element method results in the following second-order system of equations,

$$\begin{bmatrix} M_{uu} & 0 \\ 0 & 0 \end{bmatrix} \begin{pmatrix} \ddot{u} \\ \ddot{\theta} \end{pmatrix} + \begin{bmatrix} 0 & 0 \\ C_{\theta u} & C_{\theta\theta} \end{bmatrix} \begin{pmatrix} \dot{u} \\ \dot{\theta} \end{pmatrix} + \begin{bmatrix} K_{uu} & K_{u\theta} \\ 0 & K_{\theta\theta} \end{bmatrix} \begin{pmatrix} u \\ \theta \end{pmatrix} = \begin{pmatrix} F_u \\ F_\theta \end{pmatrix} \tag{3}$$

where u is the displacement vector and θ is the thermal fluctuation vector from a reference temperature. Submatrices M_{uu}, K_{uu} and $C_{\theta\theta}, K_{\theta\theta}$ are the standard mass and stiffness matrices which arise from the purely mechanical or thermal problem and submatrices $K_{u\theta}, C_{\theta u}$ represent the coupling between the mechanical and thermal domains.

In HiQLab, the perturbative structure of the underlying coupled thermoelastic problem is exploited in evaluating the eigenfrequencies of the system. A special model reduction technique which preserves the structure of the system of equations is also implemented for fast and accurate transfer function evaluation.

D. Electromechanically coupled systems

The simulation of resonators actuated piezoelectrically or electrostatically requires solving the coupled electromechanical equations, consisting of the standard balance of linear momentum equation and Maxwell's equations. Since the time scale corresponding to electrical potentials are orders of magnitude smaller than those of the mechanical domain, electrostatics are assumed. The discretized system of equations has the form,

$$\begin{bmatrix} M_{uu} & 0 \\ 0 & 0 \end{bmatrix} \begin{pmatrix} \ddot{u} \\ \ddot{\phi} \end{pmatrix} + \begin{bmatrix} K_{uu} & K_{u\phi} \\ K_{\phi u} & K_{\phi\phi} \end{bmatrix} \begin{pmatrix} u \\ \phi \end{pmatrix} = \begin{pmatrix} F_u \\ F_\phi \end{pmatrix} \tag{4}$$

where u, ϕ are the displacement and electrical potential vectors, and submatrices M_{uu}, K_{uu} and $K_{\phi\phi}$ are the standard mass and stiffness matrices which arise from the purely mechanical or electrostatics problem. The coupling between the mechanical and electrical domains, which occurs from piezoelectricity or electrostatic coupling, are represented by the submatrices $K_{u\phi}, K_{\phi u}$.

The electromechanical analysis can be combined with PML and the thermal equations to introduce anchor loss and TED as sources of damping which affect Q.

IV. Numerical Examples

HiQLab has previously been shown to accurately simulate anchor loss in bulk radial resonators [9]. In this section we demonstrate the ability of HiQLab in simulating TED, resonator optimization, and the modeling of internal dielectric drives.

A. Free-Free Beam

Modeling of TED is shown by simulating the Free-Free Beam (FF-Beam) fabricated and measured by Hsu et al [14]. The device is 2D planar and designed to resonate in an in-plane flexural mode. The vibrational mode that we are interested in evaluating the Q of is shown in Figure 3, where the color represents the thermal fluctuations from a reference temperature. The Q for this device is computed from an eigenfrequency computation of a 2D plane-stress analysis where TED is considered. The measured Q is 10743 and and the simulated value is 13423. Taking into consideration the fact that exact geometrical and material parameters of the experimental device are uncertain, the simulated Q yields satisfactory predictions.

B. Ring resonator

The ability to evaluate the effect of TED on Q from the transfer function is exhibited in this example. The structure we select is a 2D planar ring structure shown in Figure 4. The structure is excited with a uniform radial force on the perimeter which models an electrostatic drive. Figure 4 also shows the deformation and temperature fluctuations from a reference temperature when excited at 705.50[MHz]. The resulting displacement at the perimeter is measured to evaluate the transfer function between the force and displacement, centered at this frequency. The transfer function is evaluated by both the full model (solid line) with 39K degrees of freedom (DOF) and the structure preserving reduced-order model (ROM, circles) with 21 DOF as shown in Figure 5 (top). It is clear that the transfer function from the ROM matches the full model with high-order of accuracy; see Figure 5 (bot). The plot consists of 100 data points of which it took the full model approximately 2 hours to compute as opposed to the ROM which took about a minute.

C. Checkerboard optimization

We illustrate the ability to use HiQLab with optimization algorithms by a checkerboard resonator example [13]. This design has been shown experimentally to serve as a bandpass filter. Using HiQLab to evaluate the frequency response under 2D analysis including PML anchor loss, we optimized with respect to geometrical parameters such as the width of each checker and the size and shape of the individual linking beams to match a target bandpass transfer function. The optimization was conducted with MATLAB's optimization toolbox and the Genetic Algorithm Optimization Toolbox(GAOT) [8]. Figure 6 shows one optimally designed checkerboard resonator operating in an in-plane mode. On the right hand side we show the simulated mechanical band pass characteristics of the optimized device by its Bode plot.

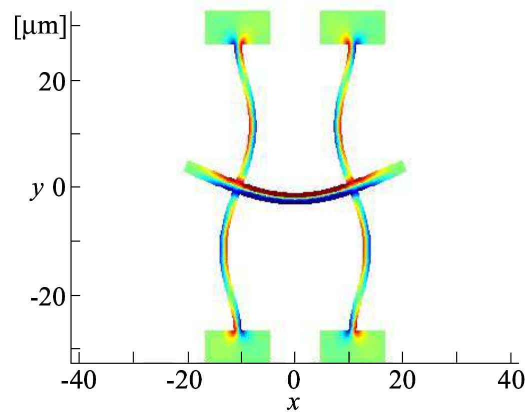

Fig. 3. Geometry and mode shape of Michigan Free-Free Beam

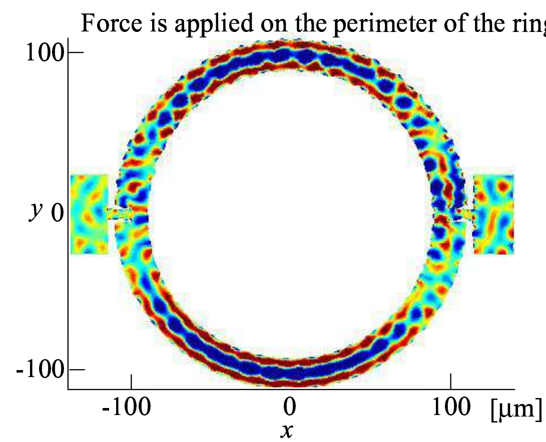

Fig. 4. Geometry, deformed shape, and thermal fluctuations of the Ring resonator at 705.50[MHz]

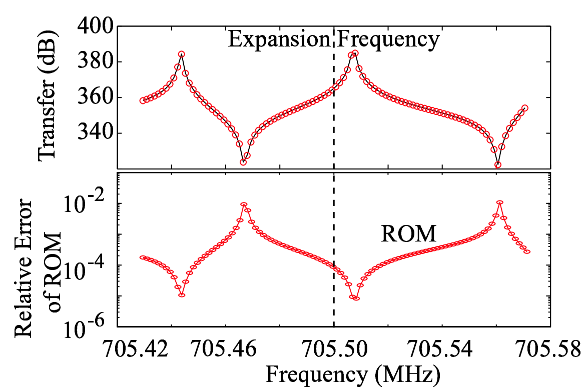

Fig. 5. Mechanical transfer function of the Ring resonator (Full and ROM)

D. Dielectric filled gap resonators

Air-gap electrostatic transduction is a popular method of actuation for high frequency resonators. Currently, research is underway, to further increase the efficiency and to reduce insertion loss by filling these air-gaps with high dielectric constant materials [15], [16]. Though this may be advantageous in terms of transduction, such an addition mechanically couples the sense and drive electrodes to the resonator, perturbing the original behavior substantially. Here we present an analysis of the Bulk Lateral Resonator (BLR) [17]. A 2D plane stress analysis is conducted on this 2D planar structure which is designed to resonate in its in-plane 3rd overtone at approximately 140.0[MHz]. The dielectric drives are taken to be 200[nm] in thickness. Figure 7 shows the mode shape of the resonator, where the color depicts the in-plane y direction displacement. Figure 8 is a plot of the transfer functions of the device when the relative permitivity of the dielectric within the filled gap is varied (ϵ_0 is the permitivity of free air). It can be clearly seen that by increasing the permitivity, the insertion loss decreases, and Q increases.

V. Summary and Future Work

HiQLab, a FEA-based tool to simulate high frequency resonators and evaluate the effect of damping due to anchor loss and TED, has been presented. The effectiveness and capabilities of the software have been exhibited by comparison with experimental results as well as predicting behavior of devices that may be fabricated in the near future.

Future work will focus on expanding the capability of the software: to simulate a wider range of resonators, incorporate other sources of damping mechanisms such as air damping, and to be able to evaluate problems of larger computational expense. Currently the software runs on sequential architecture which limits the size of the problems that can be analyzed.

HiQLab is open source, which can be freely downloaded [1].

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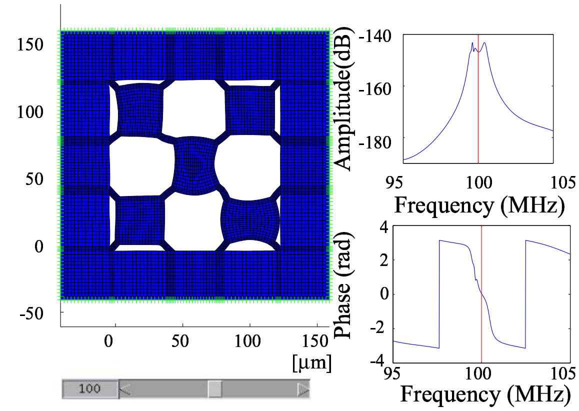

Fig. 6. Mode shape and Bode plot of an optimal design

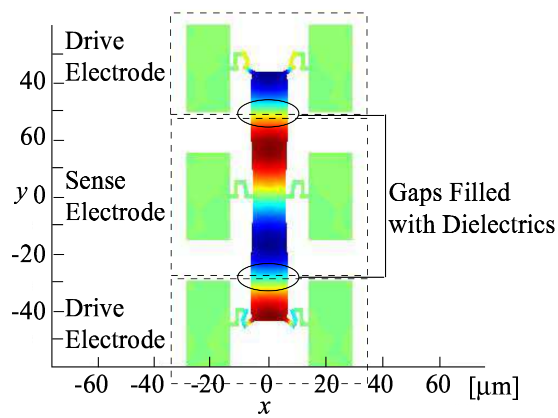

Fig. 7. Geometry and mode shape of BLR at 140.050[MHz]

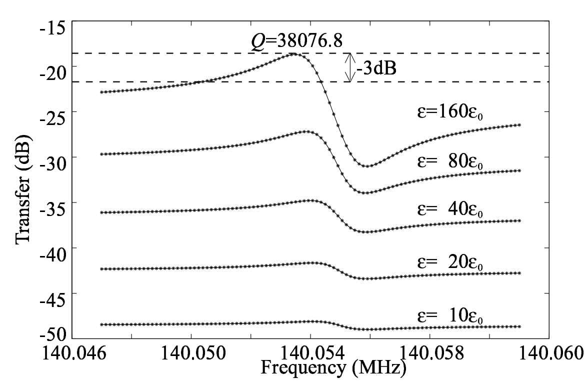

Fig. 8. Transfer Function of the BLR with varying permitivity