A highly efficient simulation technique for piezoelectric energy harvesters

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Abstract. This paper presents a new numerical technique which is aimed at obtaining fast and accurate simulations of piezoelectric beams, used in inertial energy harvesting MEMS. The execution of numerical analyses is greatly important in order to predict the actual behaviour of MEMS device and to carry out the optimization process on the basis of Design of Experiments (DOE) techniques. In this paper, a refined, yet simple, model is proposed with reference to the multi-physics problem of piezoelectric energy harvesting by means of laminate cantilevers. The proposed model is calibrated and validated with reference to 3D finite element analyses.

1. Introduction
The application of piezoelectric materials is continuously increasing, with different possible uses of both “direct” (conversion of mechanical into electric energy) and “indirect” effect. The latter is applied in actuators, e.g. in the case of micropumps [1]; one of the most promising application of “direct” effect is energy harvesting [2]. In recent times, the concept of energy harvesting has been applied to Micro-Electro-Mechanical Systems (MEMS), with similar functioning principles [3], [4]: an additional broadening of applications can be forecast in the next future, with the immediate corollary of a fundamental need for improved computational tools.

In this paper, a simple 1D model is built in order to simulate piezoelectric thin beams and plate harvesters. Starting from the fully coupled 3D constitutive equations of piezoelectricity, appropriate hypotheses are introduced to model strains and stresses so that the 1D model takes into account the 3D effects. The theoretical model is founded on an enrichment of the Euler-Bernoulli kinematic field, with some additional strain contributions in order to introduce some three-dimensional effects: the obtained model is denoted by Modified Transverse Deformation (MTD). The modification is based on the width-to-length ratio and is driven by some considerations on the 3D behaviour of piezoelectric films. Such an enriched model is unprecedented, to the Author's knowledge, and allows the user to obtain reliable results in a negligible time.

The model is applied to some specific examples referred to inertial energy harvesters, see figure 1. A simple resistance $R$ is considered in the electric circuit attached to the piezoelectric element. The numerical solution is obtained making use of a specific discretisation of both the displacement and the voltage fields. The validation is obtained by the critical comparison with the results of full 3D computations.

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2. Description of the proposed model

The cantilever harvester is a piezo-laminated beam clamped at one end section and free to oscillate on the other side. The dynamic of the laminated beam can be easily modelled by employing standard beam theories for laminated composites. Herein, Classical Lamination Theory (CLT) [5] is employed and the kinematics of the beam section is described through Euler-Bernoulli hypothesis (i.e. plane sections orthogonal to the neutral axis remain orthogonal to the same after deformation).

The reference system is centred on the neutral axis of the beam and on the built-in end section. The $x_1$ axis lies along the beam’s length, so that it ranges between 0 and $L$; the $x_2$ axis is along the beam’s width and ranges between $-b/2$ and $b/2$; finally, the $x_3$ axis is across the beam’s thickness $h$. The Euler-Bernoulli kinematic model, in its original form, depends on the transverse displacement $w(x_1)$ only. In this paper, we consider a suitable modification in order to obtain the Modified Transverse Deformation (MTD) model (further details can be found in [6]). The final model, in terms of the displacement components $s_j$, reads:

$$
\begin{align*}
    s_1 &= -x_3 \frac{dw}{dx_1}; \\
    s_2 &= \hat{s}_2 (x, \Lambda); \\
    s_3 &= w + \hat{s}_3 (x, \Lambda)
\end{align*}
$$

(1)

The additional functions depend on a geometric parameter $\Lambda = L/b$, which represents the transverse slenderness of the beam, i.e. the ratio of the beam’s length and the beam’s width. The chosen model should fulfil the standard requirements for a beam theory: the in-the-thickness stress must be null, $T_{33}=0$; the in-plane stress must be $T_{22}=0$ at $x_2 = \pm b/2$. The MTD model aims at obtaining a variable response for different transverse slenderness: when $\Lambda \to 0$ the beam is infinitely wide and the strain condition $S_{22}=0$ must be verified; on the other hand when $\Lambda \to \infty$ the beam is extremely narrow and $T_{22}=0$ has to be guaranteed. These features can be obtained if the strain component $S_{22}$ is modified through the multiplication times a “transversal shape function” $f_\Lambda$:

$$
    f_\Lambda = \left[1 - A(\Lambda)\right] \left[\frac{2x_3}{b}\right]^{a(\Lambda)} + A(\Lambda)
$$

(2)

where $A$ and $B$ depend on two fitting parameters, $a_\Lambda$ and $b_\Lambda$:

$$
    A = \frac{\Lambda^{a_\Lambda}}{\Lambda^{a_\Lambda} + b_\Lambda}; \quad B = 1 + \frac{1}{\Lambda}
$$

(3)

3. Governing equations

The governing equations for the piezoelectric problem can be obtained by using the dissipative form of Euler-Lagrange equations:

$$
\frac{d}{dt} \left( \frac{\partial L}{\partial q_i} \right) - \frac{\partial L}{\partial q_i} + \frac{\partial D}{\partial \dot{q}_i} = 0
$$

(4)
where $D$ is the dissipation function and $L$ is the Lagrangian function which is given by suitably combining the kinetic energy $K$, the internal energy $E$ and the external work $Y$: $L = K - (E - Y)$. An approximate solution is sought starting from some hypotheses on the unknown fields. First, the displacement field is expressed on the basis of a single time-variant parameter $W$, given a suitable shape function $\psi_w$:

$$w(x_t) = \psi_w(x_t) W(t) \quad (5)$$

Second, the electric potential is assumed to be linear across the thickness $t_p$ of the piezoelectric layer and constant along the beam length, so that the electric field is uniform: $E_3 = V(t)/t_p$. The electric charge $q$, collected by the electrodes, is managed by an external circuit, which provides the power supply for the self-powered electronic device. Different schemes of circuitries are investigated in [7]. The harvester provides AC voltage and the simplest solution is the coupling with an external load resistance. The final system of equations reads:

$$m\ddot{W} + c_\alpha \dot{W} + k_\alpha W - \Theta_{yx} V = F_{ax}$$
$$k_\alpha \dot{V} + \Theta_{xy} W + R V = 0 \quad (6)$$

4. Numerical results

In order to validate the model developed in section 2, a 3D FE model has been developed with the commercial code ABAQUS. The comparison between the numerical solution of the 3D model and of the proposed beam model is used in order to calibrate the parameters $a_\lambda$ and $b_\lambda$, by using some simple static analyses; afterwards, the validity of MTD hypotheses has been checked with reference to quasi-static and dynamic analyses. The comparative analyses have been performed with a 2-layer cantilever (2 μm PZT on 6 μm polysilicon substrate) without tip mass. The beam length is $L = 1000$ μm, the width is parametric and varies from $b = 50$ μm to $b = 5000$ μm. The lower surface of the PZT layer is grounded, from the electric point of view, while the potential on the upper surface is constrained to be uniform in order to reproduce the presence of electrodes. Table 1 reports the material properties of the layers.

| Table 1. Material parameters values ($\varepsilon_0 = 8.854 \times 10^{-12}$ F/m). |
|-----------------|---------|-----|-----|-----|-----|-----|
|                 | $\rho$ [g/cm$^3$] | $E$ [GPa] | $\nu$ [-] | $\varepsilon_{31}$ [N/mV] | $\varepsilon_{33}$ [N/mV] | $\varepsilon_{33}^0$ [N/mV] |
| PZT             | 7.70    | 100 | 0.30 | -12 | 20  | 2000 |
| PolySilicon     | 2.33    | 148 | 0.33 | 0   | 0   | 0    |

4.1. Static analyses

Open circuit static analyses have been performed with a tip load $f_c = 1$ μN/μm at the beam free edge. After the convergence analysis, it has been possible to select the optimal FE mesh for the 3D model, which has been discretised by using brick elements with quadratic displacement fields. The tip displacement and the voltage at the free electrode are evaluated through various 1D models, namely: a classical beam theory, which entails null transverse deformation (NTD); a classical plate theory, which shows null transverse stress (NTS); the MTD theory. The two calibration parameters $a_\lambda$ and $b_\lambda$ have been computed through fitting on these static analyses. Their final values are $a_\lambda = 0.8$ and $b_\lambda = 2.2$. The obtained results show that the MTD model correctly describes the variation in stiffness and, most importantly, the variation of the upper electrode voltage, which is strictly connected to the coupling coefficient.
4.2. Quasi-static analyses

Quasi-static analyses have been performed; a smooth step load, until the maximum value 1 μN/μm, followed by a constant plateau has been considered. Parametric analyses have been performed varying the load resistance. A peak power generation is obtained for an optimal value of load resistance which inversely depends on the capacitance of the device. All models predict the same optimal load resistance as ABAQUS. The same analysis has been performed for different values of width and the peak power per unit width, computed at the optimal load resistance, has been collected in figure 2a for all models. It is shown that the MTD model correctly predicts the harvester performances for the whole range of length-beam ratios that have been considered. On the other hand, null transverse stress and deformation models always under- and overestimate voltage and power, respectively. As shown by figure 2b the mean error on the power generation can be reduced from barely 30% to less than 5% considering both models. It can also be concluded that wider cantilever harvesters not only recover more power, which is obvious, but also have a higher power density than narrower beams.

![Figure 2. a) Peak power generation at optimal $R$ and b) error on power generation.](image)

4.3. Dynamic analyses

Free oscillation analyses have been performed on the same cantilever structure introduced previously. As before, the beam is quasi-statically moved to a certain position but in this case it is suddenly released activating free oscillations. The width is fixed to $b = 200$ μm while the load resistance $R$ and the mechanical quality factor $Q$ are varied in order to carry out parametric analyses.

A first significant result is that while the 1D code takes less than 3 seconds to complete the analysis, ABAQUS requires 5 hours 25 minutes and 23 seconds to produce the same results. Satisfactory agreement is obtained, in spite of a slight mismatch between the oscillation frequencies. Such a difference, which is due to the simplicity of the 1D model, can be appreciated by considering the Fourier transform of the displacement. Moreover, one finds that ABAQUS is able to capture the second eigen-frequency, which produces a small oscillation of the peak values of the responses. This effect originates from higher order resonance modes which are completely neglected in the 1D model since only a single shape function has been employed.

The results of parametric analyses at varying $R$ show that the MTD model better reproduces numerical results than null transverse stress and deformation models. The effect of the mechanical quality factor has been examined. Except for exceptionally low values of $Q$, the peak power generation remains more or less constant. In spite of this, the mechanical damping has a strong influence on the performances of the harvester in terms of overall harvested energy. In fact, the total energy which is collected is reduced as $Q$ decreases. The energy harvested is also affected by the
choice of the resistance. It has to be noted that the peak power generation and the peak energy harvested do not occur at the same load resistance.

5. Conclusions
The main objective of this paper was represented by the implementation of a simulation tool, which merge the simplicity of Classical Lamination Theory with the unavoidable 3D effects due to the finite width of the beam. The answer is represented by an improved theory, so-called Modified Transverse Deformation, which includes the effect of the transverse strain so that boundary conditions and limit stress and strain configurations are recovered. The accuracy of the proposed model has been validated by means of critical comparison with fully 3D analyses, carried out by means of a commercial finite element code. The MTD model allows for considerable computational savings vis-à-vis 3D FE dynamic analyses, with a reasonable degree of accuracy. Once validated, the MTD model can be employed for the characterization and for the optimal design of realistic MEMS harvesters. As an example, a multi-layer model can be introduced in order to include the electrodes, which are usually constituted of different highly conductive materials. The piezoelectric thickness varies between 0.1 and 4 µm; the cantilever width is \( b = 1000 \) µm and the beam's length is \( L = 1000 \) µm. Figure 3 shows that interesting values of peak power can be obtained by means of an impulsive excitation.

![Figure 3](image_url)

**Figure 3.** a) Total energy harvested and b) peak and mean power generation as a function of PZT thickness for an impulsive cantilever harvester

6. References
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