Computational Modelling of the Layered Piezoelectric Composites and Analysis of their Electro-Mechanical Response upon Harmonic Vibrations

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Abstract: Currently, a generation of electric power from alternative sources of energy, especially from ambient vibrations, is becoming a very hot topic. Devices converting mechanical energy into an electrical one are called energy harvesters and are often based on the piezoelectric phenomenon. For the optimal adjustment of such an energy converter in the given application, it is necessary to have its computational model, which is able to describe all key aspects of its operation. Thus, this work focuses on the development of such a complex computational tool, which is able to globally describe the electromechanical response of the studied piezoelectric harvester operating in the form of a cantilever multilayer ceramic beam with piezoelectric layers. Such a multilayer structure is subjected to a kinematic excitation during its operation and also contains thermal residual stresses coming from the manufacturing process. The derived computational model utilizes the classical laminate theory to determine the static electromechanical response of the structure. Hamilton's variational principle and the theory of beam vibrations were employed to obtain electromechanical response of the structure upon steady-state vibrations. The complex computational model is also capable of estimating the apparent fracture toughness of a given multilayer structure using the weight function method. The output of derived computational model is validated with FE simulations and available experimental results. This master's thesis also presents an application of the derived computational model in the optimization of a particular multilayer beam to obtain maximal electrical power output and to maximize its resistance to surface crack propagation and a potential brittle fracture. This goal is achieved by means of a suitable adjustment of thermal residual stresses in particular layers of the considered structure (controlled by used materials and by thicknesses of particular layers). Keywords ceramic laminate, piezoelectricity, analytical model, FEM, Ansys, classical laminate theory, vibrations of beams, Hamilton's variational principle, weight functions.

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I. Introduction

Currently, a generation of electric power from alternative energy sources is becoming a very hot topic. The electric power is needed to power various devices and the way of powering using wires is not always a feasible solution. Another option could be the usage of batteries; however, they provide electric power only for a limited time after which they need to be either recharged or replaced. Presently, there is an effort on developing such devices, that can power themselves using ambient sources of energy. The most widely known sources are without doubts wind, water or the sun. However, another interesting way to obtain energy is the conversion of mechanical energy from ambient vibrations. These vibrations can be caused e.g. by machine operation, a traffic passing over a bridge or even a movement of a human body. Devices, which can convert mechanical energy into an electrical one, are called energy harvesters. These devices employ various physical phenomena to energy conversion, such as electromagnetism, electrostatics, magnetostriction or piezoelectricity. The design of a specific energy harvester is then heavily dependent on the chosen physical phenomenon.

The piezoelectric harvester is usually a simple multilayer structure operating as a converter of mechanical energy into an electrical one. Thanks to used materials and a simple construction, it can be used also in a harsh environment. A certain disadvantage of this type of converters consists in the relatively low conversion efficiency, where only a small fraction of the input mechanical energy is converted into a usable electrical energy. A typical design of such a piezoelectric energy harvester is shown in Fig 1.1; the harvester has a form of the multilayer beam structure with a substrate in the center and piezo-ceramic layer(s) on the outside. The whole structure is designed to be as much compliant as possible to allow large deflections, i.e. large strains in the piezo layer. On the other hand, one has to be careful with the magnitude of the applied loading, since these layers are prone to a brittle fracture, which can lead to a malfunction of the whole system.



Fig 1. A typical example of a simple piezoelectric harvester [1].

This work focuses on piezoelectric harvesters in the form of a multilayer ceramic structure made of outer protective ceramic layers and inner piezoelectric layers. The aim of the multilayer design is to significantly improve the resistance of the harvester to extension of surface cracks inside the laminate by means of thermal residual stresses. To this purpose, a complex computational model is required to analyze mechanical, electrical and fracture mechanics characteristics of such a multilayer structure. This work describes the derivation of such a computational model and also contains application of the derived model in the optimization of electromechanical response of a particular multilayer cantilever beam subjected to a kinematic excitation.

II. Basics of piezoelectricity and review of key literature

A. Piezoelectric phenomenon

Piezoelectricity is an ability of certain materials to produce an internal electric field when subjected to mechanical deformation. This phenomenon was first observed by brothers Curie in 1880 on crystals of tourmaline, quartz, topaz, cane sugar and Rochelle salt [4] and named as direct piezoelectric effect. One year later, Lipmann deduced from fundamentals of thermodynamics that there also must be a converse phenomenon, upon which the crystals deform when an electric field is applied. The same year but later, this statement was experimentally proved by Curie brothers and now the converse effect is known as indirect piezoelectric effect. If a particular material shall exhibit piezoelectric properties, it needs to have a certain type of crystallographic symmetry [4]. It is known that piezoelectric properties vanish if a crystal possesses a center of symmetry. Out of 32 known crystallographic classes, there are 20 non-centro symmetric ones that can exhibit piezoelectric behavior. Among these 20 classes, there are 10 pyroelectric ones, which have a unique polar axis and contain a built-in polarization. If this polarization can be reversed by an external, sufficiently strong electric field, the crystal is called ferroelectric. Ferroelectric materials are used in technical applications due to their ability to change polarization by applying an external electric field. Piezoelectric materials are known to lose their piezoelectric properties upon reaching a certain temperature called Curie point. The reason lies in the loss of dipole moment due to changes in the crystal structure, which causes the crystal to gain a center of symmetry., Letter file.

B. Piezoelectric materials

The Piezoelectric materials are all non-conductive, i.e. they are dielectric [7]. There are manymaterials exhibiting the piezoelectric behavior, either natural or man-made. These can be sorted into following groups:

- \Box crystals,
- $\hfill\square$ synthetic ceramics,
- \Box polymers.
- 1 Piezoelectric crystals

This group contains materials like topaz, Rochelle salt, tourmaline and its most famous representative, quartz. Their notable features over other piezoelectric materials are excellent frequency stability upon varying ambient temperature and negligible deviation of their properties upon aging [8]t. Please do not revise any of the current designations.

2 Piezo-ceramics

Ferroelectric piezo-ceramics are a typical representative of man-made piezoelectric materials. They are widely used in many technical applications due to excellent mechanical properties, being chemically inert and inexpensive to manufacture [11]. The most commonly manufactured composition is called PZT (lead zirconia titanate), which is made of mixture of lead zirconate (PbZrO3) and lead titanate (PbTiO3) [12]

3 Piezo-polymers

Piezo-polymers represent a group of materials suitable for biomedical applications, since they are not as brittle and hard as previously mentioned materials. They can be divided into three groups [15]:

- □ bulk polymers,
- □ voided charged polymers,
- □ composites

III. Applications of piezoelectric materials

Applications of piezoelectric materials can be divided into four main groups [18]:

 \Box Generators – They can be either single-layered (these are used to generate anelectric spark across the electrode gap, they are small in size and simple) or multi-layered (these produce a significantly higher current output than their single-layered counterparts and can be used as solid-state batteries for electronic circuits).

 \Box Sensors – These are devices that convert measured physical parameter like pressure or acceleration into an electrical signal. Sensors made of piezo-ceramics are resistant to negative effects of electromagnetism and radiation, which makes them suitable for various environments.

 \Box Actuators – These devices are meant to convert an electric signal into a precisely controlled displacement of the component that can be used to fine-adjust e.g. machining tools, lenses or mirrors.

 $\begin{tabular}{ll} \hline & Transducers - These devices convert electrical energy into mechanical energy, typically in the form of a sound. The effect can be reversed so that sound waves make the transducer generate an electric signal.r you. \end{tabular}$

C. Modelling of the piezoelectric effect in the FE system Ansys

In the commercial FE system Ansys, the piezoelectric effect can be found under coupled field analysis problems. The piezoelectric effect is modelled via linear constitutive relations in the following matrix form.

$$\begin{cases} \{T\} \\ \{D\} \end{cases} = \begin{bmatrix} c^{E} \end{bmatrix} & [e] \\ [e]^{T} & -[\epsilon^{S}] \end{bmatrix} \begin{cases} \{S\} \\ -\{\mathcal{E}\} \end{cases} ,$$

where {T} is a mechanical stress vector, {D} is a electric flux density vector, [cE] is a common elasticity matrix from structural fundamentals, [e] is a piezoelectric stress matrix defined as [e] = [cE][d] and [S] is a permittivity matrix evaluated at constant mechanical strain. The permittivity at constant mechanical strain can be calculated from the permittivity at constant mechanical stress as follows: $[S] = [T\int] - [e]\int T[d]$. Following current-technology coupled-field elements (in FE system Ansys) support the piezoelectric effect in static, modal, harmonic and transient analyses : PLANE223 – an 8-node quadrilateral element suitable for 2D problems,• SOLID226 – a 20-node brick element suitable for 3D problems,• SOLID227 – a 10-node tetrahedron element suitable for 3D problems.•

However, the user must transfer the piezoelectric and anisotropic elasticity matrices from IEEE standard to Ansys input [24] as shown in Fig 2. In a piezoelectric matrix, the highlighted rows simply swap, whereas in an elasticity matrix, some elements near diagonal are in addition shuffled. One can clearly see that this only affects shear components of both matrices.



Fig 2 Changing of input piezoelectric and elastic characteristics from IEEE standard to Ansys format.

D. Comparison of the analytical model

The output of the developed analytical model is compared with the results of an experiment described in. In this experiment, a piezoelectric bimorph shown in Fig 3 excitation is equal to 1g (1g = 9.81 m/s2). The experiment maps how the values of the generated electrical power and values of the bimorph's free end velocity change with a varying forcing frequency upon different values of the connected resistive load. The acceleration amplitude ü0 can be transformed into a displacement amplitude according to the following relation:

$$u_0 = \frac{\ddot{u}_0}{\left(2\pi f\right)^2} \; .$$

Piezoelectric layers are 0.26 mm thick and are made of PZT-5A. Between piezoelectric layers, there is also a 0.14 mm thick substrate made of brass. The bimorph has an experimentally determined damping ratio br = 0.027. Material properties of used materials



Fig 3 A beam used in the experiment.

Piezoelectric layers of the used beam are, however, electrically connected in series and authors of the article use a resistive load Rl, which is connected to both layers simultaneously. This poses a problem for the developed analytical model, since it assumes both that piezoelectric layers are connected electrically in parallel and that each layer has its own resistive load. Fundamentals of electric circuits for elements connected in series state, that the electric current flowing through the i-th element is the same for all elements in such a circuit. This can be mathematically written for the used bimorph as

$$\underbrace{IR}_{1^{\text{st}} \text{ layer } 2^{\text{nd}} \text{ layer }} = IR_l \ .$$

From the equation we receive that each layer needs to have its own resistive load R = RI/2. This value of resistive load is subsequently used in the developed analytical model to obtain desired results. The comparison of experimental results with the output of the analytical model is shown in Fig 4. The experiment tracks how the maximal value of generated electrical power and the velocity of the beam's free end change with a varying forcing frequency. The results are displayed for three different values of used resistive load: $1 \text{ k}\Omega$, $33 \text{ k}\Omega$ and $470 \text{ k}\Omega$. The graphs show a good match between the output of the analytical model and obtained experimental results for all three used resistive loads. Discrepancies exist upon the first natural frequency. Therefore, the developed analytical model can be used without any restrictions



Fig 4 The comparison of electrical power and velocity of the free end of the beam obtained experimentally [52] and using the developed analytical model for: a) $Rl = 1 k\Omega$; b) $Rl = 33 k\Omega$; c) $Rl = 470 k\Omega$

IV. Conclusion

Aim to develop a complex computational model that enables analysis of mechanical, electrical and fracture mechanics behavior of a multilayer structure with piezoelectric layers operating in the form of a cantilever beam subjected to a kinematic excitation. The following functionalities were required from the model:

determination of the electromechanical response of a multilayer structure with piezoelectric layers, subjected to a static mechanical loading and to thermal residual stresses; determination of the steady-state electromechanical response of a multilayer structure with piezoelectric layers subjected to a time-harmonic kinematic excitation (simulating harmonic vibrations); estimation of the multilayer structure resistance to propagation of potential surface cracks under given thermal and mechanical loading conditions.

At first, a computational model of the multilayer structure, which is able to determine response to a static mechanical loading, thermal loading and to an applied external electric field was developed using the classical laminate theory. Upon the creation of the model, it was found that the piezoelectric properties of individual materials make the laminate behave stiffer. This phenomenon can be explained by a conversion of some amount of work done by external forces into the energy of the internally generated electric field in piezoelectric layers. The effect of the externally applied electric field was found to be analogous to the effect of a temperature change (since it causes the plate to change its dimensions). The output of the developed computational model of the laminate was compared with an output of the FE model, where a perfect match in both results was obtained. Then, the output of the analytical model was validated with an experiment, which mapped the deflection of a cantilever beam's free end as a function of the intensity of an applied external electric field. An excellent match was obtained for relatively weak external electric fields, where the deflection of the beam's free end is linearly dependent on the intensity of an applied external electric field. In the next step, a computational beam model of the multilayer structure for analysis of its dynamical characteristics and behavior was developed using Euler-Bernoulli beam theory and Hamilton's variational principle. This model is able to determine the first natural frequency and the steady-state response of the multilayer beam subjected to a kinematic excitation upon harmonic vibrations.

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