Modelling of Ultrasonic Wave Propagation in Integrated Piezoelectric Structures under Residual Stress

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***Abstract*—When thick film technology is employed, like tape casting or screen-printing, a non uniform shrinkage appear due to the difference of thermal expansion coefficient between the film and the substrate. It implies the presence of residual stress into the film. Hence, this paper presents models which take into account this phenomenon. At first, the modified Christoffel equations for a piezoelectric material under external stress are presented. A numerical study of its influence is carried out on the slowness curves and coupling coefficients of a PZT-based material. It is showed that a lateral residual stress could couple pure transverse mode to piezoelectricity because of a slight rotation of the polarisation vector. In a second part, modified Christoffel tensor is used to calculate the dispersion curves of Lamb waves in a piezoelectric plate. The Lamb modes are found to be sensitive to the residual stress. In a third part, these results are extended to a piezoelectric film laid down on a substrate in order to model the importance of these phenomena on the behaviour of an integrated structure.**

Index Terms - Piezoelectricity, Residual Stress, Coupling Coefficients, Guided Waves

I. INTRODUCTION

For past thirty years, sensors, electromechanical actuators and transducers are increasing their application fields thanks to the use of piezoelectric ceramics, especially lead zirconate titanates (PZT) [1]-[2]. In many cases, these devices are based on piezoelectric ceramic thick or thin films that are most often submitted to high internal residual stress [3]-[4]. Due to non linear effects, it is well known that piezoelectric characteristics are significantly affected by the presence of high mechanical stress through a shift of material properties from their stress-free values [5]-[6]. Moreover, studies of stress-induced effects on the propagation of elastic waves are of great interest in the field of non-destructive testing .

In this paper, we propose to study and highlight several effects of an initial mechanical stress on bulk and guided waves in a PZT medium. For this, the modified constitutive equations of a pre-stressed piezoelectric material are first presented. Then, these equations are used to derive the formalism of slowness curves, associated electromechanical coupling coefficients, Lamb waves and surface acoustic waves in a PZT medium. In the second part, numerical examples are given first for a Pz27 medium as far as slowness curves are concerned. Then, a Pz27 plate and Pz27 film laid down on a Si substrate are considered to study the modifications with the stress on Lamb waves and surface acoustic waves, respectively.

II. THEORETICAL CONSIDERATIONS

A. Constitutive equations for a general pre-stressed piezoelectric media

For a continuous medium under deformation, the deformation and motion of a material point can be described through the coordinate x_k:

$$x_k = x_k(X_K, t)\text{, k = 1, 2, 3 and K= I, II, III} \tag{1}$$

where X denotes a particle coordinate in the undeformed configuration, called the natural state, and x is the coordinate at the final state. It results of the superimposition of the finite initial displacement, $\boldsymbol{u}^0$, due to the applied mechanical stress with the infinitesimal displacement, $\boldsymbol{u}$, of the wave motion. The subscripts K and k denote the components in the Lagrangian coordinate system in the natural state and the Eulerian coordinate system at the final state, respectively and t denotes time. Eq. (1) represents a mapping of the natural configuration on the pre-deformed one. Using the theorem of superposition for static and dynamic values, and neglecting all the higher order terms, the constitutive equations for a piezoelectric material in a pre-stressed state are [7], [8]:

$$(\tilde{\sigma}_{ij} + u_{i,k}\sigma^0_{jk})_{,j} = \rho_0 \ddot{u}_i \tag{2}$$

$$\tilde{D}_{i,i} = 0 \tag{3}$$

where

$$\tilde{\sigma}_{ij} = \tilde{C}_{ijkl} u_{k,l} + \tilde{e}_{mij}\Phi_{,m} \tag{4}$$

$$\tilde{D}_m = \tilde{e}_{mij} u_{i,j} - \tilde{\varepsilon}_{mn}\Phi_{,n} \tag{5}$$

$$\tilde{C}_{ijkl} = C_{ijkl} + (C_{ijnl}\delta_{km} + C_{ijklmn})u^0_{m,n} + e_{mijkl}\Phi^0_{,m} + C_{njkl}\delta_{im}u^0_{m,n} \tag{6}$$

$$\tilde{e}_{mij} = e_{mij} + (e_{mjl}\delta_{ik} + e_{mijkl})u^0_{k,l} - l_{mnij}\Phi^0_{,n} \tag{7}$$

$$\tilde{\varepsilon}_{mn} = \varepsilon_{mn} + l_{mnij}u^0_{i,j} - \varepsilon_{mnp}\Phi^0_{,p} \tag{8}$$

The symbol (~) means that corresponding variables are defined in the pre-deformed state.

B. Slowness curves and coupling coefficients

The previous relations allow defining the slowness curves and the coupling coefficients for a pre-stressed piezoelectric material. By defining the unstiffened and stiffened phase velocities respectively as:

$$V = \sqrt{C/\rho} \text{ and } \tilde{V} = \sqrt{(M + \tilde{e}^2/\tilde{\varepsilon})/\rho} \tag{9}$$

where $M_{ijkl} = \tilde{C}_{ijkl} + \delta_{ik}\sigma^0_{jl}$,

In Eqs. (9), all variables in the numerator depend on the direction of propagation.

We define the electromechanical coupling coefficient as [9]:

$$K = \sqrt{\tilde{k}^2/(1+\tilde{k}^2)}\text{, with } \tilde{V} = V(1+\tilde{k}^2)^{1/2} \tag{10}$$

C. Propagation of Lamb waves in a pre-stressed transversely isotropic piezoelectric plate

A pre-stressed transversely isotropic piezoelectric plate which is oriented according to the axes defined in Fig. 1 is considered. Piezoelectric Lamb modes are polarized in the (Ox_1, Ox_3) plane. In the following, we will only consider Lamb modes with a direction of propagation along Ox_1. If a small initial displacement field is assumed, one can consider the symmetry of the plate to be unchanged. Thus, the following analysis will be given in the case of a transversely isotropic symmetry for which shear horizontal (SH) modes and Lamb modes are uncoupled. Indeed, SH modes are non piezoelectric and are polarized along the Ox_2 axis. Only the developments corresponding to the case of metallised surfaces are given entirely.

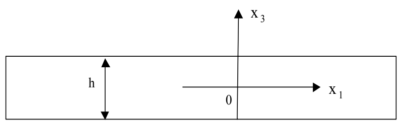

Fig. 1. Schematic of the piezoelectric plate with the coordinate system.

Using the constitutive equations given in the section A, and writing the mechanical and electrical boudary conditions leads to the constitutive equations of Lamb waves in pre-stressed transversaly isotropic piezoelectric plate:

$$N_S = 0 \text{ and } N_A = 0$$

where the first and second equations correspond to solutions for symmetric and antisymmetric Lamb modes, respectively, with:

$$N_S = T_1^1 G_1 \,/\tan(\gamma\alpha_1) - T_1^3 G_3 \,/\tan(\gamma\alpha_3) + T_1^5 G_5 \,/\tan(\gamma\alpha_5) \quad (11)$$

$$N_A = T_1^1 G_1 \tan(\gamma\alpha_1) - T_1^3 G_3 \tan(\gamma\alpha_3) + T_1^5 G_5 \tan(\gamma\alpha_5) \quad (12)$$

$$R_1^p = \frac{\Psi_{14}\Psi_{13} - (\Psi_{11} - \rho V^2)\Psi_{34}}{\Psi_{13}\Psi_{34} - (\Psi_{33} - \rho V^2)\Psi_{14}} \quad (13)$$

$$R_2^p = \frac{\Psi_{34}\Psi_{13} - (\Psi_{33} - \rho V^2)\Psi_{14}}{(\Psi_{33} - \rho V^2)\Psi_{44} - \Psi_{34}^2} \quad (14)$$

with

$$\Psi_{ik} = M_{i3k3}\alpha^2 + (M_{i1k3} + M_{i3k1})\alpha + M_{i1k1},\ i,k = 1,2,3 \quad (15)$$

$$\Psi_{i4} = \tilde{e}_{3i3}\alpha^2 + (\tilde{e}_{1i3} + \tilde{e}_{3i1})\alpha + \tilde{e}_{1i1},\ i = 1,3 \quad (16)$$

$$\Psi_{44} = -[\tilde{\varepsilon}_{33}\alpha^2 + (\tilde{\varepsilon}_{13} + \tilde{\varepsilon}_{31})\alpha + \tilde{\varepsilon}_{11}] \quad (17)$$

$$T_1^p = \tilde{C}_{3311} + \sigma_{31}^0 R_1^p + (\tilde{C}_{3333} + \sigma_{33}^0)\alpha_p R_1^p + \tilde{e}_{333}\alpha_p R_2^p \quad (18)$$

$$T_2^p = \sigma_{31}^0 + (\tilde{C}_{1313} + \sigma_{33}^0)\alpha_p + \tilde{C}_{1331} R_1^p + \tilde{e}_{113} R_2^p \quad (19)$$

$$T_3^p = \tilde{e}_{311} + \tilde{e}_{333}\alpha_p R_1^p - \tilde{\varepsilon}_{33}\alpha_p R_2^p \quad (20)$$

$$G_1 = R_2^3 T_2^5 - R_2^5 T_2^3 \quad (21)$$

$$G_3 = R_2^1 T_2^5 - R_2^5 T_2^1 \quad (22)$$

$$G_5 = R_2^1 T_2^3 - R_2^3 T_2^1 \quad (23)$$

The (α_i) are the roots of the six-degree polynomial secular equation:

$$\left|\Psi_{ik} - \rho V^2 \delta_{ik}\right| = 0 \quad (24)$$

with $\alpha_i = -\alpha_{i+1}$, i=1, 3, 5

Similar developments were led for a pre-stressed piezoelectric film laid down on a substrate. They are not presented here, but can be easily derived by taking into account the boundary conditions between the film and the substrate.

III. Numerical results

All results are presented for a PZT material, Pz27, a soft composition from Ferroperm Piezoceramics, Denmark, which presents a 6mm symmetry. The influence of a tensile stress on its acoustical properties is studied. Literature reports hysteresis loops in piezoelectric ceramics under dynamic uniaxial stress [9][10] which prevents to measure and define third order piezoelastic parameters. Moreover, since experimental values of the modified piezoeleastic tensor are uncompleted [5][6], we have chosen to describe the general behaviour of ultrasonic waves in a pre-stressed PZT material with the natural parameters. This implies to consider an initial deformation field small enough to be neglected. In order to satisfy this assumption, the applied stress value will be of a few tenths up to 1% of the elastic parameter C_{11}. Although the stress values close to from 1% of C_{11} represent a limit case to neglect the initial deformation field, some numerical results are given for this percentage in order to better illustrate some effects. It is assumed that the initial stress possesses only one component along one of the three axes and the initial electrical potential is null.

A. Slowness curves and electromechanical coupling coefficients

Fig. 2(a) represents the slowness curves of Pz27 material as a function of the elevation angle θ, without stress. Continuous curves take into account piezoelectricity, whereas dashed ones are calculated without the piezoelectric coefficients. Fig. 5 shows the associated longitudinal KL and transverse KT1, KT2 coupling coefficients. Due to the symmetry of the material, these curves are all the same whatever the azimutal angle φ is. In Fig. 2(a), there is no piezoelectric coupling with the pure transverse mode (T2) (polarization along x_1) since the two curves, with and without piezoelectricity, are superimposed. Thus, the shear coupling coefficient KT2 is equal to zero for any incident and azimutal angle as shown in Fig. 2(b).

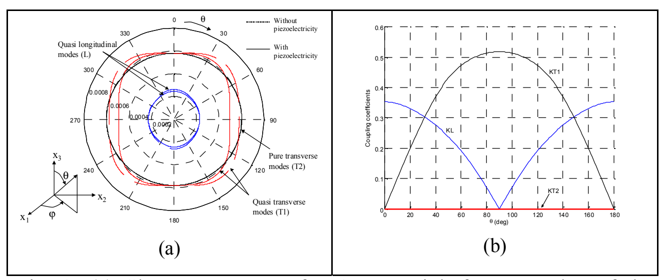

Fig. 2. (a) Slowness curves of Pz27 material, for any value of the azimutal angle φ and without external stress; (b) associated electromechanical coupling coefficients without external stress.

Now, consider a tensile stress $\sigma^0 = \sigma^0_{x_2}$ applied in the x_2 direction, which corresponds to azimutal and incident angle values both equal to 90 degrees. Figs. 3 (a-d) show the slowness curves for azimutal angles φ equal to 0, 30, 60 and 90 degrees, respectively. Due to the symmetry of the material and the small stress effect compared to the free-stress slowness values, only a quarter of the slowness curves are plotted. For clarity, the legend of each mode was not repeated but they can be identified easily from Fig. 2(a) by tracking their evolution in Fig. 3(a) to 3(d). In all cases, the modifications of slowness curves are given for a stress value equal to 1% of the elastic parameter C_{11}.

It can be observed that there is no influence of the applied stress σ^0 in the (Ox_1, Ox_3) plane, corresponding to φ = 0, since Fig. 3(a) is identical to Fig. 2(a) with σ^0=0. For the other φ values, all slowness curves are gradually modified when φ reaches 90°. For each φ value, the influence of the stress is null for θ = 0, and increases with θ with a maximum reached in the x_2 direction, for θ = 90°. The most significant result consists in the non-zero piezoelectric coupling of the pure transverse mode with non zero residual stress as it can best be observed on Fig. 3(d) for φ = 90° since this cross section contains the total applied stress. This non zero piezoelectric coupling, KT2, can be explained by a slight rotation of the corresponding polarisation vector. This can be verified using Eq. (28) if the initial displacement field is not neglected.

The changes in the values of the coupling coefficients with stress values are plotted in Fig. 4(a-d) as a function of θ, for the four azimutal angle values φ = 0, 30, 60, 90 degrees. In each case, four values of σ^0 were used, 0%, 0.25%, 0.5% and 1% of C_{11}, respectively.

A non zero coupling coefficient of the pure transverse mode appears for non zero stress and φ≠0. The general tendency consists in having an increase of the coupling coefficients with the stress. The largest coefficients are observed at the azimutal angle φ=0. Nevertheless, for each value of φ, for some elevation angles θ, the coupling coefficients of the quasi longitudinal and quasi shear mode differ from zero.

B. Dispersion curves of a pre-stressed Pz27 plate

We will consider a stress applied in the same direction as the direction of propagation x_1. In Fig. 5(a) are plotted the dispersion slowness curves of a Pz27 plate of 1mm thickness and for frequencies up to 5 MHz in the case of short-circuit boundary conditions. Since the variations of slowness with residual stress are relatively small compared to their initial values, only the results for an applied residual stress of 1% of C_{11} are compared with no stress case.

In these curves, each mode tends obviously toward the same limit, with and without stress, when the slowness tends toward zero. This means that the cut-off frequencies are not modified by the presence of the stress.

The slowness values tend to decrease when an external stress is applied. This means that the initial stress slightly increases the velocities for all modes, with variations of a few tens of m/s, depending both on the mode and the frequency considered. At a frequency of 1 MHz, the variation of the A0 Lamb mode is 47 m/s, whereas this variation is 69 m/s for the S0 mode. On the other hand, at 0.1 MHz, the variation of the A0 mode velocity is around 73 m/s whereas this variation tends toward a limit value of 53m/s for frequencies above 4 MHz.

Another result is detailed in Fig. 5(b) which shows the variations of the A0 mode velocity for small frequency-thickness product values. In order to keep frequency values around one MHz, they were chosen between 0.05 to 3 MHz, with a plate thickness of 10 µm. The A0 mode is plotted as a function of frequency for stress values equal to 0, 0.528, 1.06 and 1.47 GPa. The latter value corresponds to an applied stress equal to 1% of C_{11}. At low frequency-thickness product values, the velocity of A0 strongly depends on the applied stress. Here, the stress is not expressed in percentage of C_{11} since it allows the zero frequency limit of the velocity, which is given by $V(A_0) = \sqrt{\sigma^0 / \rho}$, to be determined [12]. Below approximately 0.2 MHz, the velocities for non zero stress tend to be constant, which make possible the measurement of the applied stress if the working frequency-thickness product is around 2 MHz*µm.

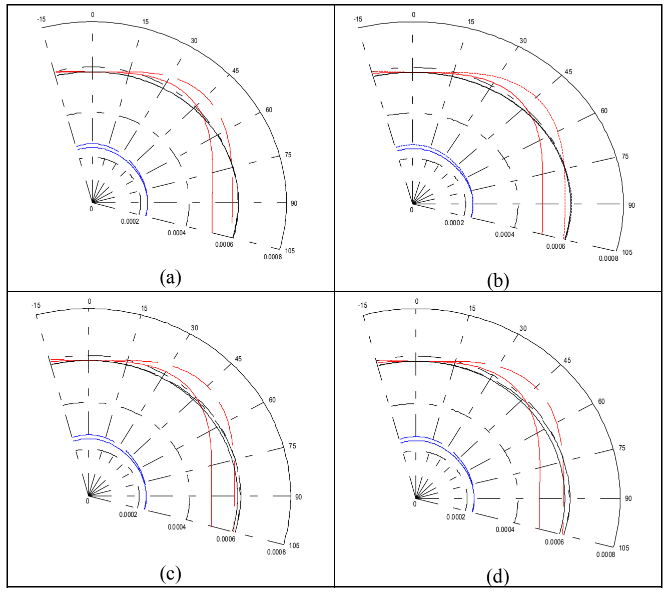

Fig. 3. Slowness curves for $\sigma^0_{x_2}$ = 1% of C_{11}, (a) φ = 0°, (b) φ = 30°, (c) φ = 60°, (d) φ = 90°.

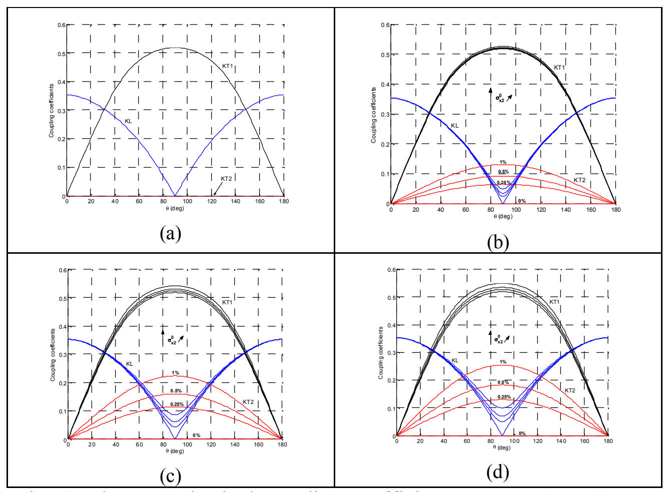

Fig. 4. Electromechanical coupling coefficients KL, KT1, KT2 as a function of elevation angle θ, (a) φ = 0°, (b) φ = 30°, (c) φ = 60°, (d) φ = 90°.

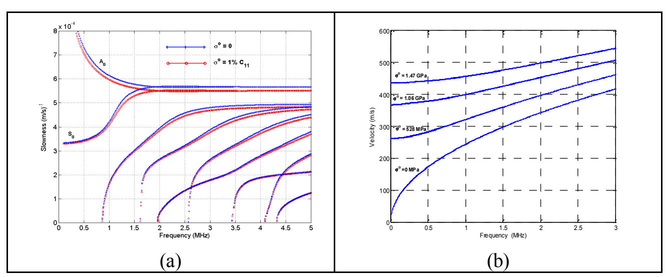

Fig. 5 (a) Dispersion slowness curves, for $\sigma^0 = 0$ and $\sigma^0 = 1\%$ of C_{11}; (b) A0 mode velocity for different values of the applied stress.

C. Dispersion curves of a Pz27 film on a Si substrate

The influence of a pre-stress on Surface Acoustic Waves (SAW) generated in a 10 µm Pz27 film laid down on a Si substrate is studied. As in the previous section, a pre-stress value of 1% of C_{11} is applied in the same direction as the direction of propagation x_1. In Fig. 6 are plotted the corresponding SAW velocities for frequencies up to 400 MHz in the case of short-circuit boundary conditions (metallized surfaces) of the film. The SAW represented here stand only for the first Rayleigh modes. They do not contain the Love modes since, as in the case of the Pz27 plate, the symmetry of both the film and the substrate allows to have uncoupled relations between Love modes and Rayleigh modes.

As in the case of Lamb waves, the general influence of the applied stress consists in an increase of the phase velocity of the modes with the stress. The cut-off frequencies are clearly not modified by the presence of the stress since each mode, with and without stress, tends toward the same limit velocity for the same cut-off frequency. As the stress is localised into the film, its influence on velocities grows up with the frequency, since the properties of the film tend to dominate. When the frequency is high enough, the increase of velocity for each mode becomes constant.

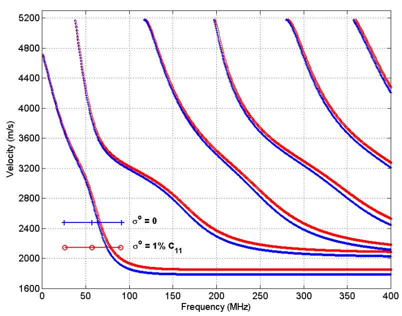

Fig. 6. Surface Acoustic Wave velocities in a 10 µm thickness Pz27 layer on Si substrate.

IV. CONCLUSIONS

In this paper, some acoustical effects of an applied external stress on a PZT transversely isotropic material were analysed. Analytical results showed that the piezoelectric tensors of the pre-stressed material are modified from their zero applied stress value. Although the third order parameters are theoretically needed, they were neglected by considering small initial displacements. These modified constitutive equations were then used to calculate the slowness curves, Lamb The stress tends to increase the coupling coefficient values, and the quasi longitudinal coupling coefficient KL no longer possesses zero values. The numerical studies of the Lamb modes highlight their sensitivity to stress. Even if the general tendency is the increase of the velocity values with the stress, it was observed that each mode has its own behaviour which is also function of the frequency. In particular, cut-off frequencies are not modified. It is also possible to measure the applied stress if a small frequency-thickness product, around 2 MHz*µm, is used. In the last part, a 10 µm thickness Pz27 film laid down on a Si substrate was studied. The presence of the stress does not modify the cut-off frequencies and the limit phase velocities near them. Moreover, the influence of the stress increases with the frequency, since the properties of the film dominate for high frequency values. The formalism presented here takes into account a tensor of applied stress. Hence, it is also possible to characterize the influence of an applied stress with spatial components.

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