Modelling of ferroic material behaviour of piezoelectrics: Characterisation of temperature sensitive functional properties

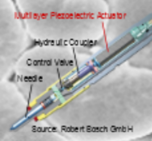
Hannes Grünbichler[1], Josef Kreith[2], Raúl Bermejo[1,2], Peter Supancic[1,2] and Robert Danzer[1,2]

[1] Institute for Structural and Functional Ceramics, University of Leoben, Franz-Josef-Straße 18, 8700 Leoben, Austria
[2] Materials Center Leoben Forschung GmbH, Roseggerstraße 12, 8700 Leoben, Austria
Corresponding author's email address: hannes.gruenbichler@unileoben.ac.at

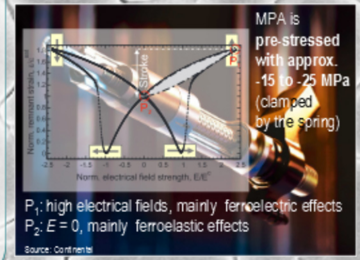
Introduction

Modern piezoelectric devices like low-voltage actuators consist of stacks of piezo-ceramic layers with interdigitated metallic electrodes in between. During application mechanical stresses are inherent loading scenarios of such electro-mechanical converters. ***A deep knowledge of the coupling*** phenomena ***among*** the field-type quantities such as ***mechanical stresses, electrical field strengths and temperature is absolutely necessary*** to guarantee demanded structural and functional integrity.

Theoretical simulations are the only way to obtain these (in detail unknown) physical relevant field-quantities within MPAs. Hence, for FE-simulations of the highly nonlinear piezoelectric material behavior, basic modelling parameters have to be determined. ***Usually,*** the ***constitutive material laws*** implemented into FEA-tools ***are parameterised by experiments*** under distinct thermo-electro-mechanical loading conditions ***performed on homogenous bulk ceramics to evaluate pure material properties***.



Source: Robert Bosch GmbH



P_1: high electrical fields, mainly ferroelectric effects
P_2: $E = 0$, mainly ferroelastic effects

Source: Continental

Material of study

RE_2O_3-$PbTiO_3$-$PbZrO_3$ ternary phase system incorporating approximately 2–3 % of the rare earth oxide in the vicinity of the morphotropic phase boundary (MPB) of PZT in the tetragonal range. The rare earth in the composition acts as a donor to make the material "soft."

Density:	7.85 ± 0.01 kg·m^{-3}
Average grain size:	1.4 ± 0.1 µm
Porosity:	1.4 ± 0.1 %
Hardness (HV1):	3.9 ± 0.1 GPa
Toughness:	0.9 ± 0.1 MPa·m^{½}
Average strength:	100 ± 10 MPa

Theoretical frame: the model

The basic assumption in order to model the nonlinear piezo-electricity is the additive decomposition of the dielectric displacement and total strain into *reversible* and *remnant*, contributions, respectively.

history-dependent anisotropy

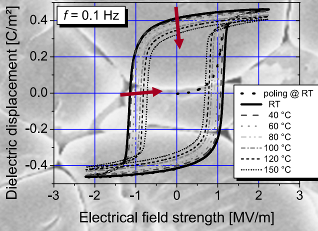
$$\overset{\leftrightarrow}{\varepsilon} = \overset{\leftrightarrow}{\varepsilon}^{rev} + \overset{\leftrightarrow}{\varepsilon}^{rem} \qquad \overset{\leftrightarrow}{\varepsilon}^{rev} = \overset{\leftrightarrow}{\overset{\leftrightarrow}{C}} \cdot\cdot \overset{\leftrightarrow}{\sigma} + \boxed{\overset{\leftrightarrow}{\vec{d}}^{T}} \cdot \vec{E}$$

$$\vec{P} = \vec{P}^{rev} + \vec{P}^{rem} \qquad \vec{P}^{rev} = \overset{\leftrightarrow}{\vec{d}} \cdot\cdot \overset{\leftrightarrow}{\sigma} + \boxed{\overset{\leftrightarrow}{\kappa}} \cdot \vec{E}$$

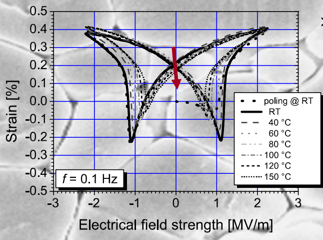
The constitutive law utilised in this work is ***based on concepts of plasticity***; ***sc. a switching criterion, an associated flow rule and purely kinematic hardening*** to describe the cyclic response. Hence, the evolution equations are defined on the basis of switching criteria. For pure ferroelectric behaviour such an evolution equ. is given by:

$$\dot{\vec{P}}^{\vec{E}} = Tr_1\left(f^{\vec{E}}\right) \cdot Tr_2\left(h^{\vec{E}}\right) \cdot \frac{\dot{\vec{E}}}{c^{\vec{E}}\left(P^{\vec{E}}\right)}$$

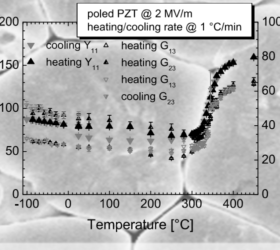
Experimental: measurements



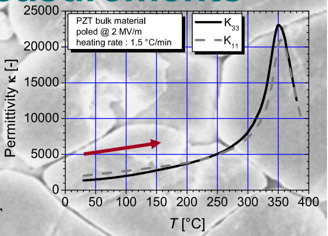
At heightened temperatures the coercive and remnant quantities diminish (cf. the corresponding shift inwards) but the values for the permittivity and the piezoelectric voltage coefficient (slope becomes steeper) increase.



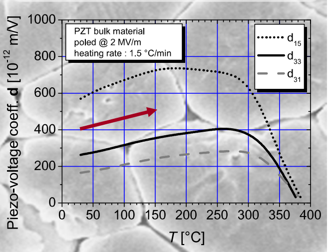
Material properties as function of temperature



The effective elastic modulus is nearly constant up to the Curie temperature, i.e. approx. 350 °C, where the phase transition takes place. Here, the elastic modulus doubles the value at room temperature (RT). The symbols ▲, ▼ represent the heating and cooling period, respectively.

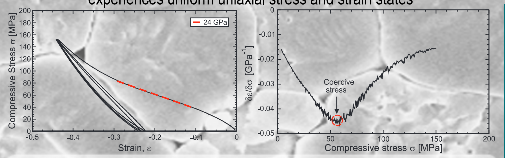


Dependence on temperature of the permittivity and the piezoelectric voltage coefficients; dynamically measured (kHz-range). At evaluated temperatures these quantities increase significantly up to close to Curie temperature.



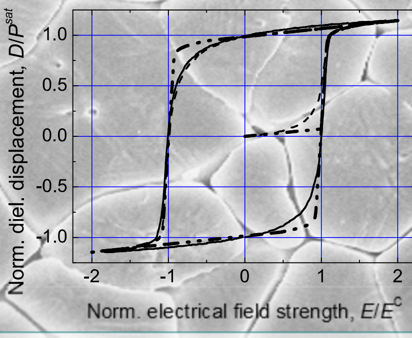
Ferroelastic measurements:

An aspect ratio of nearly 5:1 ensures that the significant central region of the sample experiences uniform uniaxial stress and strain states

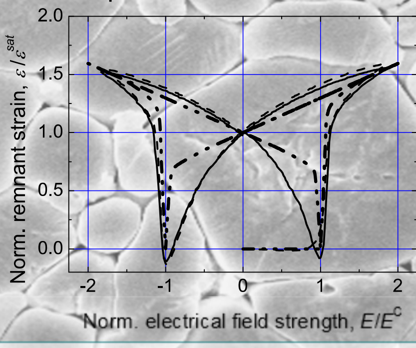


Uniaxial compression tests were performed on piezoceramic bodies (3.5 × 5 × 25 mm³). The stress-strain loops indicate the strongly non-linear ferroelastic behaviour. At coercive stress a maximum of domains align perpendicular to the external applied mechanical load (the value of the tangent modulus reaches a minimum at this point).

Modelled vs. measured dielectric loops of a moderate pre-stressed PZT-ceramic



Modelled vs. measured butterfly loops of a moderate pre-stressed PZT-ceramic



Results and conclusions

Comparison of the computed results (dashed-double-dotted) with the experiments (dashed; line). The dashed line indicates the poling loop of a native "virginal" material at ambient temperature and the solid line a 2nd bipolar loop.

In this study basic modelling-parameters have been determined enabling the parameterisation of the chosen constitutive law. A comparison of the modelled loops with the experiments shows consistency in the basic model assumptions for ambient temperatures. In future, the strong temperature dependence of the modelling parameters will be taken into account. For moderate pre-stressed MPAs (indeed the coercive stress is three times the typical pre-stress of a multilayer piezoelectric actuator stack) this model is satisfactory for describing their behaviour. In future investigations the ferroelastic, thermal coupling effects and a combination of both the isotropic and kinematic hardening will be furthermore considered.

Acknowledgements

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