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Electro-mechanical crack systems: bound theorems, dual finite elements and error estimation

C.C. Wu [a,*], Q.Z. Xiao [b]

[a] School of Naval Architecture and Ocean Engineering, Shanghai Jiao Tong University, Shanghai 200240, China
[b] School of Engineering, Cardiff University, Cardiff CF24 0YF, UK

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Abstract

Because of the complexity of piezoelectric crack problems, it is hard to obtain closed-form solutions, and numerical methods are largely resorted to. Hence, the upper/lower bound estimation of piezoelectric fracture parameters is of theoretical and practical importance. in this paper, the path-independent integral I, which is the dual of the J-integral, for electro-mechanical coupling crack systems, is presented. The related bound theorems are established for J and I. Piezoelectric dual finite elements are presented for the numerical implementation of the bound analysis. Moreover, an error estimator is presented for the assessment of numerical accuracy of the piezoelectric fracture parameters.

Keywords: Bound theorem; Crack; Dual finite element; Error estimation; Path-independent integral; Piezoelectric

1. Introduction

As an electro-mechanical coupling material, a piezoelectric ceramic is brittle and likely to crack at all scales from domains to devices. Under mechanical and/or electrical loading, it can fail prematurely due to the propagation of flaws or defects induced during the manufacturing process and by the in-service electro-mechanical loading. Hence, it is necessary to understand, and be able to analyze, the fracture characteristics of piezoelectric materials so as to predict reliable service life for the electro-mechanical coupling system.

* Corresponding author. Tel.: +86 21 54747161; fax: +86 21 54743044.
E-mail address: ccwu@sjtu.edu.cn (C.C. Wu).

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Electro-mechanical modeling of piezoelectric fracture is complicated by the fact that piezoelectric materials exhibit electro–elastic coupling behavior as well as anisotropy behavior. Among the theoretical studies of cracked piezoelectric bodies (see e.g. Chen et al., 1998; Chen and Karihaloo, 1999; and reviews by Zhang et al., 2001; and Chen and Lu, 2002), permeable and impermeable conditions on the crack faces by Parton (1976) and Deeg (1980), respectively, are most commonly adopted. Whichever condition is adopted on the crack faces, it is hard to get the exact solutions except for a few simple cases, and numerical methods are often resorted to (Kumar and Singh, 1996).

In the finite element (FE) analysis, the piezoelectric element of Allik and Hughes (1970) has been employed in a large body of literature on linear electro-mechanical materials and/or structures. In this element the basic variables, the displacement and electric potential are taken to be linear interpolations, hence it is an isoparametric/compatible model. A further discussion on the piezoelectric model has been presented by Landis (2002). In recent years, it has been found that the hybrid FE shows ideal numerical behavior in the nonlinear electro-mechanical coupling analysis (see e.g. Ghandi and Hagood, 1997). To capture the characteristic singularity at the crack tip, Wu et al. (2001) presented a piezoelectric hybrid model and simulated singular fields of a series of crack problems.

For the conventional elastic–plastic fracture problem, bound analyses for the path-independent integrals have been suggested by Wu et al. (1998, 1999). In this paper, the upper/lower bound approach will be extended to the piezoelectric fracture. To this end, the following topics will be considered for the electro-mechanical coupling system: (1) Dual path-independent integrals for the piezoelectric cracks; (2) Bound theorems for the dual crack parameters; (3) Dual piezoelectric FEs for the implementation of the upper/lower bound theorem; and finally (4) error estimation for the obtained numerical solutions.

2. Dual path-independent integrals for electro-mechanical systems

Piezoelectric solids that have zero body forces and are free of electric charges are considered. The path independent J-integral suggested by Rice (1968) has been extended to the piezoelectric crack analysis by Pak (1990) and Suo et al. (1992). It is formulated as

$$J(u_i,\varphi)=\int_S\left[H(\varepsilon_{ij},E_i)\mathrm{d}x_2-\left(\sigma_{ij}n_j\frac{\partial u_i}{\partial x_1}+D_jn_j\frac{\partial\varphi}{\partial x_1}\right)\mathrm{d}s\right]\tag{1}$$

where u_i, σ_{ij} and $\varepsilon_{ij}=(u_{i,j}+u_{j,i})/2$ are displacements, stresses and strains, respectively, and x_i are the Cartesian coordinates. S is a contour surrounding the crack tip in anticlockwise direction from the lower face to the upper face of the crack. n_j are direction cosines of the outward unit normal on S, and ds is an infinitesimal arc length along S. D_i and φ are the electric displacement and the electric potential, respectively. The electric enthalpy density

$$H(\varepsilon_{ij},E_i)=\tfrac{1}{2}c^{\mathrm{E}}_{ijkl}\varepsilon_{ij}\varepsilon_{kl}-\tfrac{1}{2}\in^{\varepsilon}_{ij}E_iE_j-e_{ikl}\varepsilon_{kl}E_i\tag{2}$$

where $E_i=-\varphi_{,i}$ are the electric field strengths, c^{E}_{ijkl} are the (short circuit) material elastic stiffness constants measured at constant electric field, $\in^{\varepsilon}_{ij}$ are the (sandwiched) dielectric constants measured at constant strain, and e_{ikl} are the piezoelectric stress constants. The corresponding constitutive relationships are

$$\sigma_{ij}=c^{\mathrm{E}}_{ijkl}\varepsilon_{kl}-e_{kij}E_k\quad\text{and}\quad D_i=e_{ikl}\varepsilon_{kl}+\in^{\varepsilon}_{ik}E_k\tag{3}$$

The system potential energy functional can be formulated as

$$\Pi_{\mathrm{p}}(u_i,\varphi)=\int_v H(\varepsilon_{ij},E_i)\mathrm{ad}v-\int_{S_s}\overline{T}_iu_i\mathrm{d}s+\int_{S_w}\bar{q}_s\varphi\mathrm{d}s\tag{4}$$

v denotes the domain of the two-dimensional body. S_s denotes the boundary portion on which the prescribed traction $\overline{T}_i$ is acting and S_w denotes the boundary portion on which the prescribed surface charge density $\bar{q}_s$ is acting. The charge density is defined as $q = -D_i n_i$. Thus, integral (1) can be zexpressed as

$$J(u_i, \varphi) = -\mathrm{d}\Pi_\mathrm{p}/\mathrm{d}a \tag{5}$$

i.e. the energy release rate for the piezoelectric crack system. Here, a denotes crack length. In order to build the dual of $J(u_i, \varphi)$, initially we consider the dual of Rice's J, i.e. the complementary energy release rate of Wu et al. (1998, 1999):

$$I^*(\sigma_{ij}, u_i) = \int_S \left[-B(\sigma_{ij})\mathrm{d}x_2 + \sigma_{i2}\frac{\partial u_i}{\partial x_j}\mathrm{d}x_j\right] \tag{6}$$

where $B(\sigma_{ij})$ is the complementary energy function. The above path-independent integral I^* defined for the conventional elastic–plastic materials can easily be extended to piezoelectric cracks by adding only the electric energy induced by the electric field D_i and φ. In this way, the desired piezoelectric crack parameter, which is the dual of Pak's J in Eq. (1), can be formulated as

$$I(\sigma_{ij}, u_i, D_i) = \int_S \left[-G(\sigma_{ij}, D_i)\mathrm{d}x_2 + \left(\sigma_{i2}\frac{\partial u_i}{\partial x_j} + D_2\frac{\partial \varphi}{\partial x_j}\right)\mathrm{d}x_j\right] \tag{7}$$

where the complementary electric enthalpy density

$$G(\sigma_{ij}, D_i) = \tfrac{1}{2}s^D_{ijkl}\sigma_{ij}\sigma_{kl} - \tfrac{1}{2}\beta^\sigma_{ij}D_iD_j + g_{kij}\sigma_{ij}D_k \tag{8}$$

s^D_{ijkl} are the (open circuit) material elastic compliance constants measured at constant electric displacement, β^σ_{ij} are the (free) dielectric insulating rate constants measured at constant stress, and g_{ikl} are the piezoelectric potential constants. The constitutive relationships (3) can be rewritten as

$$\varepsilon_{ij} = s^D_{ijkl}\sigma_{kl} + g_{kij}D_k \quad \text{and} \quad E_i = -g_{ijk}\sigma_{jk} + \beta^\sigma_{ij}D_j \tag{9}$$

it is easy to verify that

$$H(\varepsilon_{ij}, E_i) + G(\sigma_{ij}, D_i) = \sigma_{ij}\varepsilon_{ij} - D_iE_i \tag{10}$$

For a given piezoelectric crack system, the following relationship

$$I(\sigma_{ij}, u_i, D_i) = \mathrm{d}\Pi_\mathrm{c}/\mathrm{d}a \tag{11}$$

can be verified by the method used by Wu et al. (1998). In (11) the system complementary energy functional

$$\Pi_\mathrm{c}(\sigma_{ij}, D_i) = \int_v G(\sigma_{ij}, D_i)\mathrm{d}v - \int_{S_u} \overline{u_i}\sigma_{ij}n_j\mathrm{d}s - \int_{S_\varphi} \overline{\varphi}D_jn_j\mathrm{d}s \tag{12}$$

where S_u denotes the boundary portion on which the prescribed displacements $\bar{u}_i$ are acting and S_φ denotes the boundary portion on which the prescribed electric potential $\bar{\varphi}$ is acting.

With the use of the divergence theorem, we have

$$\int_v H(\varepsilon_{ij}, E_i)\mathrm{d}v = \tfrac{1}{2}\oint_{\partial v}(T_iu_i - q\varphi)\mathrm{d}s = \int_v G(\sigma_{ij}, D_i)\mathrm{d}v \tag{13}$$

where ∂v represents the boundary of domain v.

3. Bound theorems

For conventional homogenous elastic or elastic–plastic materials, bound analyses for crack parameters have been suggested by Wu et al. (1998, 1999). These analyses can be extended to electro-mechanical systems. It is well known, various upper/lower bound analyses depend on the positive definiteness of a given mathematical/physical parameter. For the present piezoelectric system, the related electric enthalpy and complementary electric enthalpy densities are both assumed to be positive definite, i.e.

$$H(\varepsilon_{ij}, E_i) > 0 \quad \text{and} \quad G(\sigma_{ij}, D_i) > 0 \tag{14}$$

3.1. Lower bound theorem for $J(u_i, \varphi)$

For a given piezoelectric crack system with homogeneous boundary constraints $\bar{u}_i|_{S_u} = 0$, $\bar{\varphi}|_{S_\varphi} = 0$, the approximate J-integral based on the potential energy principle takes the lower bound of its actual one:

$$J(\widetilde{u}_i, \widetilde{\varphi}) \leqslant J(u_i, \varphi) \tag{15}$$

Here, (u_i, φ) and $(\widetilde{u}_i, \widetilde{\varphi})$ are respectively the actual solution and the solution given by the displacement-electric potential compatible FE.

Proof. Let $\widetilde{u}_i = u_i + \delta u_i$ and $\widetilde{\varphi} = \varphi + \delta\varphi$. δu_i and $\delta\varphi$ are respectively the virtual displacement and electric potential, which satisfy u_i/φ homogeneous boundary conditions. Thus the approximate potential energy can be expressed as

$$\Pi_{\mathrm{p}}(\widetilde{u}_i, \widetilde{\varphi}) = \Pi_{\mathrm{p}}(u_i, \varphi) + \delta\Pi_{\mathrm{p}} + \delta^2\Pi_{\mathrm{p}} \tag{16}$$

Here, $\delta\Pi_{\mathrm{p}} = 0$ corresponds to the stationary condition of the system potential energy, and

$$\delta^2\Pi_{\mathrm{p}} = \Pi_{\mathrm{p}}(\widetilde{u}_i, \widetilde{\varphi}) - \Pi_{\mathrm{p}}(u_i, \varphi) = \int_v H(\delta u_i, \delta\varphi)\mathrm{d}v \geqslant 0 \tag{17}$$

In accordance with relationship (5),

$$J(\widetilde{u}_i, \widetilde{\varphi}) = -\frac{\mathrm{d}}{\mathrm{d}a}\Pi_{\mathrm{p}}(\widetilde{u}_i, \widetilde{\varphi}) = -\frac{\mathrm{d}}{\mathrm{d}a}\left[\Pi_{\mathrm{p}}(u_i, \varphi) + \delta^2\Pi_{\mathrm{p}}\right] = J(u_i, \varphi) + \delta^2 J \tag{18}$$

and

$$J(u_i, \varphi) = -\frac{\mathrm{d}}{\mathrm{d}a}\Pi_{\mathrm{p}}(u_i, \varphi) = \frac{\mathrm{d}}{\mathrm{d}a}\int_v H(u_i, \varphi)\mathrm{d}v \geqslant 0 \tag{19}$$

$$\delta^2 J = -\frac{d}{da}\delta^2\Pi_{\mathrm{p}} = -\frac{\mathrm{d}}{\mathrm{d}a}\int_v H(\delta u_i, \delta\varphi)\mathrm{d}v \tag{20}$$

Note that (13) has been used in (19). Observing that $H(u_i, \varphi)$ and $H(\delta u_i, \delta\varphi)$ are of the same form, a comparison of (19) and (20) shows that $\delta^2 J \leqslant 0$, and it follows from (18) that the inequality (15) must be true. □

3.2. Upper bound theorem for $I(\sigma_{ij}, u_i, D_i)$

For a given piezoelectric crack system with homogeneous boundary constraints $\bar{u}_i|_{S_u} = 0$, $\bar{\varphi}|_{S_\varphi} = 0$, the approximate solution to the I-integral based on the complementary energy principle takes the upper bound of its actual one:

$$I(\widetilde{\sigma}_{ij}, \widetilde{u}_i, \widetilde{D}_i) \geqslant I(\sigma_{ij}, u_i, D_i) \tag{21}$$

where (σ_{ij}, u_i, D_i) and $(\widetilde{\sigma}_{ij}, \widetilde{u}_i, \widetilde{D}_i)$ are respectively the actual solution and the solution given by the stress-electric displacement equilibrium FE.

Proof. Let $\widetilde{\sigma}_{ij} = \sigma_{ij} + \delta\sigma_{ij}$ and $\widetilde{D}_i = D_i + \delta D_i$. $\delta\sigma_{ij}$ and δD_i are the virtual stresses and electric displacements, respectively. we have

$$\Pi_c(\widetilde{\sigma}_{ij}, \widetilde{D}_i) = \Pi_c(\sigma_{ij}, D_i) + \delta\Pi_c + \delta^2\Pi_c \tag{22}$$

Here, $\delta\Pi_c = 0$ corresponds to the functional stationary condition. Moreover, accounting for the homogeneous constraints $\bar{u}_i|_{S_u} = 0$ and $\bar{\varphi}|_{S_\varphi} = 0$ the first and third terms on the right hand side of (22) becomes (see Eq. (12))

$$\Pi_c(\sigma_{ij}, D_i) = \int_v G(\sigma_{ij}, D_i)\mathrm{d}v \tag{23}$$

$$\delta^2\Pi_c = \int_v G(\delta\sigma_{ij}, \delta D_i)\mathrm{d}v \tag{24}$$

together with Eqs. (22)–(24), Eq. (11) becomes

$$I(\widetilde{\sigma}_{ij}, \widetilde{u}_i, \widetilde{D}_i) = \frac{\mathrm{d}}{\mathrm{d}a}\Pi_c(\widetilde{\sigma}_{ij}, \widetilde{D}_i) = I(\sigma_{ij}, u_i, D_i) + \delta^2 I \tag{25}$$

$$I(\sigma_{ij}, u_i, D_i) = \frac{\mathrm{d}}{\mathrm{d}a}\Pi_c(\sigma_{ij}, D_i) = \frac{\mathrm{d}}{\mathrm{d}a}\int_v G(\sigma_{ij}, D_i)\mathrm{d}v \geqslant 0 \tag{26}$$

$$\delta^2 I = \frac{\mathrm{d}}{\mathrm{d}a}\delta^2\Pi_c = \frac{\mathrm{d}}{\mathrm{d}a}\int_v G(\delta\sigma_{ij}, \delta D_i)\mathrm{d}v \tag{27}$$

Observing that both $G(\sigma_{ij}, D_i)$ and $G(\delta\sigma_{ij}, \delta D_i)$ have the same form, a comparison of (26) and (27) results in $\delta^2 I \geqslant 0$, and it follows from (25) that the inequality (21) must be true. □

4. Limitations on the bound analysis

It should be noticed that the above bound theorems are conditional for piezoelectric fracture. The lower bound theorem for J depends on the positive definiteness of the electric enthalpy density: $H(\varepsilon_{ij,\mathrm{E}i}) > 0$; and the upper bound theorem for I depends on the positive definiteness of the complementary electric enthalpy density: $G(\sigma_{ij}, D_i) > 0$. The complexity lies in that the positive definiteness of H and/or G depends on the electric loading. In the case of large electric loading (E_i and/or D_i) the electric enthalpy or complementary electric enthalpy density, is likely to lose its positive definiteness, so that the bound theorems no longer hold.

Take a mode I crack as an illustrative example, the energy release rate can be expressed as (Park and Sun, 1995)

$$G = \tfrac{1}{2}\pi[A\sigma_\infty^2 + B\sigma_\infty D_\infty - CD_\infty^2] \tag{28}$$

in which σ_∞ and D_∞ are the respective mechanical and electric loading far from the crack tip. Then the non-negativity condition, $G > 0$ leads to the following requirement for the loading ratio $\rho = D_\infty/\sigma_\infty$

$$A + B\rho - C\rho^2 > 0 \tag{29}$$

The inequality (29) shows the limitations on the bound theorems, alluded to above.

5. Piezoelectric finite elements

As for the plane fracture problem, the 4-node piezoelectric isoparametric/compatible element, denoted as PZT-Q4, can easily be formulated in terms of the assumed bilinear displacement and electric potential. The resulting model can be employed to estimate the lower bound of $J(u_i, \varphi_i)$ as mentioned in the lower bound theorem. On the other hand, for $I(\sigma_{ij}, u_i, D_i)$, its upper bound should be estimated by the stress-electric displacement equilibrium element of Fraeijs de Veubeke type (Fraeijs de Veubeke, 1965). Unfortunately it is hard to obtain a reliable equilibrium model for 2D/3D problems because numerical difficulties, such as element rank deficiency, cannot be avoided. On the other hand, for equilibrium models using only the stress as primary variables (see e.g. Duflot and Nguyen-Dang, 2002), which satisfy *a priori* the equilibrium and constitutive equations and approximate only the compatibility equations, the recovery of displacements is troublesome. One faces the problem of how to implement the upper bound theorem for $I(\sigma_{ij}, u_i, D_i)$.

It is observed that the Reissner functional $\Pi_R(u_i, \sigma_{ij}, \varphi, D_i)$ of EerNisse (1983) reduces to the complementary energy functional $\Pi_c(\sigma_{ij}, D_i)$ in (12) after the enforcement of equilibrium constraints $\sigma_{ij,j} = 0$ and $D_{i,i} = 0$. Therefore, the hybrid model based on $\Pi_R(u_i, \sigma_{ij}, \varphi, D_i)$ will be equivalent to the equilibrium model based on $\Pi_c(\sigma_{ij}, D_i)$ when the $\sigma_{ij} \sim D_i$ equilibrium equations are enforced on the element.

A 4-node piezoelectric hybrid element can be developed from the Reissner principle of EerNisse (1983). The element displacements and electric potential are assumed as bilinear interpolations:

$$\begin{Bmatrix} u \\ v \\ \varphi \end{Bmatrix} = \frac{1}{4}\sum_{i=1}^{4}(1+\xi_i\xi)(1+\eta_i\eta)\begin{Bmatrix} u_i \\ v_i \\ \varphi_i \end{Bmatrix} = \mathbf{N}\mathbf{q}, \quad \mathbf{q} = \{u_1, v_1, \varphi_1, \ldots, u_4, v_4, \varphi_4\}^{\mathrm{T}}, \quad \mathbf{u} = \begin{Bmatrix} u \\ v \end{Bmatrix} \tag{30}$$

where (ξ_i, η_i) represent the isoparametric co-ordinates of node "i" with the global co-ordinates $(x_i, y_i), i = 1,2,3,4$. (u_i, v_i, ϕ_i) are the displacements and electric potential at node "i". The stress mode of Pian and Sumihara (1984) is adopted as the element trial stresses

$$\boldsymbol{\sigma} = \begin{Bmatrix} \sigma_x \\ \sigma_y \\ \tau_{xy} \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 & a_3^2\xi & a_1^2\eta \\ 0 & 1 & 0 & b_3^2\xi & b_1^2\eta \\ 0 & 0 & 1 & a_3b_3\xi & a_1b_1\eta \end{bmatrix}\begin{Bmatrix} \beta_1 \\ \vdots \\ \beta_5 \end{Bmatrix} = \mathbf{P}_m\boldsymbol{\beta}_m \tag{31}$$

wherein the element geometric parameters are

$$\begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \\ a_3 & b_3 \end{bmatrix} = \frac{1}{4}\begin{bmatrix} -1 & 1 & 1 & -1 \\ 1 & -1 & 1 & -1 \\ -1 & -1 & 1 & 1 \end{bmatrix}\begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ x_3 & y_3 \\ x_4 & y_4 \end{bmatrix}$$

The element electric displacement is initially assumed to be a linear function of the element $\xi - \eta$ coordinates. After introducing an energy consistency condition (Liu and Wu, 1999), it can be optimized into the form

$$D = \begin{Bmatrix} D_x \\ D_y \end{Bmatrix} = \begin{bmatrix} 1 & 0 & a_3\xi & a_1\eta \\ 0 & 1 & b_3\xi & b_1\eta \end{bmatrix}\begin{Bmatrix} \beta_6 \\ \vdots \\ \beta_9 \end{Bmatrix} = \mathbf{P}_e\boldsymbol{\beta}_e \tag{32}$$

In terms of the element trial functions (30)–(32), Reissner energy functional (EerNisse, 1983) for an individual element can be formulated as (boundary terms are ignored for simplicity, as they are identical to the isoparametric/compatible model)

$$\Pi_{\mathrm{R}}^{e}(\mathbf{u},\boldsymbol{\sigma},\varphi,\mathbf{D}) = -\int_{v^e}[G(\boldsymbol{\sigma},\mathbf{D}) - \boldsymbol{\sigma}^{\mathrm{T}}(\partial\mathbf{u}) - \mathbf{D}^{\mathrm{T}}(\nabla\varphi)]\mathrm{d}v \tag{33}$$

$\partial\mathbf{u}$ is the element strain, and ∇ the gradient operator. Substitution of the element trial functions (30)–(32) into Eq. (33) results in

$$\Pi_{\mathrm{R}}^{e}(\boldsymbol{\beta},\mathbf{q}) = \boldsymbol{\beta}^{\mathrm{T}}\mathbf{G}\mathbf{q} - \tfrac{1}{2}\boldsymbol{\beta}^{\mathrm{T}}\mathbf{H}\boldsymbol{\beta} \tag{34}$$

$$\mathbf{G} = \int_{v^e}\mathbf{P}^{\mathrm{T}}(\partial\mathbf{N})\mathrm{d}v, \quad \mathbf{H} = \int_{v^e}\mathbf{P}^{\mathrm{T}}\mathbf{S}\mathbf{P}\mathrm{d}v \quad \text{and} \quad \mathbf{P} = \begin{bmatrix}\mathbf{P}_m & \mathbf{0}_{3\times4}\\ \mathbf{0}_{2\times5} & \mathbf{P}_e\end{bmatrix}, \quad S = \begin{bmatrix} s & g^{\mathrm{T}} \\ g & -\beta^{\sigma}\end{bmatrix} \tag{35}$$

wherein $\partial\mathbf{N}$ is the element generalized strain matrix. The functional stationary condition $\delta\Pi_{\mathrm{R}}^{e}(\boldsymbol{\beta},\mathbf{q}) = 0$ with respect to $\boldsymbol{\beta} = \begin{Bmatrix}\boldsymbol{\beta}_m \\ \boldsymbol{\beta}_e\end{Bmatrix}$ results in $\mathbf{H}\boldsymbol{\beta} = \mathbf{G}\mathbf{q}$. After condensing $\boldsymbol{\beta}$ functional (34) becomes

$$\Pi_{\mathrm{R}}^{e} = \tfrac{1}{2}\mathbf{q}^{\mathrm{T}}\mathbf{K}^{e}\mathbf{q} \tag{36}$$

with element stiffness matrix

$$\mathbf{K}^{e} = \mathbf{G}^{\mathrm{T}}\mathbf{H}^{-1}\mathbf{G} \tag{37}$$

In view of the fact that it is difficult to build a stress–electric displacement equilibrium element directly, the penalty-equilibrium technique developed by Wu and Cheung (1995) for conventional mechanical materials is employed here. Functional $\Pi_{\mathrm{R}}^{e}(u_i,\sigma_{ij},\varphi,D_i)$ is generalized as

$$\Pi_{\mathrm{RG}}^{e} = \Pi_{\mathrm{R}}^{e} - \alpha\left(\int_{v^e}\sigma_{ij,j}\sigma_{ij,j}\mathrm{d}v + \int_{v^e}D_{i,i}D_{i,i}\mathrm{d}v\right) \tag{38}$$

where the penalty factor α is taken to be a large constant (e.g. 10^4). In terms of the assumed element trial functions (30)–(32), the functional (38) can be formulated as

$$\Pi_{\mathrm{RG}}^{e}(\boldsymbol{\beta},\mathbf{q}) = \boldsymbol{\beta}^{\mathrm{T}}\mathbf{G}\mathbf{q} - \tfrac{1}{2}\boldsymbol{\beta}^{\mathrm{T}}\mathbf{H}\boldsymbol{\beta} - \alpha\boldsymbol{\beta}^{\mathrm{T}}\mathbf{H}_{\mathrm{p}}\boldsymbol{\beta} \tag{39}$$

where the penalty equilibrium matrix is

$$\mathbf{H}_{\mathrm{p}} = \int_{v^e}(\partial^{\mathrm{T}}\mathbf{P})^{\mathrm{T}}(\partial^{\mathrm{T}}\mathbf{P})\mathrm{d}v \quad (\partial^{\mathrm{T}} \text{ is the equilibrium differential operator}) \tag{40}$$

In this way, the equilibrium equations, $\sigma_{ij,j} = 0$ and $D_{i,i} = 0$, are enforced within the element in a penalty sense, so that the functional $\Pi_{\mathrm{R}}^{e}(u_i,\sigma_{ij},\varphi,D_i) \Rightarrow \Pi_{\mathrm{c}}^{e}(\sigma_{ij},D_i)$, and the complementary energy functional is available. It turns out that the hybrid element based on Π_{R}^{e} will degenerate into a stress equilibrium model based on Π_{c}^{e} and can be used to implement the upper bound theorem. The resulting penalty-equilibrium element is called as PZT-PS(α).

In the numerical calculations using the isoparametric element (e.g. PZT-Q4), the traction free and electric displacement free conditions on the crack surface cannot be imposed. On the other hand, these homogeneous traction/electric displacement conditions can easily be imposed by the present hybrid element since the stress and electric displacement are independently assumed in the element formulation. Numerical solutions by hybrid elements are more stable and the accuracy of the singular stress/electric displacement in the crack tip region is significantly improved (Wu et al., 2001).

6. Error estimation

Liebowitz et al. (1998) investigated the development of an adaptive FE method for fracture related problems based on the Zienkiewicz and Zhu (1987) stress recovery based error estimator.

A more natural way for crack problems is to estimate directly the error of fracture parameters. Wu et al. (1999) presented an error estimator for Rice's J-like crack parameters based on the bound theorems. Here the formula will be extended to electro-mechanical crack problems.

Let $\delta u_i = \widetilde{u}_i - u_i$ be the displacement error and $\delta\varphi = \widetilde{\varphi} - \varphi$ the electric potential error induced by using the assumed displacement-electric potential FE(e.g. PZT-Q4). in accordance with the lower bound theorem (15), the exact error for J-integral must be

$$J(\delta u_i, \delta\varphi) = J(\widetilde{u}_i, \widetilde{\varphi}) - J(u_i, \varphi) \leqslant 0 \tag{41}$$

and the absolute error is then

$$|J(\delta u_i, \delta\varphi)| = J(u_i, \varphi) - J(\widetilde{u}_i, \widetilde{\varphi}) \tag{42}$$

Let $\delta\sigma_{ij} = \widetilde{\sigma}_{ij} - \sigma_{ij}$ be the stress error and $\delta D_I = \widetilde{D}_I - D_I$ the electric displacement error induced by using the stress-electric displacement (penalty) equilibrium element (e.g. PZT-PS(α)). In accordance with the upper bound theorem (21) the exact error for I-integral should be

$$I(\delta\sigma_{ij}, \delta u_i, \delta D_i) = I(\widetilde{\sigma}_{ij}, \widetilde{u}_i, \widetilde{D}_i) - I(\sigma_{ij}, u_i, D_i) \geqslant 0 \tag{43}$$

and the absolute error

$$\left|I(\delta\sigma_{ij}, \delta u_i, \delta D_i)\right| = I(\widetilde{\sigma}_{ij}, \widetilde{u}_i, \widetilde{D}_i) - I(\sigma_{ij}, u_i, D_i) \tag{44}$$

The relative errors corresponding to Eqs. (42) and (44) can be expressed as

$$\Delta_J = \frac{|\, J(\delta u_i, \delta\varphi) \,|}{J(u_i, \varphi)} \quad \text{and} \quad \Delta_I = \frac{|\, I(\delta\sigma_{ij}, \delta u_i, \delta D_i) \,|}{I(\sigma_{ij}, u_i, D_i)} \tag{45}$$

respectively. These errors are, however, difficult to calculate in practical applications since the exact value of J or I is generally not available. In order to develop an error estimator that is easy to calculate, an alternative relative error formula is defined as the following:

$$\Delta_{J-I} = \frac{|\, J(\delta u_i, \delta\varphi) \,| + |\, I(\delta\sigma_{ij}, \delta u_i, \delta D_i) \,|}{J(u_i, \varphi) + I(\sigma_{ij}, u_i, D_i)} \tag{46}$$

wherein the reference solution is chosen as

$$J(u_i, \varphi) + I(\sigma_{ij}, u_i, D_i) = J(\widetilde{u}_i, \widetilde{\varphi}) + I(\widetilde{\sigma}_{ij}, \widetilde{u}_i, \widetilde{D}) - [J(\delta u_i, \delta\varphi) + I(\delta\sigma_{ij}, \delta u_i, \delta D_i)] \tag{47}$$

As $J(\delta u_i, \delta\varphi) \leqslant 0$ and $I(\delta\sigma_{ij}, \delta u_i, \delta D_i) \geqslant 0$ are small quantities, the last term in Eq. (47) can be ignored, so that Eq. (47) becomes

$$J(u_i, \varphi) + I(\sigma_{ij}, u_i, D_i) \approx J(\widetilde{u}_i, \widetilde{\varphi}) + I(\widetilde{\sigma}_{ij}, \widetilde{u}_i, \widetilde{D}_i) \tag{48}$$

Substituting Eqs. (42), (44) and (48) into (46), and noting that for the exact solutions, $J(u_i,\varphi) - I(\sigma_{ij},u_i,D_i) = 0$, the relative error formula (46) becomes

$$\Delta_{J-I} \approx \frac{I(\widetilde{\sigma}_{ij}, \widetilde{u}_i, \widetilde{D}_i) - J(\widetilde{u}_i, \widetilde{\varphi})}{I(\widetilde{\sigma}_{ij}, \widetilde{u}_i, \widetilde{D}_i) + J(\widetilde{u}_i, \widetilde{\varphi})} \tag{49}$$

When the FE size tends to zero, i.e. $h \to 0$, the convergence of FE results guarantees that $J(\widetilde{u}_i, \widetilde{\varphi}) \to J(u_i, \phi)$, and $I(\widetilde{\sigma}_{ij}, \widetilde{u}_i, \widetilde{D}_i) \to I(\sigma_{ij}, u_i, D_i)$, hence the above relative error $\Delta_{J-I} \to 0$. The error estimation formula (49) depends on the numerical solutions to J and I only, so it is easy to implement in the crack parameter assessment.

In the case of pure mechanical loading, D_i and $\widetilde{\varphi}$ will disappear from formula (49), one then has the following error estimation formula of Wu et al. (1999) for pure mechanical crack problems

$$\Delta_{J-I} = \frac{I(\widetilde{\sigma}_{ij}, \widetilde{u}_i) - J(\widetilde{u}_i)}{I(\widetilde{\sigma}_{ij}, \widetilde{u}_i) + J(\widetilde{u}_i)} \tag{50}$$

7. Numerical examples

In numerical calculations, the piezoelectric isoparametric/compatible element PZT-Q4 and the piezoelectric penalty-equilibrium element PZT-PS(α) are employed to estimate J and I, respectively. A center cracked square panel CCP (Fig. 1) with pure mechanical loading or mechanical-electrical mixed loading is considered. traction-free and impermeable (i.e. having zero electric displacement) boundary conditions are assumed on the crack faces. plane strain conditions are considered in the numerical computations. only a quarter of the specimen (shaded part) needs to be considered because of symmetry. The material properties of PZT-4 and PZT-5H are listed in Table 1.

To inspect the convergence behavior of the numerical solutions of J and I, three meshes with different densities, as shown in Fig. 2, are considered for each material. Two independent integration paths (Fig. 2) are used simultaneously. The value of J/I is taken to be the average of results from these two paths. Numerical results are shown in Figs. 3 and 4. for the finite specimen considered, no theoretical solution is available. The "exact solution" in Figs. 3 and 4 illustrates the converged value of J or I with mesh refinement. It can be seen that for mechanical and/or electrical loadings, the J-solutions by the PZT-Q4 compatible element always converge to the exact one from below. On the contrary, the I-solutions by the PZT-PS(α) penalty-equilibrium element always converge to the exact one from above. These numerical solutions demonstrate the bound theorems.

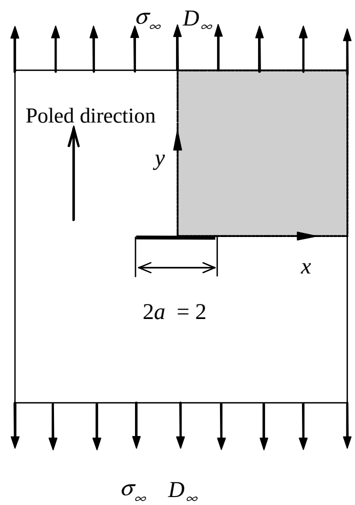

Fig. 1. Center cracked square panel (CCP) with side length of 8.

Table 1
Material constants for PZT-4 and PZT-5H (C_i: 10 GNm^{-2}, e_i: cm^{-2}, $\in_i$: μCV^{-1}m^{-1})

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	e_{31}	e_{33}	e_{15}	$\in_{11}$	$\in_{33}$
PZT-4	13.9	7.7	7.43	11.3	2.56	−6.98	13.84	13.44	6.00	5.47
PZT-5	12.6	5.5	5.30	11.7	3.53	−6.50	23.30	17.00	15.1	13.0

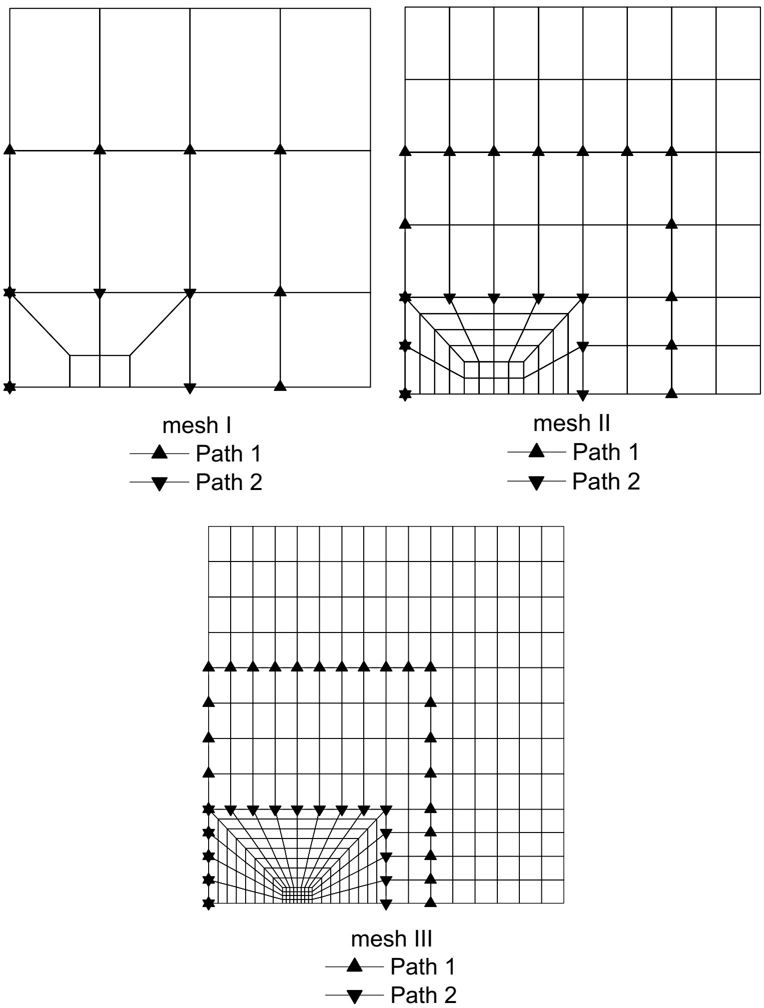

Fig. 2. The employed FE meshes and the selected integral paths.

The error estimation formula (49) is implemented to estimate the relative error of the numerical solutions for the piezoelectric CCP–specimen. The results listed in Tables 2 and 3 clearly show that the relative error converges to zero with an increase in the employed elements. These numerical tests exhibit the efficiency of the proposed error estimation.

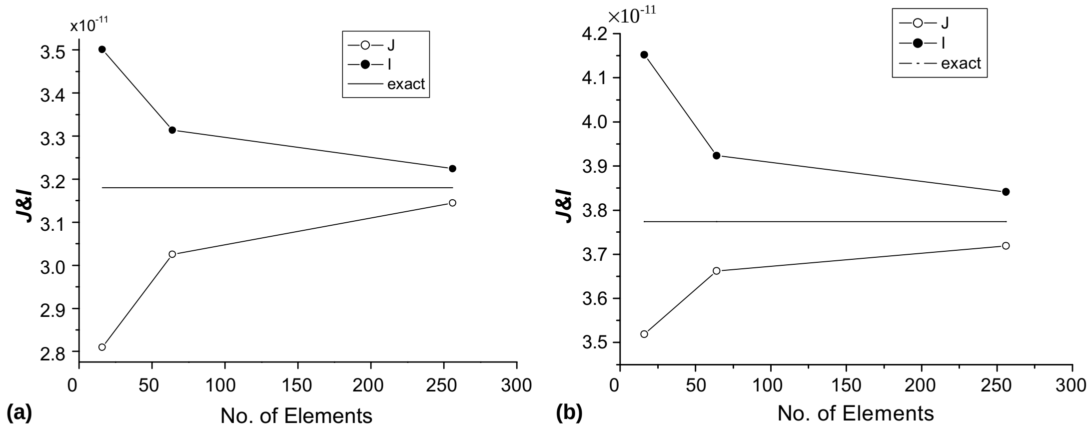

Fig. 3. Convergence of J and I with mesh refinement (PZT-4). (a) load 1: $D_\infty = 0$, $\sigma_\infty = 1.0$; (b) load 2: $D_\infty = 1.0 \times 10^{-10}$,$\sigma_\infty = 1.0$.

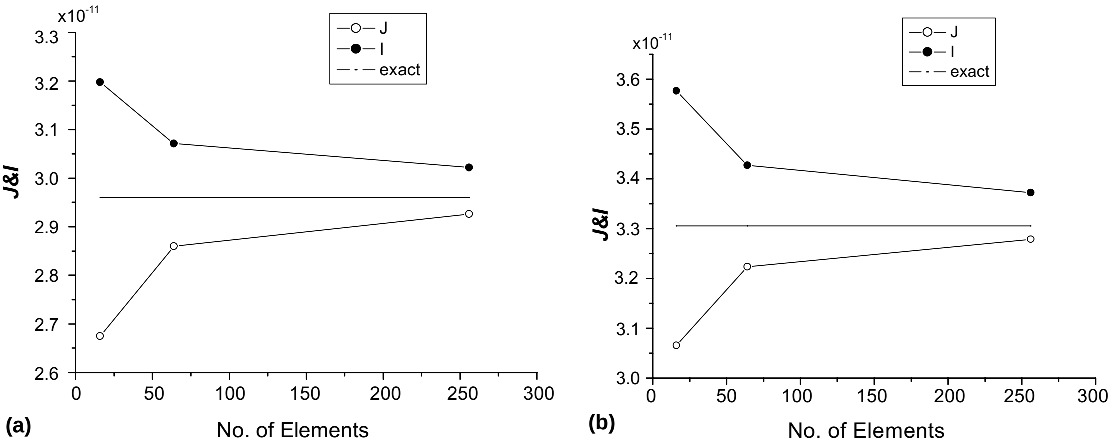

Fig. 4. Convergence of J and I with mesh refinement (PZT-5H). (a) load 1: $D_\infty = 0$, $\sigma_\infty = 1.0$; (b) load 2: $D_\infty = 1.0 \times 10^{-10}$,$\sigma_\infty = 1.0$.

Table 2
Relative Error Δ_{J-I} (%) for CCP (PZT-4)

	Mesh I (16 elements)	Mesh II (64 elements)	Mesh III (256 elements)
Load 1: $D_\infty = 0$, $\sigma_\infty = 1.0$	10.968	4.549	1.248
Load 2: $D_\infty = 1.0 \times 10^{-10}$, $\sigma = 1.0$	8.261	3.438	1.614

Table 3
Relative error Δ_{J-I} (%) for CCP (PZT-5H)

	Mesh I (16 elements)	Mesh II (64 elements)	Mesh III (256 elements)
Load 1: $D_\infty = 0$, $\sigma_\infty = 1.0$	8.901	3.560	1.606
Load 2: $D_\infty = 1.0 \times 10^{-10}$, $\sigma_\infty = 1.0$	7.694	3.068	1.409

8. Conclusions

The proposed *I*-integral, as the dual of the *J*-integral, makes the dual analysis for piezoelectric fracture possible. Under the precondition (14) the following bound relationships are available:

$$J(\widetilde{u}_i, \widetilde{\varphi}) \leqslant J(u_i, \varphi) = I(\sigma_{ij}, u_i, D_i) \leqslant I(\widetilde{\sigma}_{ij}, \widetilde{u}_i, \widetilde{D}_i) \tag{51}$$

The lower bound of J can be estimated by the piezoelectric compatible element PZT-Q4.

The upper bound of I can be estimated by the piezoelectric penalty-equilibrium hybrid element PZT-PS(α), proposed in the present work.

The proposed error estimation formula (49) makes a quantitative error estimation to the crack parameter without requiring any reference solutions. It is easier to implement than the exact relative error formula (45).

This study considered only linear piezoelectric elasticity. Obviously it is straightforward to extend it to nonlinear piezoelectric elasticity. The coefficient 1/2 in Eqs. (2),(8), and (13) needs to be replaced by the ratio of the strain energy density to the product of stresses and strains for the particular material. Moreover, the ratio of the strain energy density to the complementary energy density needs to be introduced in (49).

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References

Allik, H., Hughes, T.J.R., 1970. Finite element method for piezoelectric vibration. Int. J. Numer. Meth. Engng. 2, 151–157.

Chen, Z.T., Karihaloo, B.L., 1999. Dynamic response of a cracked piezoelectric ceramic under arbitrary electro-mechanical impact. Int. J. Solids Struct. 36, 5125–5133.

Chen, Y.H., Lu, T.J., 2002. Cracks and fracture in piezoelectrics. Adv. Appl. Mech. 39, 121–215.

Chen, Z.T., Yu, S.W., Karihaloo, B.L., 1998. A Griffith crack moving along the interface of two dissimilar piezoelectric materials. Int. J. Fract. 91, 197–203.

Deeg, W.F., 1980. The analysis of dislocation, crack and inclusion problems in piezoelectric solids. Ph.D. dissertation, Stanford University, CA.

Duflot, M., Nguyen-Dang, H., 2002. Dual analysis by a meshless method. Commun. Numer. Meth. Engng. 18, 621–631.

EerNisse, E.P., 1983. Variational method for electro vibration analysis. IEEE Trans. J. Sonics Ultrason 14, 59–67.

Fraeijs de Veubeke, B., 1965. Displacement and equilibrium models in the finite element method. In: Zienkiewicz, O.C., Holister, G. (Eds.), Stress Analysis, Chapter 9. Wiley, 197, p. 145, Reprinted in Int. J. Numer. Meth. Engng. 2001; 52: 287–342.

Ghandi, K., Hagood, N.W., 1997. A hybrid finite-element model for phase transition in nonlinear electro-mechanically coupled material. In: Varadan, V.V., Chandra, J. (Eds.), Smart Structures and Materials 1997 (Proc. of SPIE Vol. 3039). SPIE, Washington, pp. 97–112.

Kumar, S., Singh, R.N., 1996. Crack propagation in piezoelectric materials under combined mechanical and electrical loadings. Acta Mater. 44, 173–200.

Landis, C.M., 2002. A new finite-element formulation for electromechanical boundary value problems. Int. J. Numer. Meth. Engng. 55, 613–628.

Liebowitz, H., Sandhu, J.S., Menandro, F.C.M., Lee, J.D., 1998. Smart computational fracture of materials and structures. In: Cherepanov, G.P. (Ed.), Fracture: a Topical Encyclopedia of Current Knowledge. Malabar, Krieger Pub Co, Florida, pp. 526–541.

Liu, M., Wu, C.C., 1999. Numerical analysis of crack-tip fields of piezoelectric media by hybrid finite element. Chinese Sci. Bull. 44, 995–998.

Pak, Y.E., 1990. Crack extension force in a piezoelectric material. ASME J. Appl. Mech. 57, 647–653.

Park, S.B., Sun, C.T., 1995. Effect of electric field on fracture of piezoelectric ceramics. Int. J. Fract. 70, 203–216.

Parton, V.Z., 1976. Fracture mechanics of piezoelectric materials. Acta Astronaut. 3, 671–683.

Pian, T.H.H., Sumihara, K., 1984. Rational approach for assumed stress finite elements. Int. J. Numer. Meth. Engng. 20, 1685–1695.

Rice, J.R., 1968. A path-independent integral and the approximate analysis of strain concentration by notches and cracks. ASME J. Appl. Mech. 35, 376–386.

Suo, Z., Kuo, C.-M., Barnett, D.M., Willis, J.R., 1992. Fracture mechanics in piezoelectric material. J. Mech. Phys. Solids 40, 739–765.

Wu, C.C., Cheung, Y.K., 1995. On optimization approach of hybrid stress elements. Finite Element Anal. Des. 21, 111–128.

Wu, C.C., Sze, K.Y., Huang, Y.Q., 2001. Numerical solutions on fracture of piezoelectric materials by hybrid element. Int. J. Solids Struct. 38, 4315–4329.

Wu, C.C., Xiao, Q.Z., Li, Z.R., 1999. Fracture estimation: bound theorem and numerical strategy. In: Cheng, F.Y., Gu, Y. (Eds.), Computational Mechanics in Structural Engineering: Recent Developments (Proceedings of the Second Sino-US Joint Symposium/Workshop on Recent Advancement of Computational Mechanics in Structural Engineering, May 25–28, 1998, Dalian, China). Elsevier, pp. 349–360.

Wu, C.C., Xiao, Q.Z., Yagawa, G., 1998. Dual analysis for path integrals and bounds for crack parameter. Int. J. Solids Struct. 35, 1635–1652.

Zhang, T.Y., Zhao, M.H., Tong, P., 2001. Fracture of piezoelectric ceramics. Adv. Appl. Mech. 38, 147–289.

Zienkiewicz, O.C., Zhu, J.Z., 1987. A simple error estimator and adaptive procedure for practical engineering analysis. Int. J. Numer. Meth. Engng. 24, 337–357.