THIN-FILM COMPOSITE RESONATORS ON CRYSTALLINE SUBSTRATES

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Abstract—Telecommunications systems depend on high stability frequency sources. For mobile uses such as cell phones, size and cost are severe additional constraints. We describe a class of composite piezoresonators that are comprised of piezoelectric thin films deposited on crystalline plate substrates [1] oriented to obtain very low temperature coefficients of frequency (TCFs) for the composite structure. Specifically described are high-frequency bulk acoustic wave resonators (HBARs) comprised of piezoelectric thin films on AT- and BT-cut quartz substrates. An example design for a 2.1 GHz composite resonator is provided.

I. INTRODUCTION

Some current applications of resonant acoustic devices are: Wireless transceivers; PCS handsets; VCOs; CDMA filters; and MEMS/MOMS devices. Manufacturability, miniaturization, performance, and cost are the drivers that govern realizability of these components. One of the main environmental performance drivers is temperature coefficient of frequency (TCF) over an extended range, such as –55°C to +90°C. Piezoelectric thin films deposited on commercial quartz substrates yield composite resonators that are simultaneously miniaturizable, low cost, and virtually insensitive to temperature-induced frequency changes.

II. COMPOSITE AND THIN-FILM RESONATORS

Composite resonators were first used by Prof. S. Quimby. He and his students used rods of quartz as the piezodriver in a compound resonator to infer properties of a material to which it was bonded [2]. In this paper a thin-film piezoelectric is used to drive a quartz plate substrate to temperature-compensate the composite resonator; see Fig. 1. References [3]-[8] give a sampling of subsequent developments of thin-film and composite resonators. Sliker [4] mentions the possibility of using CdS on quartz to achieve a zero temperature coefficient of frequency (TCF).

The general case of acoustic plane waves propagating in crystals leads to trirefringence, with three distinct wave speeds and particle displacement vectors. In the case we consider, the situation is much simpler. The TCFs of virtually all solid materials are negative, ranging approximately from –20 to –120 x 10⁻⁶/K. In order to offset this behavior of the thin-film piezoelectric, we choose one of the very few cases of a positive TCF to effect the compensation, viz., the pure shear mode of rotated-Y-cut quartz plates, for angles between the AT- and BT-cuts; see Fig. 2.
Fortunately, the technology of this resonator type has advanced markedly [9] since its discovery [10], so that accurately oriented quartz substrates are readily available at realistic prices.

In order to make use of the positive TCF of the quartz substrate in the simplest manner, it is necessary that the piezoelectric thin-film layer properties be such that it drives the pure shear mode in the quartz without introducing coupling to other modes. Inasmuch as many suitable piezofilms, such as zinc oxide and piezoceramics, exhibit either 6mm or 4mm symmetry [11]-[12], this may be accomplished in either of two configurations: 1) polar axis of piezoelectric film in the plane of the film, and parallel to the quartz digonal axis, with applied driving field in the thickness direction (thickness-excitation, TE case), or 2) polar axis of piezoelectric film normal to the plane of the film, with applied driving field parallel to the quartz digonal axis, (lateral-excitation, LE case) [13]; see Fig. 3.

III. MATERIAL PROPERTIES

References [1] and [14]-[16] contain numerical values for candidate materials; their Van Dyke matrices are found in [11]. Point groups 6mm and 4mm share the same matrices, except that in 4mm the stiffness $c_{12}$ is independent. We assume that the piezoelectric thin film has symmetry 6mm or 4mm. Then the pure shear mode that exists for the TE case has effective stiffness $c_{44}' = c_{44} + (\varepsilon_{13})^2/\varepsilon_{11}$ and piezocoupling coefficient $k_{12} = |\varepsilon_{13}|/\sqrt{(c_{44} \cdot \varepsilon_{11})}$ [13]. Material values selected for the composite resonator simulated here are given in Table I. The piezoelectric velocity has purposely been reduced to approximately one-half of what is ordinarily found in practice; this is done to increase the velocity contrast for the sake of the simulation. Likewise, $k = k_{12}$ values chosen are 85%, which is rather high, but not out of the range of 4mm single crystals, and a more usual 45%, to show effects of variations in coupling [14]-[15].

Quartz input values and the rotational formulas used to obtain Fig. 2 are found in [17].

![Table I. Thin-Film and Quartz Substrate Values](image)

IV. NETWORK OF COMPOUND RESONATOR

We assume application of “energy-trapping” rules [18], which make the one-dimensional approximation a practicality in almost all situations. Then, on a per-unit area basis, Fig. 4 shows the network for a composite layered acoustic resonator structure. Acoustic transmission line characteristic impedances $(Z)$ equal the product of mass density $(\rho)$ and acoustic velocity $(v)$, and equivalent electrical lengths $(\theta)$ equal the radian frequency times length $(l)$, divided by acoustic velocity. In Fig. 4, the quantity $n$ equals $kv\sqrt{(\rho C_0/l)}$. Resonance frequencies of the composite are determined conjointly by the acoustic properties of the two wave propagation media, as well as by the impedance presented at the electrical port. Reference [19] contains additional details relating to equivalent networks.

![Figure 4. Method of computing input admittance of thickness-excited composite resonator.](image)

With $f_p$, $f_s$, and $f_c$ the fundamental frequencies of the piezofilm alone, the substrate alone, and the composite resonator, respectively, a simple transit-time argument yields the approximate relation $1/f_c = 1/f_p + 1/f_s$. Whereas the symmetry of the film alone would require that only odd harmonics be excited, the asymmetric composite resonator exhibits both even and odd harmonics. Defining $\eta = Z_s/Z_p = \sqrt{\rho_s/\rho_p}$, and applying standard network procedures to the circuit of Fig. 4 with the formulas therein, we find for the normalized input impedance seen at the electrical port [5]:

$$[Z_{in}(TE) \cdot (j\omega C_0)] = 1 - k^2[\tan(\theta_s)/(\theta_p)] \cdot [\eta \tan(\theta_s) + 2 \tan(\theta_p/2)]/[\eta \tan(\theta_s) + \tan(\theta_p)].$$

(1)
Figure 5. Composite resonator TCFs for various assumed TCFs of quartz substrate, assuming the piezofilm TCF is $-100 \times 10^{-6}/K$.

In the case of lateral-field excitation (LE) the corresponding relation for input impedance is:

$$\frac{Z_{in}(LE)}{(j\omega C_0 L)} = 1 + \frac{k_L^2 [\tan(\theta_p/2)/\theta_p]}{\tan(\theta_s)/\theta_p + \zeta \tan(\theta_p)} \cdot \left\{ 1 + \frac{1/2 \tan(\theta_p/2) \tan(\theta_p) \tan(\theta_s)}{\tan(\theta_s) + \zeta \tan(\theta_p)} \right\}. \quad (2)$$

V. SIMULATIONS

Assuming a TCF for the piezofilm of $-100 \times 10^{-6}/K$, and coupling coefficient of 85%, we find in Fig. 5 results of simulations for three values of TCF of the quartz substrate: $+10$, $0$, and $+4 \times 10^{-6}/K$. Plotted are the variations of the fundamental resonance frequency of the composite. Because of the piezoelectric nature of the device, one must distinguish between the resonance $f_{cR}(M)$ and antiresonance $f_{cA}(M)$ frequencies at harmonic $M$ and their TCFs [20]. The slopes in Fig. 5 are slightly shifted at the antiresonance frequency. Tables II and III give the frequencies of the first six harmonics.

The linear sensitivity coefficients $S$ are defined as:

$$TC_c = [(\Delta TC_c/\Delta TC_p)_{TC_p=0}] \cdot TC_s + \left[(\Delta TC_c/\Delta TC_p)_{TC_P=0}\right] \cdot TC_p = S_c \cdot TC_s + S_p \cdot TC_p \quad (3)$$

The $S$ are functions of material, harmonic, and thickness ratios, as well as frequency position on the impedance circle (e.g., resonance or antiresonance points). For a given combination of these parameters, (3) permits determination of the requisite value of $TC_c$, which in turn, yields the necessary quartz orientation angle from Fig. 2. Subscripts c, p, and s denote composite, piezofilm, and substrate, respectively, and $S_c + S_p = 1$. Effective piezocoupling factor of the composite is given by [5]:

$$k_{ce} = \sqrt{\frac{\phi}{\tan(\phi)}}; \quad \phi = \left(\frac{\pi}{2}\right)\left(\frac{f_{cR}(M)}{f_{cA}(M)}\right) \quad (4)$$

VI. 2.1GHz RESONATOR EXAMPLE

A simple methodology for obtaining approximate design frequencies is given below. Then the material properties of the thin-film and substrate yield thicknesses and quartz theta angle for obtaining a zero TCF, or indeed, any desired value of TCF within reasonable limits.

<table>
<thead>
<tr>
<th>M</th>
<th>$f_{cR}(M)$</th>
<th>$f_{cA}(M)$</th>
<th>$k_{c}(M)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>87.374886(^a)</td>
<td>88.433691</td>
<td>17.086(^a)</td>
</tr>
<tr>
<td>2</td>
<td>166.727541</td>
<td>176.562469</td>
<td>36.072</td>
</tr>
<tr>
<td>3</td>
<td>235.492427</td>
<td>264.226393</td>
<td>49.142</td>
</tr>
<tr>
<td>4</td>
<td>312.710256</td>
<td>351.519652</td>
<td>49.477</td>
</tr>
<tr>
<td>5</td>
<td>400.804459</td>
<td>438.767195</td>
<td>44.297</td>
</tr>
<tr>
<td>6</td>
<td>492.957177</td>
<td>526.324131</td>
<td>38.340</td>
</tr>
</tbody>
</table>

\(^a\) $f$ in MHz, $k_c$ in %.

<table>
<thead>
<tr>
<th>M</th>
<th>$f_{cR}(M)$</th>
<th>$f_{cA}(M)$</th>
<th>$k_{c}(M)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>88.338,624(^a)</td>
<td>88.433691</td>
<td>5.147(^a)</td>
</tr>
<tr>
<td>2</td>
<td>175.818,902</td>
<td>176.562469</td>
<td>10.172</td>
</tr>
<tr>
<td>3</td>
<td>261.900,451</td>
<td>264.226393</td>
<td>14.673</td>
</tr>
<tr>
<td>4</td>
<td>346.877,623</td>
<td>351.519652</td>
<td>17.933</td>
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<tr>
<td>5</td>
<td>431.985,958</td>
<td>438.767195</td>
<td>19.378</td>
</tr>
<tr>
<td>6</td>
<td>518.424,137</td>
<td>526.324131</td>
<td>19.101</td>
</tr>
</tbody>
</table>

\(^a\) $f$ in MHz, $k_c$ in %.

Operating frequency $f_{spec}$ is a specification. One may then choose an even integer $M = (P+N)$ and a small odd integer $P$ (odd because of the asymmetry of the piezoelectric traction). Example: $f_{spec} \sim 2.100$ GHz and $M = 24$. Then the composite will experience resonances approximately every $f_{cR}(1) = f_{spec}/M = 2100/24 = 87.5 \sim 88$ MHz (this will be modified somewhat by the $Z$ ratio). Choosing $P = 3$ yields $f_p = f_{spec}/P = 2100/3 = 700$ MHz (in the simulations $f_p \sim 723.75$ MHz, because $t_p$ was chosen for convenience to be 1 $\mu$m). Finally, $f_{s}(1) = f_{spec}/N = 2100/21 = 100$ MHz. Because the substrate is stress-free at its lower boundary plane, this condition will be reflected at the film-substrate interface at 100 MHz intervals. We thus satisfy the Diophantine relation: $M \cdot 88 = N \cdot 100$, with $3\lambda/2$ in the film, and $21\lambda/2$ in the substrate; $N/P = 7 \sim$ mass ratio. The displacements versus thickness are shown in Fig. 6, computed from the terminal mechanical currents. Displacements (currents) across the interface are continuous, but stress is not, because of the piezoelectric tractions. Formulas for the computation are in [21]. Table IV shows pertinent...
parameters at this harmonic for two values of piezofilm coupling factor; sensitivities are $S_\alpha = 0.89$ and $S_\beta = 0.11$. For typical piezoceramics, losses will not limit GHz operation of composites [22]. Reference [8] cites an ACN 2.14 GHz resonator with $Q = 900$, and $k = 25.5\%$.

### TABLE IV. 2.1 GHz Compound Resonator Values

<table>
<thead>
<tr>
<th>$M$</th>
<th>$k$</th>
<th>$f_{CR}(M)$</th>
<th>$f_{CA}(M)$</th>
<th>$k_c(M)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>85</td>
<td>2.099,860\textsuperscript{a}</td>
<td>2.105,710</td>
<td>9.87\textsuperscript{a}</td>
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<tr>
<td>24</td>
<td>45</td>
<td>2.105,916</td>
<td>2.108,222</td>
<td>5.18</td>
</tr>
</tbody>
</table>

\textsuperscript{a} $f$ in GHz; $k$, $k_c$ in %.

Figure 6. Mechanical displacements in 2.1 GHz, 24\textsuperscript{th} harmonic composite resonator.

### VII. CONCLUSIONS

Telecommunications and electronics require low-cost resonators and filters at gigahertz frequencies. Piezoelectric films satisfy the cost and frequency objectives, but have unacceptable temperature coefficients. Piezoelectric thin films on low-cost quartz substrates are shown to form temperature-compensated composite resonators. Compensation requires particular combinations of quartz cuts and piezofilm orientations. Design rules are sketched, and applied to an example of a temperature-compensated 2.1 GHz composite resonator.

### REFERENCES