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Analysis of contributions of nonlinear material constants to temperature-induced velocity shifts of quartz surface acoustic wave resonators

Haifeng Zhang [a,*], John A. Kosinski [b], Lei Zuo [c]

[a] Department of Engineering Technology, University of North Texas, Denton, TX 76207, United States
[b] MacAulay-Brown, Inc., Advanced Technology Group (ATG), Dayton, OH 45430, United States
[c] Department of Mechanical Engineering, Virginia Tech., Blacksburg, VA 24061, United States

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ABSTRACT

In this paper, we examine the significance of the various higher-order effects regarding calculating temperature behavior from a set of material constants and their temperature coefficients. Temperature-induced velocity shifts have been calculated for quartz surface acoustic wave (SAW) resonators and the contributions of different groups of nonlinear material constants (third-order elastic constants (TOE), third-order piezoelectric constants (TOP), third-order dielectric constants (TOD) and electrostrictive constants (EL)) to the temperature-induced velocity shifts have been analyzed. The analytical methodology has been verified through the comparison of experimental and analytical results for quartz resonators. In general, the third-order elastic constants were found to contribute most significantly to the temperature-induced shifts in the SAW velocity. The contributions from the third-order dielectric constants and electrostrictive constants were found to be negligible. For some specific cases, the third-order piezoelectric constants were found to make a significant contribution to the temperature-induced shifts. The significance of each third-order elastic constant as a contributor to the temperature-velocity effect was analyzed by applying a 10% variation to each of the third-order elastic constants separately. Additionally, we have considered the issues arising from the commonly used thermoelastic expansions that provide a good but not exact description of the temperature effects on frequency in piezoelectric resonators as these commonly used expansions do not include the effects of higher-order material constants.

1. Introduction

The temperature-frequency effect of SAW resonators describes the resonant frequency shift that occurs when the resonator is subjected to a temperature field. This phenomenon is critical for two aspects: (1) for SAW resonator applications, frequency should not be affected by temperature change and therefore, the temperature-frequency effect should be minimized; (2) for SAW temperature sensor applications, the temperature-frequency effect should be maximized to achieve the best sensitivity.

The optimal design of SAW resonators/temperature sensors relies on three major factors: the optimal selection of a substrate material, the optimal selection of the substrate cut angles, and the optimal selection of the surface wave propagation direction. These three major factors cannot easily be optimized without accurate modeling techniques. Models of the temperature-velocity effect for quartz SAW resonators has been reported by several investigators [1–4]. Schulz et al. have calculated the SAW temperature-velocity effect for a variety of crystal cuts and the calculations exhibited a satisfactory match to then-available experimental results [1]. Sinha and Tiersten have improved Schulz's model and presented improved temperature-velocity calculations [2]. Zhang and Wang have performed calculations to select optimal substrate and crystal cuts angles for both quartz and $LiTaO_3$ [3]. Notably, Their model included all nonlinear material constants. As an alternative, Ma and Shi [4] have reported a simplified model for the calculation of the temperature-velocity effect for SAW quartz resonators.

Formally, the calculation of the temperature-velocity effect requires the inclusion of all linear (elastic, piezoelectric, and dielectric constants) and nonlinear material constants (the third-order elastic constants (TOE), third-order piezoelectric constants (TOP), third-order dielectric constants (TOD) and electrostrictive

* Corresponding author.
E-mail address: haifeng.zhang@unt.edu (H. Zhang).

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constants (EL)). However, the calculations published in [1–4] included only the TOE and/or did not analyze the potential contributions of the TOP, TOD, and EL. Therefore, the influence of TOP, TOD, and EL on the temperature-velocity effect is unknown at this point. In addition, even though it is known that the TOE dominates the temperature-velocity effect, the specific contributions of each third-order elastic constant to the temperature frequency/velocity effect is unknown as well.

In this work, we have applied the perturbation integral theory developed by Tiersten [5] to calculate the temperature-velocity effect for a quartz SAW resonator with X-cut, Y-cut, and AC-cut orientation. We have included all linear and nonlinear material constants of quartz and temperature derivatives for the second-order elastic, piezoelectric and dielectric constants in the calculations. The new calculations match well with previous experiment results [1]. In addition, we have analyzed the contributions of each group of nonlinear material constants to the temperature-velocity effect, and have also analyzed the contributions from each of the TOE to the temperature-velocity effect for the X-cut quartz SAW resonator. The results quantify the contributions of each group of nonlinear material constants to the temperature-velocity effect. Based on the insights gained in performing the calculations, we also offer a suggestion for future calculations of the temperature-velocity effect of quartz SAW resonators.

This paper is organized as follows. In the next section, the temperature-velocity/frequency effect is introduced and the perturbation integral approach is described in Section 3. The description of the unperturbed surface acoustic wave and the temperature effect are presented in Section 4, and the results are shown in Section 5. Section 6 summarizes the conclusions.

2. Temperature-velocity/frequency effect of quartz saw resonators

The temperature-frequency effect is caused by intrinsic nonlinear material properties of a single crystal. The nonlinear material properties are characterized by the third-order material constants including the third-order elastic, piezoelectric, dielectric, and electrostrictive constants. A detailed description of this phenomenon requires the theory of infinitesimal fields superposed on finite biasing fields [6], which describes the influence of a biasing effect (such as mechanical stress, electrical field, and temperature) on the natural frequency of piezoelectric resonators. For most (but not all) cases of interest, the shifted value of the natural frequency can be estimated by the first-order perturbation integral [5], which is described in the next section.

3. Perturbation integral

The resonant frequency of a resonator depends on its geometry, material constants, and boundary conditions. The geometry changes slightly when a crystal resonator is subjected to a temperature field. In this case, the material constants may be characterized as effective constants, which will change with the temperature field. Thus, a resonant frequency will shift with the temperature. The shifted value may be estimated accurately by the perturbation theory. The equations used to estimate the first-order perturbation of a specific mode can be found from [5] and are shown below:

$$\Delta V_M = V - V_M = \frac{1}{2V_M\xi^2\int\rho_0(u_1^M u_1^{M^*} + u_2^M u_2^{M^*} + u_3^M u_3^{M^*})dV} \times \left(\int \hat{c}_{K\alpha L\gamma} u^M_{\gamma,K} u^{M^*}_{\alpha,L} + 2\hat{e}_{KL\gamma}\phi^M_{,K} u^{M^*}_{\gamma,L} - \hat{\varepsilon}_{KL}\phi^M_{,K}\phi^{M^*}_{,L}\right)dV, \quad (1)$$

where

$$\hat{c}_{K\alpha L\gamma} = T^0_{KL}\delta_{\alpha\gamma} + c_{K\alpha LN}\omega_{\gamma,N} + c_{KNL\gamma}\omega_{\alpha,N} + c_{K\alpha L\gamma AB}S^0_{AB} + k_{AK\alpha L\gamma}E^0_A + \frac{dc_{K\alpha L\gamma}}{dT}(T - T_0) \quad (2)$$

$$\hat{e}_{KL\gamma} = e_{KLM}\omega^0_{\gamma,M} - k_{KL\gamma AB}S^0_{AB} + b_{AKL\gamma}E^0_A + \frac{de_{KL\gamma}}{dT}(T - T_0) \quad (3)$$

$$\hat{\varepsilon}_{KL} = b_{KLAB}S^0_{AB} + \chi_{KLA}E^0_A + \frac{d\varepsilon_{KL}}{dT}(T - T_0), \quad (4)$$

with

$$b_{AKL\gamma} = b_{ABCD} + \varepsilon_0\delta_{AB}\delta_{CD} - \varepsilon_0(\delta_{AC}\delta_{BD} + \delta_{AD}\delta_{BC}).$$

In Eqs. (1)–(4), V_M is the unperturbed surface wave velocity, V is the perturbed surface wave velocity, and ΔV_M is the surface wave velocity shift. Here, $\hat{c}_{K\alpha L\gamma}$, $\hat{e}_{KL\gamma}$, and $\hat{\varepsilon}_{KL}$ are the effective elastic, piezoelectric, and dielectric constants respectively u^M_γ is a specific wave mode in the unperturbed condition, and ϕ^M is the electrical potential for this specific mode. $u^{M^*}_\gamma$ and ϕ^{M^*} are their conjugate counterparts. T^0_{KL}, S^0_{AB}, and E^0_A are the initial stress, strain and electrical field respectively with $\omega_{\gamma,N}$ defining the displacement gradient. $c_{K\alpha LN}$, e_{KLM}, and ε_{KL} are the second-order elastic, piezoelectric, and dielectric constants. $c_{K\alpha L\gamma AB}$, $k_{AK\alpha L\gamma}$, and χ_{KLA} are the third-order elastic, piezoelectric, and dielectric constants respectively, and b_{KLAB} are the electrostrictive constants. ε_0 is the permittivity of free space.

4. Unperturbed surface wave and temperature effect

Consider a quartz SAW resonator as shown in Fig. 1. A rectangular coordinate system is chosen with the x_3 axis normal to the crystal surface and the x_1 axis in the direction of the surface wave propagation. The general solution for a surface wave propagating along a crystal surface with an arbitrary cut angle (Euler angle) can be found in [7]. The solution may be written as follows:

$$U_i = \sum_{i=1}^{4} A^{(i)}\beta_i^{(j)} e^{-\frac{\alpha(j)\omega X_3}{V_s}} e^{\frac{i\omega(t-X_1)}{V_s}}, \quad j = 1, 2, 3 \quad (5)$$

$$\varphi = \sum_{i=1}^{4} A^{(i)}\beta_4^{(j)} e^{-\frac{\alpha(j)\omega X_3}{V_s}} e^{\frac{i\omega(t-X_1)}{V_s}}, \quad j = 1, 2, 3 \quad (6)$$

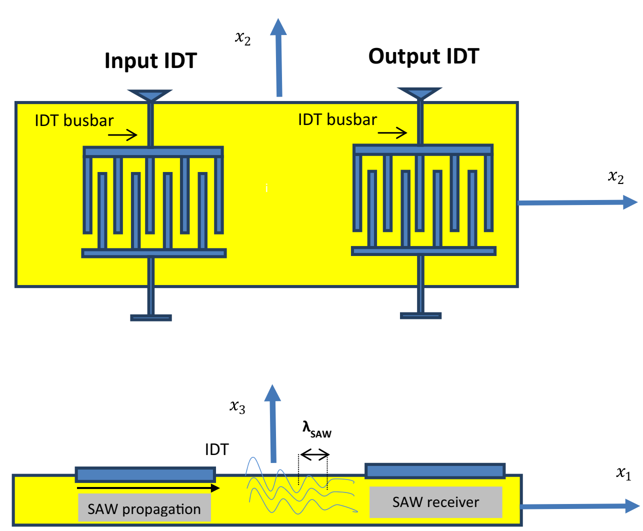

Fig. 1. The model of the temperature-velocity effect of a SAW quartz resonator.