Three-dimensional BEM for piezoelectric fracture analysis

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Abstract

A boundary element approach with quadratic isoparametric elements, quarter-point elements and singular quarter-point elements for three-dimensional crack problems in piezoelectric solids under mechanical and electrical loading conditions, is presented in this paper for the first time. The procedure is based on Deeg’s fundamental solution for anisotropic piezoelectric materials, and the classical extended displacement boundary integral equation. Stress and electric displacement intensity factors are directly evaluated as system unknowns, and also as functions of the computed nodal displacements and electric potentials at crack faces. Special attention is paid to the fundamental solution evaluation. Several three-dimensional crack problems in transversely isotropic bodies under mechanical and electrical loading conditions are analysed. Numerical solutions computed for prismatic cracked 3D plate problems with a plane strain behaviour are in very good agreement with their corresponding 2D BE solutions. Results for a penny shape crack in a piezoelectric cylinder are presented for the first time. The proposed approach is shown to be a simple, robust and useful tool for stress and electric displacement intensity factors evaluation in piezoelectric media.

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1. Introduction

Piezoelectric materials produce an electric field when deformed and undergo deformation when subjected to an electrical field. Since the mid of the 20th century, there have been piezoelectric ceramics with a piezoelectric ratio between electric field and mechanical stress (and between mechanical strain and electric displacement), two orders of magnitude higher than that of natural piezoelectric materials. These materials have become the basic ingredient for construction of sensors, transducers, actuators and adaptive structures. Lead zirconate titanate (PZT) is the most widely used piezoceramic and polyvinylidene fluoride (PVDF) the most extended piezopolymer. They were first produced in 1946 and 1969, respectively. Modelling of piezoelectrics is complicated by the fact that they exhibit not only electro-elastic coupling but anisotropic behaviour as well. Piezoelectric effect can only appear in crystals that lack a centre of symmetry; therefore, they are always anisotropic.

Piezoelectric materials are brittle, and due to manufacturing process and complex electromechanical loads, they are likely to develop cracks. The understanding and evaluation of the fracture process in piezoelectric materials are crucial to the advancement of modern intelligent material systems. Among the most significant publications on the field of piezoelectric materials fracture mechanics, one can cite the works of Barnett and Lothe [1], Deeg [2], Pak [3], Suo et al. [4], Sosa [5], Park and Sun [6] and Wu et al. [7].

It is well known that the Boundary Element Method (BEM) presents significant advantages over other numerical techniques for the analysis of fracture mechanics problems. This fact has led to the publication of several BE approaches for the analysis of cracks in piezoelectric solids in the last few years. The main difficulties in the field are related to derivation and integration of fundamental solutions for two- and three-dimensional static and dynamic problems. Pan [8] presented a single domain BE formulation for 2D static crack problems. He derived the fundamental solution using the complex variable function method [9–11] and computed the hypersingular integrals using a numerical quadrature. Liu and Fan [12] established some of the basic equations in
a rigorous way and addressed the question of degeneration for cracks and thin shell-like problems. Rajapakse and Xu [13] and Xu and Rajapakse [14] used Lekhnitskii’s formalism and distributed dislocation modelling to derive special Green’s functions for an infinite medium containing a crack. They studied different crack geometries including branched cracks. Denda and Lua [15] developed a BEM formulation using Stroh’s formalism to derive the fundamental solution but they did not show any numerical result. Davi and Milazo [16] presented a multidomain approach based on the conventional BE formulation. The fundamental solution was obtained by a variant of Lekhnitskii’s functions method similar to that used by Rajapakse and Xu [13,14]. All these papers deal with 2D domains.

Few papers on BE formulations for three-dimensional piezoelectric solids have been published. Back in 1995, Chen and Lin [17] presented a three-dimensional BEM based on Green’s functions evaluated numerically from integrals derived from the Fourier transform. They solved a simple problem using constant elements but the evaluation of integrals required cumbersome computations [17] and was done only for quasi-isotropic materials. Dunn and Wienecke [18] obtained closed-form Green’s functions for transversely isotropic piezoelectric solids and Zhao et al. [19] a 3D fundamental solution for displacement and electric potential discontinuity that was applied to the case of a circular crack in an infinite domain [20,21]. Pan and Tonon [22] derived 3D Green’s functions for anisotropic piezoelectrics using the Radon transform and evaluating the resultant contour integral by residue calculus and numerical computation of an eighth-order polynomial. All the poles are assumed to be simple and derivatives of the Green’s functions are evaluated numerically. Liew and Liang [23] presented Green’s functions for transversely isotropic piezoelectric bimaterials based on Ding et al. [24] solution for distinct eigenvalue materials and applied them to the solution of the problem of cavities in an infinite domain. Ding and Liang [25] and Ding et al. [26] presented a BE approach based on simplified fundamental solutions for transversely isotropic piezoelectric solids and applied it to problems with simple geometry and boundary conditions. Recently, Chen [27,28] has presented a hypersingular integral equation approach based on Ding and Liang [25] fundamental solution for transversely isotropic materials with distinct eigenvalues. The hypersingular integral equations are solved analytically for a penny-shaped crack in an infinite domain. A method of series expansion with numerical evaluation is used by these authors for other simple geometry planar cracks in infinite media. The above works either deal with Green’s functions evaluation with or without simplifications are restricted to certain type of materials, or are limited to infinite domain geometries. Attention should be paid also to the paper by Hill and Farris [29] where the general fundamental solution is obtained using the Radon transform as in Deeg’s work [2] and some simple numerical examples are analysed using quadratic boundary elements.

In the present paper, a general Boundary Element approach for three-dimensional fracture mechanics problems in piezoelectric solids is presented. The procedure is based on Deeg’s fundamental solution for anisotropic piezoelectric materials, and the classical extended displacement boundary integral equation, which is discretized using quadrilateral and triangular quadrilateral elements. The crack surface is represented by standard quadratic elements except for elements containing the crack front which are nine-node quadrilateral quarter-point elements. These elements are able to represent exactly the crack displacement and electric potential near the front. Elements next to the crack front containing the stress/electric displacement singularity are singular quarter-point elements whose shape functions are those of the standard elements divided by the square root of the distance to the front. By doing so, the electric displacement and stress intensity factors (ESIF) can be directly computed as system unknowns at the crack front. They can also be computed from the crack opening displacement and the electric potential increment at quarter-point nodes inside the crack. The boundary element approach presented in this paper is the 3D piezoelectric counterpart of the approaches presented by Ariza et al. [30], Saez et al. [31] and Martinez and Dominguez [32], for 3D isotropic elastic, 3D anisotropic elastic, and 2D isotropic elastic crack problems, respectively. Several three-dimensional crack problems in transversely isotropic bodies under mechanical and electrical loading conditions are analysed.

2. Basic piezoelectricity equations

Under static loading, the linear equilibrium conditions for piezoelectric materials can be written as two separate equations, one for conservation of momentum and the other for conservation of electric charge. Both can be written in a condensed notation developed by Barnett and Lothe [1] as

$$\sum_{i,j} a_{ij} + b_J = 0$$

where the lower case indices can take values 1–3, the upper case indices can take values 1–4, $\sum_{i,j}$ is the stress–electric displacement matrix, defined as

$$\sum_{i,j} = \begin{cases} \sigma_{ij} & \text{for } J = 1, 2, 3 \\ D_i & \text{for } J = 4 \end{cases}$$

and $b_J$ is the body load vector containing the three force components and the fourth component is minus the electric charge. It is noted that $J=j$ for 1, 2, or 3, the repeated indices indicate summation and the commas differentiation.
The constitutive equations are written as

\[ \mathbf{\Sigma}_{ij} = E_{ijkl} Z_{kl} \]  

(3)

where \( E_{ijkl} \) is the electroelastic constant matrix

\[ E_{ijkl} = \begin{cases} 
C_{ijkl} & \text{for } J, K = 1, 2, 3 \\
\epsilon_{ij} & \text{for } J = 1, 2, 3, K = 4 \\
-\epsilon_{ikl} & \text{for } J = K = 4 
\end{cases} \]  

(4)

The elastic constants are measured at constant electric potential, the piezoelectric constants are measured either at constant displacement or constant electric potential, and the dielectric constants are measured at constant displacements. These constants satisfy the following symmetry relations:

\[ C_{ijkl} = C_{jikl} = C_{jikl}, \quad \epsilon_{ij} = \epsilon_{ji}, \quad \epsilon_{il} = \epsilon_{li} \Rightarrow E_{ijkl} = E_{jikl} \]  

(5)

In general, a total of 45 independent material constants are possible (21 elastic, 18 piezoelectric and 6 dielectric). The formulation presented in this paper allows for this general case. Nevertheless, most piezoelectric materials are elastically transversely isotropic with a total number of independent constants equal to 10 (5 elastic, 3 piezoelectric and 2 dielectric).

The elastic strain–electric field matrix \( Z_{kl} \) takes the form:

\[ Z_{kl} = \begin{cases} 
\phi_{kl} & \text{for } K = 1, 2, 3 \\
\phi_{l} & \text{for } K = 4 
\end{cases} \]  

(6)

The elastic displacement–electric potential vector \( U_K \) is defined as

\[ U_K = \begin{cases} 
u_k & \text{for } K = 1, 2, 3 \\
\phi & \text{for } K = 4 
\end{cases} \]  

(7)

and the elastic traction–normal charge flux vector \( P_K \) as

\[ P_K = \begin{cases} 
p_k = \sigma_{kj} \cdot n_j & \text{for } K = 1, 2, 3 \\
q = D_r \cdot n_i & \text{for } K = 4 
\end{cases} \]  

(8)

The piezoelectric matrices introduced above are neither tensors nor vectors. They do not obey the transformation relations in the combined form.

By substitution of Eqs. (3) and (6) into Eq. (1) and taking into account the definition of strain in terms of displacements \( \epsilon_{ij} = 1/2(\mathbf{u}_{ij} + \mathbf{u}_{ji}) \), one obtains a system of differential equations which must be solved in reference to boundary conditions. Both mechanical and electrical boundary conditions must be applied for a well-posed piezoelectric boundary value problem. The essential boundary conditions are

\[ \mathbf{u}_t = \tilde{\mathbf{u}}_t \quad \text{on } \Gamma^a \]  

(9)

\[ \phi = \tilde{\phi} \quad \text{on } \Gamma^\phi \]  

(10)

where \( \tilde{u}_t \) and \( \tilde{\phi} \) are the known displacements and electric potentials on the boundaries \( \Gamma^a \) and \( \Gamma^\phi \), respectively. The natural boundary conditions are written as

\[ \sigma_{kj} n_j = p_i = \tilde{p}_i \quad \text{on } \Gamma^r \]  

(11)

\[ D_r n_i = q = \tilde{q} \quad \text{on } \Gamma^q \]  

(12)

where \( \tilde{p}_i \) and \( \tilde{q} \) are the known tractions and normal electric charge flux on the boundaries \( \Gamma^r \) and \( \Gamma^q \), respectively. For a well-posed problem, at each boundary point, either displacement or traction and potential or normal charge flux must be prescribed.

3. Boundary integral equation

Based on the extended reciprocal relation for piezoelectric media, a boundary integral equation for a point inside or on the boundary of a piezoelectric body under zero internal forces and electric charge conditions, can be written as

\[ C_{ij} U_j + \int_G P_{ij} U_j d\Gamma = \int_G U_{ij} P_j d\Gamma \]  

(13)

where \( U_j \) and \( P_j \) are the extended displacement and extended traction column matrices, respectively; \( U_{ij} \) and \( P_{ij} \) are the fundamental solution extended displacement and extended traction matrices, respectively, and \( C_{ij} \) is the local tensor at point \( i \) such that \( C_{ij} = (1/2) \delta_{ij} \) for smooth boundary points and \( C_{ij} = \delta_{ij} \) for internal points.

The fundamental solution matrices can be obtained from the anisotropic piezoelectric bodies Green’s function derived by Deeg [2], which is written in terms of an integral over a unit spherical surface as

\[ G_{MR}(x - x') = \frac{1}{8\pi^2 r} \int_{|z|=1} (zz)^{-1} \delta(z \cdot t) dS(z) \]  

(14)

where \( x' \) is the collocation point, \( x \) is the observation point, \( r = |x - x'| \) is the distance between those two points and \( t \) is a unit vector in the direction of \( x - x' \). The function \((zz)_{JM}\) is defined as

\[ (zz)_{JM} = z_j E_{JMn} z_n \]  

(15)

Consider a coordinate system defined by three mutually orthogonal vectors \( \mathbf{t} - \mathbf{m} - \mathbf{n} \) as shown in Fig. 1. The spherical angles are defined over the ranges \( 0 \leq \theta \leq \pi \) and \( 0 \leq \psi \leq 2\pi \). Let us define a unit vector \( \mathbf{z}^* \) as

\[ \mathbf{z}^* = z[\theta = (\pi/2), \psi] \]  

(16)

This vector \( \mathbf{z}^* \) lies in the \( \mathbf{m} - \mathbf{n} \) plane and represents all vectors \( \mathbf{z} \) that are perpendicular to \( \mathbf{t} \), such that \( \mathbf{z}^* \cdot \mathbf{t} = 0 \).
Eq. (14) can now be written in a more simplified form as
\[
G_{MR}(rt) = \frac{1}{8\pi r} \int_{0}^{2\pi} (z^* z^*)_{MR}^{-1} d\omega
\]  
(17)
where \( \omega \) is the integration angle shown in Fig. 1, with the vector \( m \) along the line \( \omega = 0 \). This function can be evaluated once the collocation point \( x' \), and the observation point \( x \) are known.

It can be observed from Eq. (17) that the fundamental solution consists of two parts. The first one \( \frac{1}{r} \) depends only on the distance between the observation and the collocation point. The second
\[
\int_{0}^{2\pi} (z^* z^*)_{MR}^{-1} d\omega
\]  
(18)
depends on the material properties and on the orientation of \( t \). This line integral does not contain singularities and can be computed by a standard Gauss quadrature.

In order to evaluate tractions and normal electric flux, the derivatives of \( G_{MR}(rt) \) are required. The general form of these derivatives is:
\[
\frac{\partial G_{MR}}{\partial x_1 \partial x_2 \ldots \partial x_n}(x - x') = \frac{1}{8\pi^2|x - x'|^{n+1}} \oint_{|z|=1} \left\{ \frac{z_2 \ldots z_n (zz)^{-1}}{|z|} \right\} \delta^{(n)}(z \cdot t) d\mathcal{S}(z)
\]  
(19)

The above integral becomes a line integral when \( z = z^* \):
\[
\frac{\partial G_{MR}}{\partial x_1 \partial x_2 \ldots \partial x_n}(x - x') = \frac{(-1)^n}{8\pi^2|x - x'|^{n+1}} \int_{0}^{2\pi} \frac{\partial z^*}{\partial (z \cdot t)} \left\{ \frac{z_2 \ldots z_n (zz)^{-1}}{|z|} \right\} \bigg|_{z = z^*} d\omega
\]  
(20)

In particular, the first integral can be written as
\[
\frac{\partial G_{MR}}{\partial x_i}(rt) = -\frac{1}{8\pi^2 r^2} \int_{0}^{2\pi} [I_i(z^* z^*)_{MR}^{-1} - z^*_i F_{MR}^*] d\omega
\]  
(21)
where
\[
F_{MR}^* = (z^* z^*)_{MR}^{-1} [n_0^*(z^* z^*)_{MN}^{-1} (z^* t)_{QN} + (z^* t)_{QN}]
\]  
(22)

The terms \( (z^* t)_{QN} \) and \( (z^* t)_{QN} \) are obtained from expression (15), and satisfy the following symmetry relation for transversely isotropic materials
\[
(z^* t)_{QN} = (z^* t)_{QN}
\]  
(23)

The fundamental solution extended displacement matrix and extended traction matrix are obtained from \( G_{MR}(x - x') \) as
\[
U^*_I(x - x') = G_{IJ}(x - x')
\]  
\[
P^*_I(x - x') = E_{kJMn} \frac{\partial G_{MI}(x - x')}{\partial x_a} n_k
\]  
(24)

Eq. (24) gives the values of the extended displacements and tractions for a unit load along direction \( I \). In the case of \( I = 4 \), these expressions give elastic displacements or tractions \( (J = 1-3) \) and electric potential or normal charge flux \( (J = 4) \) at \( x' \) when a unit point charge is applied at \( x \).

### 4. Three-dimensional cracks in piezoelectric solids

Mechanical boundary conditions at crack surfaces in piezoelectric solids can be clearly established without much difficulty. Crack surfaces are tractions free as long as no contact exists or a pressure is not prescribed inside the crack. However, electrical boundary conditions at crack surfaces are not that easily established. Some authors assumed perfectly permeable crack surfaces [33]. On the contrary, Deeg [2] and Pak [3] proposed zero normal charge flux as electrical boundary conditions at both crack surfaces, i.e.
\[
D^+_n = D^-_n = 0
\]  
(25)

In these boundary conditions there are two simplifying assumptions: (i) there is no external charge at any of the crack surfaces, and (ii) the electrical induction of the void between both crack surfaces is zero. In the present paper, the electrical boundary conditions defined by Eq. (25) are assumed.

The problem of an infinite transversely isotropic piezoelectric solid under uniform mechanical or electrical load applied at infinity containing a plane crack of infinite width and length equal to \( 2a \) perpendicular to the material axis of symmetry (Fig. 2), can be solved by assuming [3] an extended displacement of the form
\[
U_K = A_K f(m \cdot x + p n \cdot x)
\]  
(26)
where \( m \) and \( n \) are two normal unit vectors in the plane perpendicular to the crack front.

Expression (26) satisfies the equilibrium equation
\[
\sum_{ij} \sigma_{ij} = 0
\]  
(27)
It can be shown [2] by substitution of Eq. (26) into Eq. (27) that a non-trivial solution for \( A_K \) exists provided that

\[
|\langle mn \rangle_{JK} + p|\langle mn \rangle_{JK} + (mn)_{JK} + p^2(mn)_{JK}| = 0
\]  

Using Stroh’s formalism [34], the above equation can be expressed in terms of the following eigenvalue problem

\[
|\mathbf{N} - p_a \mathbf{I}| = 0
\]  

where \( \mathbf{N} \) is an \( 8 \times 8 \) real matrix defined as

\[
\mathbf{N} = \begin{bmatrix}
(mn)^{-1}(mn) & (mn)^{-1} \\
(nm)(nm)^{-1}(nm) & (nm)(nm)^{-1}
\end{bmatrix}
\]  

and \( \mathbf{I} \) is the \( 8 \times 8 \) unit matrix. Corresponding to each eigenvalue \( p_a \) there is an eigenvector that can be written in the following way:

\[
\xi_a = \begin{bmatrix} A_a \\ I_a \end{bmatrix}
\]  

It is shown in Ref. [1] that the eigenvectors are independent of the base vectors \( \mathbf{m}, \mathbf{n} \). The problem represented by Eqs. (29)–(31) can be solved in terms of only the material constants:

\[
|C_{1121} + p[C_{1122} + C_{1222}] + p^2C_{1222}| = 0
\]  

(32)

By using Eqs. (29) and (32) one can obtain the eigenvalues and eigenvectors of the problem. For each one of the four eigenvalues with positive imaginary part one obtains the \( 4 \times 4 \) \( \mathbf{A} \) and \( \mathbf{L} \) matrices given by [4,8]:

\[
\sum_{j=1}^{4} \left[ C_{112j} + p_K[C_{112j} + C_{122j}] + p_K^2C_{122j} \right] A_{jk} = 0
\]  

\[
L_{jk} = \sum_{j=1}^{4} \left[ C_{112j} + p_KC_{122j} \right] A_{jk}
\]  

The extended stress field along the crack line can be written as [3]

\[
\sum_{ij} \sigma_{ij}(x_1, 0)n_i = \sum_{ij} \sigma_{ij}^\infty |x_1| \sqrt{x_1^2 - a^2} / \sqrt{x_1^2 - a^2}
\]  

\[
\begin{cases}
\sigma_{ij}^\infty n_i |x_1| / \sqrt{x_1^2 - a^2} & i = 1, 2, 3; J = 1, 2, 3 \\
D_{ij}^\infty n_i |x_1| / \sqrt{x_1^2 - a^2} & i = 1, 2, 3; J = 4
\end{cases}
\]  

(35)

and the extended displacement field as

\[
U_j(x_1, 0) = H_{ij} \sum_{n} \sigma_{ij}^\infty \sqrt{a^2 - x_1^2}
\]  

\[
\begin{cases}
H_{ij} \sigma_{ij}^\infty n_i \sqrt{a^2 - x_1^2} & i = 1, 2, 3; J = 1, 2, 3 \\
H_{ij} \sigma_{ij}^\infty n_i \sqrt{a^2 - x_1^2} & i = 1, 2, 3; J = 4
\end{cases}
\]  

(36)

where

\[
H = 2 \text{Re}(Y)
\]  

(37)

and

\[
Y = iA\mathbf{L}^{-1}
\]  

(38)

Expressions (35) and (36) show a space variation of the electric variables of the same type as that of the elastic variables as expected from the linear coupling of both problems given by the constitutive equations.

The extended stresses for different angles \( \theta \) near the crack front (Fig. 2) can be written as

\[
\sum_{ij} \sigma_{ij}(r, \theta)n_i = \frac{K_P}{2\pi r} A_{ij} + \text{higher order terms}
\]  

(39)

where \( K_P \) are the Electric displacement and Stress Intensity Factors (ESIF) and \( A_{ij} \) gives the angular variation of stress components and electric displacement near the front. It can be written as

\[
A_{ij} = \frac{E_{ijkm}B_{SP}^\infty}{4\pi i} \sum_{a=1}^{8} \pm A_{ka} L_{Sa} (m_a + p_a n_a)
\]  

\[
\times \sqrt{\cos \theta + p_a \sin \theta}
\]  

(40)

where

\[
B_{SK} = B_{KS} = - \frac{1}{4\pi i} \sum_{a=1}^{8} \pm L_{Ka} L_{Sa}
\]  

(41)

The summations in the last two equations can be reduced to four terms since the eigenvalues are grouped in four conjugated pairs.

According to Eq. (39), one can obtain the \( K_P \) ESIF as the limit of tractions and normal charge flux at the crack front for \( \theta = 0 \), using the following equation.
\[
\lim_{r \to 0} \sum_{i,j} n_i = \frac{K_J}{\sqrt{2\pi r}} \tag{42}
\]

or using the expression for extended displacements near the front for \( \theta = \pm \pi \)

\[
U_J(r) = \sqrt{\frac{2r}{\pi}} \text{Re}[Y] K_J \tag{43}
\]

where \( Y \) is the matrix defined by Eq. (38). Note that the \( K \) vector components in Eqs. (42) and (43) are \( K = \{K_{II}, K_I, K_{III}, K_{IV}\}^t \), where \( K_I, K_{III}, K_{IV} \) are elastic SIF and \( K_{IV} \) is the Electric Displacement Intensity Factor.

5. Boundary element formulation and implementation

Using vector notation, the boundary integral equation can be written as

\[
C^i U^i + \int P^i U \, d\Gamma = \int U^* P \, d\Gamma \tag{44}
\]

where \( U \) and \( P \) are extended displacements and traction \( 4 \times 1 \) matrices, respectively, and \( C^i, U^i, \) and \( P^* \) are \( 4 \times 4 \) matrices.

The boundary of the body is divided as usual into NE elements. Extended displacements and tractions over the boundary elements are written in terms of their nodal values and shape functions. The system matrices are obtained by integration over the boundary elements of the fundamental solution matrices times the shape functions.

The boundary element representation of three-dimensional crack problems in piezoelectric bodies is done following the same steps as for elastic media [30,31]; (1) the domain under consideration is divided into subdomains by cutting it by a section through the crack; (2) each subdomain is analysed by the BEM; and (3) the subdomains are coupled using equilibrium and compatibility elastic and electrical relations. When the crack is in a plane of symmetry, the problem can be solved by studying only one subregion with the adequate symmetry boundary conditions.

The elements used in the present paper are standard nine-node or six-node quadratic elements except for those with one side at the crack front. Among these elements, the ones inside the crack surface (non-singular tractions or electric charge flux) are quarter-point elements and those extending inside the material are singular quarter-point elements. The quarter-point element (Fig. 3) is a quadrilateral with all its nodes on a plane. The displacement–potential representation over this element, with quadratic shape functions and the mid-side nodes located at one quarter of its width, is able to reproduce the first three terms of the displacement–potential actual behaviour in the proximity of the front, including the term varying with the square root of the distance to the crack front [30].

The singular quarter-point elements have one side along the crack front and are part of the boundary extending inside the material (Fig. 4). Shape functions with a \( 1/\sqrt{r} \) singularity at the crack front are used for tractions representation over this type of elements. To do so, the standard quadratic shape functions are divided by the square root of the distance to the crack front. Thus, the polynomial representation of tractions over these elements includes a term depending on the distance to the crack front as one over the square root of this distance. The tractions and normal charge flux nodal values of at nodes along the crack front represent, except for a constant, the ESIF at those nodes. A detailed description of quarter-point and singular quarter-point elements for three-dimensional elasticity problems, can be seen in Refs. [30,31].

Integration of the fundamental solution extended tractions or displacements times the shape function, over the
boundary elements, is done numerically. The fundamental solution terms for piezoelectric problems include a singular part of the same type as in the elastic problem (1/r for extended displacement and 1/r^2 for extended tractions) multiplied by a non-singular integral over a unit circumference (see Eqs. (17) and (21)) which can be evaluated numerically for any pair of collocation–observation points. This integral depends only on the orientation of the vector connecting those two points. Since the extra terms are non-singular, the same numerical approach as for isotropic and anisotropic elastic problems can be used to evaluate the system matrix. This procedure is a standard Gauss quadrature when there is not singularity involved, and a quadrature with some mapping of the integration domain when a singularity exists. Singularities appear when the collocation point belongs to the integration element, when the integration element is a singular quarter-point element, and when the combination of both occurs. A detailed description of the numerical approach, except for the integral along the unit circumference, can be seen in [30].

The numerical evaluation of the integral over a unit circumference (Eq. (18)) is rather time consuming. Twenty points along the circumference are used

\[
\int_0^{2\pi} (z^* \bar{z})^{-1}_{MR} \, dz = \frac{\pi}{10} \sum_{k=1}^{20} (z^* \bar{z})^{-1}_{MR_k} \tag{45}
\]

Evaluation of each term of the type \((z^* \bar{z})^{-1}_{MR}\) requires some manipulation. The \(z^*\) vector in the local coordinates system is:

\[
z^*(t) = \begin{pmatrix} z^*_m \\ z^*_n \\ z^*_t \end{pmatrix} = \begin{pmatrix} \cos \left(\frac{k \pi}{10}\right) \\ \sin \left(\frac{k \pi}{10}\right) \\ 0 \end{pmatrix} \quad k = 1 \ldots 20 \tag{46}
\]

It must be changed to the Cartesian basis by a transformation of the type

\[
z^*(x) = L^T \cdot z^*(t) \tag{47}
\]

where \(L^T\) is the cosines matrix of the unit vectors \(m-n-t\) in terms of \(x_1-x_2-x_3\). Vector \(t\) is uniquely defined by the collocation and the observation points and \(m, n\) are two unit normal vectors perpendicular to \(t\).

Once \(z^*(x)\) is known for an integration point, \((z^* \bar{z})^{-1}_{MR}\) is evaluated by means of Eq. (15). The resulting 4×4 matrix is then inverted and substituted into Eq. (45).

In order to reduce the computer time for evaluation of the integrals in Eq. (45), an interpolation approach can be implemented. Since those integrals depend only on the direction of vector \(t\), one can evaluate them for values of angles \(\varphi\) and \(\psi\) every 5° and interpolate linearly for intermediate angles (Fig. 5). Due to symmetries existing in the fundamental solution, only angles 0° ≤ \(\varphi\) ≤ 90° and 0° ≤ \(\psi\) ≤ 90° must be considered. The above interpolation gives accurate results for any values of \(\varphi\) and \(\psi\). By using this interpolation integration strategy, the computer time is reduced by a factor of 22. A problem with 1048 degrees of freedom runs in 40 s in a PC type computer with a 3 GHz processor.

6. Stress–electric displacement intensity factor evaluation

Once the extended displacement and traction nodal values have been computed by solution of the boundary element system of equations, the ESIF can be obtained directly from the traction nodal values at the crack front. Assuming \(x_3\) is the material axis of symmetry perpendicular to the crack plane, and \(x_2\) is tangent to the crack front line at the point where node \(k\) is located, the ESIF components at this point (Fig. 4) are given by the extended traction components nodal values

\[
K_I = p_t^k \sqrt{2\pi L} \quad K_{II} = p_t^k \sqrt{2\pi L} \\
K_{III} = p_t^k \sqrt{2\pi L} \quad K_{IV} = p_t^k \sqrt{2\pi L} \tag{48}
\]

where \(L\) is the singular quarter-point element length in the direction perpendicular to the crack front (Fig. 3). The above expressions are obtained by simple comparison of the \(1/\sqrt{r}\) term of the extended tractions representation over the singular element, and the term of the same order in the actual stresses given by Eq. (42).

A second procedure for ESIF evaluation can be obtained using the crack opening displacement/potential at quarter-point nodes (Fig. 4). Given a node on the crack front where the ESIF is desired, the computed extended values of the displacement at the quarter-point next to it, is made equal to the expression of the extended displacement at the same node in terms of the ESIF (Eq. (43)). By doing so, one obtains

\[
\int_0^{2\pi} \left( z^* \bar{z} \right)^{-1}_{MR} \, dz = \frac{\pi}{10} \sum_{k=1}^{20} \left( z^* \bar{z} \right)^{-1}_{MR_k} 
\]
\[
\begin{bmatrix}
K_{II} \\
K_{III} \\
K_I \\
K_{IV}
\end{bmatrix} = \sqrt{\frac{2\pi}{L}} \text{Re}(Y)^{-1} \begin{bmatrix}
U_1^i \\
U_2^i \\
U_3^i \\
U_4^i
\end{bmatrix}
\] (49)

where \( Y \) is given by Eq. (38).

7. Numerical examples

To validate the technique presented in this paper, several three-dimensional crack problems in piezoelectric materials have been analysed. In all cases the boundary is discretized using standard quadratic quadrilateral and triangular elements except for those in the two rows next to the crack front. The elements in the row next to the front and inside the crack are quarter-point elements. The elements in the row next to the front and outside the crack are singular quarter-point elements.

The number of results for 3D fracture mechanics problems in piezoelectrics available in the literature is very small. Because of that some simple problems which can be represented by a 2D model will be studied first. The material of all the solids analysed in this paper is a PZT-4 ceramic whose properties are given in Table 1.

7.1. Prismatic plate with central through crack

A rectangular prismatic plate with a central crack is assumed to be under two possible loading conditions: (1) uniform traction on two opposite sides; and (2) uniform electrical normal charge flux on the same two opposite sides. The geometry of the problem is shown in Fig. 6, where \( 2a = 2H = W/2 = 4t \). Owing to the problem symmetry, only one quarter of the problem has to be discretized. Mechanical and electrical symmetry boundary conditions are applied to the discretized subregion. Plane strain conditions are simulated by prescribing zero normal displacement, zero shear traction and zero normal charge flux on the two faces perpendicular to the \( x \)-axis.

The external face perpendicular to the \( y \)-axis is left free of mechanical and electrical charge. The crack faces boundary conditions are: zero internal traction and zero normal charge flux. The problem was solved with the two different meshes shown in Fig. 7. One consists of 80 elements, with 4 elements along half of the crack. The other consists of 128 elements, with 6 elements along half of the crack. The present results are compared with those obtained by Garcia-Sanchez et al. [35] with a 2D mixed boundary element

<table>
<thead>
<tr>
<th>Material</th>
<th>PZT-4</th>
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<tr>
<td>Elastic constants (( \times 10^{10} ) N/m²)</td>
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<tr>
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</tr>
<tr>
<td>( C_{12} )</td>
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<td>( C_{44} )</td>
<td>2.56</td>
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<tr>
<td>Piezoelectric constants (C/m²)</td>
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</tr>
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<td>( e_{31} )</td>
<td>−6.98</td>
</tr>
<tr>
<td>( e_{33} )</td>
<td>13.84</td>
</tr>
<tr>
<td>( e_{15} )</td>
<td>13.44</td>
</tr>
<tr>
<td>Dielectric constants (( \times 10^{-9} ) C/(V m))</td>
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</tr>
<tr>
<td>( \varepsilon_{11} )</td>
<td>6.00</td>
</tr>
<tr>
<td>( \varepsilon_{33} )</td>
<td>5.47</td>
</tr>
</tbody>
</table>

Fig. 6. Prismatic plate with central crack.

Fig. 7. Boundary element meshes for prismatic plate with crack: (a) 80 element mesh; (b) 128 element mesh.
formulation and a mesh containing 15 quadratic elements along the crack. Fig. 8 shows displacement and potential values along the crack face obtained with the 128 elements discretization, for the two different load cases. The results fully agree with those obtained using the 2D model. Values of the $K_I$ and $K_{IV}$ ESIF computed along the crack front for the two different loading conditions and using both the extended tractions Eq. (48) and the extended crack opening displacement Eq. (49) are shown in Fig. 9. Results are normalized with respect to the applied traction $\sigma_z$ and the electric displacement $D_z$ having the same numerical value as $\sigma_z$ in the first case, and with respect to the applied electric displacement $D_z$ and the traction $\sigma_z$ having the same numerical value as $D_z$ in the second case. It can be seen from this figure that both expressions give accurate values of the ESIF. The computed ESIF values at the front crack mid-node are: $K_I = 1.8077 \sigma_z \sqrt{\pi a}$ and $K_{IV} = 1.6211 D_z \sqrt{\pi a} 10^{-8}$ for the uniform traction loading, and $K_I = 0.1721 \sigma_z \sqrt{\pi a} 10^{-8}$ and $K_{IV} = 1.1601 D_z \sqrt{\pi a}$ for the uniform electric displacement loading. Values of crack surface displacements due to electrical loading and of crack surface potential due to mechanical tractions obtained with the 80 elements mesh present a maximum 4% difference with respect to the same quantities evaluated with the 2D model. Similar differences are obtained for the $K_{IV}$ ESIF due to uniform traction loading conditions and the $K_I$ SIF due to uniform electrical displacement loading conditions. Other values computed using the 80 elements mesh present smaller differences with respect to the 2D results.

7.2. Prismatic plate with two edge cracks

A prismatic solid with two edge cracks is studied next. The geometry of the problem is shown in Fig. 10, where $2a=2H=W/2=4t$. As in the previous example, only one quarter of the problem has to be discretized. Mechanical and electrical symmetry boundary conditions are applied to the discretized subregion. Plane strain conditions are considered. The problem was solved using the same 128 elements meshes of the previous example (Fig. 7b), the only
difference being that the vertical plane of symmetry and the traction–electric displacement free face conditions are interchanged. Results for the crack face displacement and electric potential, for the two loading cases, can be seen in Fig. 11. Normalized values of $K_I$ and $K_{IV}$ for the two loading cases are computed using the nodal extended traction values (Eq. (48)) at the crack front mid-node. The computed ESIF values are:

$$K_I = 2.294 \sigma_z \sqrt{\pi a}$$
$$K_{IV} = 2.707 D_z \sqrt{\pi a} \times 10^{10}$$

for the uniform traction loading, and

$$K_I = 0.1384 \sigma_z^* \sqrt{\pi a} \times 10^{-8}$$
$$K_{IV} = 1.159 D_z \sqrt{\pi a}$$

for the uniform electric displacement loading.

### 7.3. Cylinder with symmetrical penny shape internal crack

A cylinder with a symmetrical penny shape internal crack is subject to a uniform traction $\sigma_z = 1$ Pa, or to a uniform electrical displacement $D_z = 1$ C/m$^2$, at the two opposite faces. The geometry of the problem is shown in Fig. 12, where $H = R = 2a$. The quadratic boundary element mesh for one-eighth of the problem is represented in Fig. 13. Symmetry boundary conditions are applied to the discretized region. The crack face is represented by four rows of elements with the same width. The elements in the fourth row are quarter-point elements. Those in the fifth row are singular quarter-point elements. The material properties are the same as for the two previous problems. Computed displacement and potential values along the crack radius for the two load cases are shown in Fig. 14. The computed ESIF values are:

$$K_I = 0.691 \sigma_z \sqrt{\pi a}$$
$$K_{IV} = 0.075 D_z \sqrt{\pi a} \times 10^{10}$$

for the uniform traction loading, and

$$K_I = 0.0181 \sigma_z^* \sqrt{\pi a} \times 10^{-8}$$
$$K_{IV} = 0.663 D_z \sqrt{\pi a}$$

for the uniform electric displacement loading. To the authors knowledge, there are no previous results for this problem in the literature.

### 8. Conclusions

A boundary element approach with quadratic isoparametric elements, quarter-point elements and singular quarter-point elements for three-dimensional crack problems in piezoelectric solids under mechanical and electrical loading conditions, has been presented in this paper for the first time. Stress and electric displacement intensity factors are evaluated as system unknowns and also as functions of the computed nodal displacements and electric potentials. Special attention has been paid to development of a simple and efficient numerical integration approach for fundamental solution evaluation and integration over the boundary elements.
Solutions to several three-dimensional crack problems in transversely isotropic bodies under mechanical and electrical loading conditions have been presented. Numerical solutions computed for prismatic cracked 3D plate problems with a plane strain behaviour are in very good agreement with their corresponding 2D BE solutions. Results for a penny shape crack in a piezoelectric cylinder are presented for the first time.

The proposed approach is very robust and easy to implement. The computed results are very accurate even when a relatively small number of elements are used to represent the crack and its proximity.

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References