A partition of unity-based multiscale approach for modelling fracture in piezoelectric ceramics

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SUMMARY

The development of models for a priori assessment of the reliability of micro electromechanical systems is of crucial importance for the further development of such devices. In this contribution a partition of unity-based cohesive zone finite element model is employed to mimic crack nucleation and propagation in a piezoelectric continuum. A multiscale framework to appropriately represent the influence of the microstructure on the response of a miniaturized component is proposed. It is illustrated that using the proposed multiscale method a representative volume element exists. Numerical simulations are performed to demonstrate the constitutive homogenization framework. Copyright © 2009 John Wiley & Sons, Ltd.

Received 5 March 2009; Revised 22 September 2009; Accepted 25 September 2009

KEY WORDS: partition of unity method; cohesive zone models; micro systems; computational homogenization

1. INTRODUCTION

The electromechanical coupling in piezoelectric ceramics makes such materials applicable for sensing and actuating purposes. Piezoelectric ceramics, such as lead zirconate titanate (PZT), are especially used in micro electromechanical systems (MEMS). Examples of such devices are accelerometers and inkjet printer heads. Unfortunately, due to the brittleness of piezoelectric ceramics, these components are sensitive to damage. Numerical tools to assess damage in these materials and its influence on the performance of the devices are therefore of crucial importance for the further development of electromechanical devices.

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Contract/grant sponsor: BSIK programme

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Over the past decades numerical simulation of fracture in piezoelectric ceramics has primarily been based on linear elastic fracture mechanics models [1–3]. The use of either impermeable or permeable boundary conditions has been studied extensively. In the former case charge-free boundaries are used, whereas in the latter case continuity requirements for the electric field and electric flux density are employed. The permeable crack assumption was demonstrated to be the most appropriate [4, 5]. The definition of a failure criterion that correctly mimics the influence of an electric field has also been addressed frequently. The fracture criterion proposed in Reference [6] has been demonstrated to be in good agreement with experimental observations. Improvements to this fracture criterion by incorporation of non-linear effects have been suggested [7, 8] as well as models for simulating fatigue in piezoelectric ceramics [9]. Recently, the partition of unity concept has been employed for the enrichment of crack tip fields in piezoelectric ceramics [10].

The above-mentioned studies have primarily focussed on the study of fracture in relatively large specimens, i.e. specimens with dimensions in the order of centimetres. In that case, the size of the process zone, i.e. the zone in which gradual degradation of the material takes place, is negligible compared with the size of the specimen. Linear elastic fracture mechanics is in these situations a very useful tool for modelling fracture. When the size of the specimen is downscaled, as is the case for MEMS, the process zone remains in the same order of magnitude, whereas the specimen size can decrease with one or more orders of magnitude. The process zone is then no longer negligible compared with the specimen size, which restricts the applicability of linear elastic fracture mechanics. In that case, a cohesive zone approach to model fracture is more appropriate.

In this work a partition of unity-based cohesive zone formulation is used to model fracture in PZT. Electromechanical constitutive laws are used to describe the constitutive behaviour of the specimens. Failure in PZT is characterized by very small process zones (in the order of 10 micrometres), requiring an enormous amount of finite elements for the discretization of a macroscale component (and consequently a substantial amount of computational effort). Although in this case the partition of unity-based cohesive zone formulation is not very efficient, the model remains valid. The validity of the formulation for macroscale components allows for model verification based on macroscale experiments. The experiments discussed in Reference [6] are considered as a benchmark for the proposed model.

Upon miniaturization of a component, the influence of the microstructure on the performance of the device increases. Appropriate prediction for the performance of piezoelectric MEMS requires numerical models that correctly incorporate microscale effects that are generally omitted in macroscale analyses. Full-resolution modelling of the microscale is, however, often impractical from a computational effort point of view. In order to incorporate the effect of the complex microstructure, a computational homogenization procedure is employed in this work. The main feature of computational homogenization is to describe the macroscopic constitutive behaviour using finite element models on the microscale, rather than to use analytic constitutive laws [11, 12]. This approach implies that an additional finite element model is solved in all macroscopic integration points, which remains computationally expensive (although use can be made of parallel computing). In order to further reduce the required computational effort, linear constitutive behaviour is assumed in the bulk material. The coefficients for this linear material behaviour are obtained only once, prior to simulation, by means of numerical homogenization. As a consequence, microscopic finite element models are only used for the homogenization of the cohesive behaviour of the material.
This paper is organized as follows. In Section 2 the partition of unity-based discretization of
the electromechanical equilibrium equations is discussed. The electromechanical constitutive laws
are also introduced in this section. Macroscopic numerical simulations are performed in Section 3
to demonstrate some important properties of the proposed formulation. In Section 4 a homogen-
ization framework to incorporate the effect of the microstructure is outlined. The computational
homogenization framework is then applied to some numerical experiments in Section 5. Finally,
conclusions are drawn in Section 6.

2. PARTITION OF UNITY-BASED CRACK MODELLING IN PIEZOELECTRIC CONTINUA

The partition of unity approach for modelling cohesive fracture [13, 14] is commonly used to
simulate crack growth in arbitrary directions in a solid material. Application of the partition of
unity method to crack propagation problems, in which multi-physical phenomena are incorporated,
has recently been studied in, e.g. [15], where the influence of a fluid on crack propagation is
considered.

Here, a partition of unity-based cohesive zone formulation is derived for a two-dimensional
piezoelectric body, \( \Omega \subset \mathbb{R}^2 \), subject to mechanical and electric boundary conditions as schematically
shown in Figure 1. A crack, represented by the internal boundary \( \Gamma_d \), splits the body into two parts,
\( \Omega^+ \) and \( \Omega^- \) (satisfying \( \Omega = \Omega^+ \cup \Omega^- \)). The discussion is here restricted to a single crack, but can be
extended to the case of multiple cracks [16]. The formulation is extendible to the three-dimensional
case [17], but the algorithmic implementation of such an extension is not straightforward.

2.1. Kinematical formulation

The state of the body in Figure 1 is determined by a displacement field, \( u_i \) (with \( i = 1, 2 \)), and
electric potential field, \( \Phi \). A linear description of the kinematics of the body is employed, hence
assuming small displacements and displacement gradients. Upon formation of a crack, \( \Gamma_d \), discrete
jumps in both the displacement field and the electric potential field occur. These jumps are caused
by the decreased stiffness and permittivity of the fractured material. Appropriate description of
these jumps requires the formulation of a discontinuous basis for both fields, given by

\[
u_i = \bar{u}_i + \mathcal{H}_{\Gamma_d} \tilde{u}_i \quad \text{and} \quad \Phi = \bar{\Phi} + \mathcal{H}_{\Gamma_d} \tilde{\Phi}
\]

(1)

Figure 1. Schematic representation of an electromechanical domain \( \Omega \) with a crack \( \Gamma_d \).
with $\mathcal{H}_{\Gamma_d}$ being the Heaviside function, defined as
\[
\mathcal{H}_{\Gamma_d}(x) = \begin{cases} 
1 & \forall x \in \Omega^+ \\
0 & \forall x \in \Omega^- 
\end{cases}
\] (2)

Both fields in Equation (1) are decomposed into a continuous part (denoted by $\bar{\square}$) and a discontinuous part (denoted by $\tilde{\square}$). The displacement jump, $[u_i]$ and potential jump, $[\Phi]$ over the crack are given by
\[
[u_i] = \tilde{u}_i \quad \text{and} \quad [\Phi] = \tilde{\Phi}
\] (3)
respectively. Under the assumption of linear kinematics, the engineering strain is regarded as an appropriate measure for the deformation of the bulk material. This engineering strain and equivalent electric field are given by
\[
\varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad \text{and} \quad E_i = -\frac{\partial \Phi}{\partial x_i}
\] (4)
respectively.

In this contribution, the finite element method is used for the discretization of both the electric and the mechanical field. It was demonstrated by Babuška and Melenk [18] that a discontinuous field $f(x)$ can be discretized using continuous finite element shape functions $\phi_i(x)$ in combination with multiple enhanced basis functions $\gamma_j(x)$ according to
\[
f(x) = \phi_i(x)[\tilde{a}_i + \gamma_j(x)\tilde{a}_{ij}]
\] (5)
with $\tilde{a}_i$ and $\tilde{a}_{ij}$ being the nodal degrees of freedom. Discretization of the fields in Equation (1), which requires only one enhanced basis function $\mathcal{H}_{\Gamma_d}$, yields
\[
\mathbf{u}(x) = \mathbf{N}(x)\tilde{\mathbf{a}} + \mathcal{H}_{\Gamma_d}\mathbf{N}(x)\bar{\mathbf{a}} \quad \text{and} \quad \Phi(x) = \mathbf{M}(x)\tilde{\mathbf{b}} + \mathcal{H}_{\Gamma_d}\mathbf{M}(x)\bar{\mathbf{b}}
\] (6)
where the displacement field and the electric potential field are described in terms of nodal displacement vectors, $\tilde{\mathbf{a}}$ and $\bar{\mathbf{a}}$, and nodal potential vectors, $\tilde{\mathbf{b}}$ and $\bar{\mathbf{b}}$. The matrices $\mathbf{N}(x)$ and $\mathbf{M}(x)$ are arrays containing the shape function. Note that, in order to stay as close as possible to the actual implementation, the use is made of matrix-vector notation in the case that the discretized problem is discussed. Similarly as the approximation of the displacement field and electric potential field, the strain field and electric field (4) are expressed in terms of the nodal vectors as
\[
\varepsilon(x) = \mathbf{B}(x)\tilde{\mathbf{a}} + \mathcal{H}_{\Gamma_d}\mathbf{B}(x)\bar{\mathbf{a}} \quad \text{and} \quad \mathbf{E}(x) = \mathbf{C}(x)\tilde{\mathbf{b}} + \mathcal{H}_{\Gamma_d}\mathbf{C}(x)\bar{\mathbf{b}}
\] (7)
where Voigt notation is used to reduce the order of the rank two strain tensor. The matrices $\mathbf{B}(x)$ and $\mathbf{C}(x)$ contain the gradients of the finite element shape functions.

2.2. Electromechanical equilibrium equations and boundary conditions

In the absence of body forces and charges, the displacement field and electric potential field as given in Equation (1) are governed by the quasi-static equilibrium equations
\[
\frac{\partial \sigma_{ij}}{\partial x_j} = 0 \quad \text{and} \quad \frac{\partial D_i}{\partial x_i} = 0
\] (8)

where $\sigma_{ij}$ and $D_i$ denote the Cauchy stress and electric flux density, respectively. Note that the repeated indices imply summation over that index. In order to be solved, these equilibrium equations are supplemented with the boundary conditions

\begin{align*}
t_i &= \tilde{t}_i \quad \forall x \in \Gamma_t, \quad q = \tilde{q} \quad \forall x \in \Gamma_q \\
u_i &= \tilde{u}_i \quad \forall x \in \Gamma_u, \quad \Phi = \tilde{\Phi} \quad \forall x \in \Gamma_{\Phi}
\end{align*}

(9)

The weak form of both partial differential equations (8) is then obtained as

\begin{align*}
\int_{\Omega} \sigma_{ij} \delta \epsilon_{ij} \, d\Omega + \int_{\Gamma_t} t_i \delta \tilde{u}_i \, d\Gamma_t &= \int_{\Gamma_t} \tilde{t}_i \delta u_i \, d\Gamma_t \\
\int_{\Omega} D_i \delta E_i \, d\Omega + \int_{\Gamma_q} q \delta \tilde{\Phi} \, d\Gamma_q &= \int_{\Gamma_q} \tilde{q} \delta \Phi \, d\Gamma_q
\end{align*}

(10)

(11)

with $\delta \square$ being the arbitrary admissible perturbations of the same form as the corresponding fields (1) and satisfying the essential boundary conditions on $\Gamma_u$ and $\Gamma_{\Phi}$.

Following the derivation by Wells and Sluys [14], discrete equilibrium equations are obtained using the finite element discretization presented in (6) and (7)

\begin{align*}
\int_{\Omega} B^T \sigma \, d\Omega &= \int_{\Gamma_t} N^T_t \tilde{t} \, d\Gamma_t \\
\int_{\Omega^+} B^T \sigma \, d\Omega + \int_{\Gamma_d} N^T_t \tilde{t} \, d\Gamma_d &= 0 \\
\int_{\Omega} C^T D \, d\Omega &= \int_{\Gamma_q} M^T \tilde{q} \, d\Gamma_q \\
\int_{\Omega^+} C^T D \, d\Omega + \int_{\Gamma_d} M^T q \, d\Gamma_d &= 0
\end{align*}

(12)

Note that four equations are obtained due to the fact that the admissible mechanical and electric fields in (10) and (11) are composed of a regular part and an enhanced part (according to Equation (6)). As according to Equation (7), the enhanced part of the strain and the electric field (denoted by the $\tilde{\square}$-notation) is equal to zero on $\Omega^-$, the volume integrals in the second and fourth term in (12) are only taken over $\Omega^+$. In Equation (12) it is also assumed that no boundary conditions are imposed at the intersection of the discontinuity with the boundary (at $\Gamma \cap \Gamma_d$).

In this work, the equilibrium equations (12) are non-linear since the constitutive relations for the traction $t$ and surface charge density $q$ are non-linear. An additional source of non-linearity is present due to the fact that the discontinuity boundary $\Gamma_d$ evolves according to a failure criterion. The set of non-linear equations is solved incrementally by means of Newton–Raphson iterations. Energy-release rate control [19] is used to trace the equilibrium path. In this control, the amount of dissipated energy is used to let the crack evolve gradually. Force control is used in advance of crack nucleation, as no energy is dissipated until then.

2.3. Constitutive behaviour

The evaluation of the integrals in Equation (12) requires the Cauchy stress, electric flux density, mechanical traction and surface charge density to be known. These quantities are related to
the mechanical displacement field and electric potential field (1) by means of electromechanical constitutive laws.

2.3.1. Bulk constitutive behaviour. The mechanical Cauchy stress and electric flux density are related to the engineering strain and electric field using linear piezoelectricity [20]. Using Voigt notation, this can be written as

\[
\begin{bmatrix}
\sigma \\
D
\end{bmatrix} = \begin{bmatrix}
H & -e^T \\
e & \lambda
\end{bmatrix} \begin{bmatrix}
e \\
E
\end{bmatrix}
\]

(13)

In this expression, \(H\) is the Hookean matrix for a material under plane strain and \(\lambda\) is the permittivity tensor. The actual electromechanical coupling is a consequence of the piezoelectric matrix \(e\). The specific shape of \(e\) depends on the type of piezoelectric material and is discussed in Section 3.

2.3.2. Cohesive law. The cohesive behaviour of cracks is prescribed by the cohesive law introduced in [21]. A mechanical cohesive law is enhanced with electric relations by assuming the crack to behave like a parallel plate capacitor, relating the traction and surface charge density on a crack to the crack opening and potential jump by

\[
\begin{bmatrix}
t \\
qu
\end{bmatrix} = \begin{bmatrix}
I \\
-e_p H_{cp}^{-1}
\end{bmatrix} t_{mech} - E_{cp} \begin{bmatrix}
e^T_{cp} \\
\lambda_{cp}
\end{bmatrix} + \begin{bmatrix}
\frac{1}{2} \tilde{\lambda}_{cp} E_{cp}^2 n \\
0
\end{bmatrix}
\]

(14)

where

\[
H_{cp} = (1 - \omega)N^T H N, \quad e_{cp} = (1 - \omega)n^T e N, \quad \lambda_{cp} = \lambda_\infty + (1 - \omega)(n^T \tilde{\lambda} n - \lambda_\infty)
\]

(15)

In this expression, \(n\) is the normal vector of the crack plane and \(N\) is a matrix that projects the Voigt form of a second-order tensor on the crack plane (\(t_i = \sigma_{ij} n_j \Rightarrow t = N^T \sigma\)). Damage is taken into account by the scalar damage parameter \(\tilde{\lambda}_{cp}\) and \(\lambda_\infty\) is the permittivity after a crack has fully opened. The definition of the scalar damage parameter is based on the mechanical traction-opening law, \(t_{mech}\), as proposed in [14]. The normal and shear traction for this law are given by

\[
t_{mech,n} = t_{0,n} \exp \left( - \frac{t_{ult}}{\mathcal{G}_c} \right) \quad \text{and} \quad t_{mech,s} = \exp (h_s \kappa) (t_{0,s} + k_s \tilde{u}_s)
\]

(16)

In this mechanical law, \(\kappa\) is a history parameter defined as the maximum achieved value of the normal opening, \(\tilde{u}_n\), up to the current time instant. The loading condition is checked using the Kuhn–Tucker conditions. The cohesive load unloads with the secant stiffness corresponding to the history parameter. The parameters \(t_{0,n}\) and \(t_{0,s}\) are the normal and shear traction in the undamaged state (\(\kappa = 0\)) with zero opening (\(\tilde{u} = 0\)), respectively. Furthermore, \(\mathcal{G}_c\) is the mechanical fracture toughness and \(t_{ult}\) the prescribed ultimate traction. The parameter \(h_s\) governs the degradation of the shear stiffness \(k_s\) and is here directly related to the damage in the normal direction by taking \(h_s = -t_{ult}/\mathcal{G}_c\). The initial value for the shear stiffness \(k_s\) is assumed to be equal to the initial shear stiffness of the Xu–Needleman law [22]. Finally, note that the cohesive law as used in Reference [14] has been adapted slightly in order to ensure the traction continuity condition \(t(0) = t_0\) in the undamaged state.
2.4. Failure criterion

In Reference [6] a linear elastic fracture mechanics approach is used to predict the ultimate load of a piezoelectric specimen under combined mechanical and electric loading. The crack-closure method [23] is used to determine the maximum fracture energy. It is observed that a failure criterion based on the mechanical fracture toughness yields the best representation of the experimentally observed dependence of the maximum load on the electric field strength.

In contrast to the fracture energy criterion used for the singular crack model considered in Reference [6], a failure criterion based on the local stress state of the system is required for the proposed partition of unity-based cohesive zone formulation. Both the position of the crack and the angle at which the crack propagates (or nucleates) are determined on the basis of a local stress representation. The failure criterion is here based on the mechanical stress, which is defined as

\[
\sigma_{\text{mech}} = H\varepsilon = H\left[I + H^{-1}\varepsilon^T\lambda^{-1}\varepsilon\right]^{-1}H^{-1}(\sigma + \varepsilon^T\lambda^{-1}D)
\]  

(17)

Following the argumentation in Reference [6], this mechanical stress is assumed to be a more appropriate failure measure than the total stress. The reason for this is that piezoelectric materials, as a consequence of the electric contributions to the stress, can experience a zero stress state while being deformed. As a consequence, using the total stress as a failure measure can indicate that a specimen is significantly deformed, but does not experience any cracking. This counterintuitive behaviour is not experienced when using the mechanical stress as a failure indicator, as it is directly related to the strain. The reason for not using the strain directly as a failure measure is that, in contrast to the mechanical stress, it cannot be related directly to the (mechanical) fracture strength, which is a material parameter suitable for experimental determination. Note also that the mechanical stress is only used as a failure indicator. Mechanical equilibrium remains based on the total stress. As a consequence, the model can predict failure under pure electric loading. A comparison of the failure criterion based on the mechanical stress with a criterion based on the total stress is presented in Section 3.

Using the mechanical stress (17), the failure criterion is constructed as

\[
\text{failure} = \begin{cases} 
\text{true} & \text{max} (\sigma_{\text{mech}}) > \sigma_{\text{ult}} \\
\text{false} & \text{otherwise}
\end{cases}
\]  

(18)

in which \(\sigma_{\text{mech}}\) is a second-order tensor containing the principal stresses of \(\sigma_{\text{mech}}\), and \(\sigma_{\text{ult}}\) is an ultimate value for the maximum mechanical principal stress. Generally, the ultimate stress \(\sigma_{\text{ult}}\) coincides with the fracture strength \(\sigma_{\text{ult}}\), which is a parameter of the cohesive zone models. When the criterion (18) is satisfied, a crack propagates (or nucleates) perpendicular to the direction of the maximum mechanical principal stress.

For stability reasons, the direction of propagation of a crack is commonly based on a smoothed stress measure around a crack tip [24]. The instance of propagation should, however, be based on a non-smoothed crack tip stress in order to avoid delayed crack growth. In this work, both effects are achieved by determining the stress and electric flux density at the crack tip using

\[
\sigma = V_R \sigma_0 V_R^{-1} \quad \text{and} \quad D = \frac{||D_0||}{||D_R||} D_R
\]  

(19)

where \(V_R\) contains the normalized eigenvectors of the smoothed stress \(\sigma_R\), \(\Sigma_0\) is a diagonal matrix containing the eigenvalues of the approximated local stress \(\sigma_0\) and \(D_0\) is an approximation of the
local electric flux density. The local estimates are based on their values in the integration point closest to the crack tip. The smoothed stress and electric flux density are determined using

\[\sigma_R(x) = \frac{\int_{y \in \Omega} \sigma(y) \exp \left(-\frac{\|x-y\|^2}{l_R^2}\right) d\Omega}{\int_{y \in \Omega} \exp \left(-\frac{\|x-y\|^2}{l_R^2}\right) d\Omega}\]

and

\[D_R(x) = \frac{\int_{y \in \Omega} D(y) \exp \left(-\frac{\|x-y\|^2}{l_R^2}\right) d\Omega}{\int_{y \in \Omega} \exp \left(-\frac{\|x-y\|^2}{l_R^2}\right) d\Omega}\]

(20)

with \(l_R\) being the macroscale smoothing length, which is typically three times the element length in the process zone.

Comparison of numerical and experimental results, as discussed in detail in the next section, demonstrates that a propagation criterion based on (17) overestimates the influence of the electric field on the propagation instance. A likely cause of this discrepancy is that around a crack tip as well as around an initial notch, the magnitude of the piezoelectric tensor is overestimated. In reality, the high stresses involved in manufacturing the initial notch locally cause domain switching \[25\]. When domain switching occurs, the polarization direction of domains that exist within the grains is altered. As a consequence, the effective piezoelectric effect experienced is smaller than expected from computations assuming an undamaged (i.e. not affected by domain switching) piezoelectric tensor.

In this work, this diminished influence of the electric field is accounted for by the introduction of a third measure for the electric flux density, \(D_p\), corresponding to the averaging length \(l_p\) upon which the propagation electric flux density is based. As a consequence, Equation (17) is then written as

\[\sigma_{\text{mech}} = H[I + H^{-1}e^T \lambda^{-1} e]^{-1} H^{-1} \left(\sigma + \frac{\|D_p\|}{\|D_R\|} e^T \lambda^{-1} D\right)\]

(21)

A reduction in the electric field dependence is then accomplished by taking the smoothing length for the electric flux density \(l_p\) considerably larger than that used for the stresses, \(l_R\). This is the case since the stress peak around a crack tip will be smoothed out more using a larger smoothing radius. The ratio \(\|D_p\|/\|D_R\|\) will then become smaller, consequently decreasing the influence of the electric flux density \(D\) on the mechanical stress \(\sigma_{\text{mech}}\). This heuristic incorporation of the phenomenon of domain switching in the model is a limiting factor for its applicability. Incorporation of a more advanced description of domain switching is a topic of future research.

Upon propagation (or nucleation) of a crack, a corrective load step is performed, i.e. the previous step is recomputed, in order to ensure that the determined solution is in equilibrium. The necessity of this corrective step is a consequence of the explicit nature of the crack propagation algorithm.

3. MACROSCALE EXPERIMENT

The finite element formulation as presented in the previous section is tested using benchmark experiments. Following the approach in Reference \[6\], experimental results for a compact tension specimen are used to fit unknown material and geometry parameters. A three-point bending test with varying initial crack position is then considered to test the proposed method. The numerical results for that case are compared with the experimentally obtained results presented in Reference \[6\].
Table I. Parameters used for numerical simulations, the permittivity of vacuum is \( \varepsilon_0 = 8.8542 \times 10^{-12} \text{ N/V}^2 \).

The poling direction corresponds with index 1.

<table>
<thead>
<tr>
<th>Elastic constants (GPa)</th>
<th>( H_{11} )</th>
<th>113.0</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( H_{22} )</td>
<td>139.0</td>
</tr>
<tr>
<td></td>
<td>( H_{33} )</td>
<td>25.6</td>
</tr>
<tr>
<td></td>
<td>( H_{12} )</td>
<td>74.3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Dielectric constants (( \text{N/V}^2 ))</th>
<th>( \varepsilon_{11} )</th>
<th>617.8( \varepsilon_0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \varepsilon_{22} )</td>
<td>677.6( \varepsilon_0 )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Piezoelectric constants (( \text{N/V/mm} ))</th>
<th>( e_{11} )</th>
<th>13.84 \times 10^{-3}</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( e_{12} )</td>
<td>-6.98 \times 10^{-3}</td>
</tr>
<tr>
<td></td>
<td>( e_{23} )</td>
<td>13.44 \times 10^{-3}</td>
</tr>
</tbody>
</table>

The specimens considered are composed of PZT-4 (lead zirconate titanate, Pb\((Zr_xTi_{1-x})O_3\)), which is one of the most commonly used piezoelectric ceramics. A significant piezoelectric effect is obtained after poling [26] when the PZT is in the phase boundary (MPB), i.e. \( x \approx 0.5 \). The bulk parameters for this material, poled in the \( x_1 \) direction, are given in Table I. The matrices required for the evaluation of the bulk constitutive behaviour (13) are then constructed as

\[
H = \begin{bmatrix}
H_{11} & H_{12} & 0 \\
H_{12} & H_{22} & 0 \\
0 & 0 & H_{33}
\end{bmatrix}, \quad
\varepsilon = \begin{bmatrix}
e_{11} & e_{12} & 0 \\
0 & 0 & e_{23}
\end{bmatrix}
\quad \text{and} \quad
\kappa = \begin{bmatrix}
\varepsilon_{11} & 0 \\
0 & \varepsilon_{22}
\end{bmatrix}
\]

Note that the piezoelectric tensor is described by only three parameters, which is in accordance with its class 6 mm symmetry [20]. The fracture strength and fracture toughness are taken from the literature as \( t_{ult} = 80 \text{MPa} \) [27] and \( G_c = 2.34 \times 10^{-3} \text{N/mm} \) [6], respectively.

3.1. Compact tension specimen

The considered compact tension specimen with a thickness of 5.1 mm and a 0.46 mm thick initial crack is shown in Figure 2. The specimen is poled in the vertical direction and is immersed in a tub filled with silicon oil with permittivity \( \varepsilon_\infty = 2.5\varepsilon_0 \). A direct current power supply is attached to electrodes on the top and bottom of the specimen. Mechanical loading is performed by two steel hinges that are moved apart by the application of a force \( F \). The modulus of elasticity and Poisson ratio of these hinges are taken as 200 GPa and 0.3, respectively.

As mentioned in the introduction, the brittleness of the material causes the process zone to be small compared with the specimen size [21]. In fact, the process zone is even observed to be small compared with the size of the initial notch. As a consequence, the ultimate load is significantly influenced by the shape of the initial notch. To vary the shape of the crack tip, the eccentricity \( \varepsilon \) of the ellipse shown in Figure 2 is modified. To correctly predict the experimentally measured fracture load, the notch eccentricity is taken as \( \varepsilon = 4.5 \). For the same reason, the averaging length \( l_p \) is taken as 150 \( \mu \text{m} \), which is of the same order of magnitude as the notch width.

The model is discretized using 3249 nodes and 6083 linear triangular elements (Figure 2), with 3 degrees of freedom per node, yielding a system with 9747 degrees of freedom. The mesh
Figure 2. Schematic representation (with all units in millimetres) and finite element mesh of a compact tension specimen with an applied electric field. The specimen has a thickness of 5.1 mm and is poled in the vertical direction.

Figure 3. Force versus dissipated energy curve for the compact tension specimen with no external electric field applied ($V = 0$V).

is significantly refined near the crack tip in order to have an appropriate discretization of the process zone. The averaging length $l_R$ is taken as 2.5 $\mu$m, which equals the characteristic element size near the crack tip, and is experienced to yield stable solutions. Prior to crack nucleation, the forces $F$ are stepwise increased by 5.1 N (i.e. 1 N per mm thickness). After nucleation, energy release rate control is employed with a maximum dissipation increment of $1 \times 10^{-9}$ J.

As a consequence of the brittleness of the material, visualization of the response by a force–displacement (separation of the two hinges) curve is not meaningful due to the severe snapback that occurs. A better visualization of the response of the structure is obtained by plotting the force versus the amount of energy dissipated (Figure 3). Note that using the selected values for the notch eccentricity and electric flux density smoothing parameter, a fracture load of 92.8 N is found in the absence of an external electric field (with $V = 0$V), which is in agreement with the experimental results.

The influence of the discretization is studied by mesh refinement. The result is predominantly influenced by the mesh size around the crack tip, which is parameterized by the mesh length, $l_c$. The
Figure 4. Dependence of fracture load on the strength of the applied electric field for the compact tension specimen as obtained experimentally (▲), numerically without smoothing of the electric flux density (○), numerically with smoothed electric flux density (+) and numerically using a failure criterion based on the total stress (●).

previously discussed mesh with \( l_e = 0.0025 \) was refined to \( l_e = 0.0015 \), the ultimate load obtained for this mesh equals 93.4 N, which differs from the coarser mesh result by less than 1%.

In Figure 4 the influence of the externally applied potential difference on the fracture load is shown. As can be seen, the numerical results closely resemble the experimentally obtained results for all measurement voltages except for the one at 5 kV/cm. The highly non-linear behaviour for that measurement point, which is also observed for even higher electric field strengths [6], is not captured by the model. Correct representation of this behaviour would require incorporation of additional non-linear phenomena in the model, such as domain switching.

As already mentioned in Section 2.4, the averaging length \( l_\rho \) is necessary to correctly predict the dependence on the external electric field. This is illustrated in Figure 4 by means of a numerical simulation without the additional smoothing of the electric flux density. The notch eccentricity, which is then the only remaining parameter to be tuned, is taken as \( \epsilon = 2.65 \). As can be seen, this simulation significantly overpredicts the influence of the external electric field. For completeness, also in Figure 4 the fracture load dependence on the external electric field is plotted while using a fracture criterion based on the total Cauchy stress \( \sigma \) (in contrast to the mechanical stress \( \sigma_{\text{mech}} \)). A notch eccentricity of \( \epsilon = 2.73 \) is used in this case. As can be observed, this fracture criterion significantly underestimates the effect of the external electric field.

3.2. Three-point bending specimen

The three-point bending test as shown in Figure 5 is considered as a second application of the proposed model. Specimens with a 4 mm long initial crack at an offset of 0, 2 and 4 mm are studied. The initial cracks have been made in the same way as that of the compact tension specimen. Therefore, it is assumed that the geometry of the initial crack tip is the same. The specimens are poled in the horizontal direction. Besides the notch eccentricity \( \epsilon \), the smoothing parameter \( l_\rho \) found to be appropriate for the compact tension specimen is used for the simulation of the three-point bending experiment.

For all specimens the ultimate load is computed for the various electric field strengths. The results of the finite element simulations are compared with the experimental data as shown in...
Figure 5. Schematic representation (with all units in millimetres) of a three-point bending specimen with an applied electric field. The specimen has a thickness of 5.1 mm and is poled in the horizontal direction.

Figure 6. Dependence of fracture load on the strength of the applied electric field for the three-point bending specimen with a centred crack (top-left), 2 mm off-centred crack (top-right) and 4 mm off-centred crack (bottom) as obtained experimentally (▲) and numerically (+).

Figure 6. For negative and zero electric fields, the finite element method is capable of approximating the experimentally obtained results with approximately 10% accuracy. For positive electric fields it correctly predicts the downward trend of the maximum load, but the accuracy is limited.
The most important difference between the experimental results and the numerical results is the dependence on the electric field strength. This dependence is significantly overestimated by the finite element result. As already mentioned in the previous section, this dependence is dictated by the averaging length $l_p$. The optimization of the values for the notch eccentricity and averaging length to better fit the electric field dependence is possible, but is beyond the scope of this work.

4. MULTISCALE CONSTITUTIVE MODELLING

The partition of unity-based framework for modelling fracture in piezoelectric components, as introduced in Section 2, requires the provision of bulk and cohesive constitutive laws. For the macroscale experiments carried out in Section 3, the analytical relations (13) and (14) are used for this purpose. These constitutive laws can be characterized as rather phenomenological. Alternatively, homogenization methods can be applied to derive micromechanically motivated cohesive laws for the macroscale framework.

The goal of this section is to derive homogenization laws for the constitutive behaviour of a piezoelectric continuum, such that the complex behaviour of the microscale is appropriately described on the macroscale. The considered microstructure is a piezoelectric polycrystal, which upon loading fails intergranularly. It is emphasized that the proposed framework is not restricted to this specific micromodel and can be applied to other types of microstructural geometry and microscale non-linear behaviour. In order to clearly distinguish the two scales, the superscripts $^{\square M}$ and $^{\square m}$ are used to indicate if a quantity belongs to the macroscale or microscale, respectively.

For a proper description of a multiscale constitutive model, it is of crucial importance to realize that the failure description is fundamentally different on the two scales. On the macroscale, a cohesive segment is only inserted upon satisfaction of a failure criterion. We assume that the material behaves linearly until crack nucleation and hence energy is only dissipated after the insertion of a cohesive segment. In contrast, the interfaces on the microscale are present throughout the complete simulation since they represent the grain boundaries. Upon loading, the microscale model gradually loses strength due to damage accumulation in these grain boundary interfaces. As a consequence, an obvious definition for the moment of failure is not available on the microscale.

The pre-failure non-linear behaviour of the microscale cannot be represented by the macroscale formulation. Therefore, it is assumed that the macroscale constitutive behaviour prior to the insertion of a cohesive segment can be described on the basis of homogenized microscale properties in the undeformed state. This assumption is advantageous from a computational effort point of view, as these homogenized properties are obtained in a relatively cheap pre-processing step. The appropriateness of this assumption fully depends on the relative importance of the grain boundary opening prior to macroscale crack insertion. This assumption will further be commented on the numerical simulations section.

4.1. Homogenization of bulk constitutive behaviour

The bulk constitutive behaviour is described by the microscale model schematically shown in Figure 7. Note that for notational convenience a single grain boundary $F_{gb}$ is considered, which splits the microstructure into two parts. The derivation presented here, however, remains fully valid.
for the multiple grain boundary case. The microscale displacement and electric potential field are decomposed as

\[
\begin{align*}
\mathbf{u}_m^i &= \left( \langle \varepsilon_{ij}^m \rangle_{\Omega^m} \mathbf{x}_j^m + \mathbf{\dot{u}}_m^i + \mathcal{H}_{gb} \mathbf{\dot{u}}_m^i \right) \\
\Phi_m^i &= -\left( \langle E_{ri}^m \rangle_{\Omega^m} \mathbf{x}_r^m + \mathbf{\Phi}_m^i + \mathcal{H}_{gb} \mathbf{\Phi}_m^i \right)
\end{align*}
\] (23)

with \( \mathcal{H}_{gb} \) being defined similarly as in Equation (2). The boundary conditions for the micro model are then given in terms of the microscopic fluctuation fields \( \mathbf{\dot{u}}_m^i \). On the four control nodes (I–IV), both the mechanical displacement fluctuations and electric potential fluctuations are equal to zero. Moreover, the fluctuation fields are periodic from the left to the right edge and from the bottom to the top edge (as indicated by the dotted lines in Figure 7). From these boundary conditions, it follows that the homogenized engineering strain \( \langle \varepsilon_{ij}^m \rangle_{\Omega^m} \) and homogenized electric field \( \langle E_{ri}^m \rangle_{\Omega^m} \) are defined as the volume average of the corresponding microscopic fields

\[
\begin{align*}
\langle \varepsilon_{ij}^m \rangle_{\Omega^m} &= \frac{1}{wh} \int_{\Omega^m} \varepsilon_{ij}^m \, d\Omega^m \\
\langle E_{ri}^m \rangle_{\Omega^m} &= \frac{1}{wh} \int_{\Omega^m} E_{ri}^m \, d\Omega^m
\end{align*}
\] (24)

in which \( w \) and \( h \) are the micro model width and height, respectively. This is proven by differentiation of (23) and substitution in (24), while making use of Gauss’ theorem in combination with the boundary conditions mentioned above.
The definition of the homogenized stress and electric flux density then follows by the consideration of the Hill–Mandel energy condition [28] for both the mechanical and electric contributions

\[
\langle \sigma_{ij}^m \rangle_{\Omega^m} \delta(\varepsilon_{ij}^m)_{\Omega^m} = \frac{1}{wh} \int_{\Omega^m} \sigma_{ij}^m \delta \varepsilon_{ij}^m \, d\Omega^m
\]

\[
\langle D_i^m \rangle_{\Omega^m} \delta(E_i^m)_{\Omega^m} = \frac{1}{wh} \int_{\Omega^m} D_i^m \delta E_i^m \, d\Omega^m
\]

(25)

Using microscale equilibrium these expressions are rewritten as

\[
\langle \sigma_{ij}^m \rangle_{\Omega^m} \delta(\varepsilon_{ij}^m)_{\Omega^m} = \frac{1}{wh} \int_{\Gamma^m} t_i^m \delta u_i^m \, d\Gamma^m
\]

\[
\langle D_i^m \rangle_{\Omega^m} \delta(E_i^m)_{\Omega^m} = \frac{1}{wh} \int_{\Gamma^m} q_m^m \delta \Phi_m \, d\Gamma^m
\]

(26)

which can be rewritten by using the decompositions in Equation (23) as

\[
\langle \sigma_{ij}^m \rangle_{\Omega^m} \delta(\varepsilon_{ij})_{\Omega^m} = \frac{1}{wh} \int_{\Gamma^m} t_i x_j^m \, d\Gamma^m \delta(\varepsilon_{ij})_{\Omega^m}
\]

\[
\langle D_i^m \rangle_{\Omega^m} \delta(E_i)_{\Omega^m} = -\frac{1}{wh} \int_{\Gamma^m} q_m x_i^m \, d\Gamma^m \delta(E_i)_{\Omega^m}
\]

(27)

where the use is made of the anti-periodicity of the traction and surface charge density corresponding to the periodic boundary conditions for the displacements and electric potential. From this expression, the macroscopic stress and electric flux density follow as:

\[
\langle \sigma_{ij}^m \rangle_{\Omega^m} = \frac{1}{wh} \int_{\Gamma^m} t_i x_j^m \, d\Gamma^m = \frac{1}{bh} \int_{\Omega^m} \sigma_{ij}^m \, d\Omega^m
\]

\[
\langle D_i^m \rangle_{\Omega^m} = -\frac{1}{wh} \int_{\Gamma^m} q_m x_i^m \, d\Gamma^m = \frac{1}{bh} \int_{\Omega^m} D_i^m \, d\Omega^m
\]

(28)

Hence, it follows that the homogenized kinetic properties are the volume averages of the microscopic quantities, when use is made of the boundary conditions specified. Furthermore, note that the homogenized stress tensor is symmetric by the virtue of the equilibrium of moments.

For given values for the homogenized strain \( \langle \varepsilon_{ij}^m \rangle_{\Omega^m} \) and electric field \( \langle E_i^m \rangle_{\Omega^m} \), Equation (23) can be used to determine the corresponding microscale boundary conditions. Equation (28) can then be used to determine the microscopic stresses and electric flux densities. The (possible) non-linear behaviour of the microscale prior to macroscopic crack nucleation then generally leads to non-linear constitutive behaviour. This is obviously not desirable from a computational effort point of view, as a microscopic finite element simulation is then required for each evaluation of the stresses and electric flux densities. As in the present work, the non-linearities of the bulk material are assumed to be of minor importance compared with the non-linearities coming from...
the fracture process, an additional assumption is made by assuming linear bulk behaviour based on the homogenized material tangent in the undeformed state (denoted by $\square|_0$)

$$\begin{align*}
\sigma_{ij}^M &= \frac{\partial \langle \sigma_{ij}^m \rangle}{\partial \langle \varepsilon_{kl}^m \rangle} \varepsilon_{kl}^M + \frac{\partial \langle \sigma_{ij}^m \rangle}{\partial \langle E_k^m \rangle} E_k^M \\
D_i^M &= \frac{\partial \langle D_i^m \rangle}{\partial \langle \varepsilon_{kl}^m \rangle} \varepsilon_{kl}^M + \frac{\partial \langle D_i^m \rangle}{\partial \langle E_k^m \rangle} E_k^M
\end{align*}$$  \hspace{1cm} (29)

The tangents are computed by multiple evaluations of the stresses and electric flux densities using the microscale stiffness matrix in the undeformed state. As these operations are performed in a pre-processing step, their influence on the overall computational cost is negligible. During the macroscopic finite element simulation, the bulk stresses and electric flux densities are computed by the evaluation of Equation (29).

4.2. Homogenization of cohesive behaviour

For the homogenization of the bulk behaviour, the volume averages of the fields describing the kinematics are used as homogenized kinematical quantities. Based on this choice the corresponding averaging schemes for the kinetic quantities were derived by exploiting the Hill–Mandel energy condition. In the case of homogenization of the cohesive behaviour, a similar approach is troublesome, as an obvious choice for a crack opening averaging scheme is missing. However, as it is possible to find an obvious expression for the homogenized traction and surface charge density, the original procedure is inverted here. Given the averaging scheme for the kinetics, the corresponding homogenization rules for the kinematics are derived using the Hill–Mandel energy condition.

To derive an homogenization scheme for the macroscopic crack opening and macroscopic potential jump, the microscale model shown in Figure 7 is considered. The macroscopic traction and surface charge density are defined as the projection of the homogenized stress and electric flux density on the fracture plane, yielding

$$\begin{align*}
t_i^M &= \langle \sigma_{ij}^m \rangle \Omega = n_i^M \\
q^M &= -\langle D_i^m \rangle \Omega = n_i^M
\end{align*}$$  \hspace{1cm} (30)

with $n_i^M$ being the normal to the macroscopic crack, which coincides with the $x_1^m$ direction on the microscale. The (generally anisotropic) microscale material tangents are rotated in accordance with the direction of the macroscopic cohesive segment. In the present work, the microscale geometry is not adjusted to the direction of the crack, hence assuming isotropy in the geometry of the microstructure. For problems where this assumption is violated, e.g. if the microstructure is columnar, the rotation of the geometry also needs to be taken into account. Substitution of the earlier derived expressions (28) for $\langle \sigma_{ij}^m \rangle \Omega$ and $\langle D_i^m \rangle \Omega$ in Equation (30) then yields

$$\begin{align*}
t_i^M &= \frac{1}{h} \int_{\Gamma_i^m} t_i^m d\Gamma_i^m \\
q^M &= \frac{1}{h} \int_{\Gamma_i^m} q_i^m d\Gamma_i^m
\end{align*}$$  \hspace{1cm} (31)
For the case considered here the Hill–Mandel energy condition reads

\[
\sigma_{ij}^M \delta \varepsilon_{ij}^M + \frac{1}{w} t_i^M \delta u_i^M = \frac{1}{w h} \int_{\Gamma_m} t_i^m \delta u_i^m \, d\Gamma^m
\]

\[
D_i^M \delta E_i^M + \frac{1}{w} q^M \delta \Phi^M = \frac{1}{w h} \int_{\Gamma_m} q^m \delta u \Phi^m \, d\Gamma^m
\]  \hspace{1cm} (32)

As can be seen, this expression is composed of a part concerning the internal work of the bulk material and a part representing the work performed by the cohesive surface. Using the boundary conditions, the boundary integrals in Equation (32) are rewritten as

\[
\frac{1}{w h} \int_{\Gamma_m} t_i^m \delta u_i^m \, d\Gamma^m = \frac{1}{w} t_i^M \delta u_i^M
\]

\[
\frac{1}{w h} \int_{\Gamma_m} q^m \delta u \Phi^m \, d\Gamma^m = \frac{1}{w} q^M \delta \gamma^M
\]  \hspace{1cm} (33)

with \(u_i^M\) and \(\gamma^M\) being the displacement and potential of the bottom right control node (node II), respectively. Substitution of Equation (33) in Equation (32) then yields

\[
t_i^M \delta u_i^M = w \sigma_{ij}^M \delta \varepsilon_{ij}^M + t_i^M \delta u_i^M
\]

\[
q^M \delta \gamma^M = w D_i^M \delta E_i^M + q^M \delta \Phi^M
\]  \hspace{1cm} (34)

Note that for the boundary conditions used, the macroscopic stress and electric flux density as given in (28) can be written as

\[
\sigma_{ij}^M = \frac{\delta j_1}{h} \int_{\Gamma_B} t_i^m \, d\Gamma^m + \frac{\delta j_2}{w} \int_{\Gamma_C} t_i^m \, d\Gamma^m = \Delta_{ijkl} t_k^M
\]

\[
D_i^M = -\frac{\delta i_1}{h} \int_{\Gamma_B} q^m \, d\Gamma^m - \frac{\delta i_2}{w} \int_{\Gamma_C} q^m \, d\Gamma^m = -\delta_i^M q^M
\]  \hspace{1cm} (35)

in which \(\delta_{ij}\) is the Kronecker delta and \(\Delta_{ijkl} = \delta_{i1} \delta_{j1} \delta_{k1} + (\delta_{i1} \delta_{j2} + \delta_{i2} \delta_{j1}) \delta_{k2}\) is a third-order tensor. Moreover, using

\[
\delta \varepsilon_{ij}^M = \frac{\partial \varepsilon_{ij}^M}{\partial \sigma_{kl}^M} \delta \sigma_{kl}^M + \frac{\partial \varepsilon_{ij}^M}{\partial D_k^M} \delta D_k^M
\]

\[
\delta E_i^M = \frac{\partial E_i^M}{\partial \sigma_{kl}^M} \delta \sigma_{kl}^M + \frac{\partial E_i^M}{\partial D_k^M} \delta D_k^M
\]  \hspace{1cm} (36)

it follows that

\[
t_i^M \delta u_i^M = w t_i^M \left[ \Delta_{jkl} \frac{\partial \varepsilon_{jk}^M}{\partial \sigma_{kl}^M} \Delta_{pm} \right] \delta t_i^M - w t_i^M \left[ \Delta_{jkl} \frac{\partial \varepsilon_{jk}^M}{\partial D_k^M} \right] \delta q^M + t_i^M \delta u_i^M
\]

\[
q^M \delta \gamma^M = -w q^M \left[ \Delta_{jkl} \frac{\partial \varepsilon_{jk}^M}{\partial \sigma_{kl}^M} \Delta_{pm} \right] \delta t_i^M + w q^M \left[ \Delta_{jkl} \frac{\partial \varepsilon_{jk}^M}{\partial D_k^M} \right] \delta q^M + q^M \delta \Phi^M
\]  \hspace{1cm} (37)
As Equation (37) should hold for any value of the macroscopic traction and surface charge density, it follows that

\[
\delta v_i^M = w \left[ \Delta_{jki} \frac{\partial \epsilon^M_{jk}}{\partial \sigma^M_{m0}} \right] \delta \gamma^M - w \left[ \Delta_{jki} \frac{\partial \epsilon^M_{jk}}{\partial D^M_1} \right] \delta q^M + \delta \tilde{u}_i^M
\]

\[
\delta \gamma^M = -w \left[ \frac{\partial E^M_{1}}{\partial \sigma^M_{jk}} \right] \Delta_{jki} \delta \gamma^M + w \left[ \frac{\partial E^M_{1}}{\partial D^M_1} \right] \delta q^M + \delta \Phi^M
\]

This equation is then rewritten as

\[
\delta v_i^M = w \left[ \Delta_{jki} \frac{\partial \epsilon^M_{jk}}{\partial \sigma^M_{m0}} \right] \Delta_{jki} \delta \gamma^M - w \left[ \Delta_{jki} \frac{\partial \epsilon^M_{jk}}{\partial D^M_1} \right] \delta q^M + \delta \tilde{u}_i^M + \delta \tilde{u}_i^M
\]

\[
\delta \gamma^M = -w \left[ \frac{\partial E^M_{1}}{\partial \sigma^M_{jk}} \right] \Delta_{jki} \delta \gamma^M + w \left[ \frac{\partial E^M_{1}}{\partial D^M_1} \right] \delta q^M + \delta \Phi^M
\]

with

\[
\delta \tilde{u}_i = w \left[ \Delta_{jki} \left( \frac{\partial \epsilon^M_{jk}}{\partial \sigma^M_{m0}} \frac{\partial \epsilon^M_{jk}}{\partial \sigma^M_{m0}} \frac{\partial \epsilon^M_{jk}}{\partial \sigma^M_{m0}} \right) \Delta_{jki} \right] \delta \gamma^M - w \left[ \Delta_{jki} \left( \frac{\partial \epsilon^M_{jk}}{\partial D^M_1} \frac{\partial \epsilon^M_{jk}}{\partial D^M_1} \frac{\partial \epsilon^M_{jk}}{\partial D^M_1} \right) \right] \delta q^M
\]

\[
\delta \Phi = -w \left[ \left( \frac{\partial E^M_{1}}{\partial \sigma^M_{jk}} \frac{\partial E^M_{1}}{\partial \sigma^M_{jk}} \frac{\partial E^M_{1}}{\partial \sigma^M_{jk}} \right) \Delta_{jki} \right] \delta \gamma^M + w \left[ \frac{\partial E^M_{1}}{\partial D^M_1} \frac{\partial E^M_{1}}{\partial D^M_1} \frac{\partial E^M_{1}}{\partial D^M_1} \right] \delta q^M
\]

Here, it is assumed that after macroscopic crack nucleation, i.e. the part where the homogenization scheme is used, the non-linearity in \( \delta v_i^M \) and \( \delta \gamma \) is fully covered by the macroscopic jump. Hence, it is assumed that \( \delta \tilde{u}_i^M \) and \( \delta \Phi \) are zero. Making this assumption allows to rewrite (39) as

\[
\tilde{v}_i^M = w \left[ \Delta_{jki} \frac{\partial \epsilon^M_{jk}}{\partial \sigma^M_{m0}} \right] \Delta_{jki} \gamma^M - w \left[ \Delta_{jki} \frac{\partial \epsilon^M_{jk}}{\partial D^M_1} \right] q^M + \tilde{u}_i^M
\]

\[
\gamma^M = -w \left[ \frac{\partial E^M_{1}}{\partial \sigma^M_{jk}} \right] \Delta_{jki} \gamma^M + w \left[ \frac{\partial E^M_{1}}{\partial D^M_1} \right] q^M + \Phi^M
\]

The material derivatives in this expression can be directly related to those used for the bulk constitutive behaviour in Equation (29). Moreover, \( \tilde{u}_i^M \) and \( \Phi^M \) are computed at the moment of nucleation, i.e. when \( \tilde{u}_i^M = \Phi^M = 0 \). As both \( v_i^M \) and \( \gamma^M \) are functions of the macroscopic traction \( \tilde{t}_i^M \) and macroscopic surface charge density \( q^M \), Equations (41) are merely a set of non-linear equations. Hence, for a given macroscopic crack opening \( \tilde{u}_i^M \) and macroscopic potential jump \( \Phi^M \), the corresponding traction and surface charge density can be computed. Equations (41) thus serve as constitutive laws for the interfaces.

The microscale model is discretized using the finite element method to yield a system of the form

\[
f_{int}^m (\mathbf{u}^m) = \mathbf{A} \tau
\]
with \( \mathbf{f}_{\text{int}}^m \) and \( \mathbf{a}^m \) being the \( n \)-dimensional microscopic electromechanical internal force vector and microscopic electromechanical nodal displacement vector, respectively. The homogenized electromechanical external loads

\[
\mathbf{\tau} = \mathbf{h} \begin{pmatrix} \mathbf{t}^M \\ \mathbf{q}^M \end{pmatrix}
\]

are mapped on the microscopic external load vector by the matrix \( \mathbf{A} \). As \( \mathbf{\tau} \) has three components, representing the horizontal and vertical components of the homogenized traction and the homogenized surface charge density, the system (42) consists of \( n \) equations and \( n + 3 \) unknowns. In order to close this system three additional equations are obtained from (41).

By virtue of the microscale boundary conditions it then follows that the microscopic displacement of the control node can be written as:

\[
\begin{pmatrix} \mathbf{v}^M \\ \mathbf{\gamma}^M \end{pmatrix} = \mathbf{A}^T \mathbf{a}^m
\]  

(44)

Using this expression along with the loading vector (43), Equation (41) is written as

\[
\mathbf{A}^T \mathbf{a}^m = \frac{\mathbf{w}}{\mathbf{h}} \mathbf{C} \mathbf{\tau} + \begin{pmatrix} \mathbf{\hat{u}}^M \\ \mathbf{\phi}^M \end{pmatrix} + \begin{pmatrix} \mathbf{\tilde{u}}^M \\ \mathbf{\tilde{\phi}}^M \end{pmatrix}
\]

(45)

with \( \mathbf{C} \) being a \( 3 \times 3 \) matrix containing the material tangents. Note that this is merely a system of three equations with the unknowns \( \mathbf{a}^m \) and \( \mathbf{\tau} \). As a consequence, this system is used to complement the system of Equations (42). The augmented system of \( n + 3 \) equations and unknowns is then solved using a Newton–Raphson procedure. In order to preserve the sparsity of the stiffness matrix of the micromodel, the augmented system is solved using the Woodbury formula [29]. Application of this formula requires the solution of four conventional microscale systems of equations. As the LU-decomposition can be reused, these solutions are obtained without much additional computational effort.

4.3. Determination of propagation instance and direction

The instance and direction of propagation of a crack are determined on the basis of the smoothed Cauchy stress as computed by Equation (20). Obviously, the microstructural influence is captured by the fact that the bulk stresses are computed by means of the homogenized constitutive relations (29). As the cohesive law is not explicitly known in the framework considered here, it is not trivial to relate the ultimate strength of the constitutive law to the propagation criterion. Therefore, a crack is propagated before the homogenized maximum strength of a micromodel is reached. The maximum principal stress is used to determine the propagation instance as well as the propagation direction. This method of crack propagation implies that after the extension of a crack, the load bearing capacity will initially further increase. As a consequence, the cohesive zone will slightly run behind the tip of the discontinuity.

As already mentioned in the previous subsection, upon insertion of a cohesive segment the micromodel is ran with the traction corresponding to the local stress state. In order to increase the robustness of the method, this external load is increased in a number of steps (typically 10).
Once the external load matches the local stress corresponding to the propagation instance, the compatibility quantities $\tilde{u}_i$ and $\Phi$ are obtained.

### 4.4. Illustration of homogenization procedure

In Section 5, the homogenization framework is applied in the partition of unity-based finite element framework discussed in Section 2. In order to clarify the homogenization procedure, the scheme is first applied to the simplified microstructure shown in Figure 8. This microstructure represents a material with columnar grains, separated by vertical grain boundaries. Moreover, the focus in this subsection is on the homogenization of the traction-opening law. Therefore, only the homogenization procedure for the mechanical constitutive behaviour is considered here.

Let the microscopic constitutive behaviour be given by

$$\sigma^m = H^m \varepsilon^m \quad \text{and} \quad t^m = \left( \frac{t^m_{\text{ult}} e}{\varphi^m_c} \right)^2 \tilde{u}^m \exp \left( - \frac{t^m_{\text{ult}} e}{\varphi^m_c} \right)$$

with $\tilde{u}^m$ being the displacement jump over the grain boundary $\Gamma_{gb}$. The traction-separation law describes the load bearing capacity of the microscale grain boundaries. Although it shows mathematical similarities with the cohesive law (16) used for the macroscale experiments, it is emphasized that this law describes a different physical phenomenon. This is reflected by the fact that Equation (46) is initially elastic, whereas Equation (16) is initially rigid.

Using the constitutive relations (46) the response of the representative volume element can be determined. The result for $H^m = 100 \text{GPa}$, $t^m_{\text{ult}} = 100 \text{MPa}$ and $\varphi^m_c = 0.01 \text{N/mm}$ is shown in Figure 9 for the three different microstructure sizes as indicated in Table II. As can be seen, the responses for the three cases differ significantly.

Following from Equations (24) and (28) the homogenized strain and stress prior to macroscopic crack opening are obtained by

$$\langle \varepsilon^m \rangle^\Omega = \frac{v^M}{w} \quad \text{and} \quad \langle \sigma^m \rangle^\Omega = \frac{F^M}{h}$$

from which the tangent is obtained as

$$\frac{\partial \langle \sigma^m \rangle^\Omega}{\partial \langle \varepsilon^m \rangle^\Omega} = \frac{w}{h} \frac{\partial F^M}{\partial v^M}$$

Figure 8. Simplified mechanical microstructure.
Figure 9. Force–displacement curve for the simplified microstructure with three different microstructure sizes as given in Table II.

Table II. Homogenized properties for various sizes of the simplified microstructure.

<table>
<thead>
<tr>
<th>$w$ (µm)</th>
<th>$h$ (µm)</th>
<th>$\frac{\partial \varepsilon^M}{\partial \varepsilon^M}$</th>
<th>$\frac{\partial \sigma^M}{\partial \varepsilon^M}$</th>
<th>$\varepsilon^M$</th>
<th>$\varepsilon^M$</th>
<th>$F_u^M$ (N)</th>
<th>$\bar{\varepsilon}^M$ (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10</td>
<td>10</td>
<td>88.1</td>
<td>88.1</td>
<td>13.7×10^{-6}</td>
<td>1.0</td>
<td>2.33×10^{-6}</td>
</tr>
<tr>
<td>2</td>
<td>20</td>
<td>10</td>
<td>44.0</td>
<td>88.1</td>
<td>27.4×10^{-6}</td>
<td>1.0</td>
<td>4.65×10^{-6}</td>
</tr>
<tr>
<td>3</td>
<td>10</td>
<td>5</td>
<td>44.0</td>
<td>88.1</td>
<td>13.7×10^{-6}</td>
<td>0.5</td>
<td>2.33×10^{-6}</td>
</tr>
</tbody>
</table>

In Table II the initial values of both the force–displacement curve slope and averaged tangent are shown. As can be seen, the initial slope depends on both the width and height of the microstructure, but the tangent does not. For the considered case, the macroscopic stress is approximated by

$$\sigma^M = \frac{\partial (\sigma^m)_{\Omega^m}}{\partial (\varepsilon^m)_{\Omega^m}} |_0 \varepsilon^M$$

(49)

More interesting is the homogenization procedure for the cohesive law. For the simple case considered, Equation (41) reads

$$v^M = w \frac{\partial (\varepsilon^m)_{\Omega^m}}{\partial (\sigma^m)_{\Omega^m}} |_0 t^M + \bar{u}^M + \tilde{u}^M$$

(50)

Assuming the macroscopic crack to be inserted at the maximum traction, $t_u^M$, yields

$$\tilde{u}^M = v^M(t^M) - w \frac{\partial (\varepsilon^m)_{\Omega^m}}{\partial (\sigma^m)_{\Omega^m}} |_0 t^M$$

(51)

For a given value of the opening, $\tilde{u}^M$, Equation (50) can be solved for $t^M$. The resulting traction-opening laws are shown in Figure 9. The traction-opening relations for microstructure 1 and 3 coincide. Microstructure 2 dissipates less energy, which is a consequence of the fact that more energy is dissipated before crack nucleation. This is a consequence of the larger displacement at zero opening, $\tilde{\varepsilon}^M$. As will be demonstrated in the next section, this difference in dissipation is negligible for the numerical simulations considered.
5. MULTISCALE SIMULATIONS

The three-point bending test with 4 mm off-centred notch as studied in Section 3 and schematically shown in Figure 5 is considered with all dimensions scaled down by a factor of 20. Hence, the studied specimen has a width of 955 μm and a height of 450 μm. A potential difference of \( V = 100 \) V is applied. The partition of unity-based framework presented in Section 2 is employed to mimic quasi-static crack growth in this component. In contrast to the macroscale experiments in Section 3, the constitutive behaviour of the component is now obtained by means of the homogenization framework presented in Section 4. In particular, Equations (29) and (41) are used to describe the bulk and cohesive constitutive behaviour, respectively. On the microscale, a polycrystalline microstructure is considered with 1 grain/μm². In this work, the polycrystal is assumed to fail due to intergranular fracture. Failure of the grain boundaries is modelled by means of an interface element-based cohesive finite element model as outlined in Reference [21]. In contrast to the microscale cohesive zone model employed in Reference [21], the mechanical cohesive behaviour is described by the microscale traction-opening law schematically shown in Figure 10. This traction-opening relation is based on the formulation of an effective traction-opening law, as used in, e.g. Reference [30]. It is here preferred over the Xu–Needleman law [22], as its initial stiffness can be adjusted independently of the fracture strength and fracture toughness.

The constitutive behaviour of the grains is described using the linear piezoelectric relations (13) with the parameters in Table I. The polarization direction corresponds with the macroscopic horizontal direction. The polarization direction on the microscale then depends on the direction of the macroscopic crack (as the microscopic coordinate system is not aligned with the macroscopic coordinate system). For the cohesive behaviour, the initial stiffness is taken as \( 1 \times 10^9 \) MPa/mm. The fracture strength and fracture toughness are taken as 40 MPa and \( 1 \times 10^{-2} \) N/mm, respectively. The mode-mixity parameter \( \beta \) and penetration stiffness \( k_p \) are assumed to be equal to 2 and \( 1 \times 10^{14} \) MPa/mm, respectively. The grain boundary thickness is approximated to be 10 nm [31]. Note that this grain boundary thickness is merely a material parameter and that the grain boundaries are modelled using zero thickness interface elements. The grain boundary permittivity is assumed to be equal to the permittivity of the bulk material in the direction of polarization.

![Figure 10. Micromechanical traction-opening law used for the derivation of the electromechanical constitutive relations for the microscale grain boundaries as outlined in Reference [21]. The \( \langle \Box \rangle \) are the Macaulay brackets and \( \beta^m \) is a mode-mixity factor. In the case of a negative opening, an additional penetration stiffness, \( k_p^m \), is used. The unloading behaviour is illustrated by the dashed line.](image-url)
For the computations presented in this paper, the only non-linearity considered on the microscale is the debonding of the grain boundaries. Although upon increasing the loading, the grain boundaries will debond, it is questionable if other damage mechanisms can be ignored. In particular, internal stresses caused by domain switching will likely affect the failure behaviour of a piezoelectric component. This will especially be the case when cyclic loading conditions are encountered. As this work focuses on the development of an efficient homogenization scheme, the microstructural model is intentionally kept relatively simple and effects such as domain switching are ignored. However, the multiscale framework presented here does not put restrictions on the microstructural complexity. Hence, phenomena such as domain switching, transgranular fracture and many others can be incorporated in the same framework. Incorporation of these phenomena in the microscale model, yielding advance micromechanically motivated homogenized cohesive laws, is a topic of future research.

5.1. Determination of the representative volume element size

In multiscale analyses, determination of an appropriate size for the microstructural model is one of the most important issues. Generally it can be stated that the size should be chosen such that:

- The microstructural domain is large enough such that the homogenized properties become independent of microstructural variations.
- The microstructural domain is small enough such that separation of scales is guaranteed. That is, over the size of the microscale domain, the homogenized kinetic and kinematic properties are practically constant.

Upon satisfaction of both conditions we speak of a representative volume element (RVE). The determination of the RVE size is here done by a priori consideration of the first condition. The second condition is checked a posteriori.

In this work square polycrystals of 2, 4, 6 and 8 μm are considered. For each size, 20 realizations are used. In order to study the appropriateness of the polycrystals for homogenization, two components of the homogenized initial tangent are studied. Moreover, the ultimate traction in normal direction and ultimate surface charge density is considered for the case that the polycrystals are loaded in the horizontal direction with an applied electric field of 1 kV/mm. The results of this size comparison study are shown Figure 11. The study of the four quantities mentioned above is assumed to be representative for the complete homogenization procedure. Moreover, the restriction of the RVE size study to the mode I case is assumed to be appropriate since for the multiscale simulations considered in the following sections, the macro cracks are observed to be mode I dominated.

The homogenized elastic and dielectric compliance components are observed to converge in the sense that the coefficient of variation tends to go to zero upon increasing the size of the polycrystal. For the 2 μm model, the coefficient of variation between 3.2 and 0.2% is noticed for the elastic and dielectric compliance component, respectively. When increasing the size to 8 μm, these coefficients decrease to 0.6% and 0.1%. Moreover, it is seen that for both quantities the mean value hardly varies. The observations for the homogenized ultimate traction and ultimate surface charge density differ from these for the compliance components. The mean values are noticed to converge to an asymptote when the microstructure size is increased to 8 μm. The decrease in ultimate values upon increasing the specimen size is explained by the fact that more crack paths become available. As the micro cracks choose the path that requires minimum energy dissipation, the required load to
rupture a polycrystal decreases when more paths become available. In addition, the coefficient of variation is noticed to diminish from 6.6 to 4.2% for the ultimate traction and from 0.9 to 0.6% for the ultimate surface charge density when increasing the size from 4 to 8 µm. The coefficient of variation of the fracture strength for the 2 µm model is not following this trend. The reason for this is that the actual randomness in microstructural geometry is constrained due to the limited size of the microstructure.

Based on the RVE size study presented above, a representative volume size of 8 µm is selected. For this size both the compliance components and the ultimate traction and surface charge density tend to converge to a stable mean value. Although a (slightly) bigger RVE size is desirable when considering the coefficient of variation of the fracture strength, the 8 µm RVE is considered as an appropriate balance between computational costs and model accuracy. Moreover, in order to appropriately represent the average microstructural response, the realization of the microstructure being closest to the mean ultimate traction is used. It should be noted that it is possible to use different representative volume elements for different macroscale integration points. Here, the same
Figure 12. Comparison of the horizontal stress contours and force–displacement curves obtained by the multiscale model (dashed curve) and by the full-resolution model (solid curve). The displacements in the contour plots are amplified by a factor of 10 and the force $F$ acts as shown in Figure 5 and is plotted versus the downward displacement of the loading point.

RVE is used everywhere in order to reduce the memory usage of the multiscale computational framework.

5.2. Verification of the multiscale model using a full-resolution simulation

In the case of unlimited computational power, the results of the multiscale model could be verified using a full-resolution model in which the complete granular microstructure is represented. However, due to the enormous amount of degrees of freedom required, such a computation cannot be performed. In order to verify the multiscale framework, a macroscopic model is considered in which the microstructure is only incorporated in the region of interest, i.e. in the area where the crack runs (see Figure 12). The granular microstructure is modelled in a zone of $4 \times 100\mu m$ at an angle of 60 degrees with the horizontal axis. In order to make a fair comparison, the crack in the multiscale model is also forced to run at this angle. Moreover, for consistency the multiscale model is here employed with a micromodel of $4 \times 4\mu m$.

Contour plots of the Cauchy stress in horizontal direction (Figure 12) show that the microscopic stress fluctuations are smeared out in the multiscale model. A comparison of the force–displacement curves for both simulations demonstrate that this averaging hardly affects the global response of the system. The ultimate load is accurately predicted by the multiscale model. The stiffness is slightly underestimated by the multiscale model. This indicates that on average the homogenized stiffness of the micro model is slightly lower than that of the considered representative volume element. The fringing grains as observed in the full-resolution simulation partially explain this mismatch.

When considering the computational effort, a significant difference between the two methods is present. With 23,214 elements (21,049 linear triangular bulk elements and 2,165 four-node linear interface elements) and 38,868 degrees of freedom, construction of the force–displacement curve for the full-resolution model requires approximately 20 times the computation time of the multiscale model with 3,811 macroscale linear triangular elements and 5,892 macroscale degrees of freedom, when using a micromodel with 268 elements (192 linear triangular bulk elements and 76 four-node linear interface elements) and 600 degrees of freedom. For both simulations just over 150 steps are required for tracing of the equilibrium paths shown in Figure 12. Moreover, it is emphasized...
that the multiscale model remains applicable in the case that the crack trajectory is not \textit{a priori} defined. For that situation the use of the full-resolution model is impractical.

5.3. Multiscale simulation

The multiscale model is now demonstrated using an 8\,\mu m micro model. On the macroscale the same mesh as used in the previous subsection is considered. On the microscale, a mesh with 708 bulk elements, 292 interface elements and a total of 2208 degrees of freedom is employed. The instance and direction of propagation are based on the principal stress obtained by Equation (19) with the smoothing length $l_R$ taken as 5\,\mu m. The simulation is performed on a single processor. It should be noted that the proposed framework is suitable for parallel computing since the majority of the computational effort is spent in solving the individual micro models.

The force–displacement curve for the experiment is shown in Figure 13. The maximum load carried by the specimen equals 2.97 N. In Figure 14, the horizontal stress contour is shown. It is observed that the cohesive zone size is considerable larger than the size of the microstructural RVE. As a consequence, the variation of the microscopic quantities over the size of the RVEs is limited. The second RVE requirement as mentioned in Section 5.1 is therefore satisfied for the case considered here. For problems where the separation of scales between the cohesive zone size and characteristic dimensions of the microstructure is smaller, the second RVE requirement becomes troublesome. The proposed framework can remain useful in such a situation, but the application of the method should be done with great caution.

In Figure 14 the electric potential over the specimen is shown. The corresponding solutions of the microscopic models are also depicted. As can be seen, the macroscopic displacement jump is caused by a fractured grain boundary. The traction-opening relations for the two microstructural models in Figure 14 are shown in Figure 15. The compatibility opening for both micromodels is in the order of magnitude of 1 nm. The corresponding amount of dissipated energy is negligible compared with the total fracture energy of the micromodels. As a consequence, the influence of the non-linear behaviour of the microscale prior to macroscopic crack nucleation is limited.

6. CONCLUSIONS

A partition of unity-based cohesive zone model for simulating failure of electromechanically coupled materials is proposed. The performance of the model is tested by means of a comparative study with a set of benchmark experiments. It has been demonstrated that the model is capable of reasonably accurate prediction of the ultimate load of various specimens with varying loading conditions. Especially, the influence of an externally applied electric field on the fracture load is well approximated for moderate values of the electric field.

The proposed cohesive zone model is also applied on a microscale specimen. In order to correctly capture the influence of the microstructure on the response of such a miniaturized component, the cohesive behaviour of a crack is obtained on the basis of a finite element model representing the granular microstructure. This constitutive multiscale framework is derived using the Hill energy condition for both the mechanical and the electric contributions. The existence of a representative volume element is shown.

A comparison of results with a full-resolution model shows the appropriateness of the proposed multiscale framework. It is demonstrated that a significant reduction in computational effort can
Figure 13. Force–displacement curve for the miniaturized three-point bending test as modelled by the constitutive multiscale framework with 8μm RVE.

Figure 14. Contour plots of the horizontal Cauchy stress (top) and electric potential field (bottom) for the miniaturized three-point bending specimen at the ultimate load. The displacements are 10 times magnified.
be achieved by using the proposed framework. Moreover, it is emphasized that the proposed framework is capable of dealing with sophisticated microscale models as well as with purely mechanical models. This offers the possibility of deriving micromechanically motivated cohesive laws that include effects such as piezoelectric domain switching. The development and assessment of such models, which is required to obtain physically more realistic behaviour, are a topic of the future research.

ACKNOWLEDGEMENTS

The MicroNed programme (part of the BSIK programme of the Dutch government) is acknowledged for supporting the research of Clemens Verhoosel.

REFERENCES


