An analytical model for the resonance frequency of square perforated Lamé-mode resonators

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Abstract

In this work, simple analytical models based on the concept of an equivalent material are used to describe the mechanical behavior of resonators perforated by a regular array of square holes, a common occurrence in several MEMS devices and sensors. This description is applied to the determination of the resonance frequency of Lamé-mode square resonators, which are frequently pursued as high-*Q* MEMS resonators. The models predictions are compared with FEM simulations and experimental data both from the literature and from measurements obtained by the authors on thick SOI MEMS resonators. The models predictions are in good accordance both with FEM results and with experimental data.

Keywords: MEMS resonators; resonant sensors; mass sensors; perforations; cellular materials; Lamé resonators.

1. Introduction

MEMS resonators are actively researched for frequency control applications, RF filters and oscillators [1, 2], as well as and chemical and biochemical sensors [3-7], aiming at substituting their discrete counterparts based on their perceived advantages in terms of batch fabrication, monolithic integration and low dimensions/low power consumption. In sensing applications, which are predominantly based on the mass (and thus resonance frequency) shift of the resonator consequent to interaction with the analyte, common figures of merit are the sensitivity and limit of detection [3, 4]. Both quantities can be defined with respect to the mass or to the concentration. For chemical sensors, the most meaningful definitions are those based on the concentration or, alternatively, on the mass per unit surface (which makes the comparison among different sensors simpler) [3, 4].

Ultimately, the sensitivity is proportional to the ratio between the analyte and resonator masses, so that to increase it, efforts need to be made to increase the former (for example by increasing the resonator active area) and to decrease the latter by reducing the resonator volume, which also has a direct effect on the resonance frequency.

In addition, the limit of detection ultimately depends on the quality factor *Q* [4]. For this reason, efforts have been made to identify high Q, high sensitivity resonating structures. Among them, Lamé-mode resonators, because of a mode-shape which exhibits only shear deformations, are expected to radically reduce one of the causes of intrinsic noise, i.e. thermoelastic damping in the resonator material [8]. Examples of Lamé-mode MEMS resonators used both as frequency references [9] and mass sensors [5] can be found in the recent literature.

In any case, whatever be the resonator type, and depending on the resonator dimensions and fabrication technology, a pattern of holes fabricated on the resonator body may be required for the release of the moving part from the substrate [10, 11]. As a general observation, resonators of substantial dimensions without holes require a back etch [5], which make the fabrication significantly more complex.

On the other hand, perforations can drastically increase the sensitivity of resonant sensors by both increasing the surface exposed to the analyte, and decreasing their volume [12, 13]. Moreover, holes are often used in phononic-crystal structures [14], which have been proposed for the creation of high-Q resonators [15, 16] and sensors [17, 18]. Also, a possible effect of holes on the temperature stability of the resonance frequency has been recently reported [19].

Whatever the reason for their introduction, holes affect the behavior of the resonator in various ways, and thus models are needed in order to predict their effect over design parameters such as the quality factor and the resonance frequency. In the specific case of Lamé-mode resonators, holes have been related to an increase in thermoelastic and anchor losses [20, 21]. In contrast, the effect of perforations on the resonance frequency has not been investigated as thoroughly, although the authors have already presented results referred to beam resonators [22].

In this work, we develop and validate two analytical models for the resonance frequency of perforated Lamé-mode resonators, restricting ourselves to the case of resonators with a square grid of square perforations (which is the most common case). The models are based on the computation of the mechanical properties of an equivalent material. A first, simple model is based on an established theory of periodic cellular solids, i.e. solids which enclose voids with a periodic structure [23, 24]. To overcome an intrinsic limit of the simple model we also developed an original, refined model which assumes a more realistic stress distribution in the elementary grid cell. The predictions of the models are compared both with the results of FEM simulations and with experimental data. Experimental resonances are extracted from the literature on the subject as well as from experimental characterization performed by the authors on Lamé-mode MEMS resonators fabricated in a thick Single-Crystal Silicon (SCS) MEMS SOI technology.

The paper is structured as follows: in section 2, the models are developed; section 3 is devoted to comparison between predictions of the models and FEM simulations for a wide range of possible hole grids. Section 4 presents the comparison with experimental data, as well as the concluding remarks.

2. Resonance frequency model

In order to investigate the resonance behavior of square Lamé-mode resonators perforated with square holes arranged in a square grid, we start from the expression for its resonance frequency in a square solid resonator [25]:

$$f_0 = \frac{1}{L}\sqrt{\frac{G_d}{2\rho}} \tag{1}$$

with L being the resonator side length, ρ the material density and G_d its shear modulus along the diagonal direction. While the direction along which the shear modulus is defined is inessential for isotropic materials, it can become relevant for anisotropic materials (such as SCS, which exhibits cubic symmetry).

In our models, the effect of perforations is included by developing equivalent material expressions for the values of ρ and G and substituting them in (1):

$$f_{0,eq} = \frac{1}{L}\sqrt{\frac{G_{d,eq}}{2\rho_{eq}}}\,. \tag{2}$$

This approach relies on the hypothesis that the grid cell dimensions are small compared to the side length L [23].

To the purpose of developing such equivalent expressions, we preliminarily define the parameters required to describe the hole pattern. We call N the number of holes along each side of the resonator. The spatial period of the grid (i.e. the side of the square grid cell) is $l_s = L/N$, while h_s is the side of the square hole, and t_s is the difference between the former and the latter (Fig. 1). A useful parameter to describe the structure of the perforations is the *filling factor* α, defined as:

$$\alpha = \frac{t_s}{l_s}. \tag{3}$$

The allowed range of α is between 1 (solid structure) and 0 (hollow structure). Once L is assigned, the resonator geometry is completely defined by the values of N and α. The aforementioned hypothesis of small cells clearly corresponds to the assumption that $N >> 1$.

The equivalent mass density is obtained, very straightforwardly, by averaging the unit cell mass over its volume, thus giving:

$$\rho_{eq} = \alpha(2-\alpha)\rho. \tag{4}$$

For the equivalent diagonal shear modulus further considerations are needed. Since the hole grid breaks the symmetry of the original structure, the perforated equivalent material shows an anisotropic behavior even if the original material did not. For simplicity, we will assume that the original solid material presents at least cubic symmetry. This choice excludes crystalline materials whose crystal structure is not cubic, such as (limiting the analysis to the case of semiconductors used in MEMS) the system $Al_xGa_{1-x}N$, which presents a hexagonal structure. On the other hand, isotropic materials (such as amorphous materials and polycrystalline silicon under fairly general conditions [26, 27]) are included, as are included crystalline silicon, germanium, the system $Al_xGa_{1-x}As$, and many other semiconductors.

The in-plane elastic properties of a cubic material can be described by three independent elastic constants [28]. A possible choice for these constants is: the Young's modulus E_p, Poisson's ratio ν_p and shear modulus G_p, all defined along the direction parallel to the resonator side. For example, in a SCS resonator oriented as in Fig. 2, the relevant constants would be the ones defined along direction [100]. For reference, their values for SCS along both [100] and [110] directions (taken from [29]) are recalled in Table 1.

As a result of the cubic symmetry, the shear modulus along the diagonal direction (refer again to Fig. 2) can be written as [30]:

$$G_d = \frac{E_p}{2(1+\nu_p)} . \tag{5}$$

As the hole grid is square, and as long as the grid is aligned with a symmetry plane of the material, cubic symmetry is retained even after the perforations, i.e. the symmetry is not reduced by the introduction of the holes. As a consequence, our models cannot be extended, as it is, to non-square grids. The equivalent material taking the holes effect into account can thus be described by three equivalent constants $E_{p,eq}$, $\nu_{p,eq}$ and $G_{p,eq}$. For the same reason, the equivalent diagonal shear modulus can be written as

$$G_{d,eq} = \frac{E_{p,eq}}{2(1+\nu_{p,eq})} \tag{6}$$

i.e. the value of $G_{d,eq}$ can be determined if $E_{p,eq}$ and $\nu_{p,eq}$ are known. Expressions for $E_{p,eq}$ and $\nu_{p,eq}$ are typically computed by loading the unit cell with a uniaxial force f (as shown in Fig. 3) and by computing the generated elongations. For small α (i.e. large holes) it has been assumed [23] that the stress σ_{xx} in areas 1 of Fig. 3 (σ_{fh}) is negligible, leading to the following expressions:

$$E_{p,eq} = \alpha E_p \qquad \nu_{p,eq} = \alpha \nu_p . \tag{7}$$

The accuracy of (7) also depends on the fact that all the segments which can be imagined as the constituents of the perforated material have a constant cross-section. As a consequence, (7) are strictly true for square holes (or, to be more accurate, for rectangular holes, a more general case not considered in this work). Among other possible hole shapes, the circle is the only other which occurs with some frequency in applications [31].

It is not difficult to show that, to ensure static equilibrium, the assumption $\sigma_{fh} = 0$ implies that the stresses in area 2 (σ_{ff}) and areas 3 (σ_h), both supposed constant in their respective areas, are equal. In the following sections we will show that the simple model of Eqs. (7) is reasonably accurate for most cases, and specifically for low α. However, to capture the full behavior of the resonance frequency for α close to one, a refined model in desirable. Specifically, we can drop the assumption $\sigma_{fh} = 0$ and suppose that the stress in that part is proportional to the stress σ_{ff} in the center of the cell through some function of α:

$$\sigma_{fh} = f(\alpha)\sigma_{ff} . \tag{8}$$

With this definition, the expressions in (7) correspond to the case $f(\alpha) = 0$. More generally, natural consistency constraints require that $f(0) = 0$ (the stress σ_{fh} becomes negligible for very large holes) and $f(1) = 1$ (in the limit of a solid material, the stress is constant throughout the material). The simplest model which obeys this constraints is a power law:

$$\sigma_{fh} = \alpha^k \sigma_{ff} \tag{9}$$

where k is a fitting parameter which will be determined from FEM data in the following section. From (8), it is possible to obtain new, refined expressions for the Young's modulus and Poisson's ratio. We can think of the cell as loaded by an average equivalent stress $\sigma_{eq} = f/l_s$, while the actual stress σ_h is $f/(\alpha l_s)$. Also, equilibrium along x requires that

$$f = l_s \sigma_{eq} = \alpha l_s \sigma_{ff} + (1-\alpha) l_s \sigma_{fh} . \tag{10}$$

The total elongation of the cell is then:

$$\Delta l_s = \alpha l_s \frac{\sigma_{ff}}{E_p} + (1-\alpha) l_s \frac{\sigma_h}{E_p} \tag{11}$$

from which an expression for the equivalent Young's modulus can be obtained:

$$E'_{p,eq} = \frac{\sigma_{eq}}{\Delta l_s / l_s} = E_p \frac{\sigma_{eq}}{\alpha \sigma_{ff} + (1-\alpha)\sigma_h} . \tag{12}$$

Finally, by putting (12), (10) and (9) together, we obtain:

$$E'_{p,eq} = \alpha \frac{1+\alpha^{k-1}(1-\alpha)}{1+\alpha^{k-1}(1-\alpha)^2} E_p . \quad (13a)$$

A similar line of reasoning leads for a formally similar expression for the Poisson's ratio:

$$\nu'_{p,eq} = \alpha \frac{1+\alpha^{k-1}(1-\alpha)}{1+\alpha^{k-1}(1-\alpha)^2} \nu_p . \quad (13b)$$

The expressions (13a-b) reduce to (7) for the limiting case $k \to \infty$ (which corresponds to $\sigma_{fh} \to 0$). Substituting either (13a-b) or (7) in (6), and in turn (6) and (4) in (2), two expressions for the resonance frequency of the holed Lamé-mode resonator ("simple" and "refined") are obtained:

$$f_{0,eq} = \frac{1}{L}\sqrt{\frac{E_p}{4(2-\alpha)\rho(1+\alpha\nu_p)}} \qquad f'_{0,eq} = \frac{1}{L}\sqrt{\frac{E_p[1+(1-\alpha)\alpha^{k-1}]}{4(2-\alpha)\rho[1+\alpha^{k-1}(1-\alpha)^2+\alpha(1+\alpha^{k-1}(1-\alpha))\nu_p]}} \quad (14)$$

If the original materials is isotropic, the expression (8) further simplifies as it is not necessary to specify the direction along which E and ν are defined, since their values are not dependent on the direction.

3. FEM Validation

In this section, resonant frequencies of Lamé-mode resonators, computed with modal FEM simulations carried out with ANSYS, will be compared to the ones predicted by (14). In order to retain consistency with the measured structures presented in the third section, simulations were performed considering SCS resonators with sides of length $L = 1$ mm, oriented along the [100] direction. The elastic constants passed to ANSYS are the ones reported in Table 1. All simulations were carried out as 2D simulations under a plane-stress hypothesis, i.e. under the hypothesis of small thicknesses. Because of the symmetry of the problem, only one fourth of the resonator has been simulated. The modal extraction has been performed with the block Lanczos method and the sparse equation solver. No boundary conditions (others than the ones necessary in order to impose the symmetry conditions) have been applied on the structure. Among the several resonance frequencies computed by ANSYS, the Lamé-mode resonance frequency has been extracted by running a comparison between the computed mode shapes and the Lamé mode shape of a solid resonator. This procedure is clarified with the aid of Fig. 4, where the simulated displacement field of the Lamé resonators for $N = 20$ and four different values of α (including the solid case $\alpha = 1$), are reported. It is evident that the displacement field in presence of holes closely resembles the one of the solid structure.

A set of simulations has been performed for filling factors α varying in the range [0.05-1] with steps of 0.05 and for a number of holes N along each side of 10, 20 and 30. Due to the significant change in the geometry of the simulated structures upon the above-mentioned changes in α and N, a meshing algorithm aimed at keeping the number of elements constant has been adopted. This number has been fixed at a minimum of 100000. The element type used was PLANE182 and all elements were rectangular with aspect ratio as close as possible to 1. In order to investigate the numerical convergence of the FEM model, a few test structures with values of N and α varying across the discussed design space have been identified and their simulation have been repeated with four times the original number of elements. In all cases, the change in resonance frequency has always been below 0.2%.

FEM simulations were also used to extract a reasonable value for k in the expression (14). Based on the assumption (9), we extracted and compared the calculated FEM stresses along x in the areas 1 and 2 of Fig. 3. Typical averaged stress profiles at varying α are shown in Fig. 5. We then fitted the averaged FEM stresses over the two areas with the least square method against a fitting function of the form (9). The fitting gave an optimal value for k of 2.85, which was used for subsequent comparisons.

In Fig. 6 the first Lamé-mode resonance frequency as a function of the filling factor α is plotted, with α and N varying in the range described above. FEM simulations, as well as the values predicted by the two models (14), are shown. To allow an easier comparison, the relative errors of (14) with respect to FEM simulations are presented in Fig. 7. The FEM data for $N = 10$, $\alpha = 0.05$ are not included because the ANSYS modal analysis yielded no discernible Lamé mode shape for those values of the parameters. As a matter of fact, at such low values of α and N the structure is more akin to a lattice of weakly coupled flexural beams than to a continuous material withstanding a pure shear deformation. Moreover, for small values of α the errors are highly dependent on N and are quickly reduced for larger values of this parameter, when the continuous approximation is more exactly satisfied.

For values of α close to 1, the simple model fails to capture the behavior of the resonance frequency, systematically underestimating the actual resonance frequency. As this error only weakly depends on N, and does not decrease for increasing N, it can be likely attributed to an intrinsic inaccuracy of the model in this zone. This limitation is overcome by the refined model, whose behavior is comparable to that of the simple model for low α, but is dramatically improved at those values of α where the effect of the stress on the lateral portions of the unit cell (areas 1 in Fig. 3) is not negligible. The relative error between the FEM results and the models remain below 6% in every case.

4. Experimental Validation and Conclusions

In this section, measurements on Lamé-mode MEMS resonators are presented and compared with the predictions of equations (14).

Resonators were fabricated on a 60 μm thick SCS layer (Tronics MEMSOI), with sides of length $L = 1$ mm, oriented along the [100] direction. T-shaped anchors placed at the corners of the square are used to anchor the structure to the substrate. Actuation and detection are performed using three capacitive electrodes placed along the resonator sides. The transduction gap is 4.2 μm. The two electrodes placed along opposite sides are used in actuation and the remaining one in detection. An optical photograph of a typical device is shown in Fig. 2.

Measurements where performed with an Agilent E5061B network analyzer in a standard two-port configuration (shown in Fig. 8). All the measurements were performed at atmospheric pressure (which is the operating environment for many resonant mass sensors [4-6]). The resonator is DC biased at 40 V, the input electrodes are driven by an AC signal V_R, and the output signal V_T is collected at the third electrode. The parasitic feedthrough signal due to the direct capacitive coupling between the input and output electrodes is numerically cancelled from the transmission spectrum by subtracting the spectrum obtained at 0 V of DC bias.

The obtained spectra were numerically least-squares fitted against the theoretical frequency response of a second-order system in order to extract the values of the resonance frequencies and quality factors. Typical spectra with their fitting curves are shown in Figs. 9 and 10. The extracted values for f_0 (and Q) from four different resonators are reported in Table 2 along with the resonators geometrical parameters and theoretical resonance frequencies based on (14). In the same table are also reported, for comparison, the same values for three different Lamé-mode resonators presented in the literature. A wide range of different filling factors (from less than 0.1 to more than 0.8) and the two different orientations [100] and [110] are explored. The predictions of the models are within a few percent from the experimental frequencies for all the resonators presented.

While the focus of this paper is on the resonance frequency of perforated resonators, it is nevertheless interesting to examine the effect of perforations on the measured quality factors, given the importance of high Q values in many applications. Specifically, in resonant mass sensors, a higher Q lowers the minimum detectable frequency shift and thus the minimum detectable mass per unit surface. However, a more detailed analysis [3, 4] shows that the limit of detection (LOD) is inversely proportional both to the quality factor and the sensitivity of the device, and the latter is significantly improved by the presence of holes. For our resonators, the measured values of Q are low (in the thousands range) if compared with values presented in the literature which are, however, typically measured in vacuum. The Q values at atmospheric pressure are more important for those applications (i.e. mass sensing) for which the resonator typically operates in air, where viscous losses are also present. Viscous losses in Lamé resonators have been attributed to slide-film damping above and below the resonator [32], as well as squeeze-film damping at the actuation electrodes [33]. As a general remark, it can be expected that the presence of holes affects the quality factor through changes in different loss mechanisms. As an example, experimental evidence that confirms a large increase in thermoelastic losses in perforated Lamé-mode resonators has been reported [20, 21]. However, due to the presence of viscous losses caused by the surrounding atmosphere, our measurements cannot confirm (or rule out) an increase in thermoelastic losses, which are masked by other loss mechanisms.

In conclusion, our models provides a very simple and computationally straightforward expression to determine the resonance frequency of Lamé-mode resonators with a square grid of square perforations, over a large range of possible dimensions of the holes. Predictions of the models are confirmed both by FEM simulations and experimental data. The models have important applicative interests in the fast design of perforated resonators for frequency reference applications, as well as for resonant sensors showing enhanced sensitivity due to the increased surface/volume ratio introduced by the holes. Moreover, the use of expressions (7) and (13a-b) can be potentially extended to other problems where a simple model for the elastic behavior of perforated structures is required.

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Table 1. Elastic constants of single-crystal silicon at room temperature for two different orientations. Data adapted from [29].

Crystal orientation	Young's modulus E_p (GPa)	Poisson's ratio ν_p (-)	Shear modulus G_p (GPa)
[100]	130.0	0.2785	79.5
[110]	169.0	0.0625	50.8

Table 2. Geometric parameters and measured resonance frequencies and quality factors for selected resonators, along with a comparison between experimental and predicted resonance frequencies.

Sample name	Reference	Material	Resonator side length L (µm)	Number of holes N	Filling factor α	Resonance frequency (MHz) Measured	Simple model (ε_r %)	Refined model (ε_r %)	Quality factor
A1	This work	[100] SCS	1000	20	0.093	2.659	2.671 (+0.45%)	2.671 (+0.45%)	1036 (air)
A2	This work	[100] SCS	1000	20	0.296	2.787	2.751 (-1.29%)	2.768 (-0.68%)	4155 (air)
A3	This work	[100] SCS	1000	30	0.283	2.795	2.745 (-1.79%)	2.761 (-1.21%)	4530 (air)
A4	This work	[100] SCS	1000	30	0.485	2.918	2.848 (-2.4%)	2.910 (-0.27%)	6838 (air)
B	[20]	[110] SCS	360	35	0.5	9.66	9.51 (-1.55%)	9.753 (0.96%)	18190 (vacuum)
C	[21]	[110] SCS	650	15	0.75	5.92	5.73 (-3.21%)	5.987 (1.13%)	115000 (vacuum)
D	[10]	[110] SCS	320	39	0.813	12.1	11.91 (-1.57%)	12.44 (2.81%)	60000 (vacuum)

Figure Captions

Fig. 1: Definition of the filling factor α.

Fig. 2: Optical micrograph of one of the fabricated structures. The orientation of the crystallographic axes is superimposed.

Fig. 3: Unit cell of a perforated resonator. Areas under different stress conditions used in deriving the refined model are marked with progressive numbers.

Fig. 4: Superposition of FEM-simulated deflected shapes at resonance at four different values of the filling factor. Clockwise starting from upper corner: $\alpha = 1$, $\alpha = 0.8$, $\alpha = 0.5$, $\alpha = 0.1$. The rest position is outlined in black.

Fig. 5: Averaged stress profiles in areas 1 (thin lines) and 2 (thick lines), as obtained from FEM simulations, for different filling factors.

Fig. 6: Comparison between models and FEM results for the resonance frequency of a square resonator made of SCS with sides $L = 1$ mm oriented along the [100] direction, as a function of the filling factor α.

Fig. 7: Relative error of the models with respect to FEM simulations.

Fig. 8: Schematic structure of the capacitive actuation and sensing scheme.

Fig. 9: Measured resonance curve of sample A1.

Fig. 10: Measured resonance curve of sample A3.