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Evaluation of the constitutive material parameters for the numerical modelling of structures with lead–zirconate–titanate thick films

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Abstract

We present a combined experimental and numerical procedure for the characterisation of thick lead–zirconate–titanate (PZT) films, which was used to obtain the material parameters for a finite-element (FE) model of a thick-film quasi-static bending actuator. Due to the lack of standardised characterisation techniques for measuring the elastic and piezoelectric properties of thick piezoelectric films, non-conventional experimental techniques were implemented as follows: nano-indentation measurements were performed to evaluate the material compliance, and an adapted substrate-flexure method was used to measure the transverse piezoelectric coefficients of the thick PZT film. Good agreement between the results from the numerical and experimental analyses validated the model and confirmed the applicability of the proposed characterisation procedure.

Keywords: Thick-film PZT; Nano-indentation test; Effective piezoelectric coefficients; Finite-element model

1. Introduction

Finite-element analysis (FEA) has proved to be very useful in the design phase of various micro-electro-mechanical system (MEMS) devices. However, straightforward usage of the simplified numerical models in which unverified material properties (such as the material parameters from the literature or producer data sheets) are used can result in an unacceptable discrepancy between the predictions and the real structure properties, so leading the designer astray. This fact is particularly important in the case of ceramic MEMS with screen-printed piezoelectric films. The main problem with modelling such structures is that the effective material properties of the piezoelectric thick films depend not only on the material composition but also on the compatibility of the film with the electrodes and substrate materials, and a number of technological parameters relating to their processing. Therefore, in order to obtain an accurate material model for a certain piezoelectric thick-film, extensive experimental work aimed at evaluating the required material parameters is necessary.

Due to the constraints imposed by the substrate, the piezoelectric coefficients of the films cannot be measured directly using standard methods [1,2]. As a solution, different static and quasi-static techniques to assess the piezoelectric parameters have been proposed [3–10]. These techniques utilise the direct piezoelectric effect, such as the normal or impulse loading methods and the substrate-flexure technique, and the indirect piezoelectric effect, such as approaches based on the use of a laser interferometer and an atomic force microscope. A pneumatic loading method has also been proposed as an alternative method for characterising piezoelectric thick-films [11,12]; this method is capable of simultaneously measuring the longitudinal and transverse piezoelectric coefficients.

Piezoelectric thick films, especially lead–zirconate–titanate (PZT), on various substrates have been widely studied for their applications in ceramic MEMS [7–14]. However, in spite of the accumulated knowledge of processing and characterisation of thick PZT films, it is still a challenge to build a numerical model that will provide good agreement between the simulations and the experimental results. Because of the lack of available experimental data, 50%-reduced piezoelectric coefficients and the

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same compliance as for the bulk PZT were assumed for the thick-film PZT material model in our previous analyses [15,16]. Even though the initial model was good at revealing trends, updating the model with experimentally obtained material parameters was necessary for further numerical prototyping.

In this paper we describe a combined experimental and numerical procedure used for characterising PZT thick films. The most novel feature of this work is an evaluation of the elastic properties of a PZT thick-film that was conducted using a nano-indentation measurement technique. Furthermore, an adaptation of the method for measuring the effective transverse piezoelectric coefficient $e_{31,f}$ of thin films [3] was implemented to improve the accuracy of characterisation of the thick films. This was achieved by taking into account the thickness of the PZT film and by considering the most appropriate position of the measured thick-film PZT patch on the cantilever structure under test. By using the experimentally evaluated material parameters a more accurate FE model of the quasi-static bending-actuator structure was built. For validation purposes an experimental set-up with an optical surface-profiler system was built; this allowed measurements of the actuator's tip displacement. These experimental results were compared to the results of the simulations and were used to assess the validity of the model and the proposed characterisation procedure.

2. Finite-element modelling

The basic electromechanical constitutive equations for the linear material behaviours are:

$$\{S\} = [s]\{T\} + [d]\{E\}, \qquad \{D\} = [d]^{\mathrm{T}}\{T\} + [\varepsilon]\{E\}, \qquad (1)$$

where $\{S\}$ and $\{T\}$ are the strain and the stress vectors, respectively, $\{D\}$ the dielectric displacement vector, $\{E\}$ the electric field vector, $[s]$ the elastic compliance matrix evaluated at a constant electric field, $[d]$ the matrix of the piezoelectric coefficients and $[\varepsilon]$ is the permittivity matrix, evaluated at a constant stress. The superscript T denotes the matrix transpose.

As is evident from Eq. (1) a FE model of a piezoelectric structure requires the elastic parameters, the piezoelectric coefficients and the permittivity to be entered in a form that the FE package expects for the piezoelectric material input. Generally, however, the piezoelectric material matrices are not fully populated, and which of the coefficients are non-zero depends on the symmetry. For a tetragonal system, class 4 mm non-oriented polycrystalline bulk material (e.g., bulk PZT), poled in the third direction, the $[s]$ matrix has to contain only five different coefficients, s_{11}, s_{12}, s_{13}, s_{44} and s_{66}, the $[d]$ matrix contains d_{31}, d_{33}, and d_{15}, and $d_{32} = d_{31}$, and $d_{24} = d_{15}$, and the $[\varepsilon]$ matrix contains ε_{11}, $\varepsilon_{22} = \varepsilon_{11}$, and ε_{33} [17]. The PZT films have the same matrix elements as crystals that belong to the hexagonal class 6 mm symmetry [18], for which the same coefficients as for the 4 mm symmetry are needed. Only $s_{66} = 2(s_{11}–s_{12})$ can be calculated. In the present case study the semi-static behaviours of a cantilever-type actuator are analysed, and for this reason only the compliance and the piezoelectric coefficients, s_{11}, s_{12}, s_{13}, s_{33}, s_{44}, and d_{31}, d_{33} and d_{15} are required to fully define the piezoelectric material model.

Notice that in the case of piezoelectric films, due to the effect of clamping to the substrate only the effective parameter values can be measured. Assuming ideal clamping, from these effective values the parameters that are appropriate for populating the upper matrix can be approximately calculated.

3. Test patterns

For experimental purposes a series of test patterns of different geometries was designed and processed on a common 250-μm thick Al_2O_3 substrate (Fig. 1a). In this way different test structures with the same material properties and the same thicknesses of PZT films were provided for measurements of the parameters needed for the numerical model. The PZT films were made by screen printing the PZT paste (PZT 53/47 composition with the addition of 2% of PGO, prepared at the Jožef Stefan Institute [13]), pre-firing at 450 °C for 60 min and firing at a peak temperature of 850 °C for 13 min in a belt furnace with a 60-min profile. The thickness of the PZT film measured on several samples was 38–45 μm. The test samples from the common substrate were then separated (Fig. 1b) and individually poled in a silicon-oil bath at 100 °C, with a continuously applied electrical field strength of 75 kV/cm perpendicular to the film plane, for 20 min.

The patterns marked as AV5 and AV6 are used to evaluate the transverse piezoelectric coefficient d_{31} and for the functional testing of the bending actuator structure. The lateral dimensions of these patterns are 24 and 4 mm (the dimensions of the PZT patches and electrodes are 12 mm × 3.6 mm) and before the measurements they were attached to the ceramic carrier to form an appropriate cantilever structure. The other test patterns that

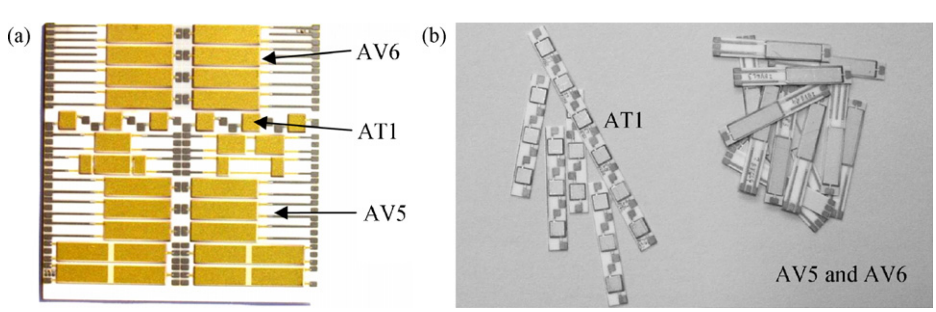

Fig. 1. (a) Different types of test patterns made on a common Al_2O_3 substrate and (b) individual test samples used for the characterisation of the PZT thick-film and the validation of the FE model.