

# THERMAL DERIVATIVES OF COMPLIANCES, PIEZOELECTRIC COEFFICIENTS AND PERMITTIVITIES IN LAGRANGIAN DESCRIPTION

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**Abstract** – The aim of this paper is to present constitutive relations expressing the strain and electric displacement as functions of Piola–Kirchoff stress tensors of the first or second kind and of material electric field. These relations are necessary to allow the use of Lagrangian (or material) description of vibrating piezoelectric devices submitted to a change of temperature. Connections between these new coefficients and the classical ones are given and numerical values for them are proposed.

## I. INTRODUCTION

The use of Lagrangian description of a piezoelectric resonator offers the advantage to use the coordinates of the reference state at the reference temperature [1,6]. By this way the boundary conditions and the orientation of the resonator with respect to the cristallographic axis are independent of the change of temperature. The treatment of this kind of problem is made by considering that the vibration is a small dynamic field superimposed to a static bias due to a temperature change. In the case of the computation of the propagation of bulk or surface acoustic waves one needs to express the first Piola–Kirchoff stress tensor and electric displacement as functions of the dynamic strain increment and material electric field [7,8]. If one wants to treat, by example, the case of low frequency resonator operating in flexure or torsional mode, the preceding relations are not convenient since the notion of fiber element used in the studies of such devices needs to express the strain versus the stress. Depending on the way the problem is treated, both kinds (first and second) of Piola–Kirchoff stress tensors may be used.

We only give here the relations between usual coefficients and new ones, but it must be mentioned that these last coefficients, as well as the associated relations, can also be defined from the derivatives of a thermodynamic potential.

## II. PRELIMINARY RESULTS

As usual we consider three states described by three sets of coordinates (see fig1):

- a natural state at a fixed temperature  $\Theta_0$ , where the coordinates of a material point are  $X_M$ .
- an initial, or intermediate state, prior to the vibration, at the current temperature  $\Theta$ , in which the material point is at the position  $\xi_\alpha$ .
- a final state, when an adiabatic vibration is superimposed on the preceding, with the associated coordinates  $y_j$ .

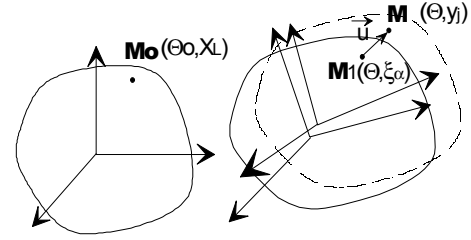


Fig. 1. Natural, initial and final states and associated axes

With these notations, the partial derivatives of coordinates are written as:

$$y_{j,L} \equiv \frac{\partial y_j}{\partial X_L}, \quad \xi_{\alpha,L} \equiv \frac{\partial \xi_\alpha}{\partial X_L}, \quad X_{M,\alpha} \equiv \frac{\partial X_M}{\partial \xi_\alpha} \quad (1)$$

Introducing the dynamic mechanical displacement  $u_\alpha$ , one can write the position of a material point at time  $t$  as :

$$y_j = \xi_\alpha(X_L) + u_\alpha(X_L, t) \delta_{j\alpha} \quad (2)$$

Let

$$E_{LM} = \frac{1}{2} (y_{j,L} y_{j,M} - \delta_{LM}) \quad (3)$$

be the total strain. It may be split into a static part  $\bar{E}_{LM}$  and a dynamic one  $\tilde{E}_{LM}$  :

$$E_{LM} = \bar{E}_{LM} + \tilde{E}_{LM} \quad (4)$$

where, by combining (2) and (3)

$$\tilde{E}_{LM} = \frac{1}{2} (\xi_{\alpha,L} u_{\alpha,M} + \xi_{\alpha,M} u_{\alpha,L}) \quad (5)$$

if only linear terms in  $u$  are retained.

Using the chain rule of differentiation, one can write

$$u_{\alpha(X_L),M} = u_{\alpha,\beta} \xi_{\beta,M} \quad (6)$$

Substituting into the above expression, one obtains

$$\begin{aligned} \tilde{E}_{LM} &= \frac{1}{2} (\xi_{\alpha,L} \xi_{\beta,M} u_{\alpha,\beta} + \xi_{\alpha,M} \xi_{\beta,L} u_{\alpha,\beta}) \\ &= \xi_{\alpha,L} \xi_{\beta,M} \left[ \frac{1}{2} (u_{\alpha,\beta} + u_{\beta,\alpha}) \right] \end{aligned} \quad (7)$$

The quantity between brackets is nothing else than the classical dynamic strain  $\tilde{S}_{\alpha\beta}$  in Eulerian description. Thus the relation between dynamic strains in Lagrangian and Eulerian descriptions is:

$$\tilde{E}_{LM} = \xi_{\alpha,L} \xi_{\beta,M} \tilde{S}_{\alpha\beta} \quad (8)$$

X

In Lagrangian description the dependent quantities which one must also consider are the first Piola–Kirchoff stress tensor  $K_{Lj}$  and the second Piola–Kirchoff stress tensor  $t_{LM}$ , the material electric field  $\tilde{W}_L$  and the electric displacement  $\Delta_L$ . If  $dA$  and  $dV$  respectively denote an elementary surface, with normal  $\mathbf{n}$ , and an elementary volume in deformed state, and  $d\bar{A}$ ,  $d\bar{V}$  and  $N$  denote the corresponding quantities in an undeformed state, they verify the identities [8]:

$$\begin{aligned} dA L_{\alpha j} n_{\alpha} &\equiv d\bar{A} K_{M\alpha} N_M \delta_{j\alpha} \\ d\dot{W} &= t_{LM} \dot{E}_{LM} d\bar{V} \equiv L_{\alpha j} \dot{S}_{\alpha\beta} dV \\ W_L dX_L &\equiv E_{\alpha} d\xi_{\alpha} \\ \Delta_L N_L d\bar{A} &\equiv D_{\alpha} n_{\alpha} dA \end{aligned} \quad (9)$$

They can also be split in two parts :

$$\begin{aligned} K_{Lj} &= \bar{K}_{Lj} + \tilde{K}_{Lj} \\ t_{LM} &= \bar{t}_{LM} + \tilde{t}_{LM} \\ W_L &= \bar{W}_L + \tilde{W}_L \\ \Delta_L &= \bar{\Delta}_L + \tilde{\Delta}_L \end{aligned} \quad (10)$$

They are related to the usual stress tensor  $L_{\alpha j}$ , electric field  $E_{\alpha}$  and electric displacement  $D_{\alpha}$  in spatial (or Eulerian) description [9]. For dynamic parts one has

$$\begin{aligned} \tilde{L}_{\alpha j} &= \frac{1}{J} \xi_{\alpha,L} \tilde{K}_{Lj} \\ \tilde{L}_{\alpha j} &= \frac{1}{J} \xi_{\alpha,L} \xi_{\beta,M} \tilde{t}_{LM} \delta_{j\beta} \\ \tilde{\Delta}_L &= \bar{J} X_{L,\alpha} \tilde{D}_{\alpha} \\ \tilde{E}_{\alpha} &= X_{L,\alpha} \tilde{W}_L \end{aligned} \quad (11)$$

where  $\bar{J} = \det[\xi_{\alpha,L}]$  denotes the Jacobian of the static deformation. If the thermal expansion of the resonator is mechanically free and if no static electric field is applied, the static parts in (10) are identically zero.

### III. RELATIONSHIP WITH RESPECT TO THE FIRST PIOLA-KIRCHOFF TENSOR

#### A. Constitutive relations

In Eulerian (usual) formalism, the usual constitutive relations are written by using the notations of this paper

$$\begin{aligned} \tilde{S}_{\alpha\beta} &= s_{\alpha\beta\lambda\mu} \tilde{L}_{\lambda j} \delta_{j\mu} + d_{\lambda\alpha\beta} \tilde{E}_{\lambda} \\ \tilde{D}_{\alpha} &= d_{\alpha\lambda\mu} \tilde{L}_{\lambda j} \delta_{j\mu} + \varepsilon_{\alpha\beta} \tilde{E}_{\beta} \end{aligned} \quad (12)$$

By putting these relations in (8) and (11–3) one obtains the constitutive relations for dynamic quantities in the form:

$$\begin{aligned} \tilde{E}_{LM} &= E_{LMN}^4 \pi \delta_{j\pi} \tilde{K}_{Nj} + E_{PLM}^3 \tilde{W}_P \\ \tilde{\Delta}_K &= E_{KL\mu}^3 \delta_{j\mu} \tilde{K}_{Lj} + E_{KL}^2 \tilde{W}_L \end{aligned} \quad (13)$$

where so-defined “effective material coefficients” are related to the usual coefficients by the relations:

$$\begin{aligned} E_{LMN\mu}^4 &= \frac{1}{J} \xi_{\alpha,L} \xi_{\beta,M} \xi_{\gamma,N} s_{\alpha\beta\gamma\mu} \\ E_{PLM}^3 &= \xi_{\alpha,L} \xi_{\beta,M} X_{P,\gamma} d_{\gamma\alpha\beta} \\ E_{KL\mu}^3 &= X_{K,\alpha} \xi_{\lambda,L} d_{\alpha\lambda\mu} \\ E_{KL}^2 &= \bar{J} X_{K,\alpha} X_{L,\beta} \varepsilon_{\alpha\beta} \end{aligned} \quad (14)$$

We may notice that the two kinds of piezoelectric coefficients respectively denoted by the superscript 3 and respectively appearing in the two relations (13) are not identical.

#### B. Symmetries with respect to the indices

It follows from relations (14) and from the symmetries of the usual coefficients with respect to the indices that

$$\begin{aligned} E_{LMN\mu}^4 &= E_{MLN\mu}^4 \\ E_{PLM}^3 &= E_{PML}^3 \\ E_{KL\mu}^3 &\neq E_{K\mu L}^3 \\ E_{KL}^2 &= E_{LK}^2 \end{aligned} \quad (15)$$

An index compression rule such as the following:

$$\begin{aligned} 11 &\leftrightarrow 1 & 22 &\leftrightarrow 2 & 33 &\leftrightarrow 3 \\ 23 &\leftrightarrow 4 & 31 &\leftrightarrow 5 & 12 &\leftrightarrow 6 \\ 32 &\leftrightarrow 7 & 13 &\leftrightarrow 8 & 21 &\leftrightarrow 9 \end{aligned} \quad (16)$$

has to be used whenever indices cannot be exchanged in a pair, whereas the classical rule

$$\begin{aligned} 11 &\leftrightarrow 1 & 22 &\leftrightarrow 2 & 33 &\leftrightarrow 3 \\ 23 &\leftrightarrow 4 & 31 &\leftrightarrow 5 & 12 &\leftrightarrow 6 \\ 32 &\leftrightarrow 4 & 13 &\leftrightarrow 5 & 21 &\leftrightarrow 6 \end{aligned} \quad (17)$$

must be used, associated by factor 2, whenever indices can be exchanged in a pair. As a consequence, the coefficients  $E^4$  can be written in form of a 6x9 matrix,  $E^3$  of a 3x6

matrix,  $E'^3$  of a 3x9 matrix and  $E^2$  of a 3x3 matrix. The compression rules are

$$\begin{aligned} E_{LMN\alpha}^4 &= \frac{1}{2}(1 + \delta_{LM})E_{PQ}^4 \\ E_{KLM}^3 &= \frac{1}{2}(1 + \delta_{LM})E_{KP}^3 \\ E_{KLM}'^3 &= E_{KR}'^3 \end{aligned} \quad (18)$$

where  $P$  corresponds to the  $(L, M)$  pair through (16), while  $Q$  and  $R$  respectively correspond to the  $(N, \alpha)$  and  $(L, M)$  pairs through (17).

### C. Case of 32 class of symmetry

The number of independent coefficients is reduced by the cristallographic symmetries. Taking into account the fact that the matrix  $[\xi_{\alpha,L}]$  is diagonal in the case of 32 class, the

$E^4$  matrix has the form:

$$\begin{bmatrix} E_{11}^4 & E_{12}^4 & E_{13}^4 & E_{14}^4 & 0 & 0 & E_{17}^4 & 0 & 0 \\ E_{12}^4 & E_{11}^4 & E_{13}^4 & -E_{14}^4 & 0 & 0 & -E_{17}^4 & 0 & 0 \\ E_{31}^4 & E_{31}^4 & E_{33}^4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2E_{17}^4 & -2E_{17}^4 & 0 & E_{44}^4 & 0 & 0 & E_{47}^4 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{47}^4 & 2E_{17}^4 & 0 & E_{44}^4 & 2E_{17}^4 \\ 0 & 0 & 0 & 0 & 2E_{17}^4 & E_{66}^4 & 0 & 2E_{14}^4 & E_{66}^4 \end{bmatrix} \quad (19)$$

There are six independent coefficients. If we choose  $E_{11}^4, E_{12}^4, E_{13}^4, E_{14}^4, E_{33}^4, E_{44}^4$ , as independent coefficients, in addition we have the relations:

$$\begin{aligned} E_{66}^4 &= E_{11}^4 - E_{12}^4 \\ E_{17}^4 X_{3,3} &= E_{14}^4 X_{1,1} \\ E_{31}^4 X_{3,3} &= E_{13}^4 X_{1,1} \\ E_{47}^4 X_{3,3} &= E_{44}^4 X_{1,1} \end{aligned} \quad (20)$$

The  $E'^3$  matrix has the form:

$$\begin{bmatrix} E_{11}'^3 & -E_{11}'^3 & 0 & E_{14}'^3 & 0 & 0 & E_{17}'^3 & 0 & 0 \\ 0 & 0 & 0 & 0 & -E_{17}'^3 & -E_{11}'^3 & -E_{14}'^3 & -E_{11}'^3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (21)$$

with the relation:  $E_{17}'^3 X_{3,3} = E_{14}'^3 X_{1,1}$

The  $E^3$  and  $E^2$  matrix have the same forms than the corresponding matrix in usual description.

### D. Thermal sensitivities of coefficients

At the reference temperature  $\Theta_0$  the new coefficients have the same values than the usual coefficients in tensorial notation. In counterpart, the introduced coefficients exhibit different thermal sensitivities. In matrix notation, the  $E^4$  and  $E'^3$  matrices have of course a different form than the corresponding  $s$  and  $d$  matrices. Their forms at the reference temperature  $\Theta_0$  are given in appendix.

The thermal expansion of coefficients is given by the formula

$$E_{LM}^k(\Theta) = E_{LM}^k(\Theta_0) \left( 1 + \sum_{n=1}^p T^{(n)} E_{LM}^k(\Theta - \Theta_0)^n \right) \quad (22)$$

where

$$T^{(n)} E_{LM}^k = \frac{1}{n!} \frac{1}{E_{LM}^k} \frac{\partial^n E_{LM}^k}{\partial \Theta^n} \quad (23)$$

The static deformation gradients are expressed in terms of usual thermal expansion coefficients  $\alpha_{ij}^{(n)}$ :

$$\xi_{\alpha,M} = \delta_{\alpha M} + \sum_n \alpha_{LM}^{(n)} \delta_{\alpha L} (\Theta - \Theta_0)^n \quad (24)$$

and, for 32 class:

$$X_{L,\alpha} = (\xi_{\alpha,L})^{-1} \quad (25)$$

The thermal coefficients of elastic coefficients  $E_{17}^4, E_{31}^4$  and  $E_{47}^4$  are related to those of  $E_{14}^4, E_{13}^4$  and  $E_{44}^4$ . From the relations (20) and by using (22,24) we obtain (using the notation:  $\alpha_{ii}^{(1)} \equiv \alpha_{ii}$ ;  $\alpha_{ii}^{(2)} \equiv \beta_{ii}$ ;  $\alpha_{ii}^{(3)} \equiv \gamma_{ii}$ ):

$$\begin{aligned} T^{(1)} E_{17}^4 &= T^{(1)} E_{14}^4 - \alpha_{11} + \alpha_{33} \\ T^{(2)} E_{17}^4 &= T^{(2)} E_{14}^4 + (\alpha_{33} - \alpha_{11}) T^{(1)} E_{14}^4 \\ &\quad - \alpha_{11} \alpha_{33} + \alpha_{11}^2 - \beta_{11} + \beta_{33} \\ T^{(3)} E_{17}^4 &= T^{(3)} E_{14}^4 + (\alpha_{33} - \alpha_{11}) T^{(2)} E_{14}^4 \\ &\quad + (\alpha_{11}^2 - \alpha_{11} \alpha_{33} - \beta_{11} + \beta_{33}) T^{(1)} E_{14}^4 \\ &\quad - \alpha_{11}^3 + \alpha_{11}^2 \alpha_{33} + \alpha_{11} (2\beta_{11} - \beta_{33}) - \alpha_{33} \beta_{11} \\ &\quad + \gamma_{33} - \gamma_{11} \end{aligned} \quad (26)$$

The relations between  $E_{31}^4$  and  $E_{13}^4, E_{47}^4$  and  $E_{44}^4, E_{17}^3$  and  $E_{14}^3$  are exactly similar to those between  $E_{17}^4$  and  $E_{14}^4$ , and are not reproduced here.

E. Numerical values computed from the thermal coefficients published by James [9].

It is possible to use literal expressions of  $T^{(n)}E_{PQ}^4$  in terms of  $T^{(n)}_{sij}$  to numerically compute  $T^{(n)}E_{PQ}^4$ . Or we can choose, as we have done, to use a software to obtain directly the Taylor expansion of (14a) when the static deformation gradients and the elastic compliances  $s_{ij}$  are expressed in forms of thermal expansions. The  $T^{(n)}_{sij}$  are computed from the  $T^{(n)}_{cij}$  given in James's paper. For consistency with the work of James, we have employed the coefficients of thermal expansion given in the reference [9]. The following values are obtained :

| PQ | First order in $10^{-6}$ | Second order in $10^{-9}$ | Third order in $10^{-12}$ |
|----|--------------------------|---------------------------|---------------------------|
| 11 | 14.37                    | 79.1                      | 72.5                      |
| 12 | -1234                    | -1510                     | -1947                     |
| 13 | -193                     | -884                      | -921                      |
| 14 | 136                      | 119                       | -340                      |
| 17 | 130                      | 114                       | -340                      |
| 31 | -199                     | -886                      | -914                      |
| 33 | 155                      | 130                       | 47.7                      |
| 44 | 204                      | 303                       | 237                       |
| 47 | 198                      | 298                       | 236                       |
| 66 | -138                     | -114                      | -173                      |

Table 1 Numerical values of  $T^{(n)}E_{PQ}^4$  calculated from the data of James

Relations (14b–14d) allow to compute the values of the  $T^{(n)}E^3$ ,  $T^{(n)}E'^3$  and  $T^{(n)}E^2$  coefficients

| PQ | $T^{(1)}E_{PQ}^3$    | $T^{(1)}E'_{PQ}^3$    |
|----|----------------------|-----------------------|
| 11 | $-1.5 \cdot 10^{-4}$ | $-1.65 \cdot 10^{-4}$ |
| 14 | $+7.2 \cdot 10^{-5}$ | $+5.2 \cdot 10^{-5}$  |
| 17 | -                    | $+4.5 \cdot 10^{-5}$  |

| PQ | $T^{(1)}E_{PQ}^2$     | $T^{(2)}E_{PQ}^2$     | $T^{(3)}E_{PQ}^2$      |
|----|-----------------------|-----------------------|------------------------|
| 11 | $+1.45 \cdot 10^{-5}$ | $+2.58 \cdot 10^{-8}$ | $-2.26 \cdot 10^{-10}$ |
| 33 | $+3.88 \cdot 10^{-5}$ | $+5.0 \cdot 10^{-8}$  | $-2.54 \cdot 10^{-10}$ |

Table 2 Numerical values of  $T^{(n)}E_{PQ}^3$ ,  $T^{(n)}E'_{PQ}^3$  and  $T^{(n)}E_{PQ}^2$  calculated from the data of James

F. Numerical values obtained from those of effective elastic coefficients in Lagrangian formalism

A second set of data can be obtained from the values of thermal derivatives of effective elastic coefficients (stiffnesses) in Lagrangian description [2]. These coefficients have been directly computed from the thermal behavior of quartz resonators and SAW delay lines, without the need of knowledge of thermal expansion coefficients. These coefficients are related the usual elastic constants (Appendix B of [2] ) from which the usual constants may be computed. In this case, to compute the numerical values of the coefficients of this paper, we have used as thermal expansion coefficients those published by Kosinsky and all [10] and used the data of Bechmann [11] for the elastic compliances.

| PQ | First order in $10^{-6}$ | Second order in $10^{-9}$ | Third order in $10^{-12}$ |
|----|--------------------------|---------------------------|---------------------------|
| 11 | 11.2                     | 96.7                      | 61.8                      |
| 12 | -1276                    | -1487                     | -1919                     |
| 13 | -298                     | -749                      | -474                      |
| 14 | 129                      | 102                       | -483                      |
| 17 | 123                      | 98.3                      | -475                      |
| 31 | -304                     | -750                      | -460                      |
| 33 | 156                      | 141                       | -86.8                     |
| 44 | 208                      | 276                       | 121                       |
| 47 | 202                      | 272                       | 128                       |
| 66 | -138                     | -87                       | -168                      |

Table 3 Numerical values of  $T^{(n)}E_{PQ}^4$  calculated from the data of ref. [2 ]

#### IV. RELATIONSHIP WITH RESPECT TO THE SECOND PIOLA-KIRCHOFF TENSOR

The relations (11b–d) allow us to express the dynamic strain tensor, as well as the dynamic electric displacement, as functions of the second Piola–Kirchhoff stress tensor. With the help of (8) and (12), we obtain

$$\begin{aligned}\tilde{E}_{LM} &= V_{LMNP}^4 \tilde{t}_{NP} + V_{KLM}^3 \tilde{W}_K \\ \tilde{\Delta}_K &= V_{KNP}^3 \tilde{t}_{NP} + V_{KM}^2 \tilde{W}_M\end{aligned}\quad (27)$$

where the new coefficients are connected to the usual coefficients by:

$$\begin{aligned}V_{LMNP}^4 &= \frac{1}{J} \xi_{\alpha,L} \xi_{\beta,M} \xi_{\gamma,N} \xi_{\delta,P} s_{\alpha\beta\gamma\delta} \\ V_{KLM}^3 &= \xi_{\alpha,L} \xi_{\beta,M} X_{K,\gamma} d_{\gamma\alpha\beta} \equiv E_{KLM}^3 \\ V_{KL}^2 &= \bar{J} X_{K,\alpha} X_{L,\beta} \varepsilon_{\alpha\beta} \equiv E_{KL}^2\end{aligned}\quad (28)$$

These coefficients have the same symmetries with respect to indices than the usual ones in Eulerian description. Thus, one can use the usual the compression of indices to rewrite (27) in matrix form. Clearly  $V_{KL}^4$  is a 6x6 matrix.,  $V_{KL}^3$  and  $V_{KL}^2$  are 3x6 and a 3x3 matrixes respectively.

Like the preceding coefficients, the values of thermal sensitivities  $T^{(n)}V_{PQ}^4$  have been calculated from the same sets of data of  $s_{ij}$  coefficients. The use of the data of James give the numerical values in table 4, while the data of [2] are reported in table 5:

| PQ | First order<br>in $10^{-6}$ | Second order<br>in $10^{-9}$ | Third order<br>in $10^{-12}$ |
|----|-----------------------------|------------------------------|------------------------------|
| 11 | 28.2                        | 92.3                         | 67.5                         |
| 12 | -1220                       | -1514                        | -1991                        |
| 13 | -185                        | -876                         | -935                         |
| 14 | 144                         | 129                          | -343                         |
| 33 | 162                         | 141                          | 44.7                         |
| 44 | 212                         | 314                          | 236                          |
| 66 | -124                        | -103                         | -183                         |

Table 4 Numerical values of  $T^{(n)}V_{PQ}^4$  calculated from the data of ref. [9]

| PQ | First order<br>in $10^{-6}$ | Second order<br>in $10^{-9}$ | Third order<br>in $10^{-12}$ |
|----|-----------------------------|------------------------------|------------------------------|
| 11 | 24.8                        | 108                          | 44                           |
| 12 | -1263                       | -1493                        | -1973                        |
| 13 | -290                        | -743                         | -493                         |
| 14 | 137                         | 111                          | -492                         |
| 33 | 164                         | 150                          | -94.9                        |
| 44 | 216                         | 285                          | 114                          |
| 66 | -125                        | -77.8                        | -190                         |

Table 5 Numerical values of  $T^{(n)}V_{PQ}^4$  calculated from the data of ref. [2]

#### V FLEXURAL BEAM

As enlightening application, we briefly show how the thermal behavior of a flexural beam resonator can be obtained in material description with the effective coefficients. The geometry of the beam is depicted on the figure 2. We assume that the flexure occurs in the  $(X_2, X_3)$  plane and that the material of the beam posses the 32 cristallographic symmetry.

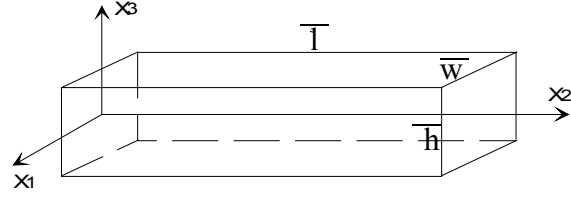


Fig. Beam in reference configuration at  $\Theta_0$

For simplicity we restrict our analysis to the Bernouilli approximation, which consist to assume that in the deformed state a cross section of the beam remains plane and perpendicular to the neutral fiber. When the Eulerian coordinates are used, this hypothesis leads to the strain component:

$$\tilde{S}_2 = \xi_3 \frac{\partial^2 u_3}{\partial \xi_2^2} \quad (29)$$

To apply the Lagrangian description we only have to express the strain  $\tilde{E}_2$  in the framework of Bernouilli hypothesis. By using the relation (8) we have

$$\begin{aligned} \tilde{E}_2 &= \xi_{2,2}^2 \xi_3 \frac{\partial^2 u_3}{\partial \xi_2^2} = \xi_{2,2}^2 \xi_3 \frac{\partial^2 u_3}{\partial X_2^2} (X_{2,2})^2 \\ \tilde{E}_2 &= \xi_3 \frac{\partial^2 u_3}{\partial X_2^2} = X_{3,3} \xi_{3,3} \frac{\partial^2 u_3}{\partial X_2^2} \end{aligned} \quad (30)$$

Neglecting the other stress components than  $\tilde{t}_2$ , the stress-strain relation is then written

$$\tilde{E}_2 = V_{22}^4 \tilde{t}_2 \quad (31)$$

The internal energy due to the flexure comes from the definition of the second Piola-Kirchoff tensor (9).

$$\begin{aligned} v_{\text{int}} &= \frac{1}{2} \int_0^L \int_A Y X_3^2 (\xi_{3,3})^2 \left( \frac{\partial^2 u_3}{\partial X_2^2} \right)^2 dX_2 d\bar{A} \\ &= \frac{I}{2} Y (\xi_{3,3})^2 \int_0^L \left( \frac{\partial^2 u_3}{\partial X_2^2} \right)^2 dX_2 \end{aligned} \quad (32)$$

where

$$Y = \frac{1}{V_{22}^4} \quad (33)$$

is the “Young modulus” and

$$I = \frac{\bar{w} \bar{h}^3}{12} \quad (34)$$

the quadratic moment of the cross section. The integration is performed on the volume of the beam in the reference state at temperature  $\Theta_0$ . The integrand in (32) is nothing else than the one in classical treatment of the vibrating beam when the Young modulus E is replaced by:

$$E \rightarrow Y(\xi_{3,3})^2 = \frac{(\xi_{3,3})^2}{V_{22}^4} \quad (35)$$

The kinetic energy is

$$\nu_K = \int_V \bar{\rho} [\dot{u}(X_L)]^2 dV \quad (36)$$

By applying Hamilton principle or Lagrange equations as usual (see textbooks), the following expression of resonant frequency is obtained:

$$\omega = \frac{\mu^2}{\bar{l}^2} \sqrt{\frac{E I}{\bar{\rho} \bar{w} \bar{h}}} = \frac{\mu \bar{h}}{\bar{l}^2} \sqrt{\frac{(\xi_{3,3})^2}{12 \bar{\rho} V_{22}^4}} \quad (37)$$

$\mu$  is a constant depending of boundary conditions. In this last expression the dimensions and the mass density are those at the reference temperature  $\Theta_0$ , and only the elastic coefficient  $V_{22}^4$  and the derivative  $\xi_{3,3}$  are functions of  $\Theta$ . Thus, with the help of (24), the first order temperature coefficient of the resonant frequency is:

$$\begin{aligned} T^{(1)}\omega &= \frac{1}{2} \left[ -T^{(1)}V_{22}^4 + 2T^{(1)}\xi_{3,3} \right] \\ &= -\frac{1}{2}T^{(1)}V_{22}^4 + \alpha_{33} \end{aligned} \quad (38)$$

Since from (28), the first order temperature coefficient of effective elastic coefficient is

$$T^{(1)}V_{22}^4 = 2\alpha_{22} - \alpha_{33} + T^{(1)}s_{22} \quad (39)$$

Eq. (38) is equivalent to

$$T^{(1)}\omega = \frac{3}{2}\alpha_{33} - \alpha_{22} - \frac{1}{2}T^{(1)}s_{22} \quad (40)$$

which is identical to the result obtained by the classical way. The second order temperature derivative is

$$T^{(2)}\omega = -\frac{1}{2}T^{(2)}V_{22}^4 + \frac{1}{4}[T^{(1)}V_{22}^4]^2 + T^{(2)}\xi_{3,3} - \frac{1}{2}[T^{(1)}\xi_{3,3}]^2 \quad (41)$$

## VI CONCLUSION

The use of Lagrangian description of resonators vibrating in mode like flexure or torsion submitted to a change of temperature can be done with the help of coefficients introduced in this paper. One of advantages of the use of these coefficients is to simplify the calculation of high order temperature sensitivities of devices when refined treatment is required like in the case of Timoshenko bar theory of flexural beam or the computation of St Venant's function of torsion of rectangular beam.

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## APPENDIX

At the reference temperature  $\Theta_0$ , the contents of the  $E^3$  matrix are the following

$$\begin{bmatrix} d_{11} & -d_{11} & 0 & \frac{1}{2}d_{14} & 0 & 0 & \frac{1}{2}d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2}d_{14} & -d_{11} & 0 & -\frac{1}{2}d_{14} & -d_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

while the contents of the  $E^4$  matrix are

$$\begin{bmatrix} s_{11} & s_{12} & s_{13} & \frac{1}{2}s_{14} & 0 & 0 & \frac{1}{2}s_{14} & 0 & 0 \\ s_{12} & s_{11} & s_{13} & -\frac{1}{2}s_{14} & 0 & 0 & -\frac{1}{2}s_{14} & 0 & 0 \\ s_{13} & s_{13} & s_{33} & 0 & 0 & 0 & 0 & 0 & 0 \\ s_{14} & -s_{14} & 0 & \frac{1}{2}s_{44} & 0 & 0 & \frac{1}{2}s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}s_{44} & s_{14} & 0 & \frac{1}{2}s_{14} & s_{14} \\ 0 & 0 & 0 & 0 & s_{14} & \frac{1}{2}s_{66} & 0 & s_{14} & \frac{1}{2}s_{66} \end{bmatrix}$$

## REFERENCES

- [1] B.Dulmet and R.Bourquin, "Lagrangian effective material constants for the modelling of thermal behavior of acoustic waves in piezoelectric crystals. I Theory" *Journ.Acoust.Soc.Am*, Vol 110(4), pp.1792-1799, Oct.2001
- [2] B.Dulmet and R.Bourquin, "Lagrangian effective material constants for the modelling of thermal behavior of acoustic waves in piezoelectric crystals. II Applications and numerical values for quartz" *Journ.Acoust.Soc.Am*, Vol 110(4), pp.1800-1807, Oct.2001
- [3] B.K.Sinha and H.F.Tiersten, "First temperature derivatives of the fundamental elastic constants of quartz", *Journ. Appl. Phys.* Vol 50, pp. 2732-2739
- [4] Y.K.Yong and W.Wei, "Lagrangian temperature coefficients of the piezoelectric stress constants and dielectric permittivity of quartz" *2000 Int. Freq. Cont. Symp.*, Proc. pp.364-372

- [5] Y.K.Yong and W.Wei, "Lagrangian versus classical formulation of frequency temperature problem in quartz resonators" *2001 Int. Freq. Cont. Symp.*, Proc. pp.828-837
- [ 6] J.Yang, "Equations for small fields superposed on finite biasing fields in thermoelectroelastic body", *IEEE Trans. Ultrason., Ferroelect., Freq. Contr.*, Vol.50, pp. 187-192.
- [7] C. Truesdell and R.A.Toupin, " The classical field theories" in *Handbuch der Physik*, Vol.III/1, Berlin ,Springer Verlag,, 1960, pp. 226-793
- [8] R.N.Thurston, "Waves in solids" *Mechanics of solids IV*, Vol. Via/4, Berlin, Springer,1974, , pp. 109-132
- [9] B.James "A new measurement of the basic elastic and dielectric constants of quartz" *1988 Ann. Symp. Freq. Cont.*, Proc. pp.146-154
- [10] J.A.Kosinski, J.G.Gualtieri and A.Ballato, " Thermal expansion of alpha quartz" *1991 Ann. Freq. Cont.Symp.* , Proc. pp .22-28
- [11] R.Bechmann, A.Ballato, T.Lukaszek, "High order temperature coefficient of the elastic stiffnesses and compliances of quartz" Proc. IRE 50, pp. 1812-1822, (1962)