Fracture analysis in piezoelectric semiconductors under a thermal load

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A B S T R A C T

In this paper, we solve the in-plane crack problem in piezoelectric semiconductors under a transient thermal load. General boundary conditions and sample geometry are allowed in the proposed formulation. The coupled governing partial differential equations (PDE) for stresses, electric displacement field and current are satisfied in a local weak-form on small fictitious subdomains. All field quantities are approximated by the moving least-squares (MLS) scheme. After performing the spatial integrations, we obtain a system of ordinary differential equations for the nodal unknowns. The influence of initial electron density on the intensity factors and energy release rate is investigated.

1. Introduction

Piezoelectric materials (PZ) have a wide range of engineering applications in smart structures and devices. Certain piezoelectric materials are also temperature sensitive, i.e. an electric charge or voltage is generated when temperature variations are exposed. This effect is called the pyroelectric effect. If a temperature load is considered in a piezoelectric solid it is needed to take into account the coupling of thermo-electro-mechanical fields. The theory of thermo-piezoelectricity was for the first time proposed by Mindlin [22]. The physical laws for thermo-piezoelectric materials were explored by Nowacki [23]. Dynamic thermoelasticity is relevant for many engineering problems since thermal stresses play an important role in the integrity of structures. The uncoupled thermoelasticity is considered here, since there is no heat production due to the strain rate, i.e. the thermoelastic dissipation. Thus, the temperature field is not influenced by mechanical deformation and the heat conduction equation can be solved first to obtain the temperature distribution. However, the coupling of mechanical and electric fields is still valid. Recently, Sladek et al. [39] analyzed non-conducting piezoelectric materials under a thermal load.

However, piezoelectric materials can be either dielectrics or semiconductors. Up to date dielectric materials are more intensively investigated than semiconductors. The analyzed problem for non-conducting PZ is simpler than for semiconductors. In piezoelectric semiconductors the induced electric field produces also the electric current. The interaction between mechanical fields and mobile charges in piezoelectric semiconductors is called the acoustoelectric effect [18,50]. An acoustic wave traveling in a PZ semiconductor can be amplified by application of an initial or biasing direct current electric field [44].
This phenomenon is utilized in many acoustoelectric devices [15,4]. In literature one can find also more sophisticated models of deformable piezoelectric semiconductors [52,53]. Lorenzi and Tiersten [52] derived governing equations for finitely deformable, polarized and magnetizable heat conducting and electrically semiconducting continuum. The model consists

<table>
<thead>
<tr>
<th>Nomenclature</th>
<th>Description</th>
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<tbody>
<tr>
<td><strong>Latin symbols</strong></td>
<td></td>
</tr>
<tr>
<td>( a )</td>
<td>crack-length</td>
</tr>
<tr>
<td>( c )</td>
<td>specific heat</td>
</tr>
<tr>
<td>( c_{ijkl} )</td>
<td>elasticity tensor</td>
</tr>
<tr>
<td>( d_{ij} )</td>
<td>carrier diffusion tensor</td>
</tr>
<tr>
<td>( e_{ijk} )</td>
<td>piezoelectric tensor</td>
</tr>
<tr>
<td>( h_{ij} )</td>
<td>dielectric tensor</td>
</tr>
<tr>
<td>( k_{ij} )</td>
<td>thermal conductivity</td>
</tr>
<tr>
<td>( n_j )</td>
<td>outward unit normal vector</td>
</tr>
<tr>
<td>( p_{ij} )</td>
<td>pyroelectric material coefficients</td>
</tr>
<tr>
<td>( p^i )</td>
<td>vector of complete basis functions</td>
</tr>
<tr>
<td>( q )</td>
<td>electric charge of electron</td>
</tr>
<tr>
<td>( t_i )</td>
<td>traction vector</td>
</tr>
<tr>
<td>( u_i )</td>
<td>elastic displacements</td>
</tr>
<tr>
<td>( u_{ik} )</td>
<td>test function</td>
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<tr>
<td>( w^a )</td>
<td>test function</td>
</tr>
<tr>
<td>( w^a )</td>
<td>weight function</td>
</tr>
<tr>
<td>( D_i )</td>
<td>electric displacements</td>
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<tr>
<td>( E_i )</td>
<td>electric field</td>
</tr>
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<td>( G )</td>
<td>energy release rate</td>
</tr>
<tr>
<td>( j_i )</td>
<td>electric current</td>
</tr>
<tr>
<td>( K_{I}, K_{II} )</td>
<td>stress intensity factors</td>
</tr>
<tr>
<td>( K_D )</td>
<td>electric displacement intensity factor</td>
</tr>
<tr>
<td>( K_s )</td>
<td>strain intensity factor</td>
</tr>
<tr>
<td>( K_E )</td>
<td>electric vector intensity factor</td>
</tr>
<tr>
<td>( M )</td>
<td>electron density</td>
</tr>
<tr>
<td>( N^a )</td>
<td>shape function associated with the node ( a )</td>
</tr>
<tr>
<td><strong>Greek symbols</strong></td>
<td></td>
</tr>
<tr>
<td>( \beta_{ij} )</td>
<td>linear thermal expansion</td>
</tr>
<tr>
<td>( \delta_{ij} )</td>
<td>Kronecker delta</td>
</tr>
<tr>
<td>( \varepsilon_{ij} )</td>
<td>strain tensor</td>
</tr>
<tr>
<td>( \phi )</td>
<td>electric potential</td>
</tr>
<tr>
<td>( \lambda_{ij} )</td>
<td>stress-temperature modulus</td>
</tr>
<tr>
<td>( \mu_{ij} )</td>
<td>electron mobility tensor</td>
</tr>
<tr>
<td>( \nu^a )</td>
<td>test function</td>
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<tr>
<td>( \rho )</td>
<td>mass density</td>
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<tr>
<td>( \sigma_{ij} )</td>
<td>stress tensor</td>
</tr>
<tr>
<td>( \tau )</td>
<td>time</td>
</tr>
<tr>
<td>( \Gamma_v )</td>
<td>boundary with prescribed displacements</td>
</tr>
<tr>
<td>( \Gamma_t )</td>
<td>boundary with prescribed tractions</td>
</tr>
<tr>
<td>( \Gamma_e )</td>
<td>boundary with prescribed electric potential</td>
</tr>
<tr>
<td>( \Gamma_{ex} )</td>
<td>boundary with prescribed normal component of the electric displacements</td>
</tr>
<tr>
<td>( \Gamma_s )</td>
<td>boundary with prescribed electron density</td>
</tr>
<tr>
<td>( \Gamma_{eb} )</td>
<td>boundary with prescribed electric current flux</td>
</tr>
<tr>
<td>( \Gamma_t )</td>
<td>boundary with prescribed temperature</td>
</tr>
<tr>
<td>( \Omega_S )</td>
<td>local subdomain</td>
</tr>
<tr>
<td>( \partial \Omega_S )</td>
<td>boundary of the local subdomain</td>
</tr>
<tr>
<td><strong>Other symbols</strong></td>
<td></td>
</tr>
<tr>
<td>( f_i )</td>
<td>partial derivative of the function ( f )</td>
</tr>
<tr>
<td>( f )</td>
<td>time derivative of the function ( f )</td>
</tr>
</tbody>
</table>
of five suitably defined interpenetrating continua. The relative displacement of the bound electronic continuum with respect to the lattice continuum produces electrical polarization, and electrical conduction results from the motion of the charged free electronic and hole fluids. However, this model seems to be complicated for treatment of wave-interaction problems. Later, Maugin and Dahar [53] derived linearized governing equations for piezoelectric semiconducting crystals on the base of fully nonlinear theory of the continuum. While more sophisticated models require more advanced computational methods, there is even no available modeling result for simpler models like the Hutson and White linear model [18].

Piezoelectric ceramics are brittle and susceptible to fracture during service. To improve the performance and to predict the reliable service lifetime of ceramic piezoelectric components, it is necessary to analyze theoretically the damage and fracture processes taking place in piezoelectric materials with consideration of the coupling effect of mechanics and electrics. Deeg [5] and Pak [25] addressed the plane and anti-plane fracture problems of an infinite piezoelectric body and obtained the closed form solutions of stress field and electric displacement field near the crack tip. There are only few papers devoted to crack problems in piezoelectric semiconductor materials. These papers concerned only the anti-plane crack problem in unbounded domain with a semi-infinite crack [43] or a finite crack [17] under stationary conditions. The Fourier transform technique was applied to reduce the problem to a pair of dual integral equations. In the present paper, we aim at analyzing the in-plane crack problem in bounded domains under a transient thermal load.

The solution of the boundary value problems for conducting piezoelectric solids requires advanced numerical methods due to the high mathematical complexity. Transient regime brings additional complications. Thus, efficient computational methods to solve the boundary or the initial-boundary value problems for piezoelectric solids are required. Notably, the finite element method (FEM) [13,12,7,19] and boundary element method (BEM) [26,20,6,14,9,10,30,34] were applied to solve general piezoelectric problems. Fracture and damage behaviours of a cracked piezoelectric solid under coupled thermal, mechanical and electrical loads were studied by Yu and Qin [45,46]. A review on fracture of thermo-piezoelectric materials was given by Qin [28]. Boundary value problems for coupled fields are complex. Analytical methods can be only applied to simple problems of thermo-piezoelectricity [41,32,33]. However, the analysis and design process of smart engineering structures with integrated piezoelectric actuators or sensors require powerful calculation tools. Up to now the FEM provides an effective technique [42,11,31] in a homogeneous medium. Rao and Sunar [29] investigated the piezothermoelastic problem of intelligent structures with distributed piezoelectric sensors and actuators and concluded that the inclusion of the thermal effects may help improve the performance characteristics of the system.

In recent years, meshless formulations are becoming popular due to their high adaptivity and low costs to prepare input and output data for numerical analyses. A variety of meshless methods has been proposed so far and some of them are also applied to PZ problems [24,21,36–39]. They can be derived either from a weak-form formulation on the global domain or on a set of local subdomains. In this paper, both the heat conduction equation and coupled electro-mechanical governing equations are satisfied in a weak form on small fictitious subdomains. The meshless Petrov–Galerkin (MLPG) method [35] is then applied to the subdomains. Nodal points are introduced and spread on the analyzed domain and each node is surrounded by a small circle for simplicity, but without loss of generality. The spatial variations of the displacement, electric potential and electron density are approximated by the moving least-squares (MLS) scheme [51]. After performing the spatial integrations, a system of ordinary differential equations for unknown nodal values is obtained. The essential boundary conditions on the global boundary are satisfied by the collocation. Then, the system of the ordinary differential equations of the second order resulting from the equations of motion is solved by the Houbolt finite-difference scheme [16] and backward difference method.

### 2. Local integral equations for piezoelectric semiconductor

Consider a homogeneous n-type piezoelectric semiconductor with electron density $M_0$ in the unloaded state with vanishing initial electric field $E_0$. Supposing the frequency of external loadings to be close to the characteristic frequency of elastic waves, one can assume quasi-static approximation for electromagnetic fields. Then, the effect of Faraday’s induction is neglected even if there is a magnetic field induced by the electric current according to the Ampere’s law. Eventually, the governing equations within the linear theory are given by the balance of momentum, Gauss’s law and conservation of charge [18]

$$
\sigma_{ij}(x, \tau) = \rho \ddot{u}_i(x, \tau), \quad D_{ij}(x, \tau) = qM(x, \tau), \quad qM(x, \tau) + J_{is} = 0,
$$

where $\ddot{u}_i, \sigma_{ij}, D_{ij}$ and $q$ are the acceleration of elastic displacements, stress tensor, electric displacement field, and electric charge of electron, respectively. The electron density and electric current are denoted by $M$ and $J_i$, respectively. Symbol $\rho$ is used for the mass density. A comma followed by an index denotes partial differentiation with respect to the coordinate associated with the index. In uncoupled thermo-elastic theory the temperature distribution is independent on mechanical and electrical fields. The governing Eq. (1) have to be supplemented by the heat conduction equation

$$
[k_{ij}(x)\theta_j(x, \tau)]_j - \rho c \dot{\theta}(x, \tau) = 0,
$$

where $k_{ij}$ and $c$ are the thermal conductivity tensor and specific heat, respectively.
For most materials the inverse thermoelastic and pyroelectric effects are very weak, i.e. the heat generation by mechanical and electrical fields can be neglected. Then, the constitutive equations \([18,50]\) need to be supplied only with thermal terms \([39]\)

\[
\begin{align*}
\sigma_{ij}(\mathbf{x}, \tau) &= c_{ijkl}(\mathbf{x}) \varepsilon_{kl}(\mathbf{x}, \tau) - \varepsilon_{iy}(\mathbf{x}) \dot{E}_y(\mathbf{x}, \tau) - \lambda_{ij}(\mathbf{x}) \theta(\mathbf{x}, \tau), \\
D_j(\mathbf{x}, \tau) &= c_{ijkl}(\mathbf{x}) \varepsilon_{kl}(\mathbf{x}, \tau) + h_{ij}(\mathbf{x}) E_j(\mathbf{x}, \tau) + p_j(\mathbf{x}) \theta(\mathbf{x}, \tau), \\
J_j(\mathbf{x}, \tau) &= qM_j(\mathbf{x}) \mu_j(\mathbf{x}) E_j(\mathbf{x}, \tau) - qd_{ij}(\mathbf{x}) M_j(\mathbf{x}, \tau),
\end{align*}
\]

(3)

where \(c_{ijkl}(\mathbf{x}), e_{ij}(\mathbf{x}), h_{ij}(\mathbf{x}), \mu_{ij}(\mathbf{x}), d_{ij}(\mathbf{x})\) and \(p_j(\mathbf{x})\) are the elastic, piezoelectric, dielectric, electron mobility, carrier diffusion and pyroelectric material coefficients, respectively. Generally, these coefficients can be dependent on Cartesian coordinates in functionally graded materials. Recall that the Joule heating (heat generated by a current passing through a resistive material), the Seebeck effect (when a temperature gradient generates an electromotive force in a conductor) as well as the Thomson effect (production of heat rate due to temperature gradient when an electric current passes through a conductor) are omitted in the considered model. The stress–temperature modulus \(\lambda_{ij}(\mathbf{x})\) can be expressed through the stiffness coefficients and the coefficients of linear thermal expansion \(\beta_{kl}\)

\[\lambda_{ij} = c_{ijkl} \beta_{kl},\]

since the thermal expansion strains are given as \(\varepsilon^\theta_{ij} = \beta_{ij} \theta\).

For an orthotropic material, the thermal expansion cannot induce shear, hence the coefficient tensor \(\beta_{kl}\) takes the form

\[\beta_{kl} = \beta_{11} \delta_{k1} \delta_{l1} + \beta_{22} \delta_{k2} \delta_{l2} + \beta_{33} \delta_{k3} \delta_{l3} .\]

The strain tensor \(\varepsilon_{ij}\) and the electric field vector \(E_j\) are related to the displacements \(u_i\) and the electric potential \(\phi\) by

\[\varepsilon_{ij} = \frac{1}{2}(u_j + u_i), \quad E_j = -\phi_j .\]

(4)

The governing Eqs. (1)–(4) are for general three-dimensional deformation/motion. In the case of certain crystal symmetries, one can formulate also the plane-deformation problems \([27]\). For instance, in the crystals of hexagonal symmetry with \(x_3\) being the 6-order symmetry axis and assuming \(u_2 = 0\) as well as the independence on \(x_2\), i.e. \((\cdot, \cdot)_2 = 0\), we have \(e_{22} = e_{23} = \varepsilon_{12} = E_2 = J_2 = 0\), \(\beta_{22} = 0\). Thus, the problem is reduced to the two-dimensional \((x_1, x_3)\)-plane as we will discuss in this paper with the coordinate vector \(\mathbf{x}\) being \(\mathbf{x} = (x_1, x_3)\).

Using the Voigt notation, the constitutive Eq. (3) are reduced to the following form

\[
\begin{bmatrix}
\sigma_{11} \\
\sigma_{33} \\
\sigma_{13}
\end{bmatrix} =
\begin{bmatrix}
c_{11} & c_{13} & 0 \\
c_{13} & c_{33} & 0 \\
0 & 0 & c_{44}
\end{bmatrix}
\begin{bmatrix}
\varepsilon_{11} \\
\varepsilon_{33} \\
2\varepsilon_{13}
\end{bmatrix} - \begin{bmatrix}
0 & e_{31} \\
0 & e_{33} \\
e_{15} & 0
\end{bmatrix}
\begin{bmatrix}
E_1 \\
E_3 \\
E_1 + 2\varepsilon_{13}
\end{bmatrix} - \lambda \theta = C(\mathbf{x})
\begin{bmatrix}
\varepsilon_{11} \\
\varepsilon_{33} \\
2\varepsilon_{13}
\end{bmatrix} - L(\mathbf{x})
\begin{bmatrix}
E_1 \\
E_3
\end{bmatrix} - \lambda(\mathbf{x}) \theta
\]

(5)

\[
\begin{bmatrix}
D_1 \\
D_3 \\
D_3
\end{bmatrix} =
\begin{bmatrix}
0 & 0 & e_{15} \\
e_{31} & e_{33} & 0 \\
e_{31} & e_{33} & 0
\end{bmatrix}
\begin{bmatrix}
\varepsilon_{11} \\
\varepsilon_{33} \\
2\varepsilon_{13}
\end{bmatrix} + \begin{bmatrix}
h_{11} & 0 & 0 \\
0 & h_{33} & 0 \\
0 & 0 & h_{33}
\end{bmatrix}
\begin{bmatrix}
E_1 \\
E_3 \\
E_1 + 2\varepsilon_{13}
\end{bmatrix} + \begin{bmatrix}
p_1 & 0 \\
0 & p_3 \\
0 & 0
\end{bmatrix}
\begin{bmatrix}
\theta = G(\mathbf{x})
\begin{bmatrix}
\varepsilon_{11} \\
\varepsilon_{33} \\
2\varepsilon_{13}
\end{bmatrix} + H(\mathbf{x})
\begin{bmatrix}
E_1 \\
E_3
\end{bmatrix} + \Pi(\mathbf{x}) \theta
\end{bmatrix}
\]

(6)

\[
\begin{bmatrix}
J_1 \\
J_3 \\
J_3
\end{bmatrix} =
\begin{bmatrix}
\mu_{11} & 0 & 0 \\
0 & \mu_{33} & 0 \\
0 & 0 & \mu_{33}
\end{bmatrix}
\begin{bmatrix}
E_1 \\
E_3 \\
E_3
\end{bmatrix} - \begin{bmatrix}
d_{11} & 0 & 0 \\
0 & d_{33} & 0 \\
0 & 0 & d_{33}
\end{bmatrix}
\begin{bmatrix}
M_1 \\
M_3 \\
M_3
\end{bmatrix} = qm_{ab} A(\mathbf{x})
\begin{bmatrix}
E_1 \\
E_3 \\
E_3
\end{bmatrix} - qF(\mathbf{x})
\begin{bmatrix}
M_1 \\
M_3 \\
M_3
\end{bmatrix}
\]

(7)

where

\[
\lambda =
\begin{bmatrix}
\lambda_{11} \\
\lambda_{33} \\
\lambda_{13}
\end{bmatrix} =
\begin{bmatrix}
c_{11} & c_{13} & 0 \\
c_{13} & c_{33} & 0 \\
0 & 0 & c_{44}
\end{bmatrix}
\begin{bmatrix}
\beta_{11} \\
\beta_{33} \\
\beta_{13}
\end{bmatrix} =
\begin{bmatrix}
\lambda_{11} \\
\lambda_{33} \\
\lambda_{13}
\end{bmatrix} .
\]

The following essential and natural boundary conditions are assumed for the mechanical fields

\[
u_i(\mathbf{x}, \tau) = \bar{u}_i(\mathbf{x}, \tau), \quad \text{on } \Gamma_u, \\
t_j(\mathbf{x}, \tau) = \bar{t}_j(\mathbf{x}, \tau), \quad \text{on } \Gamma_t, \Gamma = \Gamma_u \cup \Gamma_t .
\]

For the electrical fields, we assume

\[
\phi(\mathbf{x}, \tau) = \tilde{\phi}(\mathbf{x}, \tau), \quad \text{on } \Gamma_p , \\
Q(\mathbf{x}, \tau) = D_i(\mathbf{x}, \tau) n_i(\mathbf{x}) = \tilde{Q}(\mathbf{x}, \tau), \quad \text{on } \Gamma_q, \Gamma = \Gamma_p \cup \Gamma_q ,
\]

for the electric current fields

\[
M(\mathbf{x}, \tau) = \tilde{M}(\mathbf{x}, \tau), \quad \text{on } \Gamma_u , \\
S(\mathbf{x}, \tau) = \tilde{J}_j(\mathbf{x}, \tau) n_i(\mathbf{x}) = \tilde{S}(\mathbf{x}, \tau), \quad \text{on } \Gamma_b, \Gamma = \Gamma_u \cup \Gamma_b .
\]
and for the thermal fields
\[ \frac{\partial (x, \tau)}{\partial (x, \tau)} + \frac{\partial (x, \tau)}{\partial (x, \tau)} \mid_{\Gamma_1} = 0 \quad \text{on} \quad \Gamma_1, \]
\[ \zeta(x, \tau) \equiv \frac{\partial (x, \tau)}{\partial (x, \tau)}n_j(x) = \zeta(x, \tau) \mid_{\Gamma_2} = \Gamma_2 \cup \Gamma_3, \]
where \( \Gamma_1 \) is the part of the global boundary \( \Gamma \) with prescribed displacements, while on \( \Gamma_3, \Gamma_4, \Gamma_5, \Gamma_6 \) and \( \Gamma_7 \) the traction vector, the electric potential, the normal component of the electric displacement vector, the electron density, the electric current flux, the temperature and the heat flux are prescribed, respectively. Recall that \( Q(x, \tau) \) can be considered approximately as the surface density of the free charge, provided that the permittivity of the solid is much greater than that of the surrounding medium (vacuum).

The initial conditions for the mechanical displacements are assumed as
\[ u_i(x, \tau) |_{\tau=0} = u_i(x, 0) \quad \text{and} \quad \dot{u}_i(x, \tau) |_{\tau=0} = \dot{u}_i(x, 0) \quad \text{in} \quad \Omega. \]

As shown by Atluri et al. [2] the local weak form of the governing equations (1) can be written with
\[ \int_{\Omega} [\sigma_{ij}(x, \tau) - \rho \ddot{u}_i(x, \tau)] u_{ik}(x) d\Omega = 0, \tag{8} \]
where \( u_{ik}(x) \) is a test function and \( \Omega_i \subset \Omega \).

Applying the Gauss divergence theorem to the first integral, we obtain
\[ \int_{\partial \Omega_i} \sigma_{ij}(x, \tau) \eta_j(x) u_{ik}(x) d\Gamma - \int_{\Omega_i} \sigma_{ij}(x, \tau) u_{ik}(x) d\Omega - \int_{\Omega_i} \rho \ddot{u}_i(x, \tau) u_{ik}(x) d\Omega = 0, \tag{9} \]
where the boundary of the local subdomain \( \partial \Omega_i \) consists of three parts \( \partial \Omega_i = L_i \cup \Gamma_{iu} \cup \Gamma_{iu} \). Here, \( L_i \) is the local boundary that is totally inside the global domain, \( \Gamma_{iu} \) is the part of the local boundary which coincides with the global traction boundary, i.e., \( \Gamma_{iu} = \partial \Omega_i \cap \Gamma_1 \), and similarly \( \Gamma_{iu} \) is the part of the local boundary that coincides with the global displacement boundary, i.e., \( \Gamma_{iu} = \partial \Omega_i \cap \Gamma_2 \). Similar definitions are valid also for other fields and related integration parts.

By choosing the characteristic function as the test function \( u_{ik}(x) \) in each subdomain
\[ u_{ik}(x) = \begin{cases} \delta_{ik} & \text{at} \quad x \in \Omega_i, \\ 0 & \text{at} \quad x \notin \Omega_i, \end{cases} \]
the local weak-form (9) is converted into the following local boundary-domain integral equations
\[ \int_{L_i} \tau_i(x, \tau) d\Gamma - \int_{\Omega_i} \rho \ddot{u}_i(x, \tau) d\Omega = - \int_{\Gamma_{iu}} \ddot{u}_i(x, \tau) d\Gamma. \tag{10} \]

Eq. (10) is recognized as the overall force equilibrium conditions on the subdomain \( \Omega_i \). Note that the local integral Eq. (10) is valid for both the homogeneous and nonhomogeneous solids. Nonhomogeneous material properties are included in Eq. (10) through the elastic, piezoelectric, and thermo-elastic coefficients involved in the traction components
\[ \tau_{ij}(x, \tau) = [\sigma_{ij}(x, \tau) + \varepsilon_{ijkl}(x, \tau) \phi_k(x, \tau) - \lambda_{ij}(x, \tau) \theta(x, \tau)] n_j(x). \]

Similarly, the local weak-form of the second governing equation in (1) can be written as
\[ \int_{\Omega_i} \left[ D_{ij}(x, \tau) - qM(x, \tau) \right] \nu^i(x) d\Omega = 0, \tag{11} \]
where \( \nu^i(x) \) is a test function.

Applying the Gauss divergence theorem to the local weak-form (11) and choosing the characteristic function as the test function \( \nu^i(x) \), we obtain
\[ \int_{L_i} Q(x, \tau) d\Gamma - \int_{\Omega_i} qM(x, \tau) d\Omega = - \int_{\Gamma_{iu}} \ddot{Q}(x, \tau) d\Gamma, \tag{12} \]
where
\[ Q(x, \tau) = D_{ij}(x, \tau) n_j(x) = [\sigma_{ij}(x, \tau) + \rho_{ij}(x, \tau)] n_j(x) + \varepsilon_{ijkl}(x, \tau) \phi_k(x, \tau) - \lambda_{ij}(x, \tau) \theta(x, \tau)] n_j(x). \]

The local integral equation corresponding to the last governing equation in (1) has the form
\[ \int_{L_i} S(x, \tau) d\Gamma + \int_{\Omega_i} qM(x, \tau) d\Omega = - \int_{\Gamma_{iu}} S(x, \tau) d\Gamma, \tag{13} \]
where the electric current flux is given by
\[ S(x, \tau) = J_{ij}(x, \tau) n_j(x) = [-qM_{ij} \mu_{ij}(x, \tau) - q d_{jk} M_{jk}(x, \tau)] n_j(x). \]
The local weak-form of the heat conduction Eq. (2) can be written as
\[
\int_{\Omega} \left\{ [k_i(x)] \frac{\partial \phi(x, \tau)}{\partial r} - \rho c \phi(x, \tau) \right\} w^\varepsilon(x) \, d\Omega = 0,
\] (14)
where \( w^\varepsilon(x) \) is a test function.

Applying the Gauss divergence theorem to the local weak-form and considering the characteristic function for the test function \( w^\varepsilon(x) \), we also obtain
\[
\int_{\Omega} \zeta(x, \tau) d\Gamma - \int_{\partial \Omega} \rho c \phi(x, \tau) d\Omega = - \int_{\Gamma_d} \zeta(x, \tau) d\Gamma,
\] (15)
where the heat flux is defined as
\[
\zeta(x, \tau) \equiv k_i \frac{\partial \phi(x, \tau)}{\partial n_i}.
\]

### 3. Numerical solution in terms of the MLPG method

In the MLPG method the test and the trial functions are not necessarily from the same functional spaces. For internal nodes, the test function is chosen as a unit step function with its support on the local subdomain. The trial functions, on the other hand, are chosen to be the MLS approximations by using a number of nodes spreading over the domain of influence. According to the MLS method (see e.g. Belytschko et al. [3]), the approximation of the displacement field can be given as
\[
u^h(x) = \sum_{i=1}^{s} \mathbf{p}_i(x) a_i(x) = \mathbf{p}^T(x) \mathbf{a}(x),
\] (16)
where \( \mathbf{p}^T(x) = \{ p_1(x), p_2(x), ... p_s(x) \} \) is a vector of complete basis functions of order \( s \) and \( \mathbf{a}(x) = \{ a_1(x), a_2(x), ... a_s(x) \} \) is a vector of unknown parameters that depend on \( x \). For example, in 2-D problems
\[
\mathbf{p}^T(x) = \{ 1, x_1, x_3 \} \quad \text{for} \quad s = 3
\]
and
\[
\mathbf{p}^T(x) = \{ 1, x_1, x_3, \sqrt{r} \cos(\theta/2), \sqrt{r} \sin(\theta/2), \sqrt{r} \cos(\theta/2) \sin \theta, \sqrt{r} \cos(\theta/2) \sin \theta \} \quad \text{for} \quad s = 7,
\]
where \( r \) and \( \theta \) are polar coordinates with the crack-tip as the origin. These enriched basic functions represent all occurring terms in asymptotic expansion of displacements at the crack tip vicinity. Then, density of node distribution in such a case can be lower than in the polynomial basis functions at the same accuracy of results.

Following the approximation (16), the approximated functions for the mechanical displacements, the electric potential, electron density and the temperature can be written as Atluri [1]
\[
u^h(x, \tau) = \sum_{a=1}^{n} N^a(x) \mathbf{u}^a(\tau),
\]
\[
\phi^h(x, \tau) = \sum_{a=1}^{n} N^a(x) \phi^a(\tau),
\]
\[
M^h(x, \tau) = \sum_{a=1}^{n} N^a(x) \tilde{M}^a(\tau),
\]
\[
\delta^h(x, \tau) = \sum_{a=1}^{n} N^a(x) \tilde{\delta}^a(\tau),
\] (17)
where the nodal values \( \mathbf{u}^a(\tau) = (u^a_1(\tau), u^a_2(\tau))^T, \phi^a(\tau), \tilde{M}^a(\tau), \) and \( \tilde{\delta}^a(\tau) \) are fictitious parameters for the displacements, electric potential, electron density and the temperature, respectively, and \( N^a(x) \) is the shape function associated with the node \( a \). The number of nodes \( n \) used for the approximation is determined by the weight function \( w^\varepsilon(x) \). A 4th-order spline-type weight function is applied in the present work
\[
w^\varepsilon(x) = \begin{cases} 1 - 6 \left( \frac{d^3}{\pi^3} \right) + 8 \left( \frac{d^3}{\pi^3} \right)^3 - 3 \left( \frac{d}{\pi} \right)^4, & 0 \leq d^3 \leq r^3, \\ 0, & d^3 > r^3, \end{cases}
\] (18)
where \( d^2 = \| x - x^0 \| \) and \( r^2 \) is the size of the support domain. It is seen that the \( C^1 \) – continuity is ensured over the entire domain, and therefore the continuity conditions of the tractions, the electric charge, the electric current flux and the heat flux are satisfied. In the MLS approximation the rates of the convergence of the solution may depend upon the nodal distance as well as the size of the supporting domain \([47–49]\)). It should be noted that a smaller size of the subdomains may induce larger oscillations in the nodal shape functions \([1]\). A necessary condition for a regular MLS approximation is that at least \( m \) weight functions are non-zero (i.e. \( n \geq s \)) for each sample point \( x \in \Omega \). This condition determines the size of the supporting domain.

Then, the traction vector \( t_i(x, \tau) \) at a boundary point \( x \in \partial \Omega_s \) is approximated in terms of the same nodal values \( \hat{u}^r(\tau) \) as

\[
t^i(x, \tau) = \hat{v}_i(x, \tau) - \hat{u}^r(\tau) + \hat{v}_i(x, \tau) - \hat{m}_i(x, \tau) \sum_{a=1}^{n} \mathbf{B}^a(x) \hat{u}^a(\tau) + \hat{m}_i(x, \tau) \sum_{a=1}^{n} \mathbf{P}^a(x) \hat{p}^a(\tau).
\]  

(19)

where the matrices \( \mathbf{C}(x), \mathbf{L}(x) \) are defined in Eq. (5), the matrix \( \mathbf{G}(x) \) is related to the normal vector \( n(x) \) on \( \partial \Omega_s \) by

\[
g(x) = \begin{bmatrix} n_1 & 0 & n_3 \\ 0 & n_3 & n_1 \end{bmatrix}.
\]

and finally, the matrices \( \mathbf{B}^a \) and \( \mathbf{P}^a \) are represented by the gradients of the shape functions as

\[
\mathbf{B}^a(x) = \begin{bmatrix} N_1^a & 0 \\ 0 & N_3^a \\ N_3^a & N_4^a \end{bmatrix}, \quad \mathbf{P}^a(x) = \begin{bmatrix} N_1^a \\ \vdots \\ N_3^a \end{bmatrix}.
\]

Similarly the normal component of the electric displacement vector \( Q(x, \tau) \) can be approximated by

\[
Q^i(x, \tau) = N_i(x)G(x) \sum_{a=1}^{n} \mathbf{B}^a(x) \hat{u}^a(\tau) - N_i(x)H(x) \sum_{a=1}^{n} \mathbf{P}^a(x) \hat{p}^a(\tau) + N_i(x)G(x) \sum_{a=1}^{n} \mathbf{B}^a(x) \hat{u}^a(\tau) + N_i(x)H(x) \sum_{a=1}^{n} \mathbf{P}^a(x) \hat{p}^a(\tau).
\]

(20)

where the matrices \( \mathbf{G}(x), \mathbf{H}(x) \) are defined in Eq. (6) and

\[
N_i(x) = [n_1, n_3].
\]

Eventually, the electric current flux \( S(x, \tau) \) is approximated by

\[
S_i(x, \tau) = -N_i(x)qM_0A(x) \sum_{a=1}^{n} \mathbf{P}^a(x) \hat{p}^a(\tau) - N_i(x)qF(x) \sum_{a=1}^{n} \mathbf{P}^a(x) \hat{p}^a(\tau) + N_i(x)qM_0A(x) \sum_{a=1}^{n} \mathbf{P}^a(x) \hat{p}^a(\tau),
\]

(21)

with the matrices \( \mathbf{A}(x), \mathbf{F}(x) \) being defined in Eq. (7).

The heat flux \( \zeta(x, \tau) \) is approximated by

\[
\zeta^i(x, \tau) = k_i n_i \sum_{a=1}^{n} \mathbf{P}^a(x) \hat{p}^a(\tau) = N_i(x)\Theta(x) \sum_{a=1}^{n} \mathbf{P}^a(x) \hat{p}^a(\tau),
\]

(22)

where \( \Theta(x) = [k_{11}, k_{13}, k_{13}, k_{33}] \).

Satisfying the essential boundary conditions and making use of the approximation formulae \((17)\), we obtain the discretized form of these boundary conditions as

\[
\sum_{a=1}^{n} \mathbf{P}^a(x) \hat{p}^a(\tau) = \hat{q}(x, \tau) \quad \text{for} \quad x \in \Gamma_u,
\]

(23)

\[
\sum_{a=1}^{n} \mathbf{P}^a(x) \hat{p}^a(\tau) = \hat{d}(x, \tau) \quad \text{for} \quad x \in \Gamma_c.
\]

Furthermore, in view of the MLS-approximations \((19)-(22)\) for the unknown quantities in the local boundary-domain integral Eqs. (10), (12), (13), and (15), we obtain their discretized forms as
which are considered on the sub-domains adjacent to the interior nodes as well as to the boundary nodes on \( \Gamma_{at}, \Gamma_{sq}, \Gamma_{sb} \) and \( \Gamma_{sf} \).

Collecting the discretized local boundary-domain integral equations, together with the discretized boundary conditions for the displacements, electric potential, electron density, and the temperature, results in a complete system of ordinary differential equations, which can be rearranged in such a way that all known quantities are on the r.h.s of an equation. Thus, in the matrix form the system becomes

\[
\mathbf{A}\mathbf{F}(\tau) + \mathbf{B}\mathbf{F}(\tau) + \mathbf{C}\mathbf{F}(\tau) = \mathbf{Y}(\tau),
\]

where the vector \( \mathbf{F} \) contains all the unknowns to be solved, as listed in (23). We point out again that the system matrix has a block structure and the thermal unknowns can be solved separately from the mechanical and electric unknowns.

There are many time integration procedures for the solution of this system of ordinary differential equations. In the present work, the Houbolt method is applied. In the Houbolt finite-difference scheme [16], the “acceleration” is expressed as

\[
\mathbf{F}_{t+\Delta t} = \frac{2\mathbf{F}_{t+2\Delta t} - 5\mathbf{F}_{t} + 4\mathbf{F}_{t-\Delta t} - \mathbf{F}_{t-2\Delta t}}{\Delta \tau^2},
\]

where \( \Delta \tau \) is the time step. The backward difference method is applied for the approximation of “velocities”

\[
\mathbf{F}_{t+\Delta t} = \frac{\mathbf{F}_{t+\Delta t} - \mathbf{F}_{t}}{\Delta \tau}.
\]

Substituting Eqs. (29) and (30) into Eq. (28), we get the following system of algebraic equations for the unknowns \( \mathbf{F}_{t+\Delta t} \)

\[
\left[ \frac{2}{\Delta \tau^2} \mathbf{A} + \frac{1}{\Delta \tau} \mathbf{B} + \mathbf{C} \right] \mathbf{F}_{t+\Delta t} = \frac{1}{\Delta \tau^2} (5\mathbf{A} + \mathbf{B} \Delta \tau) \mathbf{F}_{t} + \frac{1}{\Delta \tau^2} \left( -4\mathbf{F}_{t-\Delta t} + \mathbf{F}_{t-2\Delta t} \right) + \mathbf{Y}.
\]

The value of the time step has to be appropriately selected with respect to material parameters (wave velocities) and time dependence of the boundary conditions.

---

**Fig. 1.** A central crack in a finite strip with prescribed temperatures on the outer boundary and crack surfaces.
4. Numerical examples

As numerical examples, we analyze a straight central crack in a finite strip under a thermal load. The geometry of the strip is given in Fig. 1 with the following values: \( a = 0.5 \) m, \( a/w = 0.4 \) and \( h/w = 1.2 \). On the outer boundary of the strip \( t_1 = 0, Q = 0 \) and \( t_2 = 0 = \theta_0 = 1 \) deg, while on the crack surface \( t_1 = 0, t_1 = 0, S = 0 \) and electrically impermeable boundary conditions are assumed.

Due to the symmetry of the problem with respect to both Cartesian coordinates, only a quarter of the strip is modeled. We use 930 \((31 \times 30)\) nodes equidistantly distributed for the MLS approximation of the physical quantities. The local subdomains are considered to be circular with a radius of \( r_{loc} = 0.033 \) m. The material properties correspond to aluminium nitride (AlN)

\[
\begin{align*}
c_{11} &= 403 \cdot 10^9 \text{Nm}^{-2}, & c_{12} &= 143 \cdot 10^9 \text{Nm}^{-2}, & c_{13} &= 104 \cdot 10^9 \text{Nm}^{-2}, & c_{33} &= 382 \cdot 10^9 \text{Nm}^{-2}, \\
c_{44} &= 120 \cdot 10^9 \text{Nm}^{-2}, & e_{15} &= -0.39 \text{Cm}^{-2}, & e_{31} &= -0.66 \text{Cm}^{-2}, & e_{33} &= 1.57 \text{Cm}^{-2}, \\
h_0 &= 8.854 \cdot 10^{-12} \text{C/(Vm)^{-1}}, & h_{11} = h_{33} &= 9.14 h_0, & \mu_{11} = \mu_{33} &= 3.0 \cdot 10^{-2} \text{m}^2/(Vs)^{-1}, \\
d_{11} = d_{33} &= 7.0 \cdot 10^{-4} \text{m}^2\text{s}^{-1}, & q &= 1.602 \cdot 10^{-19} \text{C}, & \rho &= 3255 \text{kg/m}^3, \\
k_{11} = k_{33} &= 150 \text{W/km}, & \beta_{11} &= 0.45 \cdot 10^{-5} \text{1/K}, & \beta_{33} &= \beta_{22} &= 0.45 \cdot 10^{-5} \text{1/K}, \\
p_1 &= 0, & p_3 &= 0.00 \text{C/km}^2, & c &= 740 \text{Ws kg}^{-1}\text{K}^{-1}.
\end{align*}
\]

Stationary boundary conditions are considered in the first example and absence of the surface free electric charge \( Q = 0 \) and the electric current flux \( S = 0 \) are assumed on the outer boundary. Variations of displacements, electric potentials and electron densities along the crack surface \( (x_3 = 0) \) for various initial electron densities \( M_0 \) are presented in Figs. 2–4, respectively.

Fig. 2. Variations of the crack-opening-displacement on the crack surface with normalized coordinate \( x_1/a \).

Fig. 3. Variations of the electric potential on the crack surface with normalized coordinate \( x_1/a \).
The presented numerical results correspond to a pure thermal load. One can observe while the initial electron density has only a small influence on the crack displacement, it strongly affects the induced electric potential. The largest value of the induced potential is for a non-conducting PZ material, and with increasing value of $M_0$, the induced electric potential decreases. Furthermore, the distribution of the electron density on the crack surface is also strongly dependent on $M_0$ value. A higher value of $M_0$ results in a higher density of electrons $M$.

For cracks in homogeneous and linear piezoelectric solids, the asymptotic behaviour of the field quantities was given in Garcia-Sanchez and Saez [9]. In the crack tip vicinity, the displacements and electric potential show the classical $1/r$ asymptotic behaviour. Hence, correspondingly, the stresses and electrical displacement exhibit $1/r$ behaviour, where $r$ is the radial polar coordinate with origin at the crack tip. The generalized intensity factors can be computed from the asymptotic expressions of the displacements and electric potential [10]

$$ K = \begin{bmatrix} K_I \\ K_{II} \\ K_D \end{bmatrix} = \sqrt{\frac{\pi}{2\Gamma}} \text{Re}(Y)^{-1} \begin{bmatrix} u_1 \\ u_3 \\ \phi \end{bmatrix}, $$

where the matrix $Y$ is determined by the material properties as shown in Garcia-Sanchez et al. [10] and

$$ K_I = \lim_{r \to 0} \sqrt{2\pi r} \sigma_{33}(r,0), \\
K_{II} = \lim_{r \to 0} 2\pi r \sigma_{13}(r,0), \\
K_D = \lim_{r \to 0} 2\pi r D_3(r,0), \\
K_F = \lim_{r \to 0} \sqrt{2\pi r} \epsilon_{33}(r,0), $$

are the stress intensity factors (SIF) $K_I$ and $K_{II}$, the electrical displacement intensity factor (EDIF) $K_D$, the strain intensity factor $K_F$, and the electric vector intensity factor $K_F$, respectively. Recall that the set of intensity factors $\{K_I, K_{II}, K_D, K_F\}$ is reducible, since having known $\{K_I, K_F\}$ one can get $\{K_{II}, K_D\}$ according to the constitutive laws (3).

For the central crack under stationary boundary conditions, non-zero values of thermal stresses occur ahead of the crack tip. Therefore, there is a finite value of the stress intensity factor. In the non-conducting PZ the stress intensity factor of pure mode I for the considered boundary conditions is $K_I^{\text{stat}} = 4.55 \times 10^4$ Pa $\cdot$ m$^{1/2}$. This value is computed from Eq. (32) by extrapolating the near-field quantities $(u_1, u_3, \phi)$ around the crack tip. Recently, Sladek et al. [38] showed that the electrical potential $\phi$ caused by a remote pure mechanical load is identical to $u_3$ caused by a remote pure electric displacement loading as a consequence of the extended Betti’s reciprocal theorem in stationary piezoelectricity [Pan [26]]. Thus, it is interesting to remark that, although a pure mechanical load would induce a finite value of electrical potential $\phi$ and $K_F$ on the electrically impermeable crack surface, the EDIF $K_D$ is still zero for this case.

We now suppose that the crack length is extended by $\delta$, then the total energy release rate (ERR) can be expressed as

$$ G = \lim_{\delta \to 0} \frac{1}{2\delta} \int_0^\delta \left[ \sigma_{ij}(x) \Delta u_i(\delta - x) + D_{ij}(x) \Delta \phi(\delta - x) \right] dx, $$

where $\Delta u_i$ and $\Delta \phi$ are the displacement and potential discontinuities on the crack faces.
Since the ERR can be expressed by the intensity factors (e.g., Tian and Rajapakse [40])

$$ G = \frac{1}{2} K^T Y K, $$

the energy release rate in our case can be expressed as
In the second example, the influence of the stationary electric current $J_0 = \pm \dot{S}(x_3 = \pm h/2)$ on the energy release rate is investigated. Results are illustrated in Fig. 5. Two different initial electron densities are considered in the numerical analyses. One can observe that the ERR is less sensitive on the electric current for PZ semiconductor as for non-conducting PZ solid, since the initial electron density $M_0 = 10^6 \text{ m}^{-3}$ can be considered as a value corresponding to a non-conducting solid. We also remark that a positive value denotes released energy, whilst a negative value represents absorbed energy.

In the final example the influence of the non-stationary boundary conditions on the physical quantities is investigated. The strip is subjected to a thermal shock with Heaviside time variation on the entire outer boundary while the crack surfaces are kept at zero temperature. The time variation of the normalized stress intensity factors for a non-conducting and semiconductor PZ solid are presented in Fig. 6. One can observe that the initial electron density has no influence on the SIF.

In non-stationary case a pure thermal load can induce finite value of the electric displacement intensity factor (EDIF). The response of the electric fields is immediate, while that of the elastic ones is taken as finite because of the finite velocity of elastic waves. The EDIF induced at a pure thermal load is presented in Fig. 7. For non-conducting PZ the character of the EDIF curve is similar to the SIF, while the EDIF evolution is exponentially growing for the conducting material. This is due to the strong influence of $M_0$ on $K_D$ as observed for electric potential at stationary boundary conditions.

5. Conclusions

The MLPG method has been successfully applied for 2-D crack problems in piezoelectric semiconductors subjected to a thermal load. Stationary and transient thermal conditions are considered in the heat conduction equation. Our numerical results reveal that initial density of electrons (carriers of electric charge in n-type PZ semiconductors) has only moderate influence on the crack displacement. However, the induced electric potential is strongly affected by the initial electron density. The largest value of the induced potential is achieved for a non-conducting PZ material.

We have also observed that the energy release rate is less sensitive on the electric current for PZ semiconductor as for almost non-conducting PZ solid. Furthermore, the initial electron density has no influence on the stress intensity factor (SIF) for a crack under a transient thermal load. In non-stationary case a pure thermal load also yields a finite value of EDIF. For non-conducting PZ, the character of the EDIF curve is similar to the SIF, while the EDIF evolution is exponentially growing for the conducting material.

The present method is promising for numerical analyses of multi-field problems like piezoelectric, electro-magnetic or thermoelastic problems. All approximated fields have $C^1$-continuity as compared to other common domain discretization methods where continuity is guaranteed only for the primary fields.

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References


