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MULTI-PHYSICS SIMULATION OF LAMINATES WITH PIEZOELECTRIC LAYERS FOR ENERGY HARVESTERS

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Summary: *In this paper, a refined, yet simple, model is considered with the aim of providing fast and insightful solutions to the multi-physics problem of piezoelectric energy harvesting by means of laminate cantilevers. The main objective is to retain a simple structural model (Euler-Bernoulli beam), with the inclusion of effects connected to the actual three-dimensional shape of the device. The obtained results are validated by the comparison with 3D analysis carried out with a commercial code, and the procedure is finally applied to the case of a realistic MEMS harvester.*

1 INTRODUCTION

The application of piezoelectric materials in “smart” composite structures is continuously increasing, with different possible uses of both “direct” (conversion of mechanical energy into electric energy) and “indirect” effect. The latter is applied for actuating purposes, e.g. in the case of micro-pumps [1]; “direct” effect is now widely used for energy harvesting, namely for obtaining an electric power by exploiting some freely available mechanical energy [2]. In recent times, the concept of energy harvesting has been applied to MEMS devices, with similar functioning principles [3]: 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. It is worth noting that such effects are really negligible if one consider the structural behaviour of a beam in the absence of piezoelectric coupling. Conversely, in the case of multi-physics simulation of harvesters, the effects connected to the actual shape of the beam involve a significant variation of the results in terms of electrical quantities.

The theoretical model is based on an enrichment of the Euler-Bernoulli kinematic field, with additional strain contributions in order to introduce some three-dimensional effects, which are specifically important for the correct evaluation of power generation of energy harvesters. The model is applied to specific examples, making use of the well-known Rayleigh-Ritz technique to obtain a reduced order model. The validation is obtained by the critical comparison with the results of full 3D computations. The new developed model is employed for the simulation of a realistic MEMS harvester, constituted of a multi-layer cantilever which includes an active thin film of lead zirconate titanate Pb(Zr,Ti)O_3 (PZT [4]). The piezoelectric layer is then attached to an external load resistance which reproduces the circuitry employed for the power management. The case of impulsive actuation is considered and some interesting conclusion on the harvesting efficiency are reached.

The paper is organized as follows. The problem of layered piezoelectric beams is presented in Section 2, with a short description of the new model. In Section 3 we present the numerical validation of the proposed method, in the case of dynamic step-by-step analyses. The case of a realistic MEMS harvester is described in Section 4. Finally, conclusions and future prospects are drawn in Section 5.

2 PROBLEM FORMULATION

The problem is formulated according to the procedure which is extensively described in our previous paper [5].

The schematic diagram of the laminate is depicted in Figure 1: L is the length, h the total thickness and b the width (not viewable in the figure). The x_3-coordinate originates in the neutral axis and is directed downwards, x_1-coordinate lies along the beam axis while the x_2-coordinate originates in the middle of the beam, so that $-b/2 \le x_2 \le b/2$.

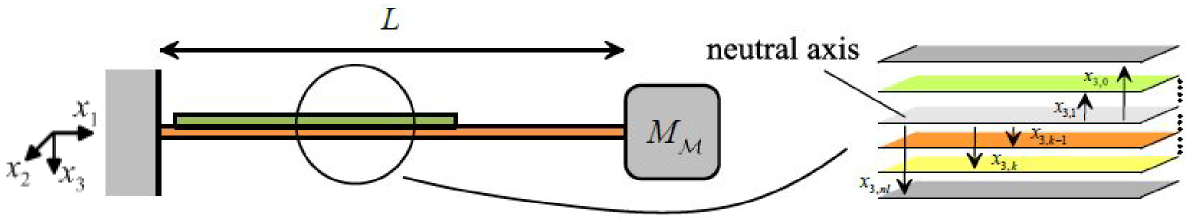

Figure 1: Scheme of a cantilever laminate.

The Classical Lamination Theory, described e.g. in [6], is modified to introduce the electro-mechanical coupling in the active layer, as thoroughly described in [1]. The standard Euler-Bernoulli kinematic model is enriched by considering some additional terms (denoted by a hat), which depend on the in-plane slenderness $\Lambda = L/b$:

$$\mathbf{s} = \begin{bmatrix} -x_3 w_3'(x_1) \\ \hat{s}_2(x_1, x_2, x_3, \Lambda) \\ w_3(x_1) + \hat{s}_3(x_1, x_2, x_3, \Lambda) \end{bmatrix} \tag{1}$$

The functions $\hat{s}_2$ and $\hat{s}_3$ should be chosen to ensure the fulfilment of the following requirements. First, as usual for the beam theory, the in-the-thickness stress is null, T_{33}=0. Second, the in-plane stress must be T_{22}=0 at $x_2 = \pm b/2$. Moreover, 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. After some algebraic manipulations (see [5] for details), one finds that the piezoelectric constitutive law can be written in the following form. In the next equations, the following symbols are used: E is the Young's modulus; ν is the Poisson's ratio; e_{31}, e_{32}, e_{33} are the piezoelectric coupling coefficients; ε_{33}^S is the dielectric permittivity of the piezoelectric material; finally, and most importantly, $f_\Lambda(x_2,\Lambda)$ is a shape function, that must be 1 when $\Lambda \to \infty$ or $x_2 = \pm b/2$ and must be 0 when $\Lambda \to 0$.

$$T_{11}=\frac{E\left(1-\nu^2 f_\Lambda\right)}{1-\nu^2}S_{11}-\left(e_{31}-\nu e_{32} f_\Lambda-\frac{\nu\left(1-\nu f_\Lambda\right)}{1-\nu}e_{33}\right)E_3$$
$$T_{22}=\left(1-f_\Lambda\right)\left(\frac{E\nu}{1-\nu^2}S_{11}-\left(e_{32}-\frac{\nu}{1-\nu}e_{33}\right)E_3\right) \tag{2}$$
$$D_3=\left(e_{31}-\nu f_\Lambda e_{32}-\frac{\nu\left(1-\nu f_\Lambda\right)}{1-\nu}e_{33}\right)S_{11}+\left(\frac{1-\nu^2}{E}\left(e_{32}-\frac{\nu}{1-\nu}e_{33}\right)^2 f_\Lambda+\frac{(1+\nu)(1-2\nu)}{E\left(1-\nu\right)}e_{33}^2+\varepsilon_{33}^S\right)E_3$$

The function $f_\Lambda(x_2,\Lambda)$ is given by:

$$f_\Lambda\left(x_2,\Lambda\right)=\left(1-A_\Lambda\left(\Lambda\right)\right)\left|\xi\right|^{B_\Lambda(\Lambda)}+A_\Lambda\left(\Lambda\right) \tag{3}$$

with ξ = $2x_2/b$ and:

$$A_\Lambda\left(\Lambda\right)=\frac{\Lambda^{a_\Lambda}}{\Lambda^{a_\Lambda}+b_\Lambda} \qquad B_\Lambda\left(\Lambda\right)=1+\frac{1}{\Lambda} \tag{4}$$

The shape function encompasses two coefficients, a_Λ and b_Λ, which are used as fitting parameters. The so-called *Modified Transverse Deformation (MTD) model* is obtained.

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathsf{L}}{\partial \dot{q}_i}\right)-\frac{\partial \mathsf{L}}{\partial q_i}+\frac{\partial \mathsf{D}}{\partial \dot{q}_i}=0 \tag{5}$$

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 W $\mathsf{L}=\mathsf{K}-(\mathsf{E}-\mathsf{W})$; the internal energy can be computed on the basis of the constitutive law described in Eqs. (2). All these functions are obtained by integration over the volume of the beam: after that operation, one finds an averaged version of the governing parameters, which accounts for the layered nature of the beam (along the thickness) and of the effect of f_Λ (which varies along the width.

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 ψ_w:

$$w_3\left(x_1\right)=\psi_w\left(x_1\right)w\left(t\right) \tag{6}$$

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:

$$E_3=v\left(t\right)/t_p \tag{7}$$

The governing equations are finally obtained:

$$\begin{aligned} &m\ddot{w}+c_M\dot{w}+k_L w-\Theta_{\chi v}v=F_{ext}\\ &k_E v+\Theta_{\chi v}w=q \end{aligned} \tag{8}$$

where m is the total inertial term; c_M is the linear mechanical damping coefficient; k_L is the linear elastic stiffness; k_E is the internal capacitance of PZT; $\Theta_{\chi v}$ is the coupling constant.

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:

$$\dot{q} = -R^{-1} v \tag{9}$$

The final system of equations reads:

$$\begin{aligned} & m\ddot{w} + c_M \dot{w} + k_L w - \Theta_{\chi v} v = F_{ext} \\ & k_E \dot{v} + \Theta_{\chi v} \dot{w} + R^{-1} v = 0 \end{aligned} \tag{10}$$

3 CALIBRATION AND VALIDATION OF THE MODEL

The calibration is referred to the two parameters a_Λ and b_Λ, which have been evaluated on the basis of open circuit static analyses with a tip load F = 1 $\mu N/\mu m$ at the beam's free edge. A 2 layers (2 µm PZT on 6 µm silicon substrate) cantilever beam has been chosen. The length is 1000 µm, the width is parametric and varies from 50 µm to 5000 µm. The material properties of the two layers are given in Table 1.

	ρ [g/cm³]	E [GPa]	ν [-]	e_{31} [N/mV]	e_{33} [N/mV]	$\varepsilon_{33\text{-}r}$ [g/cm³]
PZT	7.70	100	0.30	-12	20	2000
Si	2.33	148	0.33	0	0	0

Table 1: Material properties for the calibration and validation analyses.

The reference solutions have been obtained by means of fully 3D analyses, which have been carried out by means of the commercial software ABAQUS. By choosing a_Λ = 0.8 and b_Λ = 2.2, one finds that the mean error on the tip displacement is less than 1% and that the mean error on the electrode voltage is less than 3%. In Figures 2 and 3 we report the comparison between the proposed model and the ABAQUS outcomes. Moreover, we consider the results for the classic models (uniaxial stress and plane stress), which are valid in the two extreme situations $\Lambda\to\infty$ and $\Lambda\to 0$. In the intermediate cases, the MTD model is by far more accurate, if compared to the finite element analyses.

The model has been validated by considering a set of free oscillation analyses, that have been performed on the same structure. As before, the beam is quasi-statically moved to a certain position but now is suddenly released and left free to oscillate. The width is fixed to b = 200 μm while the load resistance R and the mechanical quality factor $Q_M = \sqrt{k_L m} / c_M$ are changed over broad intervals. The first significant result is that the 1D code took less than 3 seconds to perform the analysis, whereas ABAQUS required more than 5 hours to produce such results. This is explained by the fact that ABAQUS implements a 3D fully coupled model, with a large number of degrees of freedom, solved in implicit dynamics; conversely, the 1D model is governed by two parameters only. In spite of the big difference in terms of discretization, the 1D model shows an excellent degree of accuracy, both in the mechanical and in the electrical fields. For instance, the Fourier transform of the time-variant response allows us to appreciate the excellent accuracy of the first frequency of vibration (see Figures 4 and 5 for the displacement and the voltage, respectively). Clearly, the 1D model is not able to capture the higher modes, in view of the intrinsic limitation of the number of free parameters.

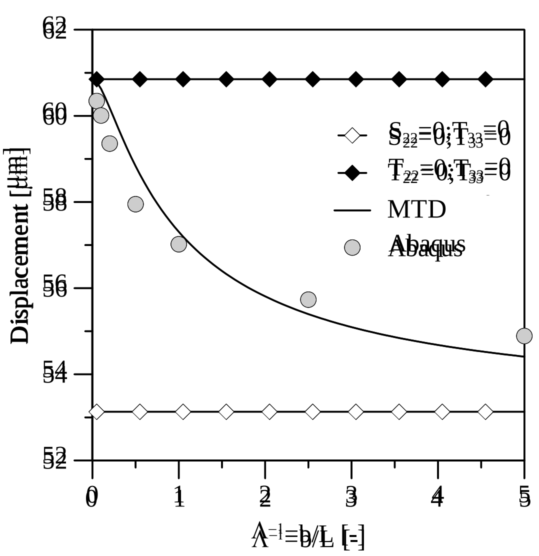

Figure 2: Open circuit static analyses: displacement.

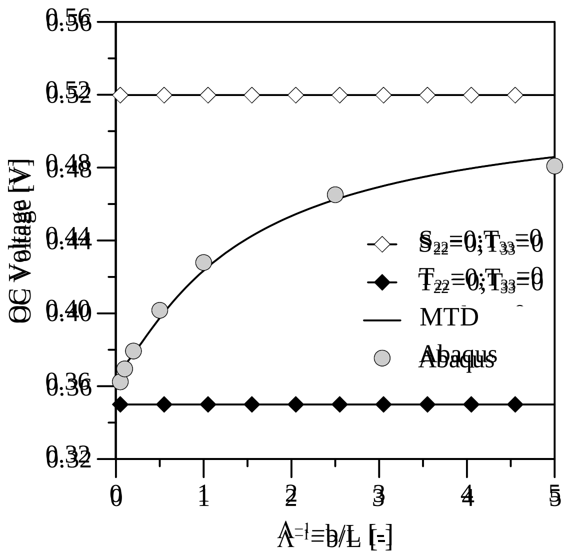

Figure 3: Open circuit static analyses: voltage.

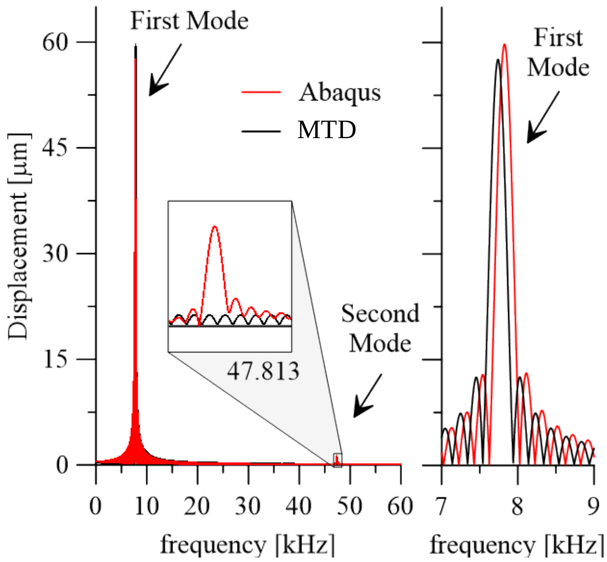

Figure 4: Frequency response of the free oscillations.

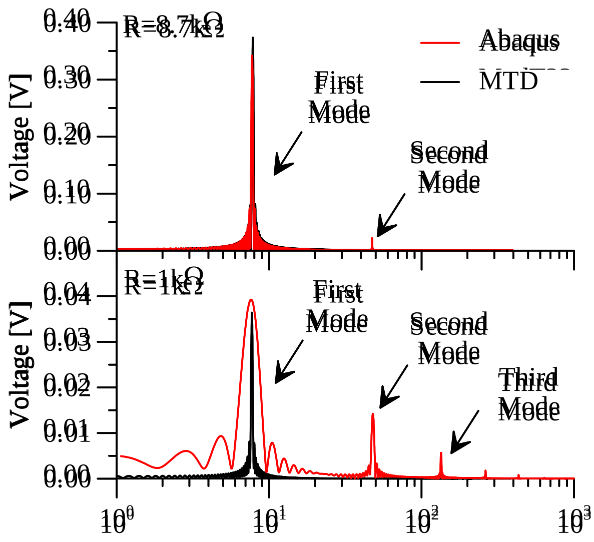

Figure 5: Frequency responses of the resulting voltage.

The good quality of the 1D solution has been confirmed also by the comparison of the most important variable for an energy harvester, namely the peak power generation during free oscillation. The results of the parametric analyses for different levels of resistance R have been collected in Figure 6. As expected, the MTD model better reproduces numerical results than plane and uniaxial stress models. The influence of the mechanical quality factor on the peak power generation is reported in Figure 7. Except for very low values of Q_M, the power is more or less constant. This does not mean that the mechanical damping has no influence on the performances. In fact, in order to see the effect of mechanical damping, the total energy harvested should be considered instead of the peak power. One finds that the total energy harvested reduces as Q_M decreases: when no mechanical damping is considered, the whole energy injected into the system is harvested; conversely, for overdamped systems the energy is almost completely dissipated due to mechanical damping, with a small amount of harvesting.

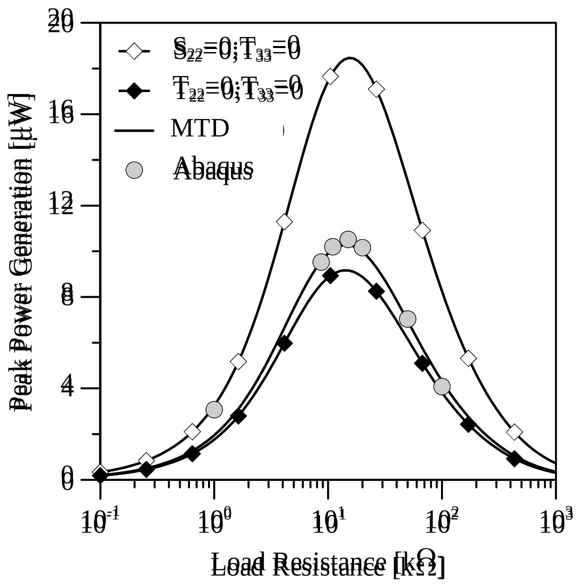

Figure 6: Influence of the circuit resistance R on the harvester performance for $Q_M = \infty$.

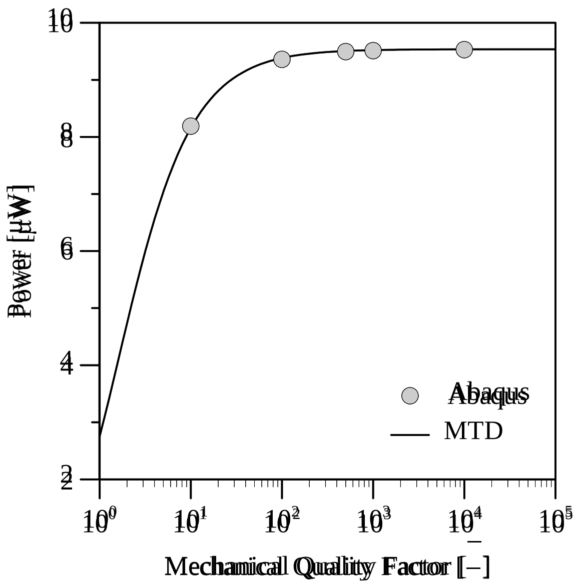

Figure 7: Influence of the mechanical damping on the harvester performance for $R = 8.7$ kΩ

4 APPLICATION TO A MEMS HARVESTER

Once validated, the model of the cantilever beam can be employed for the characterization and evaluation of the performances of cantilever harvesters. Parametric analyses with different geometrical features have been performed in order to analyse the influence of the beam length and the piezoelectric layer thickness on the harvester response. A realistic stratification is considered, including not only the structural and the active layer but also the electrodes and the passivation layers. The piezoelectric layer thickness varies between 0.5 and 2 μm; the geometrical, mechanical, piezoelectric and dielectric features are reported in Table 2, starting from the top layer. The cantilever width is fixed at b=1000 μm while the length of the beam varies between 400 μm and 2000 μm. The mechanical quality factor is supposed to be $Q_M = 500$.

		t [μm]	ρ [g/cm^3]	E [GPa]	ν [-]
SiO_2-pass	Passivation	0.30	2.33	70	0.27
Ruthenium	Electrode	0.10	4.50	447	0.30
PZT	Active	0.5-2	7.70	100	0.30
Platinum	Electrode	0.12	21.45	180	0.30
SiO_2-th	Barrier	0.62	2.33	148	0.27
PolySilicon	Structural	5.00	2.33	148	0.33
SiO_2	Passivation	0.50	2.33	148	0.27

Table 2: Geometry of the composite laminate and material properties for the realistic harvester.

The analyses are focussed on the mechanical response to an impulsive solicitation. In fact, cantilever piezoelectric beams can be used in devices which involve jump phenomena or frequency-up conversion techniques. From a general point of view, such devices are often characterised by the presence of impulsive stimulation of piezoelectric beams, which may therefore vibrate at the resonance eigenfrequency ω_r. In that way, an effective harvesting device is obtained also in the case of a huge mismatch between the frequency of the vibration source and the eigenfrequency of the cantilevers. The interested reader can find a review of frequency-up conversion techniques in [8].

The cantilever has been initially submitted to a smooth step load (tip force F_{max} = 1 μN/μm), followed by a sudden jump as it has been done in the validation section. In this way, the beam is free to oscillate until the unperturbed configuration is reached again. The external load resistance is supposed to be equal to the optimal value, that maximises the overall harvested energy. It is possible to prove that such an optimal value is $R_{opt} = (k_E\, \omega_r)^{-1}$.

The peak displacement (Figure 8), the peak voltage (Figure 9) and the peak power generation (Figure 10) are obtained just after the beam is released. Their values depend on the maximum value of the applied force and on the harvester piezoelectric characteristics. Herein, the Modified Transverse Deformation theory (MTD) has been used in order to correctly reproduce the beam behaviour for the whole range of width-length ratios. Consequently, the peak voltage and the peak power generation are not perfectly linear with respect to the beam length, as one should expect from a simple dimensional analysis. Similarly, the peak displacement is not perfectly cubic with respect to the beam length. Figure 11 shows the overall harvested energy, over the whole duration of free oscillation. Such a time lapse is arbitrarily defined by considering that the vibration is completed when the peak displacement is less than 1/100 of the initial displacement.

The most important comment on the obtained results is that the peak power seems to be high enough to provide a switch-on signal to a typical MEMS sensor: this is a good hint for the feasibility of an impulsive MEMS harvester. Moreover, it is worth noting that the power and the energy are not monotonous with respect to the PZT thickness. This happens because, while increasing the thickness of the piezoelectric layer, the total stiffness of the beam increases and the total efficiency of the harvester is lower. In fact, it is possible to show that the maximum power is attained for t_P = 1.9 μm; conversely, the maximum energy corresponds to t_P = 0.7 μm.

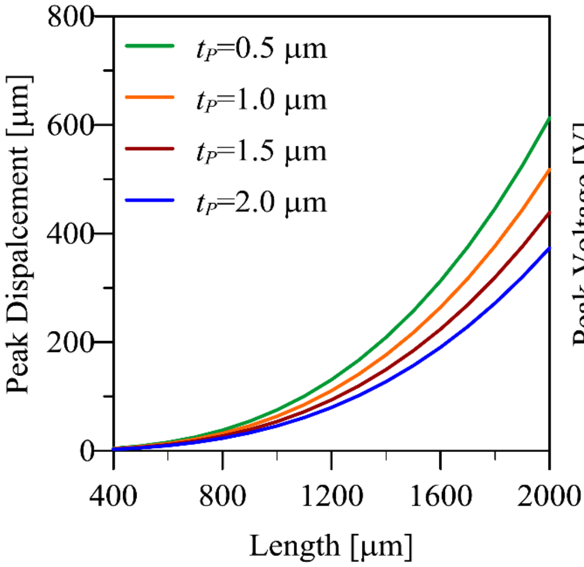

Figure 8: Peak displacement for the realistic harvester as a function of the beam length and the PZT thickness.

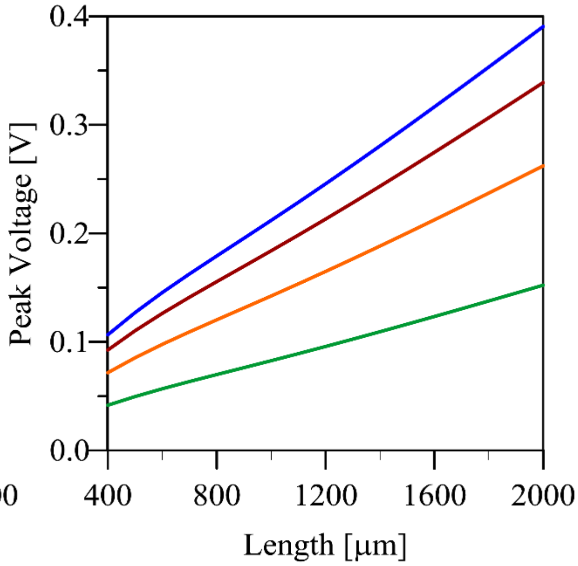

Figure 9: Peak voltage for the realistic harvester.

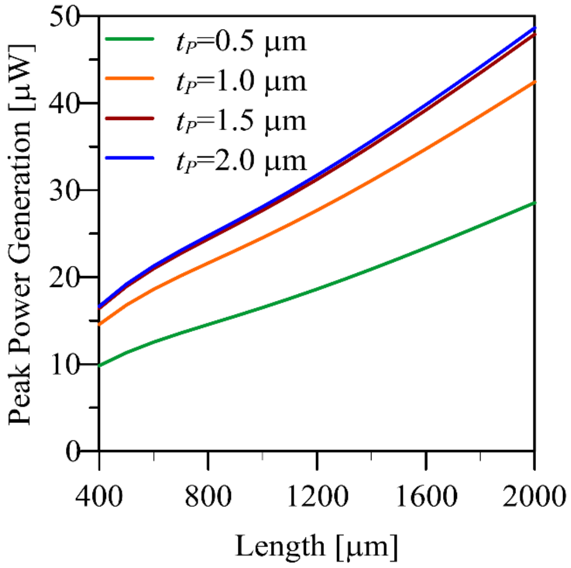

Figure 10: Peak power for the realistic harvester as a function of the beam length and the PZT thickness.

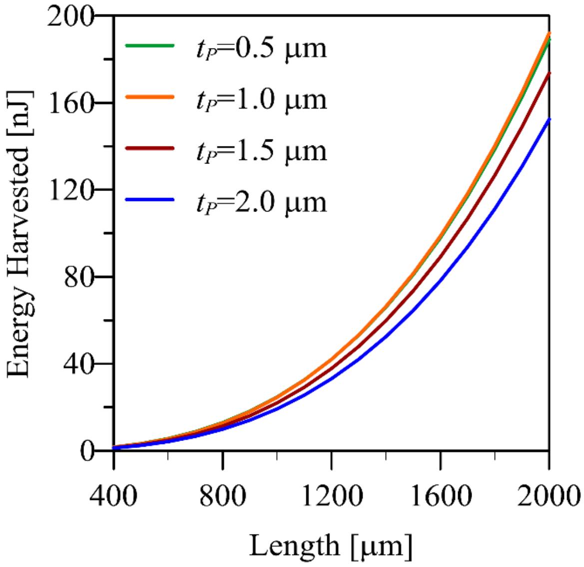

Figure 11: Overall harvested energy over the whole free oscillation for the realistic harvester.

5 CONCLUSIONS

The present paper focuses on the multi-physics analyses of composite laminates with piezoelectric layers. The main objective is 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 a mixed 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. It is worth noting that the calibration of the MTD model needs only the execution of some static FE analyses, with a reasonable computational burden. The calibrated model shows good performances if extended to the dynamic field, which is of paramount importance for the case of energy harvester. The MTD model allows for considerable computational savings vis-à-vis 3D FE dynamic analyses, with a reasonable degree of accuracy.

The proposed model has been applied to perform some parametric analyses of a realistic MEMS harvester, in the hypothesis of impulsive load and free vibrations. The analyses reveal that the cantilever piezoelectric beam has good performances when impulsively solicited; remarkable peak power generation can be obtained and the mean power generation is comparable to the one of a resonant harvester with the important advantage of being uncoupled from the source frequency. Moreover, the performances can be further increased if considering the full deformation capability of the beam. A major issue regards the technique how the impulsive force is applied. In many cases the applied force has a limit threshold which cannot be overcome (this might be due to external conditions such as the input acceleration content or the maximum transferable force of the frequency up conversion mechanism). In those cases, the beam length must be designed in order to assure the maximum performances of the harvester and this can result in big devices.

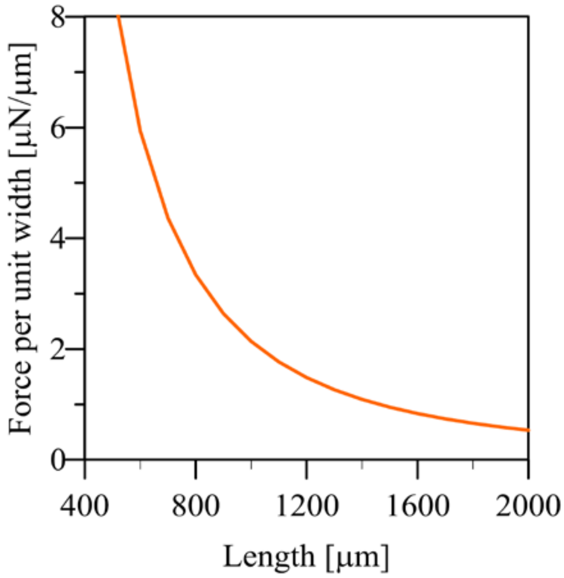

Figure 12: Maximum allowable force per unit width for a maximum displacement equal to 1/10 of the length.

A possible drawback of cantilever harvester is the presence of large displacements, which might endanger the structure itself or the surrounding elements. As an example, Figure 12 reports the tip force considering a maximum allowable displacement of 1/10 the beam length: we have checked that in this case the error between the adopted linear model versus a geometrically nonlinear one is of the order of 1%.The figure confirms that the cantilever beams can be effectively adopted as energy harvesters. In fact, the results reported in Section 4 are referred to a tip force of 1 µN/µm, which corresponds to a maximum allowable length of about 1500 µm. Account taken of the plot in Figure 10, one finds that the peak power might be larger than 35 µW, which is a reasonable value in view of the possible practical applications.

The possible application of the MTD model is not limited to cantilever harvester, but can be extended to other cases of piezoelectric beams. For example, the model can be applied to energy harvesters that exploit advanced design solutions for maximizing the conversion of energy. Such devices may involve geometric nonlinearity (see e.g. [9]), with the possible occurrence of bistable equilibrium configurations [10]. Some preliminary analyses have confirmed, also in those cases, the effectiveness of the proposed model.

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