Available online at www.sciencedirect.com

SCIENCE DIRECT®

Journal of the European Ceramic Society 25 (2005) 2467–2470

www.elsevier.com/locate/jeurceramsoc

Characterization and modelling of 3D piezoelectric ceramic structures with ATILA software

Esa Heinonen*, Jari Juuti, Seppo Leppävuori

University of Oulu, Microelectronics and Material Physics Laboratories, EMPART (Electronic Materials, Packaging and Reliability Techniques) Research Group of Infotech Oulu, Linnanmaa FIN-90570 Oulu, Finland

Available online 26 March 2005

Abstract

In this paper, the correspondence between ATILA-simulated and measured values of two piezoelectric ceramic structures, bulk and RAINBOW actuators, was determined. Modelling was started by creating a 2D wire model of the structures, after which a 3D model was created and simulation parameters were introduced (electric potentials, polarizations and boundary conditions). Harmonic type analysis was used in the simulations. The results obtained from the simulations contained information about displacements in the z-axis direction.

Displacements of the measured structures behaved nonlinearly as a function of the electric field. Accordingly, effective piezoelectric coefficients (i.e. d_{31}, d_{33}) calculated from the electric field and the displacement also changed nonlinearly. However, the displacement results acquired from simulations are linear, since the ATILA program uses a linear approach for in the calculation. This causes the modelling results to differ from the measurement results, especially when large voltages are used.

The problem was solved by modifying the constant parameters used in the simulations. In the study reported here, relative permittivity K_{33}, piezoelectric coefficient d_{33} and approximated piezoelectric coefficient d_{31} were used to obtain more accurate modelling results corresponding to the measurement results.

The differences in the z-axis displacements between the modelling (using the original material parameters) and measurement results obtained with bulk and RAINBOW actuators were 6.5–17.7% and 6.0–27.9%, respectively. With modified material parameters, the differences were 1.1–1.6% and 3.1–8.5%, respectively.

Keywords: ATILA; Actuators; PZT; Piezoelectric properties

1. Introduction

Different active materials and new actuator applications require thorough modelling before practical experiments are feasible. Modelling programs facilitate and speed up the design and development of new structures, especially optimization. The changes in different applications (i.e. size and shape) and their effects on the whole structure can be predicted, which also facilitates optimization.

The characteristics of the modelled structures are strongly dependent upon material-specific parameters. In the modelling software, parameters and modifications for designs can be altered easily and quickly. When designing the function of a component, different types of modelling software can also be used for problem-solving, particularly when the problem is perceived as difficult or nearly impossible to solve otherwise.

The aim of this paper is to define the correspondence between ATILA-simulated and measured values of piezoelectric ceramic structures. Frames for reliable simulation using the ATILA software were also determined. The modelled structures were bulk and RAINBOW actuators.

2. Experimental

The displacement measurement system used was based on Michelson's Interferometer. The z-axis displacement of the piezoelectric actuator's top surface was measured.[1,2] The

* Corresponding author. Tel.: +358 8 553 2734.
E-mail address: esa.heinonen@ee.oulu.fi (E. Heinonen).

0955-2219/$ – see front matter
doi:10.1016/j.jeurceramsoc.2005.03.083

Table 1
Material properties of the piezoelectric materials PZT-5H and PZT-5A and the elastic material lead

Material	Elastic compliance coefficients ($\times 10^{-12}$ m^2/N)					
	s_{11}	s_{12}	s_{13}	s_{33}	s_{44}	s_{66}
PZT-5H	16.5	−4.78	−8.45	20.7	43.5	42.56
PZT-5A	16.4	−5.74	−7.22	18.8	47.5	44.28

	Density (kg/m^3)	Piezoelectric coefficients ($\times 10^{-12}$ m/V)			Relative permittivity	
		d_{31}	d_{33}	d_{15}	$\varepsilon_{11}/\varepsilon_0$	$\varepsilon_{33}/\varepsilon_0$ (K_{33})
PZT-5H	7500	−274	593	741	1700	1470
PZT-5A	7750	−171	374	584	916	830

	Density (kg/m^3)	Young's modulus (N/m^2)	Poisson's ratio
Lead	11100	1.6E+10	0.45

material of the bulk actuator was PZT-5H. The RAINBOW actuator was manufactured from a commercial PZT-5A bulk disc (Morgan Electro Ceramics).[3,4] The voltage signal used in measurements was sinusoidal with an offset value of $V_{p–p}/2$ and frequencies of 100 Hz (bulk actuator) and 10 Hz (RAINBOW actuator).

The ATILA software used in this study was developed primarily to model actuators and transducers used in underwater applications.[5,6] ATILA uses FEM (Finite Element Method) to calculate the modelled structures. The software version used was 5.2.2, and it functioned in a Windows XP environment.

The modelling of all the structures was started by making a 2D wire model, which was further processed into a 3D model. The data needed for FEM calculations were also introduced, including the materials and parameters used, boundary conditions, polarizations and excitation signals. In the simulations, harmonic type analysis was used, and Cartesian polarization with Euler angles 0, 90, 0 (α, β and γ, respectively)[6] was applied to the materials; hence, the positive voltage was applied to the top surface of the structure and the ground to the bottom surface.

ATILA assumes the piezoelectric material to belong to the crystalline class 6 mm (hexagonal).[6] The material properties needed for FEM calculations are presented in Table 1. The materials used in the simulations and real structures were commercial, and the material properties were acquired from the manufacturers.[7] Some material parameters were modified during the modelling process; the modified parameters are listed in the context of each case.

2.1. Bulk actuator

In the measurement, the bulk actuator was clamped with a metal pivot (diameter 2 mm), which was attached to the bottom surface of the actuator.[2] The diameter of the bulk actuator was 10 mm and thickness 500 μm. The voltage values used in the measurements and simulations were 100–1000 V.

Table 2
Calculated d_{33} values of the bulk actuator

Voltage (V)	Displacement ($\times 10^{-9}$ m)	d_{33} values ($\times 10^{-12}$ m/V)
100	62	620
250	159	636
500	355	710
750	510	680
1000	641	641

The piezoelectric coefficients d_{33} shown in Table 2 were calculated from the displacement measurement results with formula (1).

$$d_{33} = \frac{\eta_3}{U_3} \tag{1}$$

η_3 is the displacement in the polarization direction (m) and U_3 the voltage in the polarization direction (V)

In the modelling, the actuator was clamped from the bottom surface of the clamping area, so that the displacements in the *x*-, *y*- and *z*-axis directions in that surface were zero. Two sets of simulations were calculated and compared to the measured results. In the first set, the material parameters used were those provided by the material manufacturer (Table 1). In the second set, the previously measured piezoelectric d_{33} values (Table 2) were used.

2.2. RAINBOW actuator

The edges of the RAINBOW actuator rested freely against the measurement jig. The electric field values used in the measurements and simulations were 0.5–1.25 kV/mm. The electric field values were calculated using minimum piezoelectric ceramic thickness (300 μm) at the centre of the actuator (Fig. 1). The RAINBOW actuator's relative permittivity in the polarization direction (K_{33}) was also measured as a function of the electric field, using the Radiant RTV6000HVS equipment. The measured relative permittivity values of the RAINBOW actuator can be seen in Table 3.

The radius of the RAINBOW actuator was 12.5 mm, thickness 500 μm, minimum thickness of the active mate-

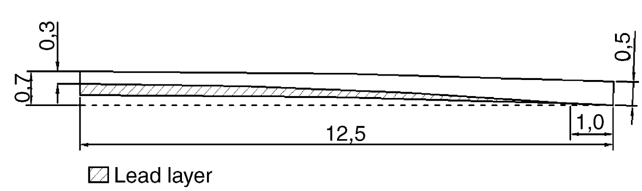

Fig. 1. 2D wire model of the RAINBOW actuator.

Table 3
Measured relative permittivity K_{33} values of the RAINBOW actuator

Electric field (kV/mm)	Relative permittivity K_{33}
0.5	1776
0.75	2597
1.0	3922
1.25	6155

Table 4
Approximated piezoelectric coefficient d_{31} values

Electric field (kV/mm)	Original d_{31} value ($\times 10^{-12}$ m/V)	Difference in displacement (%)	New d_{31} value ($\times 10^{-12}$ m/V)
0.5	−171	−16.28	−143
0.75	−171	5.98	−181
1.0	−171	17.23	−200
1.25	−171	27.94	−219

rial 300 μm at the centre and height 700 μm at the centre. On the bottom of the actuator was a 200 μm thick (at the centre) reduced lead layer, which started at 1 mm from the edge of the actuator. The 2D wire model of the RAINBOW actuator can be seen in Fig. 1.

The piezoelectric material of the actuator was PZT-5A. The passive material was elastic material lead. The properties of the reduced lead layer were assumed to be similar to those of pure lead[3] (Table 1). Clamping was applied from the edge of the actuator, so that displacement in the *z*-axis direction at that edge was zero.

Four sets of simulations were calculated and compared to the measurement results. In the first set, the material parameters given by the material manufacturer were used (Table 1). The measured relative permittivity K_{33}, shown in Table 3, was used in the second set of simulations.

The new piezoelectric coefficient d_{31} values were approximated from the first set of simulation results. The simulated *z*-axis displacements were compared to the measured results, from which a percentage difference was calculated. The acquired percentage differences were used to calculate new d_{31} values (i.e. if the difference was 5.98%, the new d_{31} value was 5.98% higher than the original). The approximated d_{31} values are shown in Table 4.

In the third set, the approximated piezoelectric coefficient d_{31} values (Table 4) were used. In the fourth set, both the measured relative permittivity values (Table 3) and the approximated d_{31} values (Table 4) were used.

3. Results and discussion

The displacements of the actuators changed nonlinearly as a function of electric field in the measurements. Therefore, the effective piezoelectric coefficients (i.e. d_{31}, d_{33}) calculated from voltage and displacement (formula (1)) change nonlinearly. When calculating displacements, the ATILA program uses constant material parameters for all electric field values (linear approach). This causes the modelling results to differ from the measurement results, especially when large voltages are used.

When the original parameters used by the ATILA program were adjusted, the correspondence between the modelling results and the measured results improved. When the measured d_{33} values were used in the case of the bulk actuator, the correspondence improved significantly, as it can be seen in Fig. 2.

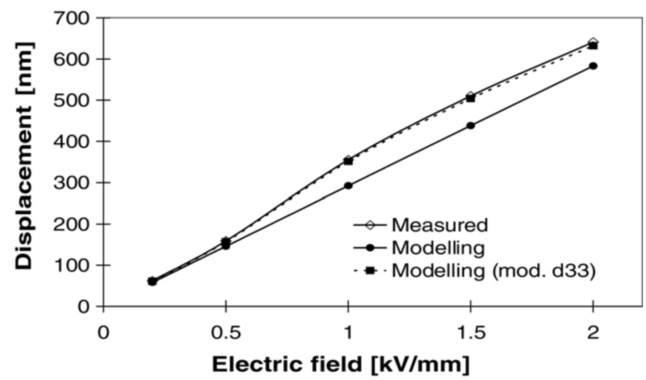

Fig. 2. Measured and modelled results of the *z*-axis displacement of the PZT-5H bulk actuator.

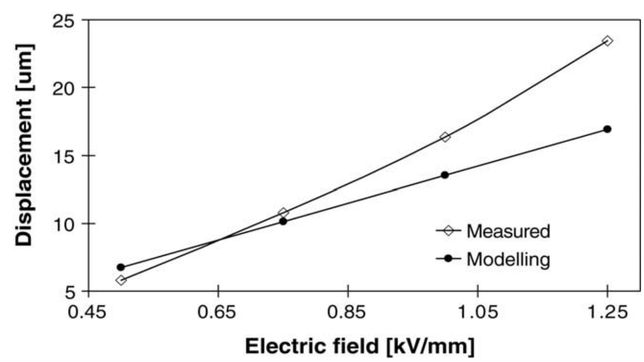

Fig. 3. Measured and modelled results of the *z*-axis displacement of the PZT-5A RAINBOW actuator (using original material parameters in simulation).

The four sets of modelling results of the RAINBOW actuator compared to the measured results are presented in Figs. 3–6. The simulation results of the RAINBOW actuator improved significantly, especially when modified d_{31} or

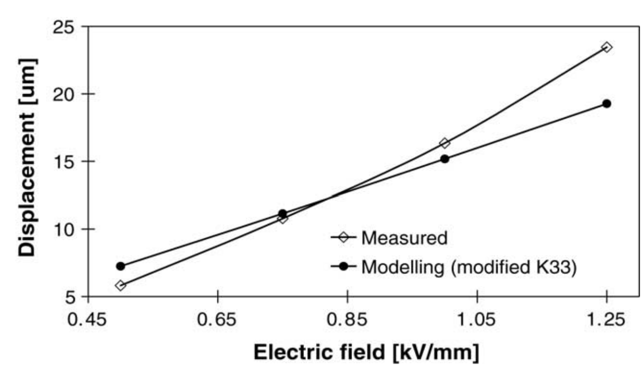

Fig. 4. Measured and modelled results of the *z*-axis displacement of the PZT-5A RAINBOW actuator (using modified K_{33} values in simulation).

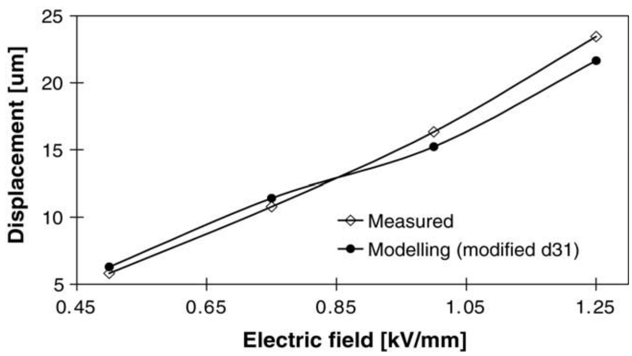

Fig. 5. Measured and modelled results of the *z*-axis displacement of the PZT-5A RAINBOW actuator (using modified d_{31} values in simulation).

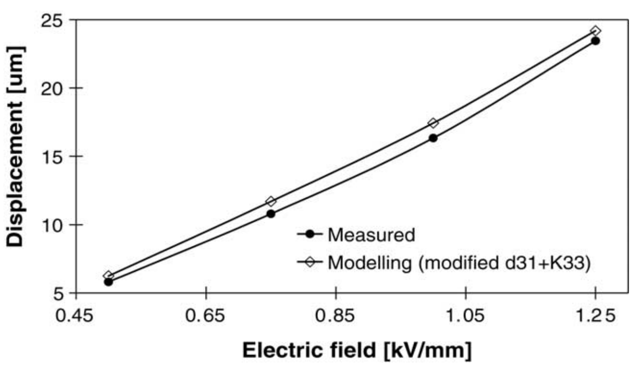

Fig. 6. Measured and modelled results of the *z*-axis displacement of the PZT-5A RAINBOW actuator (using modified $d_{31} + K_{33}$ values in simulation).

both modified d_{31} and modified K_{33} values were used, which can be seen in Figs. 5 and 6, respectively.

4. Conclusions

The linear approach of the ATILA software caused simulation results to differ from measured results, especially when large voltages were used. When measured/calculated material parameters and values approximated with feedback calculations were used, the correspondence between modelling and real results improved significantly. The differences of the *z*-axis displacements between the modelled (using the original material parameters) and measured results obtained with the bulk and RAINBOW actuators were 6.5–17.7% and 6.0–27.9%, respectively. When modified material parameters were used, the differences were 1.1–1.6% and 3.1–8.5%, respectively.

Acknowledgements

The work was performed within the project "Novel ceramic technologies in the realisation of miniature actuators and motors" (project 49830, TUKEVA programme) funded by the Academy of Finland and Finnish National Technology Agency (project 52059, PRESTO programme). The author (E.H.) also acknowledges the financial support of the Seppo Säynäjäkankaan tiedesäätiö.

References

1. Moilanen, H. and Leppävuori, S., Determination of low-voltage actuator displacements in d.c. and a.c. electric fields using an optical interferometer. *Sens. Actuators A, Elsevier Sequoia*, 1993, **37–38**, 555–560.
2. Moilanen, H. and Leppävuori, S., Laser interferometric measurements of displacement-field characteristics of piezoelectric actuators and actuator materials. *Sens. Actuators A (Phys.)*, 2001, **A92**, 236–334.
3. Juuti, J., Moilanen, H. and Leppävuori, S., Manufacturing of Rainbow actuators for displacement applications. *Proc. 2nd Euspen Int. Conf.*, 2001, **1**, 204–207.
4. Juuti, J., Heinonen, E., Moilanen, V.-P. and Leppävuori, S., Displacement, stiffness and load behaviour of laser-cut RAINBOW actuators. *J. Eur. Ceram. Soc.*, 2004, **24**(6), 1901–1904.
5. Hladky-Hennion, A. C., Bossut, R., Alkoy, S., Lopath, P. and Newnham, R. E., Finite element modeling of transduction materials with application to piezoelectric hollow sphere transducers. *Proc. IEEE Int. Frequency Control Symp.*, 1998, 709–714.
6. Cedrat Recherche, *ATILA Finite Element Analysis for Piezoelectric and Magnetostrictive Structures Version 5.2.2. User's Manual*, Inst. Sup. d'Electron. du Nord Acoustics Laboratory, Lille Cedex, France, 2003.
7. Berlincourt, D., Krueger, H. H. A. and Near, C., *Technical Publication TP-226 Properties of Piezoelectricity Ceramics*. Technical Publication, Morgan Electro Ceramics, 2003.