IUTAM Symposium on Multiscale Modelling of Fatigue, Damage and Fracture in Smart Materials
IUTAM BOOKSERIES
Volume 24

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IUTAM Symposium on Multiscale Modelling of Fatigue, Damage and Fracture in Smart Materials

Proceedings of the IUTAM Symposium on Multiscale Modelling of Fatigue, Damage and Fracture in Smart Materials, held in Freiberg, Germany, September 1–4, 2009
Preface

Multi-functional materials as piezoelectric/ferroelectric ceramics, magnetostrictive and shape memory alloys are gaining increasing applications as sensors, actuators or smart composite materials systems for promising high tech areas. One primary problem is, however, that these functional materials suffer from various mechanical and/or electromagnetical degradation mechanisms as fatigue, damage and fracture. As a consequence of field coupling effects, fabrication processes and service loads, smart materials systems are exposed to high mechanical and/or electromagnetical field concentrations under internal and external loading of static, cyclic and dynamic type. For this reason, the investigation of fatigue, damage and fracture plays a decisive role for the optimum design, reliability and durability of smart materials systems. Thus, the topic of the symposium represents an active international research area in mechanics of materials. From the experience and investigations during the last decade it has become evident that progress in this scientific discipline is only possible, if material models are based on the true physical nature of the phenomena and if theoretical predictions are verified by skilful experiments. Therefore, the scientific challenges can only be solved by

- A multi-scale modelling at several length scales from atomistic to macroscopic level
- An interdisciplinary cooperation between solid mechanics, materials science and physics

To promote the international scientific exchange in this important field, in 2006 the General Assembly of IUTAM approved the proposal to host this symposium in Freiberg, Germany and appointed the International Scientific Committee. The IUTAM Symposium (GA. 06-16) “Multiscale Modelling of Fatigue, Damage and Fracture in Smart Materials Systems” was held on September 1–4, 2009 at Technische Universität Bergakademie Freiberg, Germany, organized by the Institute of Mechanics and Fluid Dynamics.

This symposium stands in a line with former symposia on related topics held under the auspices of IUTAM in 2000 at Magdeburg and in 2004 at Beijing. The helpful assistance of the International Scientific Committee to communicate the symposium and to recommend invited speakers is thankfully appreciated.
According to the rules and tradition of IUTAM, the aim of the Symposium is to bring together internationally leading researchers working in the area of smart materials. The goal is to exchange recent scientific results, to discuss new achievement and actual problems in an open and frank atmosphere. The organizers were happy to welcome a lot of outstanding scientists in this field from all parts of the globe as well as many young researchers. In total there were 44 participants coming from 14 countries: Australia (1), Austria (3), Belgium (1), Canada (1), China (8), Great Britain (1), France (2), Germany (19), Israel (1), Italy (1), Japan (2), Slovakia (1), Ukraine (1) and USA (2). The scientific program covered 35 invited oral contributions presented in 10 sessions.

The following main topics have been addressed during the symposium:

- Development of computational methods for coupled electromechanical field analysis, especially extended, adaptive and multi-level finite element techniques in combination with boundary elements.
- Constitutive modeling of smart materials with coupled electric, magnetic, thermal and mechanical fields, especially of nonlinear dissipative hysteretic behavior. Major trend is the development of micromechanical models. Especially for ferroelectric materials and shape memory alloys the simulation of microstructure (domain switching, martensitic transformation etc.) are of paramount concern.
- Further understanding and modeling of fracture and fatigue in piezoelectric and ferroelectric ceramics, especially the modeling of fracture process zone and of electric boundary conditions at crack faces. Applications of phase field simulation and configurational mechanics.
- Reliability and durability of sensors and actuators under in service loading by alternating mechanical, electrical and thermal fields. The role of interface cracks between layers and in thin films is addressed.
- Experimental methods to measure fracture strength and to investigate fatigue crack growth in ferroelectric materials under electromechanical loading. It has been pointed out that complicated theoretical predictions have to be contrasted and verified by skillful experiments.
- New ferroelectric materials, compounds and composites with enhanced strain capabilities.

The chairman and its organizing team tried to make this IUTAM symposium not only a successful scientific meeting but an outstanding social event, too. Many thanks are due to Prof. Dr. A. Ricoeur, who carried the main workload in organizing all details of this symposium.

The Technische Universität Bergakademie Freiberg is located in the East German Federal State Saxony. Besides Dresden and Chemnitz, TU Bergakademie Freiberg is considered as the “smallest” but “smartest” among these Technical Universities. Its history started with the discovery of silver in the middle ages. The “Mining Academy” Freiberg was founded by the Saxon King in 1765 in order to promote the technologies in surveying, mining and metallurgy. Thus, TU Bergakademie Freiberg possesses a long and famous tradition as one of the oldest mountainistic universities in the world. Nowadays, TU Bergakademie Freiberg is established as modern
Technical University focusing mainly on Geoscience, Resources, Materials Science, Energy and Environmental Technologies.

Freiberg has one of the largest and most splendid mineralogical exhibitions “Terra Mineralia” in the world hosted in the old castle “Freudenstein”. The participants of the symposium enjoyed the visit very much.

Freiberg, 2009

Meinhard Kuna
Chairman of the Symposium
International Scientific Committee

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Meinhard Kuna (Chair, Germany)
Andreas Ricoeur (Germany)

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Scientific Program

Tuesday, September 01

Opening and Welcome Address by the Chairman of the Symposium M. Kuna

Fracture Mechanics I (session leader: T. Kitamura)

Leslie Banks-Sills, Yael Motola: “Failure of piezoelectric ceramics”

Gerold Schneider, A. Engert, H. Jelitto: “What do we know about crack surface charges and the difference between intrinsic and extrinsic process during fracture in ferroelectric ceramics?”

Yasuhide Shindo, Fumio Narita: “Effects of electric field and poling on fatigue behavior of PZT ceramics with single-edge crack by three-point bending”

Daining Fang, Yihui Zhang, Guanzhong Mao, Bin Liu: “Electric field induced fatigue crack growth in ferroelectric ceramics”

Shape Memory Alloys I (session leader: C. Lexcellent)

Martin F.-X. Wagner, Christian Grossmann, Marcus Young, Gunther Eggeler: “Localized deformation, mesoscopic phase interfaces and functional fatigue in pseudoelastic NiTi shape memory alloys”

**Ferroelectrics I** (session leader: R. McMeeking)

Artem S. Semenov, Albrecht C. Liskowsky, Herbert Balke: “Effective computational methods for the modeling of ferroelectroelastic hysteresis behavior”

Stephan Roth, Peter Neumeister, Artem Semenov, Herbert Balke: “Finite element simulation of the non-remanent straining ferroelectric material behaviour based on the electric scalar potential – convergence and stability”

Li Yu, Shouwen Yu, Dietmar Gross: “Constitutive behaviour of nano-particle ferroelectric ceramics”

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**Wednesday, September 02**

**Ferroelectrics II** (session leader: J. Huber)

Faxin Li: “An optimization-based computational model for polycrystalline ferroelectrics”

Ralf Müller, David Schrade, Baixiang Xu, Dietmar Gross: “Modelling of domain structure evolution in ferroelectric materials”

Qun Li, Marco Enderlein, Meinhard Kuna: “Microstructural FEM modeling of domain switching in tetragonal/rhombohedral ferroelectrics”

Sven Klinkel, K. Linnemann: “A phenomenological constitutive model for piezoelectric ceramics and magnetostrictive materials”

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**Shape Memory Alloys II** (session leader: F. Auricchio)

Christian Lexcellent, R. Laydi, V. Taillebot, P. Malecot: “Prediction of the phase transformation zone around the crack tip of a shape memory alloy exhibiting an asymmetry between tension and compression”

Thomas Antretter, Wolfgang Pranger, Thomas Waitz, Franz D. Fischer: “Martensite morphologies in nanostructured NiTi shape memory alloys – energetic considerations”

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**Fracture Mechanics II** (session leader: L. Banks-Sills)

Duc Khoi Vu, Paul Steinmann: “The concept of material forces and the coupled boundary-finite element method in electroelastostatics”
Cun-Fa Gao, Yiu-Wing Mai: “Stresses in an electrostrictive solid containing an elliptic cavity”

Eric Béchet, Meinhard Kuna: “Some numerical experiments about cracked piezoelectric media”

Qing-Hua Qin, X.Q. He, J.S. Wang: “Singularity analysis of electro-mechanical fields in angularly inhomogeneous piezoelectric composites wedges”

Thursday, September 03

Fracture Mechanics III (session leader: Y. Shindo)

Jie Wang, Marc Kamlah: “Three dimensional finite element modeling of nonlinear fracture of ferroelectric materials”

Ł. Janski, P. Steinhorst, M. Kuna: “Crack propagation simulations in piezoelectric structures with an efficient adaptive finite element tool”

Volodymyr Loboda, S.V. Kozinov: “Periodic set of interface cracks with limited electric permeability”

Fulin Shang, Yabin Yan, Takayuki Kitamura: “Interfacial delamination of PZT thin films”

Nano (session leader: J. Schröder)

Karsten Albe, Paul Erhart: “Modelling of point defects in ferroelectric materials”

Takayuki Kitamura, Takashi Sumigawa, Taisuke Sueta: “Mechanical behaviour of thin film comprised of sculptured nano-elements”

Actuators (session leader: J. Rödel)


Ayech Benjeddou, Mohammad Al-Ajmi: “Analytical homogenization of piezoceramic shear macro-fibre composites”

Hannes Grünbichler, Raúl Bermejo, Peter Supancic, Robert Danzer: “Influence of the load dependent material properties on the performance of multilayer piezoelectric actuators”
Technical Visit: Laboratories of the host Institute of Mechanics and Fluid Dynamics

Friday, September 04

Ferroelectrics III (session leader: S. Yu)

Robert McMeeking, S.M.A. Jimenez: “Models for actuation, failure and tearing of electroactive materials”

Fei Fang, W. Yang, X. Luo: “In-situ observations of multi-phase coexistence and polarization rotation under electric loadings for Pb(Mg_{1/3}Nb_{2/3})O_3-PbTiO_3 single crystals at the morphotropic phase boundary”

Jörg Schröder, Marc-André Keip: “Multiscale modeling of electromechanically coupled materials: homogenization procedure and computation of overall moduli”

Kaushik Dayal, Kaushik Bhattacharya: “A boundary element method coupled to phase field to compute ferroelectric domains in complex geometries”


Nien-Ti Tsou, Ingo Münch, John Huber: “Low energy periodic microstructure in ferroelectric single crystals”

Closing Address: M. Kuna
A Fracture Criterion for Piezoelectric Material

Leslie Banks-Sills and Yael Motola

Abstract  A fracture criterion for piezoelectric ceramics is proposed which is based upon the energy release rate and two phase angles determined from the ratio between the intensity factors. It is assumed that the crack plane is at an angle to the poling direction within a symmetry plane of the body. The special cases of a crack perpendicular and parallel to the poling direction are presented. This criterion was implemented with experimental results from the literature in which the crack faces were perpendicular to the poling direction and the applied electric field. Excellent agreement was found between the fracture curve and the experimental results.

1 Introduction

Piezoelectric ceramics are in widespread use as sensors and actuators in smart structures, despite the absence of a fundamental understanding of their fracture behavior. Piezoceramics are brittle and susceptible to cracking. As a result of the importance of the reliability of these devices, there has been tremendous interest in studying the fracture and failure behavior of such materials. To understand failure mechanisms of piezoelectric materials and maintain the stability of cracked piezoelectric structures operating in an environment of combined electro-mechanical loading, analysis of its mechanical and electrical behavior is a prerequisite.

For cracks in piezoelectric material, there are three stress intensity factors $K_I$, $K_{II}$ and $K_{III}$, representing the usual three deformation modes, and an electric flux density intensity factor $K_{IV}$. Depending on the applied load and electric field, as well as the poling direction relative to the crack faces, various modes are excited. In this paper, a fracture criterion, presented in Section 2, is proposed based upon the energy release rate and two phase angles determined from the ratio between the

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intensity factors. It is assumed that the crack plane is at an angle to the poling direction within a symmetry plane of the body. Four point bend fracture tests carried out in [1] were analyzed in [2] to obtain the non-zero intensity factors $K_I$ and $K_{IV}$. These values are used to obtain a fracture criterion for this material (PIC-151) when the crack faces are perpendicular to the poling direction and the electric field. These results are presented in Section 3.

2 Fracture Criterion

A mixed mode fracture criterion is developed for piezoelectric ceramics. This criterion is based upon the energy release rate and one or two phase angles, determined from the ratio between the intensity factors. It is assumed that the crack plane is at an angle to the poling direction with poling within a symmetry plane of the body. The special cases of a crack perpendicular and parallel to the poling direction are presented, as well.

A general expression for the energy release rate for piezoelectric ceramics was derived in [3] as

$$\mathcal{G} = \frac{1}{2} k^T L^{-1} k \tag{1}$$

where $k$ is the intensity factor vector defined as

$$k^T = [K_{II}, K_I, K_{III}, K_{IV}] \tag{2}$$

where the superscript $T$ represents transpose. The matrix $L$ is one of the Barnett–Lothe tensors [4] whose components are related to material properties. Based on Eq. 1, the energy release rate for a crack at an angle to the poling direction with poling within a symmetry plane is obtained as

$$\mathcal{G} = \frac{1}{2} \left( \hat{L}_{22}^{-1} \hat{K}_{II}^2 + \hat{L}_{11}^{-1} \hat{K}_{II}^2 + \hat{L}_{44}^{-1} \hat{K}_{IV}^2 + 2\hat{L}_{12}^{-1} \hat{K}_I \hat{K}_{II} + 2\hat{L}_{14}^{-1} \hat{K}_{II} \hat{K}_{IV} + 2\hat{L}_{24}^{-1} \hat{K}_I \hat{K}_{IV} \right). \tag{3}$$

Out-of-plane loading is omitted here. The parameters $\hat{L}_{11}^{-1}, \hat{L}_{12}^{-1}, \hat{L}_{14}^{-1}, \hat{L}_{22}^{-1}, \hat{L}_{24}^{-1}$ and $\hat{L}_{44}^{-1}$ in Eq. 3 are given by

$$\begin{align*}
\hat{L}_{11}^{-1} &= E_A^2 L_{11}^{-1} L, \\
\hat{L}_{12}^{-1} &= E_A^2 L_{12}^{-1} L, \\
\hat{L}_{14}^{-1} &= E_A e_{26} L_{14}^{-1} L, \\
\hat{L}_{22}^{-1} &= E_A^2 L_{22}^{-1} L, \\
\hat{L}_{24}^{-1} &= E_A e_{26} L_{24}^{-1} L, \\
\hat{L}_{44}^{-1} &= e_{26}^2 L_{44}^{-1} L
\end{align*} \tag{4}$$

where $L_{ij}^{-1}$ are elements of the matrix $L^{-1}$, $E_A$ and $e_{26}$ are the Young’s modulus in the poling direction and a piezoelectric coupling coefficient, respectively, and $L$ is a characteristic length of the problem. The Barnett–Lothe tensor $L^{-1}$ is ill-conditioned. Hence, it was normalized as

$$\hat{L}^{-1} = VL^{-1}V \tag{5}$$
where

\[
\mathbf{V} = \begin{bmatrix}
E_A \sqrt{L} & 0 & 0 & 0 \\
0 & E_A \sqrt{L} & 0 & 0 \\
0 & 0 & G_T \sqrt{L} & 0 \\
0 & 0 & 0 & e_{26} \sqrt{L}
\end{bmatrix}
\]

(6)

and \(G_T\) is the shear modulus perpendicular to the poling direction. In this way, the diagonal and off-diagonal elements are the same order of magnitude [5]. It is worth mentioning that the units of \(O_{ij}/NUL\) are N/m. Finally, the intensity factors in Eq. 3 are normalized according to

\[
\hat{K}_I = \frac{K_I}{E_A \sqrt{L}}, \quad \hat{K}_{II} = \frac{K_{II}}{E_A \sqrt{L}}, \quad \hat{K}_{IV} = \frac{K_{IV}}{e_{26} \sqrt{L}}.
\]

(7)

The energy release rate \(G\) may be rewritten as

\[
G = \frac{1}{2} \hat{\mathbf{L}}_{22}^{-1} \hat{\mathbf{K}}_I^2 \left( 1 + 2 \frac{\hat{L}_{24}^{-1} \hat{K}_{IV}}{\hat{K}_I} + 2 \frac{\hat{L}_{12}^{-1} \hat{K}_{II}}{\hat{K}_I} + 2 \frac{\hat{L}_{14}^{-1} \hat{K}_{II} \hat{K}_{IV}}{\hat{K}_I^2} + 2 \frac{\hat{L}_{11}^{-1} \hat{K}_{II} \hat{K}_{IV}}{\hat{K}_I^2} \right). \tag{8}
\]

Thus, it is possible to define

\[
G_I \equiv \frac{1}{2} \hat{\mathbf{L}}_{22}^{-1} \hat{\mathbf{K}}_I^2.
\]

(9)

When the crack propagates \(G = G_c\), so that

\[
G_c = G_{Ic} \left( 1 + 2 \frac{\hat{L}_{24}^{-1} \hat{K}_{IV}}{\hat{K}_I} + 2 \frac{\hat{L}_{12}^{-1} \hat{K}_{II}}{\hat{K}_I} + 2 \frac{\hat{L}_{14}^{-1} \hat{K}_{II} \hat{K}_{IV}}{\hat{K}_I^2} + 2 \frac{\hat{L}_{11}^{-1} \hat{K}_{II} \hat{K}_{IV}}{\hat{K}_I^2} \right)
\]

(10)

where

\[
G_{Ic} = \frac{1}{2} \hat{\mathbf{L}}_{22}^{-1} \hat{\mathbf{K}}_{Ic}^2.
\]

(11)

To obtain \(G_{Ic}\), values of \(G_I\) from Eq. 9 are obtained at failure for each test and averaged, as will be discussed in Section 3. Introducing two phase angles

\[
\psi = \tan^{-1} \frac{\hat{K}_{IV}}{\hat{K}_I}, \quad \phi = \tan^{-1} \frac{\hat{K}_{II}}{\hat{K}_I},
\]

(12)
Equation 10 becomes

\[ G_c = G_{Ic} \left( 1 + 2 \frac{\hat{L}_{24}^{-1}}{\hat{L}_{22}^{-1}} \tan \psi + 2 \frac{\hat{L}_{12}^{-1}}{\hat{L}_{22}^{-1}} \tan \phi + 2 \frac{\hat{L}_{14}^{-1}}{\hat{L}_{22}^{-1}} \tan \psi \tan \phi + \frac{\hat{L}_{44}^{-1}}{\hat{L}_{22}^{-1}} \tan^2 \psi \right. \]

\[ + \left. \frac{\hat{L}_{11}^{-1}}{\hat{L}_{22}^{-1}} \tan^2 \phi \right). \] 

(13)

This is a three-dimensional failure surface for the case in which the crack faces are at an angle to the poling direction and in which the critical energy release rate \( G_c \) is a function of the phase angles \( \psi \) and \( \phi \).

For a crack perpendicular to the poling direction, the component \( \hat{K}_{14} \) is zero. In addition, for symmetric applied loading and electric field, \( \hat{K}_{II} \) was found to be negligible [2]. Therefore, for this case, there is only one non-zero phase angle \( \psi \) given in Eq. 12 leading to the failure curve

\[ G_c = G_{Ic} \left( 1 + 2 \frac{\hat{L}_{24}^{-1}}{\hat{L}_{22}^{-1}} \tan \psi + \frac{\hat{L}_{44}^{-1}}{\hat{L}_{22}^{-1}} \tan^2 \psi \right). \] 

(14)

For a crack perpendicular to the poling direction, there is coupling between the first and fourth modes of fracture. This coupling is expressed by the second term in the parentheses of the right hand side of Eq. 14.

For a crack parallel to the poling direction, \( \hat{L}_{24}^{-1} \) is zero. In addition, if both the applied loading and electric field are symmetric, then \( \hat{K}_{II} \) is negligible (implying \( \phi = 0 \)) and there is nearly no coupling between modes I and IV (see [2]). Thus, the failure curve for a crack parallel to the poling direction with symmetric applied loading and electric field may be found based on Eq. 13 as

\[ G_c = G_{Ic} \left( 1 + \frac{\hat{L}_{44}^{-1}}{\hat{L}_{22}^{-1}} \tan^2 \psi \right). \] 

(15)

### 3 Fracture Tests

Tests were reported in [1] on four-point bend specimens (see Fig. 1) fabricated from the piezoelectric ceramic PIC-151. In these experiments the crack faces were perpendicular to the poling direction and both mechanical loads and electric fields were applied. The dimensions of the specimens are \( L = 24 \), \( S_1 = 20 \), \( S_2 = 10 \) mm, the width \( W = 4 \) mm and the thickness \( B = 3 \) mm (see Fig. 1). The samples were placed in a Fluorinert-liquid to prevent electric sparks; this material is dielectrically isotropic with the permittivity \( \kappa_a = 1.75\kappa_0 \).

Using the same boundary conditions applied in the tests [1], numerical analyses were carried in [2]. These included the finite element method and the interaction
energy or $M$-integral for obtaining the intensity factors. The Fluorinert-liquid within the notch was modeled as a dielectric isotropic material. Average values of $\hat{K}_I$ and $\hat{K}_{IV}$, given in Eqs. 7 and 7, respectively, with application of different loads and electric fields for all notch lengths were determined. In Eqs. 7, $E_A = 60.2$ GPa, as calculated according to material properties given in [1] and $\epsilon_{26} = 12.0$ C/m$^2$. Results for $\hat{K}_{II}$ were negligible in comparison to the other intensity factors.

Values of $\hat{K}_{IV}$ are plotted versus those of $\hat{K}_I$ and presented in Fig. 2. It is observed that values of $\hat{K}_I$ are relatively constant with respect to $\hat{K}_{IV}$. The average value of $\hat{K}_I$, obtained for all points, is $1.44 \times 10^{-5}$. This leads to an average value
of the mode I stress intensity factor $K_I = 0.86 \text{ MPa}\sqrt{\text{m}}$ and $K_{IV}$ ranges between $-0.46 \times 10^{-3}$ and $0.82 \times 10^{-3} \text{ C/m}^{3/2}$.

The fracture criterion in Eq. 14 is applied using the intensity factors in Table 6 of [2] and presented in Fig. 2. From those values and with $\hat{K}_{II} = 0$, the critical energy release rate $\mathcal{G}_c$ and the phase angle $\psi$ were calculated using Eqs. 3 and 12 for each test. It was found that some of the values of the critical energy release rate are negative or close to zero; hence, these values are not physically plausible. It is possible that this phenomenon occurs because of a large domain switching zone in the vicinity of the notch tip. This aspect of the problem will be examined in the future. The calculated points are plotted as the colored symbols in Fig. 3 omitting those points in which $\mathcal{G}_c \leq 0$. In addition, Eq. 14 is plotted as the solid curve in Fig. 3. Values below this curve are safe; for those above it, failure is expected. The value of $\mathcal{G}_{IC}$ used for this curve is given in Eq. 11. The value of $\dot{\mathcal{G}}_{IC}$ is found as the average of the values of $\dot{\mathcal{G}}_I$ at failure in Fig. 2 excluding those for which $\mathcal{G}_c$ is negative or close to zero. Its value is $1.46 \times 10^{-5}$ which is slightly different from the value shown in Fig. 2 which includes all of the tests. With $\dot{L}_{22}^{-1} = 8.151 \times 10^{10} \text{ N/m}$ a value of $\mathcal{G}_{IC} = 8.6 \text{ N/m}$ is found. Excellent agreement is observed between the experimental results and the curve. As a result of the coupling between the first and fourth modes of fracture, which is expressed by the second term in parentheses of the right hand side of Eq. 14, the fracture curve in Fig. 3 is not symmetric with respect to $\psi$. Recall that the crack faces are perpendicular to the poling direction. Furthermore, it should be emphasized that the apparent fracture toughness $\mathcal{G}_{IC}$ should not be used to predict catastrophic failure. Only the mixed mode fracture curve presented in Eq. 14 and Fig. 3 should be used to predict failure.
4 Conclusions

A fracture criterion has been presented for piezoelectric material for poling at an angle to the crack plane and within a material symmetry plane. It is based upon the energy release rate and one or two phase angles. If mode III deformation was added and/or poling would be in a more general direction, the criterion could easily be generalized with the addition of third phase angle. Experimental results [1] were used in a special case of the criterion for which the crack is perpendicular to the poling direction. Excellent agreement was observed between the fracture curve and the experimental results. Nevertheless, some values of the critical energy release rate were negative or close to zero. These points were neglected as being physically unreasonable. Future study is required to understand this behavior. The criterion presented may be used for other poling directions.

References

What Do We Know About Surface Charges on Cracks in Ferroelectric Ceramics?

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Abstract The present work investigates the static and time dependent electric potential distribution around cracks in a poled ferroelectric ceramic by Kelvin Probe Force Microscopy (KFM). In a first step a Vickers indentation crack in poled lead zirconate titanate (PZT) was subjected to static electric fields of up to 500 V/mm in poling direction, and the potential distribution around the crack was measured. In a second step, the polarity of the applied voltage was reversed against the poling direction during the measurement of the potential. Using a simple model, an effective dielectric constant of the crack, as well as the surface charge density on the crack face were calculated as a function of the distance from the crack tip, the applied field and the time. The results are discussed with reference to free charges on the crack surface, electrically induced domain switching at the crack tip and crack bridging.

1 Introduction

Ferroelectric materials are used, amongst other applications, in electro-mechanical transducer applications, converting mechanical forces into an electrical potential (direct piezoelectric effect) or vice versa (inverse piezoelectric effect). During their lifetime, ferroelectric ceramics must be capable to operate under long-term electro-mechanical loading. While they continue to find increasing use, their fracture mechanics are still investigated due to their low fracture toughness and complex material behavior. This work contributes to the understanding of the effect of electrical loading on fracture in ferroelectric ceramics.

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A crack filled with air in a dielectric material with a high permittivity, is a void with a relative dielectric constant of one in a matrix with a dielectric constant that can be up to three orders of magnitude higher. If an electrical field is applied normal to the crack surface, it will penetrate the crack. The crack shape, the crack opening displacement and the ratio of the permittivities of the crack interior and the ceramic, will determine to what extent the electric flux through the crack will be diluted, and increased ahead of the tip. For cracks in a ferroelectric ceramic, i.e. in an electromechanically coupled material, this leads to a non-linear boundary value problem. In the literature three approaches are used to describe cracks in ferroelectric materials assuming impermeable boundaries (impermeable crack), permeable boundaries with an infinite dielectric constant of the crack (permeable crack), and permeable boundaries with a dielectric constant of the crack higher than one (semi-permeable crack). Theoretical works, e.g. from Balke et al [1] using the capacitor model of Hao and Shen [2] have shown that the latter results in the most realistic representation of the electric field around the crack. However, the capacitor model proved to be energetically not consistent [3]. In consequence, Landis [4, 5] derived the so called “energetically consistent” boundary conditions along the crack faces that include electrostatic tractions, which are caused by an electric field perpendicular to the crack faces closing the crack. His improved model, that also includes surface charges on the crack faces, and an electrical discharge model within the crack, predicts that an electrical load increases the critical mechanical load for fracture. Except of the permeable crack model, all other theoretical approaches predict that the electric field applied perpendicular to the crack plane increases the critical mechanical load for crack growth [6]. These theoretical predictions could not be observed experimentally. E.g. Jelitto et al. [7–9] and Häusler [10] show that DC electric fields of 1/3 of the coercive field only influence the critical loads for crack growth to a very small extent.

Haug and McMeeking [11] showed, that screening charges on the crack surface would change the fracture behavior of the crack dramatically. Schneider et al. [12] already successfully used Kelvin Probe Force Microscopy (KFM) to study the potential distribution around an electrically loaded Vickers crack in PZT. From the results an effective dielectric constant was calculated for the crack tip. On the basis of a Griffith crack it was further shown, that a higher dielectric constant of the crack reduces the dependency of the crack tip energy release rate on an applied electric field. The present work is a continuation of the work presented by Schneider et al. [12]. It takes into account not only a single applied electric field, but different field strengths up to 500 V/mm. Besides, the potential distribution is not only analyzed at the crack tip, but to a crack length of around 60 μm. The objective was to analyze whether or not the crack could also be described by a single effective dielectric constant farther away from the tip and at different applied electric fields. This part of the work is described in more detail in the Ph.D. thesis from Felten [13]. In addition, the time response of the electric potential distribution upon a reversal of the electric field against the polarization direction was studied. The motivation for this experiment was the assumption that free charges on the crack surface would
not immediately change after the reversal of the applied voltage. The objective of all experiments was to verify the theoretical assumption of screening charges on the crack surface, trying to quantify and characterize them.

2 Samples, Experimental Setup and Methods

KFM is a scanning probe technique, which allows mapping the surface potential of a sample versus the in-plane coordinates x and y in a two-pass technique. During the first pass the topography is recorded in tapping-mode. In the second pass, the so-called interleave scan, the topography is retraced in a set lift height and the contact potential difference is measured. As the tip travels over the sample surface in lift-mode, the tip and the cantilever experience a force wherever the potential on the surface is different from the potential of the tip. The force is nullified by varying the voltage of the tip so that the tip is at the same potential as the region of the sample surface underneath it. This voltage is plotted versus the in-plane x-y-coordinates, creating the surface potential image. The principle of the KFM-mode is described e.g. by Kalinin and Bonnell [14], the resolution of KFM is discussed e.g. by Jacobs et al. [15].

The experiments were performed in a similar way as described by Schneider et al. [12]. 270 μm thin plates of a commercial soft PZT (Vibrit1100, Johnson Matthey) covered with thin gold electrodes on both sides were cut into samples of $1 \times 2 \text{cm}^2$. The plates were poled at room temperature with an electric field of 2 kV/mm. The coercive field extracted from a hysteresis measurement (room temperature, 2 kV/mm maximum field, 8.3 mHz) is around 700 V/mm. According to the data sheet the dielectric constant $\varepsilon_{33}$ of the poled material is 4,500 [16].

One thin 4 cm × 260 μm face was polished on a semi-automatic polishing machine (Saphir550, ATM GmbH) using diamond suspension down to a grain size of 0.25 μm (DP-Suspension P on MD-NAP, Struers GmbH). The material’s grain size measured with an optical microscope is around 3 μm. After polishing a Vickers indent (0.5 kg, 10 s, Vickers hardness tester 3212 preceding model of ZVH10, Zwick) was induced in the middle of the surface, producing cracks parallel to the surface edges (Fig. 1). The advantage of the indentation methodology was its easy control and simplicity concerning the experimental performance. Vickers indenters produce two basic types of crack systems: radial-median and lateral. After the diamond is removed, local residual stress states hold the cracks open [17, p. 249ff.].

The sample was fixed in a custom made holder and aligned under a Scanning Probe Microscope (SPM) in a way that the cantilever was perpendicular to the applied field, and would not electrostatically interact with the indent. The voltage was externally applied to the sample. For the measurements with constant fields two separate power supplies were used (HCN-35-12500, MCN-35-1250, FuG). For the measurements where the field was reversed, a bipolar power supply with two ports and a fast response (Pzd700, large signal bandwidth up to 15 kHz, TREK INC.) was chosen. The power supplies were controlled using a computer program (LabView®, National Instruments). Therewith the voltage was applied in a way that