Sensors and Actuators A 233 (2015) 176–183

Contents lists available at ScienceDirect

Sensors and Actuators A: Physical

journal homepage: www.elsevier.com/locate/sna

Simulation of damage in ferroelectric actuators by means of cohesive zone model

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ARTICLE INFO

Article history:
Received 22 March 2015
Received in revised form 1 June 2015
Accepted 25 June 2015
Available online 8 July 2015

Keywords:
Ferroelectric actuator
Fracture mechanics
Domain switching
Cohesive zone model
Finite element method

ABSTRACT

The reliability of smart structures and in particular of ferroelectric multilayer actuators (MLA) is essentially reduced by accumulation of damage and crack formation. Such failure processes are numerically simulated in the current research by finite element method (FEM) employing coupled electro-mechanical analyses. At first, the poling process during manufacturing of the actuator is simulated. Next, an alternating electric voltage with a constant amplitude is applied to mimic in-service conditions. In order to model the bulk material, ferroelectric user elements are implemented into the commercial software ABAQUS©, thus allowing to simulate domain switching processes. Material damage is considered by means of a cyclic cohesive zone model (CCZM). The traction-separation law (TSL) accounts for electro-mechanical interaction. It was found that the poling process of the actuator may induce crack initiation at an electrode surface, which is driven further by the cyclic electric loading. Damage accumulation is observed due to mechanical and electrical field concentrations near the electrode tip. To the best of our knowledge, it is the first coupled ferroelectromechanical modeling combined with gradual damage accumulation in smart structures which is an important step towards future optimizations of the actuator design.

1. Introduction

Piezo-(ferro-)electric multilayer actuators (MLA) are widely used in micropositioning appliances due to their precise resolutions in the sub-nanometer range, high force generation, fast response of a few microseconds, no wear and tear since a piezo actuator has no moving parts, like bearings or gears, nonsusceptibility to magnetic fields [1]. MLA, which is a stack of hundreds of ceramic layers with two electrical leads, is the most common form of piezo actuator. Electrically, a piezo actuator behaves like a capacitor. The MLA displacement is proportional to the stored electrical charge, the capacitance depends on the material properties, area and thickness of the ceramic. Severe exploitation conditions, high electromechanical field concentrations near the electrode edge and existing micro-cracks demand application of fracture mechanics methods in order to correctly predict failure or reliability of MLA. The most crucial problem is the reliability of MLA under in-service electric operation. Hereby, only by cyclic electric fields a mechanical damage and failure is induced. This phenomenon limits the lifetime of the components. Details of ferroelectric ceramics cracking can be found in reviews [2,3].

The non-linear electromechanical behavior of ferroelectric bulk ceramics is due to domain-switching phenomenon caused by high electric fields. Early finite element (FE) models of actuators were mostly focused on linear piezoelectric behavior, which is a rough approximation of inherent non-linear electromechanical properties of ferroelectrics. In many simulations the electrical and mechanical fields are actually not fully coupled. In the present investigation a micromechanical material model, based on 3D tetragonal domain switching [4], is used.

The crack propagation mechanisms in the MLA are still under investigation due to the complex non-linear interactions between microstructure and electromechanical fields at the region close to the electrode edge. Lack of accurate experimental data is a consequence of several reasons. Strain gages provide only average strains in the local area because of the large size of the gages in comparison with the thickness of ceramic layers. Therefore deformations near the electrode edge cannot be measured. On the other hand, interferometry only provides limited pattern information in the small region near the electrode edge.

Experimental observations indicate that the electric-field induced cracks initiate from the electrode edge [5–7]. In most cases they propagate along the ceramic–electrode interface.

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http://dx.doi.org/10.1016/j.sna.2015.06.030

For simulation of damage initiation and evolution the concept of cohesive zone models is quite efficient, when one or several possible damage paths with embedded cohesive elements can be introduced a priori. Arias et al. [8] made first adaptation of the classical exponential cohesive zone model to ferroelectric materials to simulate electric fatigue, whereby some physical simplifications were made. Consecutive simulations with cohesive zone elements but with piezoelectric bulk behavior were performed by Utzinger et al. [9] and Verhoosel and Gutiérrez [10].

The coupled electromechanical cyclic cohesive zone model (EMCCZM) was suggested by Kozinov et al. [11] as an extension of the previously developed pure mechanical cyclic cohesive zone elements by Roth et al. [12]. Both mechanical and electric properties of the cohesive layer are taken into account in EMCCZM. The finite element implementation as cohesive zone elements was used to track the initiation and evolution of interface cracks during mechanical loading and/or electrical cycles.

The first numerical non-linear research of actuator was done by Hom and Shankar [13]. A fundamental study of multilayer actuator response incorporating the simulation of a ferroelectric hysteresis behavior was conducted by Kamlah and Böhle [14]. Paper by Zhao et al. [7] offered certain improvements and modifications. First coupled simulation of fracture and micro-structure evolution in MLA was done by Abdollahi and Arias [15].

A first fully coupled three-dimensional electromechanical model, considering domain switching together with the cohesive zone implementation, was recently elaborated by the authors [11].

The present analysis is based on a fully coupled electromechanical simulation with a cohesive zone application. It allows not only to study stresses and electric field in the critical regions of piezoceramic devices, but also to investigate possible gradual failure of the multilayer ferroelectric actuator, which (to the best of our knowledge) is done for the first time. In the earlier papers the main effort was put on the study of the electric quantities during poling and domain reorientation, while the present research pays attention to a fracture investigation. Poling process is the first step of the simulation, then followed by a cyclic electric loading of a constant amplitude.

2. Ferroelectric materials constitutive behavior and electromechanical cyclic cohesive zone model

Details of the constitutive behavior of piezo- and ferroelectric materials and explanation about advanced electromechanical cyclic cohesive zone model can be found in [11]. In this section only the main formulae and descriptions are presented.

Constitutive equations for a ferroelectric material in a fixed rectangular coordinate system $x_k (k = 1, 2, 3)$ have the form:

$$\sigma_{ij} = C_{ijls}(\epsilon_{ls} - \epsilon^r_{ls}) - e_{sij}E_s, \quad D_i = e_{ils}(\epsilon_{ls} - \epsilon^r_{ls}) + \kappa_{is}E_s + P^r_i. \tag{1}$$

where u_k, ϵ_{ls}, ϕ, σ_{ij}, D_i, E_i are mechanical displacements, strains, electric potential, mechanical stresses, electric displacements and electric field, respectively. ϵ^r_{kl} and P^r_i are remanent strain and polarization of the polycrystal. The coefficients C_{ijls} are elastic moduli, e_{sij} are piezoelectric constants and κ_{is} are dielectric permittivities. In Eqs. (1) the indices are ranging from 1 to 3.

Ferroelectric domains are such subregions of a ceramic grain, where all elementary cells have the same dipole orientation and identical spontaneous strain ϵ^{sp}_{kl} and polarization P^{sp}_i. If the dipole orientation is changed, the process is called domain switching.

The switching criterion used for each domain species is based on requirement of energy supply to overcome energy barrier [16]:

$$\sigma_{ij}\epsilon_{ij} + \sigma_{ij}\Delta\epsilon^{sp}_{ij} + E_iD_i + E_i\Delta P^{sp}_i \geq \omega_c. \tag{2}$$

Table 1
Material constants of the PZT-5H ceramics (polarized along x_1 axis) [2].

Elastic moduli	C_{1111}	117,000	MPa
	C_{2222}, C_{3333}	126,000	MPa
	C_{1122}, C_{1133}	53,000	MPa
	C_{2233}	55,000	MPa
	C_{1212}, C_{1313}	35,300	MPa
	C_{2323}	35,500	MPa
Dielectric constants	κ_{11}	0.0151	μF/m
	κ_{22}, κ_{33}	0.0130	μF/m
Piezoelectric constants	e_{111}	23.3	C/m^2
	e_{122}, e_{133}	−6.5	C/m^2
	e_{212}, e_{313}	17.0	C/m^2
Spontaneous polarization	P^{sp}	0.3	C/m^2
Coercive field strength	E_c	0.8	kV/mm
Spontaneous strain	ϵ^{sp}	0.3	%

According to [2] the critical energy barrier for domain switching is

$$\omega_c^{\pm 90^\circ} = \sqrt{2}P^{sp}E_c, \quad \omega_c^{180^\circ} = 2P^{sp}E_c. \tag{3}$$

For tetragonal domains, 90° switching alters spontaneous strain and polarization, 180° switching leads to spontaneous polarization change with no influence on the remanent strain value. During application of a strong electric loading (poling process), the domains reorient along the direction of the electric field. After termination of the external electric loading a remanent polarization P^r as well as a remanent strain ϵ^r remain.

By means of the non-linear Eqs. (1) the polarization and strain hysteresis loops in polycrystalline ferroelectric materials are described as a result of switching in accordance with criteria (2) and (3).

The micromechanical ferroelectric model [4] was implemented by [17] as user routine for the finite element code Abaqus©. The material properties for a lead zirconate titanate PZT-5H used for the numerical simulations are presented in Table 1.

The cohesive zone approach allows to model the whole damage process starting from crack formation until complete failure. The electromechanical cyclic cohesive zone model (EMCCZM) is briefly illustrated in Fig. 1.

Normalized effective traction t and normalized effective separation δ are introduced as following:

$$t = \sqrt{t_n^2 + t_r^2 + t_s^2}/t_0, \quad \delta = \sqrt{\langle\delta_n\rangle^2 + \delta_r^2 + \delta_s^2}/\delta_0. \tag{4}$$

Here t_0 denotes maximum cohesive traction, δ_0 – critical separation at maximum cohesive traction, indices n, r and s stand for normal and two tangential quantities, $\langle\delta_n\rangle = (\delta_n + |\delta_n|)/2$.

The total energy dissipated by the cohesive element under monotonic loading conditions is defined by the formula

$$\Gamma_0 = t_0\delta_0 \int_0^\infty t(\delta)d\delta. \tag{5}$$

Γ_0 is equal to the fracture energy for the piezoelectric/ferroelectric material.

The developed CZE is three-dimensional, but in the current simulation only normal opening occurs and shear components are zero due to symmetry.

The properties of the EMCCZM are defined by the traction-separation law (TSL) $t(\delta)$ (see Fig. 2) and are listed in Table 2.

Table 2
Material constants of the cohesive zone.

Fracture energy	Γ_0	2.34	N/m
Maximum cohesive traction	t_0	80	MPa
Critical separation	$\delta_0 = \Gamma_0/(et_0)$	10.76	nm
Thickness of a grain boundary	Δ_0	5	nm
Grain boundary permittivity at failure (air)	κ_0	8.854 $\times 10^{-6}$	μF/m
Initial grain boundary permittivity	$\kappa_0\kappa_r$	0.006	μF/m