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Optimization of MEMS Piezo-Resonators

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Abstract: Single crystal silicon MEMS resonators are a potential alternative to quartz for timing and frequency control applications. Even if capacitive resonators with very high quality factors have been demonstrated and produced commercially, in order to achieve a good electromechanical coupling and admissible impedance levels, large bias voltages and submicron gaps are required. To overcome these challenges, piezotransduced bulk MEMS resonators have rapidly emerged as a valid alternative. We propose a numerical strategy to simulate dissipation mechanisms that correctly reproduce available experimental data.

Keywords: MEMS, piezoelectricity, resonators, dissipation.

1 Introduction

Among the various piezoelectric block resonators developed so far, some utilize silicon as a structural layer and a piezoelectric material as a transduction layer Rosenberg, Jaakkola, Dekker, Nurmela, Pensala, Asmala, Riekkinen, Mattila, and Alastalo (2008). However it has been observed experimentally that the presence of the piezoelectric layer may degrade the quality factor (and hence increase dissipation) considerably, a phenomenon which is somehow puzzling due to the very limited thickness of the added layer. When MEMS are packed in nearvacuum, which is typical of high frequency resonators, the mechanical dissipation is essentially connected to loss mechanisms in the solid material, and for this reason it is often called "intrinsic damping" or "solid damping". Solid damping is induced by numerous physical and chemical processes and many of them are still needing further investigation. Sources of dissipation generally include attachment losses and thermal processes like thermoelastic and, to a minor extent, Akhieser losses. Since a piezoelectric block resonator operates in one of its bulk-modes, thermoelastic damping is generally negligible and can anyway be computed with reasonable accuracy. The issue of anchor dissipation deserves specific attention. In order to predict anchor

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losses it is generally accepted that all the elastic waves radiating from the anchor of the resonator into the elastic subspace are finally dissipated. From the numerical standpoint this can be simulated using suitable absorbing conditions. Among the different options, the Perfectly Matched Layer (PML) technique has gained increasing attention and has be adapted to a fully general 3D context. Nevertheless, neither thermal effects, nor anchor losses can account alone for the measured dissipation of piezotransduced resonators. There is strong evidence that other effects should be considered for thin resonators or when, for specific reasons, the above mentioned mechanisms are negligible. This remark is strongly supported by the fact that the capacitive counterparts with similar design have demonstrated a much higher Q. Since capacitive devices contain all these loss sources the low Q measured in piezo-resonators should result from dissipation of different nature. Several experiments seem to suggest that indeed sputtered AlN is a high-Q material and that the reduction in quality factor on resonator size is found to be consistent with a surface (interface) loss mechanism. The formulation of constitutive models accounting for the physics of interface phenomena, like dislocation and defects migration, is prohibitively complicated and hence phenomenological approaches are generally privileged. However constitutive parameters of these simplified models need to be calibrated on the basis of measured data and the accuracy of the calibration procedure and of the overall analysis heavily depends on the ability to filter out of measured data all the other known sources of dissipation. The specific family of length extensional (LE) presented and analysed in Rosenberg, Jaakkola, Dekker, Nurmela, Pensala, Asmala, Riekkinen, Mattila, and Alastalo (2008) is addressed in this investigation (see Figure 1. The resonator beam, of length $L = 320\mu m$, in plane width $w = 40\mu m$ and out of plane thickness $h = 20\mu m$, is attached to the anchoring region by means of bridges of varying width w_a and length $L_a = 60\mu m$. The vibration mode ($f = 13Mhz$) is a half sinusoidal in-plane wave with a nodal point at the attachment point of the bridge. A thin (300 *nm*) layer of AlN is deposited on top of the resonator beam with variable length L_p and width $w_p = 30\mu m$. Several devices with different silicon orientations, w_a and L_p have been produced and tested. The upper electrode is represented by a thin layer of Mo (300 *nm*) which, unlike the AlN piezolayer, covers the whole upper surface of the resonator beam.

2 Analysis of dissipation

Anchor losses in MEMS originate from the fact that elastic waves radiate from the anchor of the resonator into the much larger elastic subspace and are finally dissipated before being reflected back to the anchor region. Dissipative boundary conditions, and the PML approach in primis, are gaining increasing attention in the dedicated literature. If we suppose that the resonator deforms according to the

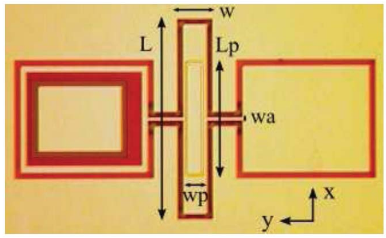

Figure 1: Length extensional resonator Rosenberg, Jaakkola, Dekker, Nurmela, Pensala, Asmala, Riekkinen, Mattila, and Alastalo (2008)

Table 1: Q_a for the LE resonator

w_a	orientation	Q_a
4	[110]	2180885
4	[100]	201452
8	[110]	473301
8	[100]	54037
20	[110]	66583
20	[100]	9430

eigenvector $\{V\}$ associated to the eigenvalue Ω_0^2, a standard result states that the quality factor is given by: $Q = \Re[\Omega_0^2]/\Im[\Omega_0^2] \simeq \Re[\Omega_0]/(2\Im[\Omega_0])$. Using a recently developed fully 3D dedicated numerical tool, the results collected in Table 1 were obtained. Quality factors Q_a are presented for different values of the bridge width w_a and orientation ([110] or [100]) of the crystalline structure along the axis the silicon resonator beam. Indeed Q_a only accounts for dissipation associated to anchor losses. Numerical results match qualitatively experimental observations (see Figures 2 and 3). Indeed larger anchor tethers (w_a) induce a stronger elastic coupling between the resonator and the substrate and higher energy dissipation; moreover, the [100] orientation is associated with a larger Poisson coefficient v_{xy} which amplifies the movement of the anchor tethers and induces important anchor losses. However, only the most dissipative case ($w_a = 20\mu m$, orientation [100]) gets quantitatively close to measurements. It is clear that anchor losses alone cannot account for the measured dissipation. Moreover thermoelastic losses are negligible even if we consider the spurious bending induced by the presence of the piezo and electrode layers. Indeed, predicted values of Q_{TED} are always well above 10^6. According to the remarks presented in the Introduction, we assume the presence of dissipative phenomena occurring at the interface between different materials following and extending an idea put forward in Hao and Liao (2010) for a 1D problem. Technological restrictions guarantee that we can always assume with good accuracy that all the interfaces are orthogonal to the z axis. Following standard theories for evolving interfaces between different phases, the interface is here assimilated to a surface (of thickness h) with intrinsic energy. Local equilibrium conditions impose continuity of σ_{i3} across the interface, while a discontinuity in $\sigma_{\alpha\beta}$ ($\alpha,\beta \in \{1,2\}$) is admissible. Displacements u_α are assumed continuous as well as the in-plane components of strains $\varepsilon_{\alpha\beta}$. Moreover, account taken of the limited thickness of piezo-layers and electrodes, we admit a state of plane stress, allowing to set $\sigma_{33} = 0$. When an interface separates two linear elastic materials the stress jump is induced by the difference $\Delta A_{\alpha\beta\gamma\delta}$ of the plane-stress stiffness matrices of the two materials:

$$\Delta\sigma_{\alpha\beta}[\mathbf{u}] = \Delta A_{\alpha\beta\gamma\delta}\varepsilon_{\gamma\delta}[\mathbf{u}] \tag{1}$$

In the present context we assume that dissipation phenomena are driven by interfacial static $\pi_{\alpha\beta}$ and kinematic $\theta_{\alpha\beta}$ variables:

$$\pi_{\alpha\beta}(\mathbf{x},t) = \Re[\Pi_{\alpha\beta}(\mathbf{x})e^{i\omega t}] \quad \theta_{\alpha\beta}(\mathbf{x},t) = \Re[\Theta_{\alpha\beta}(\mathbf{x})e^{i\omega t}]$$

The interface variables are assumed to linearly dependent: $\dot{\theta}_{\alpha\beta}(\mathbf{x},t) = \eta_1\pi_{\alpha\beta}(\mathbf{x},t)$ through the material parameter η and static variables $\pi_{\alpha\beta}$ play the role of "viscous discontinous" stresses $\pi_{\alpha\beta}(\mathbf{x},t) = \eta_2\Delta A_{\alpha\beta\gamma\delta}\dot{\varepsilon}_{\gamma\delta}[\mathbf{u}(\mathbf{x},t)]$. With these choices, the interface dissipation ΔW per cycle given by the time integral of the power exerted by static variables on the kinematic field becomes:

$$\Delta W = \int_0^T \int_S \pi_{\alpha\beta}(\mathbf{x},t)\dot{\theta}_{\alpha\beta}(\mathbf{x},t)\,dS\,dt = \pi\omega\eta\Re\left[\int_S \varepsilon_{\gamma\delta}[\mathbf{U}(\mathbf{x})]B_{\gamma\delta\lambda\rho}\varepsilon_{\lambda\rho}[\bar{\mathbf{U}}(\mathbf{x})]\,dS\right]$$

where $B_{\gamma\delta\lambda\rho} = \Delta A_{\alpha\beta\gamma\delta}\Delta A_{\alpha\beta\lambda\rho}$ is a positive definite tensor and $\eta = \eta_1\eta_2^2$.
The the 3D code employed for estimating anchor losses has been customized to include also the dissipative term. Initially we assume that only the Si-AlN interface dissipates so that a single material parameter η_{AlN} must be calibrated employing available experimental data. If we focus on Figure 2, which collects data for a constant length of the piezo layer ($L_p = 310\mu m$ and for silicon orientation [110], it appears that anchor losses have a minimal impact in the $w_a = 4\mu m$ case and hence a calibration employing these data points should be accurate. Using the average value $Q_e = 39000$ of the measured quality factors and imposing that $1/Q_e = 1/Q_a + 1/Q_d$ with Q_a taken from Table 1, we get $Q_d = 397000$ which gives a specific value of $\eta_{AlN} = 0.44910^{-10}\mu m\mu s/\mu Pa$. The identified value of η_{AlN} is now employed in a validation phase to simulate other available experimental configurations.

First we analyse the case of the LE resonator with different silicon orientation ([110] or [100]) and bridge width w_a. As before, the dissipation due to the anchor

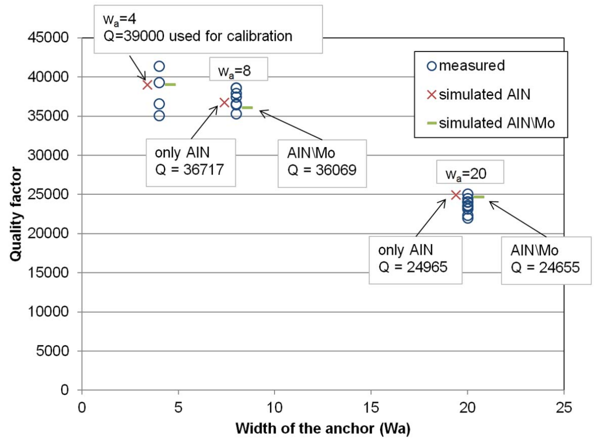

Figure 2: LE resonator: experimental data and results of simulations for different w_a; orientation [110], $L_p = 310\mu m$

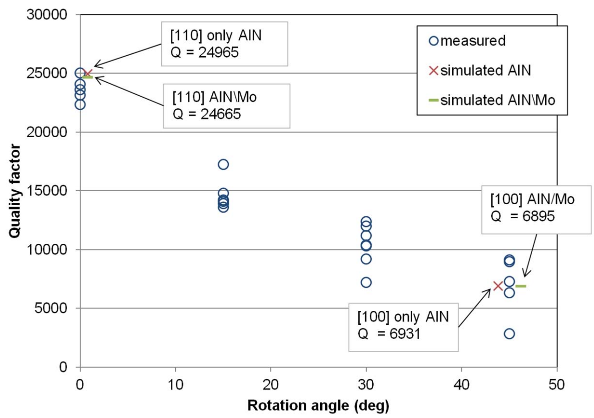

Figure 3: LE resonator: experimental data and results of simulations for different silicon orientations; $w_a = 6\mu m$; $L_p = 310\mu m$

losses is taken from Table 1 and is added to the dissipation coming from the interface according to the assumed surface law. In Figure 2 the simulation data for the [110] orientation, represented by red crosses and labelled “AlN”, are superposed to experimental measurements. The match with experimental data is surprisingly good. The same graphical comparison is performed in Figure 3 for the different orientations of silicon.

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