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MODELING TEMPERATURE SENSITIVITY OF STW USING LAGRANGIAN MATERIAL CONSTANTS

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Abstract - This paper details the computation of the speed of surface transverse waves on periodically corrugated surfaces with help of the effective lagrangian material constants referred to the natural state of the crystal. The main benefit of the method is that, at the difference of commonly encountered methods based on the perturbation theory, it allows in a single pass for a direct computation of the temperature sensitivity of the speed or of the delay up to the third order in terms of temperature, thereby giving access to the modeling of the location of turn over points in temperature-compensated cuts.

Keywords **Lagrangian constants, STW, temperature behavior.**

I. INTRODUCTION

Using material constants defined in Lagrangian description is especially efficient to compute the speed of STWs propagating on corrugated surfaces. The reason of this is quite simple : in this method, the description of the stress-free biasing state arising from thermal expansion is embedded in the definition of elastic, piezoelectric and dielectric constants, and it is no more necessary to explicitly solve this quasi-static problem together with the propagation problem itself. Putting aside the theoretical reasons to promote this method, which was extensively described in [1], we remark that, in the particular case of STW propagation on corrugated surfaces, using it significantly reduces the complexity of analysis, since the boundary conditions and the geometry as a whole must be explicitly considered only at the reference value chosen for temperature. Another benefit is that, as far as the thermal bias can be assumed as stress-free, it is immediately possible to expand all computations up to the third order in terms of temperature. Considering the wide applications of STW for resonators or resonant sensing elements, it is useful to increase the order of the expansion in terms of temperature, inasmuch as the accurate determination of the behavior of compensated cuts depends on it. We complete the method to numerically or analytically compute the thermal sensitivity of propagation speed of STWs. Results are given for quartz.

II. Bloch–Floquet analysis of propagation

Here-studied configuration is classical : as shown on Fig. 1, we analyze the propagation of transverse horizontal waves along the Z' direction of a singly rotated cut Y+θ of quartz or of a homeotype of it. Without loss of generality we can assume that the outer normal of the average plane of the boundary surface of the semi-infinite substrate lies in Y'+ direction. Accordingly we consider that the substrate is infinitely deep along Y'-. The interface plane supports a system of identical infinite grooves parallel to X axis, suggested on Fig. 2 in the particular case of a trapezoid profile. Important parameters are the period Λ of corrugations and their height h, which can be simply related to the corrugation "wavenumber" Q and a dimensionless parameter ε, as follows :

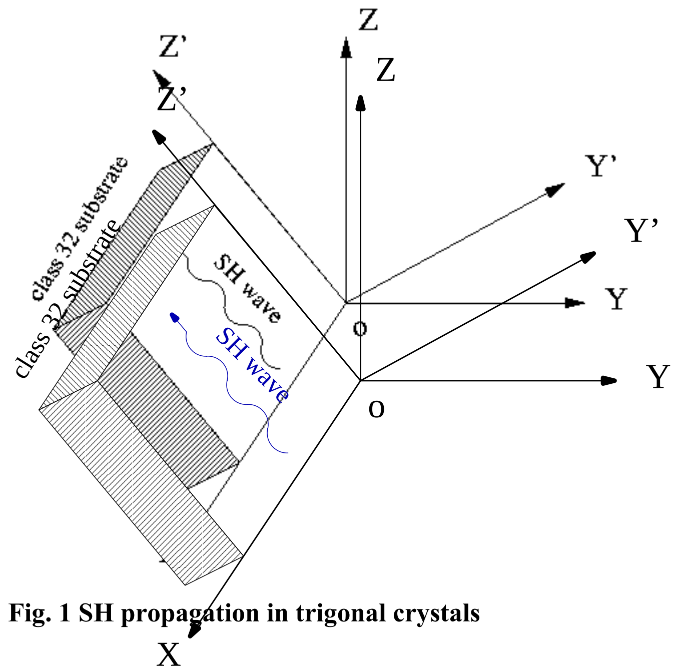

Fig. 1 SH propagation in trigonal crystals

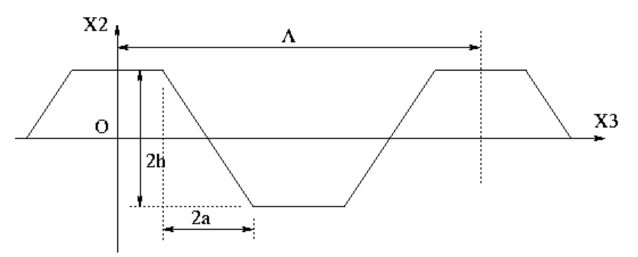

Fig. 2 Parameters of trapezoidal corrugations

$$Q = \frac{2\pi}{\Lambda} \quad y = \xi(X_3) = h\bar{\xi}(X_3) = \frac{\varepsilon}{Q}\bar{\xi}(X_3) \qquad \textbf{(1)}$$

Here, $\bar{\xi}$ is the normalized surface profile, by definition prescribed in the interval $-1 \le \bar{\xi} \le 1$. As a general rule in the lagrangian formalism, the geometry of the structure has to be known only in an arbitrarily chosen reference state, *i.e.* 25°C in our case. We use (X_1, X_2, X_3) to indicate coordinates mapping the substrate to the reference state. For instance, the way the geometric parameters *a, h, Λ* of the trapeze profile represented on Fig. 2 are affected by temperature do not need to be explicitly known since the effective material constants contain all the necessary information to account for a stress–free homogeneous temperature variation of the substrate. In this framework the dependent quantities of interest are Piola-Kirchhoff asymmetric stress tensor ***K*** and the material electric displacement ***D*** defined by the following formula

$$\begin{aligned} \sum_{L=1}^{3} n_L^0 K_{Lj} dS_0 &= F_j \quad j = 1 \ldots 3 \\ \sum_{L=1}^{3} n_L^0 D_L dS_0 &= \sigma \end{aligned} \tag{2}$$

where n^0 is the unit normal of some surface element of the matter taken in the reference state and F_j and σ respectively denote a component of the surface force and the surface charge density, existing and evaluated in the actual (final) state of the body while the surface element dS_0 is the elementary surface which consists of the small grains of matter which transform into the actual surface element when the force and the charge exist. Then the general form of the incremental equations of conservation of the quantity of movement and of the electric charge for dynamic quantities are the following

$$\begin{aligned} \sum_{L=1}^{3} \frac{\partial \tilde{K}_{L\alpha}}{\partial X_L} &= \rho_0 \frac{\partial^2 u_\alpha}{\partial t^2} \\ \sum_{L=1}^{3} \frac{\partial \tilde{D}_L}{\partial X_L} &= 0 \end{aligned} \tag{3}$$

where $\tilde{K}$ denotes the dynamic increment of the asymmetric (first) tensor of Piola-Kirchhoff, $\tilde{D}$ is the dynamic increment of the material electric displacement, and ρ_0 is indeed the mass density of the reference state, ie a constant with respect to temperature changes. Those equations pertain for infinitesimally small dynamic fields so that both mappings of the problem onto the coordinates y_j of the final state and onto the coordinates of the intermediate state ξ_α are strictly equivalent. Getting field equations written in terms of mechanical displacement and electric potential does require proper constitutive equations to account for material properties of substrate. It has been shown that those constitutive equations can be written in an effective linearized form with respect to small dynamic displacement and potential [2]

$$\begin{aligned} \tilde{K}_{L\alpha} &= G_{L\alpha M\varepsilon} \frac{\partial u_\varepsilon}{\partial X_M} + R_{K.\alpha L} \frac{\partial \varphi}{\partial X_K} \\ \tilde{D}_K &= R_{K.\alpha L} \frac{\partial u_\alpha}{\partial X_L} - N_{KL} \frac{\partial \varphi}{\partial X_L} \end{aligned} \tag{4}$$

where we classically make use of Christoffel's convention of automatic summing over all dummy indices. The latter relations introduce so–called effective lagrangian constants G (elastic) R (piezoelectric) and N (dielectric). Since we are in fact interested only by dynamic incremental quantities, we will from now on omit the superscript ~ in the rest of this paper.

For here–studied configuration it is very well known that SH straight–crested waves represented by $u_1(X_3, X_2)$ in local axes is totally uncoupled with other components of mechanical displacement, so that the following simple form of incremental balance equations pertain for a propagation problem restricted in the sagittal plane

$$\begin{aligned} \frac{\partial \tilde{K}_{21}}{\partial X_2} + \frac{\partial \tilde{K}_{31}}{\partial X_3} &= \rho_0 \frac{\partial^2 u_1}{\partial t^2} \\ \frac{\partial \tilde{D}_2}{\partial X_2} + \frac{\partial \tilde{D}_3}{\partial X_3} &= 0 \end{aligned} \tag{5}$$

Due to the asymmetric nature of both Piola-Kirchhoff stress tensor, which is self-contained in above definition (2), and of the displacement gradients $\partial u_\alpha / \partial X_L$, the reduction of indices should consider all nine possibilities [1]

$$\begin{array}{ccccccccc} 11 & 22 & 33 & 23 & 31 & 12 & 32 & 13 & 21 \\ \updownarrow & \updownarrow & \updownarrow & \updownarrow & \updownarrow & \updownarrow & \updownarrow & \updownarrow & \updownarrow \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \end{array} \tag{6}$$

Accordingly, all we need are the balance equations written as

$$\begin{aligned} \frac{\partial \tilde{K}_9}{\partial X_2} + \frac{\partial \tilde{K}_5}{\partial X_3} &= \rho_0 \frac{\partial^2 u_1}{\partial t^2} \\ \frac{\partial \tilde{D}_2}{\partial X_2} + \frac{\partial \tilde{D}_3}{\partial X_3} &= 0 \end{aligned} \tag{7}$$

together with the following subset of constitutive equations

$$\begin{aligned} K_5 &= G_{55} \frac{\partial u_1}{\partial X_3} + G_{59} \frac{\partial u_1}{\partial X_2} + R_{28} \frac{\partial \varphi}{\partial X_2} + R_{38} \frac{\partial \varphi}{\partial X_3} \\ K_9 &= G_{59} \frac{\partial u_1}{\partial X_3} + G_{99} \frac{\partial u_1}{\partial X_2} + R_{26} \frac{\partial \varphi}{\partial X_2} + R_{36} \frac{\partial \varphi}{\partial X_3} \\ D_2 &= R_{26} \frac{\partial u_1}{\partial X_2} + R_{28} \frac{\partial u_1}{\partial X_3} - N_{22} \frac{\partial \varphi}{\partial X_2} - N_{23} \frac{\partial \varphi}{\partial X_3} \\ D_3 &= R_{36} \frac{\partial u_1}{\partial X_2} + R_{38} \frac{\partial u_1}{\partial X_3} - N_{23} \frac{\partial \varphi}{\partial X_2} - N_{33} \frac{\partial \varphi}{\partial X_3} \end{aligned} \tag{8}$$

At the difference of ρ_0, ***G, R, N*** are functions of temperature. Also, they merge with usual constants ***c, e,*** ε when there is no biasing state at all, *i.e.* at the reference temperature.

Since the propagation of STW is conditioned by the existence of some periodic perturbation of the surface, we can take advantage of Floquet's theorem to search the solutions of problem as Bloch series expansion, *i.e.*, after introducing the notation

$$q_k = q_0 + kQ \quad k \in \mathrm{Z} \tag{9}$$

we get

$$\left.\begin{aligned} u_1 &= \sum_{k\in Z}\sum_{n=1}^{2} C_{k,n} u_1^{k,n} e^{j\left(\beta_k^n X_2 + q_k X_3 - \omega t\right)} \\ \varphi &= \sum_{k\in Z}\sum_{n=1}^{2} C_{k,n} \varphi^{k,n} e^{j\left(\beta_k^n X_2 + q_k X_3 - \omega t\right)} \end{aligned}\right\} \tag{10}$$

in the piezoelectric substrate, and

$$\phi = \sum_{k\in Z} \phi_k e^{j(\chi_k X_2 + q_k X_3 - \omega t)} \tag{11}$$

in the adjacent vacuum or air, if the surface is not metallized at all. Additionally, we can state that the vertical component of the k-th harmonic wavenumber must fulfill the condition $\mathrm{Im}\left(\beta_k^n\right) < 0$ for a damping into the depth of substrate, and, in the absence of reflection of the SH waves and of any excitation of other kind of waves into the bulk of the substrate, q_0 must be real below the first stopband $q_0 < Q/2$. Each harmonic k should individually obey the balance equations. Under above–mentionned conditions, solving Laplace equation in the vacuum or air adjacent to the substrate is trivial and provide with the following condition

$$\chi_k = -\left|q_k\right| \tag{12}$$

in the adjacent dielectric (if any). At the same time, after substituting the notation $\beta_k^n = q_k r_{kn}$ to normalize the vertical components of wavenumbers, the balance equations of the harmonic in the piezoelectric substrate writes as follows

$$\left.\begin{aligned} &\left[\rho_0 V_k^{\,2} - \left(G_{55} + 2G_{59} r_{kn} + G_{99} r_{kn}^{\,2}\right)\right] u_1^{kn} \\ &\qquad - \left[R_{38} + \left(R_{28} + R_{36}\right) r_{kn} + R_{26} r_{kn}^{\,2}\right]\varphi^{kn} = 0 \\ &\left[R_{38} + \left(R_{28} + R_{36}\right) r_{kn} + R_{26} r_{kn}^{\,2}\right] u_1^{kn} \\ &\qquad - \left[N_{33} + 2N_{23} r_{kn} + N_{22} r_{kn}^{\,2}\right]\varphi^{kn} = 0 \end{aligned}\right\} \tag{13}$$

where $V_k = \omega / q_k$ is the speed of the harmonic in the direction of guidance parallel to the average surface of substrate. The characteristic polynomial of this linear system yields four roots, whichfrom only two exhibit a negative imaginary part (damping behavior along $X_2 \le 0$) in the wavenumber domain of interest, that is q_0 smaller than the corresponding value q_{BG} for Bleustein-Gulyaev waves propagating onto a flat surface, with boundary conditions of the same nature, shortcut or free surface, as in here–considered problem. Therefore, due to the linearity of here–considered problem, its most general solutions are sought as a superposition of the two so-called partial solutions obeying this condition and numbered *n=1,2*, obtained from Eqs (13) for any *k*-th harmonic.

III. Treatment of Boundary Conditions

Let us define the following open–contour integrals as functions of an integer number *m* and a real or complex number α :

$$\begin{aligned} I_0(m,\alpha) &= \int_\Lambda e^{j\left(mQX_3 + \alpha\xi_{(X_3)}\right)} dX_3 \\ I_2(m,\alpha) &= \int_\Lambda n_{2(X_3)} e^{j\left(mQX_3 + \alpha\xi_{(X_3)}\right)} dX_3 \\ I_3(m,\alpha) &= \int_\Lambda n_{3(X_3)} e^{j\left(mQX_3 + \alpha\xi_{(X_3)}\right)} dX_3 \end{aligned} \tag{14}$$

where $\xi(X_3)$ is the previously–defined profile function. They will appear in a possible treatment of the boundary conditions which consists first in multiplying the left hand member of each boundary condition by $\exp\left(jlQX_3\right)$ with *l* integer, and second in integrating each obtained product over one corrugation period Λ and equating the result to zero. For instance, applying this procedure to the mechanical boundary conditions, we obtain :

$$\int_\Lambda \left[n_2 K_9 + n_3 K_5\right] e^{-jlQX_3} dX_3 = 0 \qquad \forall l \in \mathrm{Z} \tag{15}$$

Substituting previously–mentionned expressions into the latter one, we obtain an integral form of stress–free boundary conditions on a corrugated surface :

$$\begin{aligned} 0 &= \sum_{k\in \mathrm{Z}}\sum_{n=1}^{2} C_{k,n}\left[K_9^{k,n} I_2\left(k-l,\beta_k^n\right) + K_5^{k,n} I_3\left(k-l,\beta_k^n\right)\right] \\ K_5^{k,n} &= jq_k\left[\left(G_{55} + G_{59} r_{kn}\right)u_1^{kn} + \left(R_{38} + R_{28} r_{kn}\right)\varphi^{kn}\right] \\ K_9^{k,n} &= jq_k\left[\left(G_{59} + G_{99} r_{kn}\right)u_1^{kn} + \left(R_{36} + R_{26} r_{kn}\right)\varphi^{kn}\right] \end{aligned} \tag{16}$$

where $K_5^{k,n}$ and $K_9^{k,n}$ are essentially functions of q_0 and ω. Whatever are the electrical boundary conditions, it readily turns out that the terms inside brackets in above *mechanical* boundary conditions (16a) constitute the odd lines of the matrix ***M*** of a homogeneous linear system in terms of the $C_{k,n}$ -s :

$$\boxed{M_{\langle l,1|k,n\rangle} C_{|k,n\rangle} = 0} \tag{17}$$

which has to be written for all integers l appearing in (15) and which we have still to complete with even lines coming from the electrical boundary conditions. We figured out three kinds of sensible electrical boundary conditions

a) Surface with a thin and shortcut conductive coating of negligible mass effect.

This is the most simple case for the building of integral form of electrical boundary conditions. Applying the same procedure as for the mechanical boundary conditions, we get

$$\int_\Lambda \varphi_{(X_3,\xi(X_3))} e^{-jlQX_3} dX_3 = 0 \tag{18}$$

Substituting Bloch expansion (10) for the electric potential, and recalling above–defined open contour integrals, we actually obtain

$$\sum_{k\in Z}\sum_{n=1}^{2} C_{n,k}\varphi^{k,n} I_0\left(k-l,\beta_k^n\right)=0 \tag{19}$$

Accordingly, the even lines of the matrix are obviously given by

$$M_{\langle l,2|k,n\rangle} = \varphi^{k,n} I_0(k-l)\beta_k^n \tag{20}$$

b) Free, non metallized surface

This case requires a bit more manipulations to turn it into a simple equation. As a matter of fact, we must consider two conditions : firstly, the continuity of potential across the corrugated boundary surface, which can still readily be obtained applying the same multiplication–integration procedure

$$\sum_{k\in Z}\left[\phi_k I_0\left(k-l,-j\chi_k\right)-\sum_{n=1}^{2} C_{n,k}\varphi^{k,n} I_0\left(k-l,\beta_k^n\right)\right]=0 \tag{21}$$

and secondly, the continuity of $\vec{D}\cdot\vec{n}$ across the boundary

$$\int_\Lambda\left(\vec{D}\cdot\vec{n}-\varepsilon_0\frac{\partial\phi}{\partial n}\right)e^{-jlQX_3} dX_3 = 0\,. \tag{22}$$

After substituting Bloch expansion and applying the multiplication–integration procedure, we turn the latter continuity equation into :

$$\begin{aligned}0=\sum_{k\in Z}\Big\{&-\varepsilon_0\phi_k\left[jq_k I_3\left(k-l,-j\chi_k\right)+\chi_k I_2\left(k-l,-j\chi_k\right)\right]\\ &-\sum_{n=1}^{2} C_{k,n}\left[D_3^{k,n} I_3\left(k-l,\beta_k^n\right)+D_2^{k,n} I_2\left(k-l,\beta_k^n\right)\right]\Big\}\end{aligned} \tag{23}$$

where $D_2^{k,n}$ and $D_3^{k,n}$ are defined as follows :

$$\begin{aligned}D_2^{k,n} &= jq_k\left[\left(R_{28}+R_{26}r_{kn}\right)u_1^{kn}-\left(N_{23}+N_{22}r_{kn}\right)\varphi^{kn}\right]\\ D_3^{k,n} &= jq_k\left[\left(R_{38}+R_{36}r_{kn}\right)u_1^{kn}-\left(N_{33}+N_{23}r_{kn}\right)\varphi^{kn}\right]\end{aligned} \tag{24}$$

Combining Eqs (23) and(24) allows to eliminate the amplitudes of harmonics of potential ϕ_k in the surrounding dielectric, so that the combination reduces into the desired form

$$\boxed{M_{\langle l,2|k,n\rangle} C_{|k,n\rangle} = 0} \tag{25}$$

A detailed presentation of the procedure is presented in Eqs 11–13 of Ref.[2] in a quite similar case.

c) Approximation of zero electric displacement outside the substrate.

This is altogether the same level of approximation as would be used in FEA analysis of BAW resonators, which generally ignores the dielectric medium surrounding the piezoelectric device itself. The basic integral condition is :

$$\int_\Lambda \vec{D}_{(X_3,\xi(X_3))}\cdot\vec{n}_{(X_3)} e^{-jlQX_3} dX_3 = 0 \tag{26}$$

which immediately turns itself into the desired form, and gives the even lines of the homogenous linear system of boundary conditions :

$$\begin{aligned}&M_{\langle l,2|k,n\rangle} C_{|k,n\rangle} = 0\\ &M_{\langle l,2|k,n\rangle} = D_2^{k,n} I_2\left(k-l,\beta_k^n\right)+D_3^{k,n} I_3\left(k-l,\beta_k^n\right)\end{aligned} \tag{27}$$

Although it is not rigorous, this approximation provides with intermediate conditions in comparison with the treatment of the free and the shortcut surface. Thus it can be regarded as a straightforward way to quickly estimate the behavior of partially metallized substrates which are of utmost interest in practice since depositing metallic strips to trap the SH wave near the surface is actually a much more popular technique than etching the substrate without metal deposition.

IV. Roots Finding, Variant of the Method

As shown above, here–proposed method for the treatment of boundary conditions result into a determinantal equation. Since the propagation of STW is dispersive, we have to fix either ω or the ratio λ/Λ (where λ is the wavelength $\lambda=\frac{2\pi}{q_0}$) and then to vanish the determinant as a function of q_0. Thus, the proposed method is equivalent to zeroing the Fourier coefficients of the stress along the surface profile, and of involved electric quantities playing the same formal role, depending on the type of retained electrical boundary conditions. Nevertheless, the method is approximate since Bloch–Floquet analysis establishes all components of the solution as the product of $\exp(jq_0X_3)$ by a periodic function with respect to the period of corrugations Λ, according to the explicit form of Bloch expansions (10). As a direct consequence, the determinant of the linear system obtained through multiplying by each boundary condition by $\exp(-jlQX_3)$ and integrating over Λ cannot be strictly set equal to zero, since Bloch solutions are not exactly periodic with respect to Λ. Conversely, we can sustain that using orthogonality of the harmonic functions $\exp(-jlQX_3)$ to build a sequence of integral boundary conditions such as (15) is a sensible procedure to produce a best–fit approximation when the obtained determinant is minimal. In this sense, the mathematical equivalence between here–proposed method and commonly encountered Brekhovskikh expansion of the stress in terms of the profile slope is yet to be demonstrated, and has probably not to be expected.

Despite of its approximate nature, here–proposed method possesses an intrinsic advantage *i.e.* its good potential for modeling corrugations with steep, and even vertical slopes. For instance, keeping this purpose in mind, one can propose a different approximate integral form of boundary conditions by using the curvilinear abscissa along the surface profile instead of the horizontal coordinate X_3 as a main parameter for integration. This approach yields a respective substitution of the integrals defined by Eqs (14) by

$$\begin{aligned} J_0(m,\alpha) &= \int_{\overline{\Lambda}} e^{j\left(mQX_3(s)+\alpha\xi_{(s)}\right)} ds \\ J_2(m,\alpha) &= \int_{\overline{\Lambda}} n_{2(X_3)} e^{j\left(mQX_3(s)+\alpha\xi_{(s)}\right)} ds \\ J_3(m,\alpha) &= \int_{\overline{\Lambda}} n_{3(X_3)} e^{j\left(mQX_3(s)+\alpha\xi_{(s)}\right)} ds \end{aligned} \tag{28}$$

into the boundary conditions system. In above integrals, $\overline{\Lambda}$ stands for the period of the curvilinear abscissa along he actual profile, i.e. not projected onto $\vec{X}_3$ axis. The advantage is that the effect of vertical steps still remain finite in the integral boundary conditions, the drawback is that harmonic functions $\exp(-jlQX_3)$ are orthogonal over the period Λ of X_3, not over the period $\overline{\Lambda}$ of *s*. From a more practical point of view, we can remark that whenever the slope of profile remains finite, the following identities hold :

$$\begin{aligned} J_2(m,\alpha) &\equiv I_0(m,\alpha) \\ J_3(m,\alpha) &\equiv \frac{mQ}{\alpha} J_2(m,\alpha) \end{aligned} \tag{29}$$

Concluding on this issue is left for further research. At this moment, we simply point out that :

- The whole issue arises from the absence of equivalence between orthogonality and completeness. Nevertheless, it might be interesting to know that non complete bases are routinely and successfully used in FEA programs, so that we can think of developing an efficient argumentation on this issue in the near future.
- Although the integral forms of boundary conditions established in the previous section does not allow for vertical steps, they do allow for a periodic profile of steps with finite slope, where "finite" is not "small" at all.

- To remove any misunderstanding, it should be pointed out that using any of previously–presented treatments of boundary conditions is a choice which we may carry out independently from the use of effective lagrangian constants, the latter topic relating to quite another field of understanding.

V. Approximate Analytical Method

Obtaining an approximate analytical value of speed in the framework of lagrangian formalism involves some successive steps.

First, we have to completely neglect piezoelectric effect and to solve the purely mechanical problem of propagation in the sagittal plane (X_2oX_3) with free boundary condition on the plane (X_1oX_3). This step easily provides with the following closed–form expression of SSBW speed :

$$V_{SSBW} = \sqrt{\frac{G_{58} - \dfrac{G_{56}G_{89}}{G_{99}}}{\rho_0}} \tag{30}$$

Admitting that STW propagate on a corrugated non piezoelectric substrate with a speed which remains very close to V_{SSBW}, we can rewrite the procedure outlined in Secs. 6.2–6.4 of [4] with help of Piola–Kirchhoff tensor instead of regular stress. Thus, the condition for zero stress associated with pure SH vibration on a corrugated profile is given by Brekhovskikh's series expansion :

$$\left.\frac{\partial u_1}{\partial X_2} - \left(\frac{d\xi}{dX_3}\right)\frac{\partial u_1}{\partial X_2} + \xi\frac{\partial^2 u_1}{\partial X_2{}^2} + \cdots\right|_{X_2=0} = 0 \tag{31}$$

After substituting in the combination of partial derivative equations restricted to the mechanical terms and above boundary conditions in the case of simple cosine profile, a Bloch series expansion (10a) yields a dispersion equation which can be asymptotically solved for small corrugation wavenumber together with infinitesimal profile slope

$$\Lambda << \lambda$$

$$\left| \frac{d\xi}{dX_3} \right| << 1 \tag{32}$$

Rewritten with using effective material constants, the dispersion yields a closed–form expression of the vertical wavenumber component from which the speed of STW waves is easily obtained for the purely mechanical case :

$$V_{STW} = \left(1 - \frac{G_{99} \quad \left(1 - \frac{G_{59}{}^2}{G_{55}G_{99}}\right) \quad h^4 Q^2 \rho_0 \omega^2}{8 G_{55}{}^2} \right) V_{SBW} \tag{33}$$

From another hand, an asymptotic expansion can also be achieved for the propagation of SH waves onto a flat piezoelectric substrate, leading to the following closed–form expression of the speed of so–called Bleustein–Gulyaev waves whenever the piezoelectric coupling is small :

$$V_{BG} = \sqrt{\frac{G_{55}}{\rho_0} \left(1 + \eta^2 B - \frac{G_{59}{}^2}{G_{55} G_{59}} \right)} \tag{34}$$

where η is the piezoelectric coupling and *B* is a relatively cumbersome dimensionless expression, which involves effective material constants. Depending on the piezoelectric properties of crystal, *B* remains very small with respect to unity. Since it is know that the trapping of SH near the surface arising from periodic perturbations is in practice much stronger than the trapping arising from piezoelectric effect on a flat surface, assuming that the latter one exists, we can propose an approximate formula for the speed of surface transverse waves on piezoelectric substrates with cosine–corrugated surface :

$$\overline{V}_{STW} \approx V_{BG} + V_{STW} - V_{SSBW} \tag{35}$$

Of course, such formula is not rigorous because the structure of waves obtained in piezoelectric case, involving the combination of essentially mechanical and essentially dielectric partial solutions, differs from the much simpler structure of purely mechanical solutions, so that the actual shift between the actual STW and the first SSBW–step cannot be represented by a simple superposition of separate effects.

VI. Examples of Results

The interest of being able to model the high–order temperature behavior of surface transverse waves is indeed larger in the case of temperature–compensated cuts used in resonators than it probably would be in studying large passband filters.

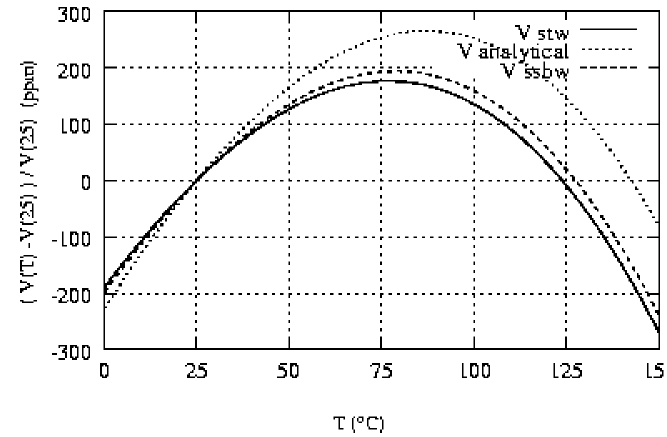

Fig. 3 Temperature behavior of SH according to the level of modeling for $Y + 37.8°$ quartz shortcut substrate.

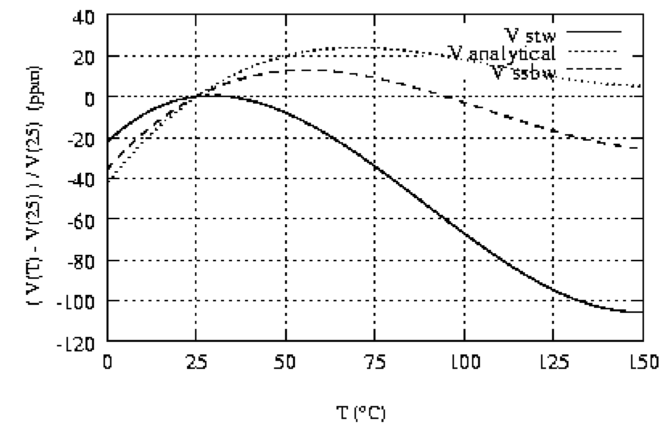

Fig. 4 Temperature behavior of SH according to the level of modeling for $Y - 50.5°$ quartz shortcut substrate.

Figs. 3 and 4 respectively propose predicted temperature characteristic of STW speed in quartz cuts near AT and near BT. The computations were achieved with $k \in [-3:3]$ while the shortcut substrate profile was assumed most symmetrical (*a=0.125*), $\lambda = 4\Lambda$ and $\lambda \approx 100h$. For BT–like cuts, the difference between the numerical model for piezoelectric substrate and the approximate analytical model is much larger than for the AT–like cut.

Complementary results are provided by Figs. 5 and 6 which respectively show the influence of groove depth and of the ratio λ / Λ on the temperature–speed characteristic. In all cases, it appears than the influence of investigated parameters is worth considering to master the optimization of resonant structures, although this task would also require to take into account the influence of the design transducer and Bragg's reflectors regions in a fully–integrated model, since the STW structure – in particular the depth of trapping inside the substrate – is by definition much more depending on periodic perturbations than the standard SAW structure.

VII. Conclusion

- Using the lagrangian formalism involving effective material constants provides with a straightforward way to modeling higher–order temperature behavior of the speed of STW onto corrugated piezoelectric substrates.
- In particular, associated with here–proposed procedure to integral boundary conditions, this formalism gives an easy access to the influence of the geometrical parameters of the corrugations onto the temperature–speed characteristic, including its curvature and turn–over points.
- Predicted results show a significant difference from the results predicted in the simpler case of SSBW and with help of here–outlined approximate analytical model.
- Here–proposed procedure for the treatment of boundary conditions is usable for grooves profiles with finite slope.
- The treatment of STW trapping occurring from metallic strips deposited onto a flat substrate can be proposed as an useful goal for further application of the lagrangian formalism to the understanding of the thermal behavior of STW resonant structures.

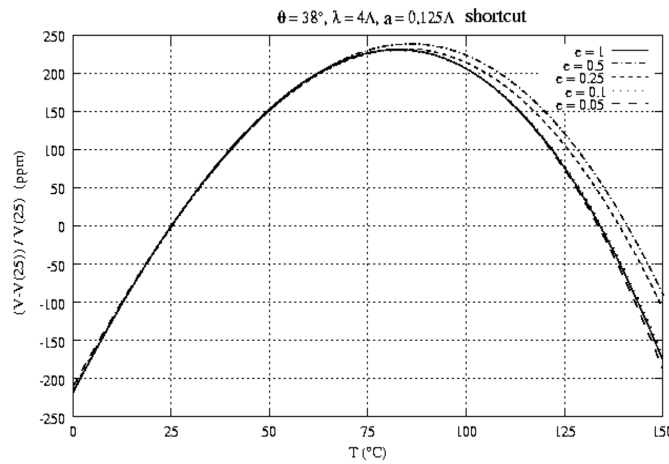

Fig. 5 Influence of height of groove on temperature characteristics.

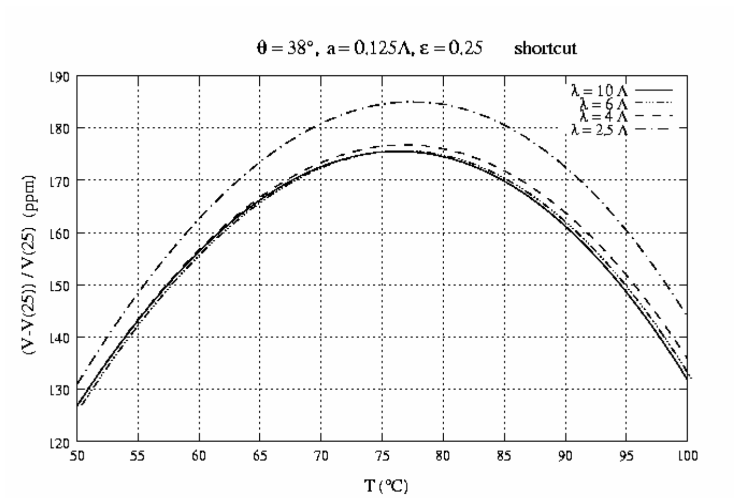

Fig. 6 Influence of λ / Λ on temperature characteristics.

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