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Design of Resonators Based on Functionally Graded Piezoelectric Materials

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Abstract: Resonators have been widely used in several fields of measurements such as instrumentations, microprocessors and others. They can be built using piezoelectric materials that have the property of converting electrical energy into mechanical energy and vice versa. Functionally Graded Materials (FGM) are advanced materials that posses continuously graded properties and are characterized by spatially varying microstructures created by nonuniform distributions of the reinforcement phase as well as by interchanging the role of reinforcement and matrix (base) materials in a continuous manner. The application of FGM concept to piezoelectric resonators design allows designing composite transducers without interface between materials (e.g. PZT and Aluminum), due to the continuous change of property values. This offer advantages such as reduction of local stress concentration, increasing bonding strength and fatigue-lifetime. Based on these ideas, this work studies the advantage of using, in resonator design, a graded piezoceramic instead of homogeneous piezoelectricity properties, by using Finite Element Method for computational simulations. Elastic and piezoelectric properties are graded along the thickness of a FGM piezoceramic. Several piezoelectric material gradations are assumed through the piezoceramic thickness. Static analysis, vibration modes and resonance frequencies are computed, examined, and compared with homogeneous piezoelectric resonators to show the improvement.

Keywords: Piezoelectric Transducers, Functionally Graded Material, Finite Element Method, Resonators, Static and Dynamic Simulation

NOMENCLATURE

$\boldsymbol{T}$ = stress tensor
$\boldsymbol{D}$ = electric displacement tensor
$\boldsymbol{E}$ = electric field vector
$\boldsymbol{c}^{E}$ = elastic tensor under short circuit conditions
$\boldsymbol{e}$ = piezoelectric deformation tensor
$\mathbf{u}$ = displacement vector
$\mathbf{F}$ = mechanical force vector
$\mathbf{Q}$ = electric charge vector
$\mathbf{M}$ = mass matrix
$\mathbf{K}$ = stiffness matrix

Greek Symbols

ε = strain
$\boldsymbol{\epsilon}$ = dielectric tensor
ε_0 = dielectric constant of free space, farads/meter
Φ = electric potential vector

Subscripts

i, j, k, l relative to tensor order
uu relative to elastic matrix
$\mathbf{u\Phi}$ relative to piezoelectric matrix
$\mathbf{\Phi\Phi}$ relative to dielectric matrix

11 indicates transverse direction
15 indicates shear direction
33 indicates longitudinal direction
31 indicates transverse direction
1, 2 indicates elastic constants on transverse directions
3 indicates elastic constants on axial direction
4, 5, 6 indicates elastic constants on shear axes

INTRODUCTION

Piezoelectric materials have the property to convert an electric energy (electric field and electric potential) into a mechanical energy (stress and strain) and vice versa. Examples of piezoelectric materials include quartz, ceramics (PZT) and polymers (PVDF). Its main applications are sensors and electromechanical actuators, as resonators in electronic equipment and acoustic applications, as ultrasound transducers, naval hydrophones, and sonars. Ultrasound transducers are used in medical imaging (Akhnak et al., 2000) and non-destructive tests. Other applications include pressure sensors; piezoelectric actuators for the structural vibration control; performance of micropositioning and micromanipulation devices as: electronic microscopy instruments; laser interferometry; cell manipulation equipment; microelectromechanical systems "MEMS"; nanotechnology and precision mechanics equipment (Kögl and Silva, 2005; Silva, 2003). A brief of piezoelectric applications is offered by Newnham and Ruschau (Newman and Ruschau, 1991).

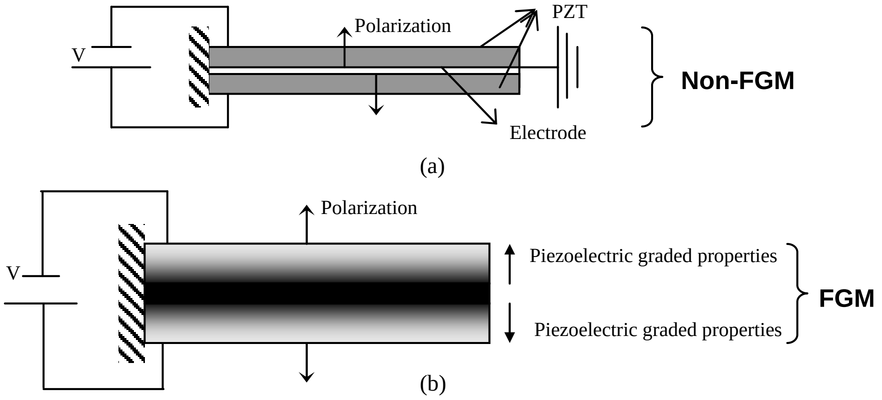
Generally, the best piezoceramics for transducers and actuators are composites, by using two or more materials (Haertling, 1994, Tomikawa et al., 1986). For instance, the bimorph piezoactuators are composed by two piezoelectric ceramic sheets in strip form bonded together with a bonding agent (usually epoxy resin) and fixed at one end to form a cantilever beam structure, see Fig. 1a. Application of an external electric field across the bimorph results in the axial contraction of one sheet and the axial extension of the other sheet. Thus, the result of the electric excitation is a mechanical deformation field that can generate a transverse beam deflection at the tip.

However, piezocomposite ceramics suffer from uneven distribution of stresses. Such drawbacks will reduce the electric-field-induced displacement characteristics, the reliability and lifetime of the piezoelectric devices. In order to extend the lifetime and to improve the reliability, the FGM (Functionally Graded Materials) concept arises as a solution for these interface-problems. Thus, in piezoceramics the new concept of FGM brings great advantages. By using the same example (see Fig. 1), the bonding agent has been replaced by a functionally graded piezoelectric material (see Fig. 1b); therefore, all properties vary along the thickness direction of the FGM bimorph in opposition to each other.

Currently, most of on-going researches related to FGM piezoelectric materials are analytical or experimental tests (Chen et al., 2000; Hauke et al., 2000; Kouvatov et al., 1999; Zuh and Meng, 1995), and the analytical models have several and large limitations due to the continuous variation of the property material (Hauke et al., 2000; Kouvatov et al., 1999). In view of this idea, in this paper a static, modal and harmonic analysis of a functionally graded piezoceramic are performed to explore the FGM potential by designing piezoelectric resonators, using Finite Element Method (FEM). These analyses are compared with results of a homogeneous piezoceramic to show FGM advantages.

In FEM modelling, the piezoceramic is modelled using a layer approach instead of a continuous material variation. This approach has a disadvantage related to the mechanical tension distribution at interfaces; however, dynamic characterization (natural frequencies, vibration modes, and others) is very close to characterization of ceramics with material continuous variation. FE softwares have no “tools” to simulate graded continuous materials for while.

The paper is built up as follow: first, it is described the FE (Finite Element) formulation of piezoelectricity. Then, some ideas, about FGM concept, are illustrated. Finally, results and some conclusions are given.



(a)

(b)

Figure 1. Example of FGM concept; a) bimorph piezo-actuator; b) bimorph piezo-actuator based on concept of functionally graded material (FGM)

PIEZOELECTRIC FINITE ELEMENTS

In this section, the piezoelectric constitutive equations are briefly described. It is assumed that the piezoelectric response is linear with electric field change, or with mechanical stress and strains. Thus, the piezoelectric behaviour is described by piezoelectric constitutive equations given by Eq. (1). They relate stress ($\boldsymbol{T}_{ij}$), strain (ε_{kl}) with electric displacement ($\boldsymbol{D}_i$), and electric field ($\boldsymbol{E}_k$) (Silva et al., 1999; Lerch, 1990):

$$\begin{aligned} \boldsymbol{T}_{ij} &= \boldsymbol{c}^{E}_{ijkl}\boldsymbol{\varepsilon}_{kl} - \boldsymbol{e}_{kij}\boldsymbol{E}_{k} \\ \boldsymbol{D}_{i} &= \boldsymbol{e}_{kij}\boldsymbol{\varepsilon}_{kl} + \in^{S}_{ik} \boldsymbol{E}_{k} \end{aligned} \tag{1}$$

where, $\boldsymbol{c}^{E}_{ijkl}$ is a fourth order elastic tensor under short circuit conditions, $\in^{S}_{ik}$ is a second order dielectric tensor, and $\boldsymbol{e}_{kij}$ is third order tensor of a piezoelectric deformation.

On the other hand, the FE piezoelectric equilibrium equations can be written based on variational principle. These equations are written considering displacement ($\boldsymbol{u}$), electric potential ($\boldsymbol{\Phi}$), mechanical forces ($\boldsymbol{F}$) and electric charges ($\boldsymbol{Q}$), on nodal points, as (Lerch, 1990):

$$\begin{aligned} \boldsymbol{M}_{uu}\ddot{\boldsymbol{u}} + \boldsymbol{C}_{uu}\dot{\boldsymbol{u}} + \boldsymbol{K}_{uu}\boldsymbol{u} + \boldsymbol{K}_{u\Phi}\boldsymbol{\Phi} &= \boldsymbol{F} \\ \boldsymbol{K}^{T}_{u\Phi}\boldsymbol{u} + \boldsymbol{K}_{\Phi\Phi}\boldsymbol{\Phi} &= \boldsymbol{Q} \end{aligned} \tag{2}$$

where $\boldsymbol{M}_{uu}$, $\boldsymbol{C}_{uu}$, $\boldsymbol{K}_{uu}$, $\boldsymbol{K}_{u\Phi}$, $\boldsymbol{K}_{\Phi\Phi}$, denote mass, damping, stiffness, piezoelectric, and dielectric matrices, respectively.

FUNCTIONALLY GRADED MATERIALS - FGM

Functionally Graded Materials (FGM) are materials that possess continuously graded properties with gradual change in microstructure (Hirai, 1996; Suresh and Mortensen, 1998), see Fig. 2. The materials are made to take advantage of desirable features of its constituent phases. For instance, in a thermal protection system, FGMs take advantage of heat and corrosion resistance, typical of ceramics, and mechanical strength and toughness, typical of metals. A soft property variation supplies advantages as local stress concentration reduction (Kim, Paulino, 2002; Suresh and Mortensen, 1998), once they do not present interface among inclusion and matrix materials, therefore, it reduces a common problem in composite materials, the crack arising or damages in these interfaces. These materials are subjected to active research in several countries, such as United States, Japan, and Germany, and recent advances in material processing have allowed manufacturing a large variety of functionally graded materials. Kieback et al. (2003) shows some FGM manufacturing processes such as powder stacking, wet to powder spraying, among others.

Recently, the concept of functionally graded materials (FGM) has been explored in piezoelectric materials to improve the properties and increase the lifetime of piezoelectric transducers (Almajid et al., 2001). In an FGM piezoceramic, usually, elastic, piezoelectric, and dielectric properties are graded along the thickness. Previous studies (Zhifei, 2002; Almajid et al., 2001) have shown that the gradation law of piezoceramic properties can influence the performance of piezoceramics, such as generated output displacements and natural frequencies. This suggests that several graded material functions can be investigated to improve FGM transducers. In the next section, results are obtained by considering several gradation functions for piezoelectric materials.

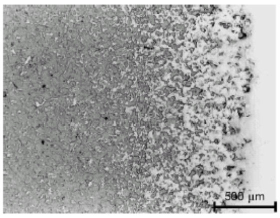


Figure 2. W/Cu FGM microstructure produced by electrochemical gradation

RESULTS

FE Model

This paper presents the modeling of a simple cylindrical piezoceramic based on FGM concept using a layer approach. Figure 3 shows the ceramic, corresponding boundary conditions for the simulations and an example of a common linear gradation function for FGM piezoceramics (next section shows the materials and properties used in FE simulations). It is used the coupled field capability of the ANSYS/Multiphysics™ product, and the cylindrical geometry is treated as an axisymmetric model using the PLANE13 element type. This model is used for static, modal and harmonic analysis solutions to understand electro-mechanical behavior and to aid to understand the FGM advantage in relation to homogeneous piezoceramics.

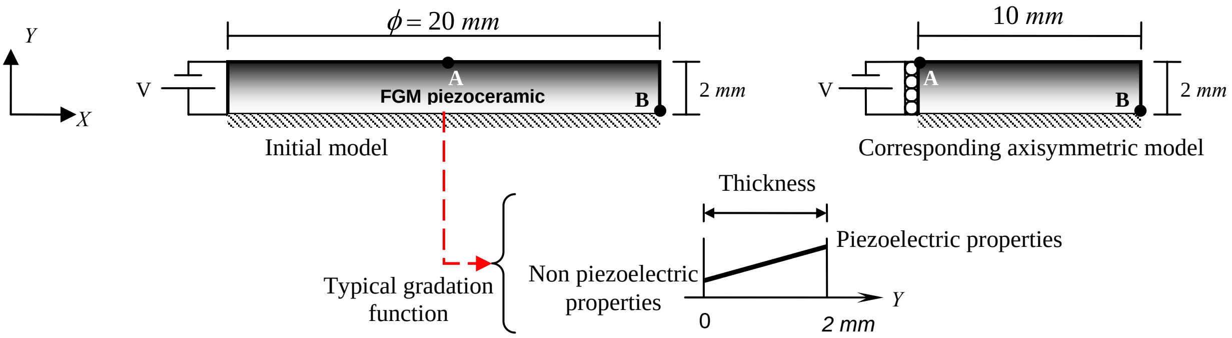
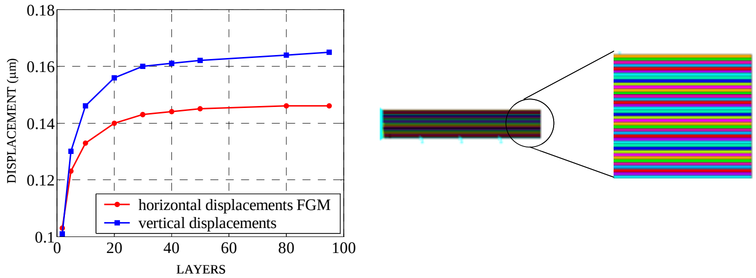


Figure 3. FE model for FGM piezoceramic simulations

Because a layer approach is used, a convergence analysis is developed. This reduces the discrepancies between continuous gradation and a layer modelling. Several simulations are conducted by discretizing into 2, 5, 10, 20, 30, 40, 50, 80, and 95 layers, by using a linear gradation function, see Fig. 5. Figure 4 shows the results. It is observed that convergence is found for 40 layers, considering horizontal displacement at point A (see Fig. 3). Thus, in following simulations 40 layers are used, due to low computational cost.



CONVERGENCE ANALYSIS

FINAL LAYER DISTRIBUTION

Figure 4. Layer convergence and final layer model (40 layers)

In FE model the electrical contacts are modeled as coupled d.o.f. sets at each electrode: upper and lower piezoceramic faces. Finally, the temperature effects are ignored in this study.

Piezoelectric material data

Most manufacturers of piezoelectric materials do not publish the material properties in a format that can be directly input to an ANSYS model. The published data must be converted and transformed to fill the necessary material matrices that ANSYS requires for piezoelectric material input. Specifically, ANSYS (ANSYS, 1998a; ANSYS, 1998b) requires a dielectric matrix, a piezoelectric matrix, and either a compliance matrix or a stiffness matrix.

The dielectric matrix defines the electrical permittivity in typical units of Farads/meter. This matrix is a 3x3, diagonal matrix for a 3D model and the data is input to ANSYS as an orthotropic material property with labels PERX, PERY, and PERZ. (In a 3D model, PERZ is the axial or polarized direction in the element coordinate system). In a 2D model, only the PERX and PERY values are entered, with PERY being the polarized direction.

The piezoelectric matrix relates the electric field to stress and typically its property values have units of Coulombs/meter². For a 3D model, this matrix is a 6x3 matrix and the data is input to ANSYS as a material data table of type, PIEZ. In a 2D model, the piezoelectric matrix has 4x2 size.

Table 1 – Dielectric constants

Property	Bottom of the ceramic (PZT-5A matrix)	Top of the ceramic (Al matrix with PZT-5A inclusions)
ε_0	8.85×10^{-12}	8.85×10^{-12}
ε^S_{11}	$916 \times \varepsilon_0$	$196 \times \varepsilon_0$
ε^S_{33}	$830 \times \varepsilon_0$	$178 \times \varepsilon_0$

Table 2 – Piezoelectric constants

Property	Bottom of the ceramic (PZT-5A matrix)	Top of the ceramic (Al matrix with PZT-5A inclusions)
e_{31}	-5.4 C/m^2	-1.02 C/m^2
e_{33}	15.8 C/m^2	3 C/m^2
e_{15}	12.3 C/m^2	2.34 C/m^2

Table 3 – Elastic constants

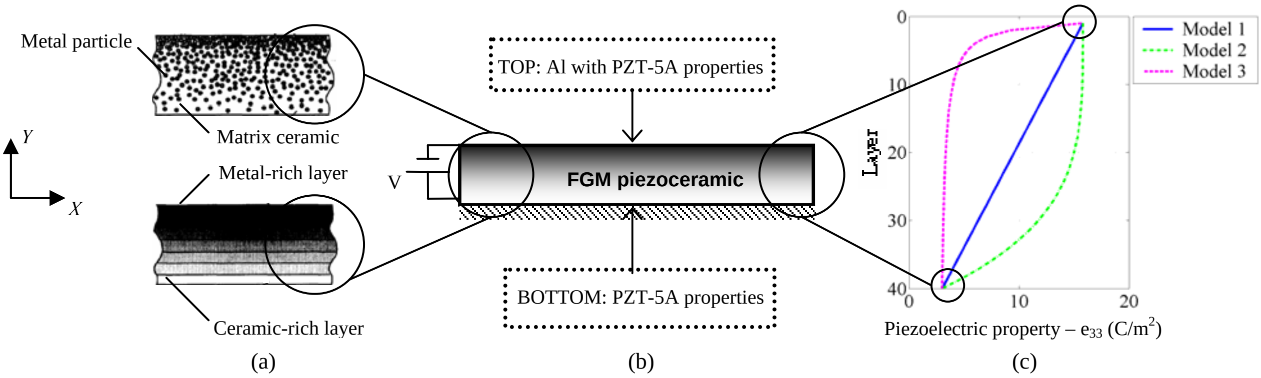
Property	Bottom of the ceramic (PZT-5A matrix)	Top of the ceramic (Al matrix with PZT-5A inclusions)
C^E_{11}	12.1×10^{10} N/m^2	6.67×10^{10} N/m^2
C^E_{12}	7.54×10^{10} N/m^2	4.16×10^{10} N/m^2
C^E_{13}	7.52×10^{10} N/m^2	4.15×10^{10} N/m^2
C^E_{33}	11.1×10^{10} N/m^2	6.12×10^{10} N/m^2
C^E_{44}	2.11×10^{10} N/m^2	1.16×10^{10} N/m^2
C^E_{66}	$0.5 \times (C^E_{11} - C^E_{12})$	$0.5 \times (C^E_{11} - C^E_{12})$

While ANSYS accepts stiffness data in terms of the Young's modulus and Poisson's ratio, it seems more usual in practice to define either the compliance matrix or the stiffness matrix for a piezoelectric coupled-field analysis. Units for compliance matrix coefficients are typically meter²/Newton, while for stiffness matrix, Newtons/meter² is commonly used. The analyst selects which matrix to input with the element option switch for the coupled-field element type, then enters the 6x6 symmetric matrix data as a material data table of type, ANEL. In a 2D model, the stiffness or compliance matrix has 4x4 size.

For the FGM piezoceramic discussed in this paper, two material property set are chosen, and the FGM ceramic disk is taken to be an inclusion/matrix type ceramic, as shown in Fig. 5a, simulated as functionally graded multilayer one, depicted in Fig. 2a. However, the distribution of FGM properties is chosen for comparison reasons within this paper only, and it may not represent the real distribution within an actual FGM as it will be subjected to fabrication constraints. Thus, the FGM piezoceramic is graded from a metal-rich layer (Aluminum matrix with PZT-5A inclusions), on top of the ceramic, up to a piezoceramic-rich layer (PZT-5A matrix), on bottom of the ceramic, see Fig. 5b. For homogeneous piezoceramic simulations only one material is used: the PZT-5A properties are chosen.

In FGM simulations, the dielectric, piezoelectric, and elastic properties are graded. Tables 1, 2, and 3 show the adopted dielectric, piezoelectric, and elastic constants, respectively, by using the ANSYS nomenclature. PZT-5A properties were obtained from Nader, (2002) and Aluminum properties from Boresi *et al*., (1993). In Tab. 1, dielectric constant of free space, ε_0, is equal to 8.85 x 10^{-12} farads/meter, and the subscript notation, 11 and 33, indicate the transverse and axial directions, respectively. In Tab. 2, these constants relate the voltage and displacement behavior of the piezoelectric material and the subscript notations indicate the transverse direction (31), the longitudinal direction (33), and the shear direction (15). Finally, in Tab. 3 the subscripts identify the transverse directions (1 and 2), the axial direction (3), and the shear axes (4, 5, and 6). Other simulation data are PZT-5A density = 7500 kg/m^3, Aluminum = 2710 kg/m^3, and damping = 3e-9.

Several gradation functions can be used. In this work, three functions are applied on graded properties. Former function is a linear function, named model 1; the second one is a *1/x* function type, which represents a quick change of properties, this model is named model 2; and the last one is a fourth order equation, which represents a more slow change of properties, named model 3, see Fig. 5c.



(a) (b) (c)

Figure 5. (a) FGM Microstructure and layer approach; (b) Material distribution on FGM piezoceramic; (c) Gradation functions used for piezoelectric constants (specifically, e_{33} constant)

Static analysis

Initially, a static analysis was developed. Thus, by using ANSYS program several simulations with several input data were conducted. Five voltages were applied: 1, 50, 100, 200, and 300V. The vertical displacements and von Mises stresses are analyzed. Figure 6 shows the vertical displacement measured at point A (showed in Fig. 3), and the maximum von Mises stress measured at point B, see Fig 3. In FGM models lower displacements are obtained when an input voltage is applied (although differences with non-FGM material is very small); because the Aluminum-PZT-5A composite (top material) have smaller piezoelectric properties and, at the same time, the PZT-5A is a high sensitivity material and does not produce large mechanical amplitudes. However, the FGM materials keep lower stress levels, see Fig. 6, even though a layer approach was used; because, the FGM material, as a whole, is a softer graded material. It is an advantage, because high stress levels accelerate the aging process of piezoelectric materials.

Modal analysis

Modal analysis of this piezoceramic involves two cases which spans the extremes of the piezoelectric coupling effect due to voltage and displacement degrees of freedom. The first case is commonly called the "resonance" condition. A constant voltage equal to zero is applied to the electrical contacts (electrodes) of ceramic disk. This is a "short-circuit" condition, where all voltage potentials are connected to ground. The second case, called "anti-resonance", applies a zero voltage only to one electrode. In this modal analysis, no structural constraint was applied.

Table 4 shows a comparison of the natural frequencies when homogeneous and FGM materials are used (in this last case, by using three graded functions). The vibration modes are calculated for resonance and anti-resonance conditions. Thus, when resonance and anti-resonance frequencies are equal, it is a mechanical mode and, when resonance and anti-resonance frequencies are different, it is a piezoelectric mode, which is our mode of interest.

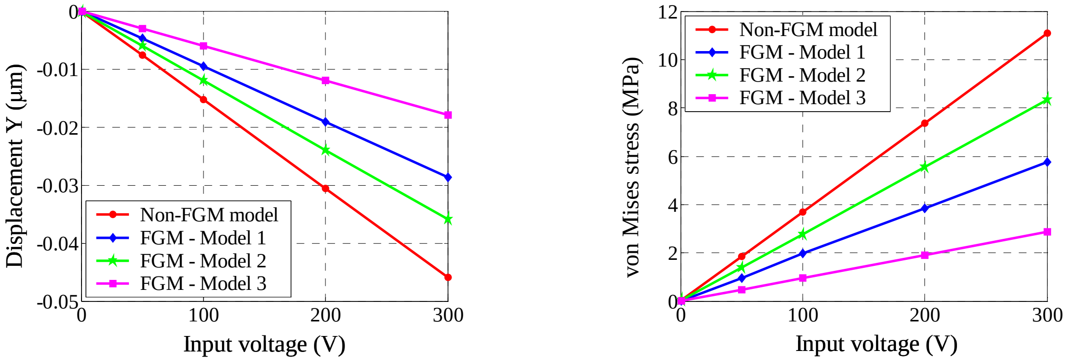


Figure 6. Vertical displacement and von Mises stress plots of FGM and non-FGM distribution

Table 4 – Results of the modal analysis

NATURAL FREQUENCIES (kHz)				
MODEL	**FIRST**	**SECOND**	**THIRD**	**FOURTH**
non-FGM	1090	3365	5705	8460
FGM model 1	889	1920	2810	3750
FGM model 2	1290	2848	4342	5940
FGM model 3	746	1542	2390	4040

Harmonic analysis (frequency response)

The same 2D axisymmetric model used in modal analysis is used for harmonic one (unrestrained simulation). The input for this simulation was a voltage amplitude imposed across the piezoelectric ceramic disk. The input varied sinusoidally between +/-1V.

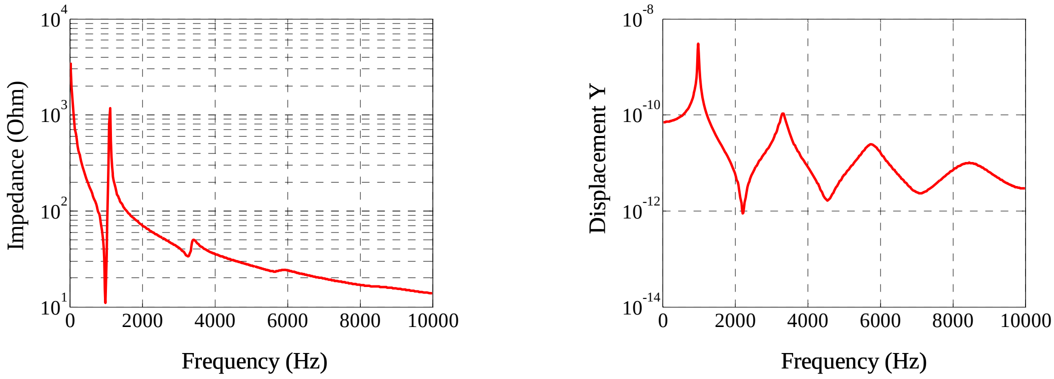


Figure 7. Electrical impedance and Y displacement curves for non-FGM transducer

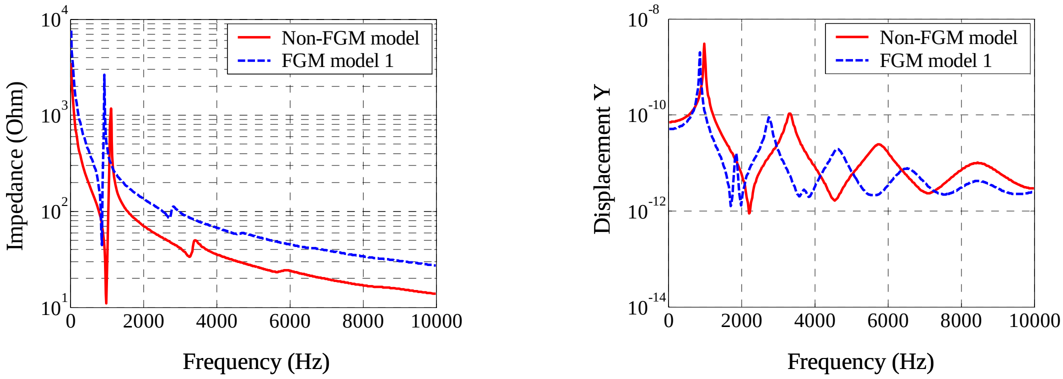


Figure 8. Electrical impedance and Y displacement curves for FGM transducer and first gradation model

The harmonic analysis was performed over a frequency range of 0-10 MHz in equal steps of 0.02 MHz. At each frequency, ANSYS computes the steady-state response of the system to a sinusoidally varying input on the ceramic disk.

A constant damping ratio was assumed over all frequencies of the harmonic analysis sweep. The result of particular interest in this solution was the electrical impedance of the transducer over the frequency sweep and the Y (vertical) displacement, both measured at point A in Fig. 3.

Figure 7 shows the electrical impedance characteristics and the Y displacement (focused on the thickness vibration modes) for the uniform piezoelectric ceramic (non-FGM) disk; and Fig. 8, 9, 10 show the impedance curve and Y displacement for several FGM models (1 up to 3), respectively.

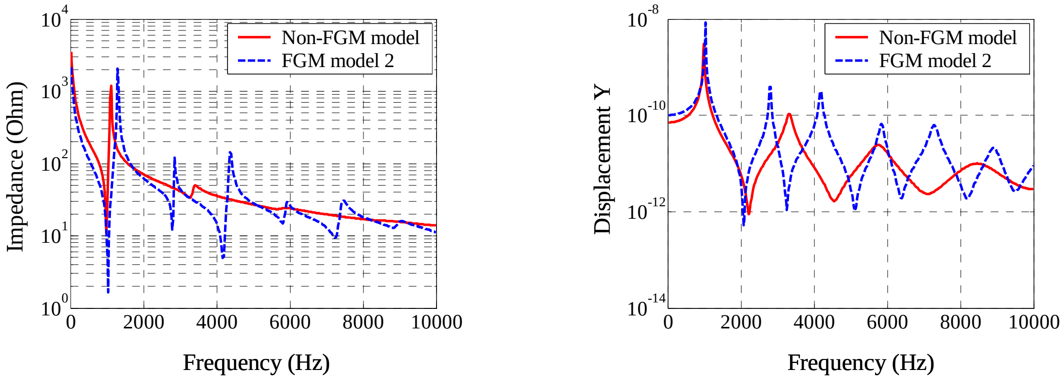


Figure 9. Electrical impedance and Y displacement curves for FGM transducer and second gradation model

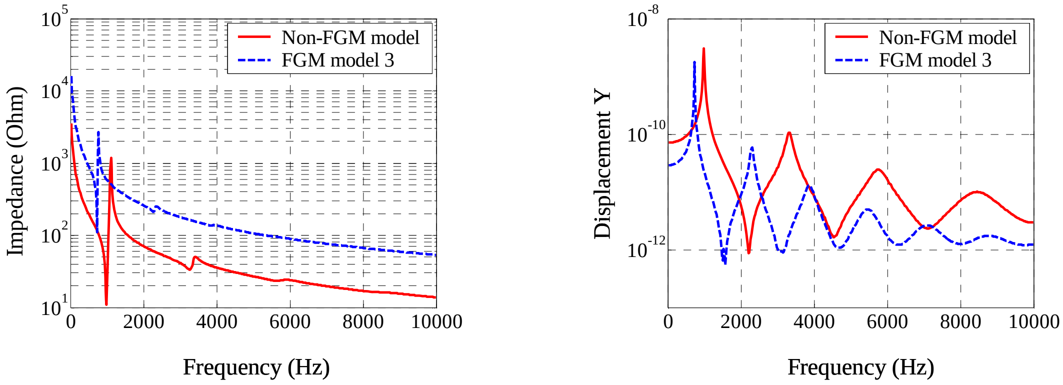


Figure 10. Electrical impedance and Y displacement curves for FGM transducer and third gradation model

The resonant responses for the odd order vibration mode appear in the non-FGM. It is noted, however, that both the even and odd order mode resonant responses tend to appear in all FGM models, see table 4. This result indicates that the FGM piezoelectric disk here examined has more versatility for resonator purposes in relation to material-homogeneous resonators; thus, it is possible more or less resonance modes in selective frequencies according to used gradation function.

CONCLUSION

The modeling of a FGM piezoceramic was carried out with considerable success, even though using layer approach. The designs were compared with homogeneous piezoceramics (non-FGM) and the influence of material gradation was analyzed. Based on results, by using FGM concept, it can be obtained lower stress levels and more resonance frequencies (even and odd modes); in other words, large improvements can be achieved in their performance characteristics.

It was observed that performance changes with type of applied gradation function; this suggests the use of optimization techniques to design it, in other words, the presented results illustrate that the piezoceramic performance can be improved by finding the optimal gradation of material properties in the FGM piezoceramics. Furthermore, it was observed lack of computational methods to model these devices and to evaluate their performance based on FGM concept, because, no FE commercial software has this concept implemented.

Based on these ideas, in a future work, it is proposed the development of FE and optimization algorithms to design new FGM piezoelectric ceramics with better performance and to explore the FGM potential. Furthermore, it would be appropriate to continue the simulations considering the transient behavior of FGM piezoceramics radiating a short pulse into water.

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