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Conservation integrals for the interfacial crack in bimaterial and layered ferroelectrics

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ABSTRACT

This paper focuses on establishing conservation integrals for nonlinear bimaterial and layered ferroelectrics. Employing the infinitesimal transformation, we obtain the invariant condition for ferroelectrics in the sense of Noether's theorem. A revised $\tilde{J}_i$-vector path-independent integral is achieved for homogeneous ferroelectrics both in the global and local coordinate systems. The path-independence of revised $\tilde{J}_1$-integral in bimaterial and layered ferroelectrics is demonstrated, with different electric crack surface conditions considered. Moreover, the crack-tip $\tilde{J}_1$-integral can be interpreted as energy release rate. Numerical simulations in layered ferroelectrics are presented to show characteristics of conservation integrals with respect to layer thickness and combined external loading.

1. Introduction

Due to strong mechanical–electric coupling effects and quick response to external excitations, bimaterial and layered ferroelectrics have various applications in smart materials and structures, such as micro-electro-mechanical systems (MEMS), ultrafast-switching room-temperature detectors, and ferroelectric random access memories [1,2]. Unfortunately, these attractive properties come with drawbacks. Cracks and flaws inevitably emerge on the interfaces of ferroelectric materials during manufacturing and serving [3]. Structural reliability concerns call for a better understanding of the fracture of bimaterial and layered ferroelectrics.

Classical routes of studying crack problems are along constructing field equations and solving corresponding boundary value problems directly (e.g., [4,5]). However, it is difficult to obtain exact solutions to ferroelectric interfacial crack problems owing to mathematic complexities. Conservation integrals provide a different way to obtain critical parameters governing the extension of cracks, which relate to clear physical concepts such as the energy release rate and require merely a contour integral far from the crack tip. Consequently, investigations on conservation integrals become a hotspot in past few decades. A comprehensive review is referred to Chen and Lu [6]. Fundamental methods of constructing conservation integrals can be classified into three categories:

(i) The first type is employing Noether's theorem. Noether [7] revealed the correspondence between conservation integrals and symmetry groups of a variational problem. Based on this cornerstone, Knowles and Sternberg [8] developed *J*-integral, *M*-integral and *L*-integral in linearized and finite elastostatics considering the invariance of the Lagrangian density under spatial infinitesimal transformations, while Fletcher [9] established conservation integrals in linear

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Nomenclature

a_{ijkl}, $\bar{a}_{ij}$, $\bar{\bar{a}}_{ijkl}$, $\bar{\bar{\bar{a}}}_{ijklmn}$, $\bar{\bar{\bar{\bar{a}}}}_{ijklmnrs}$, b_{ijkl}, c^{H}_{ijkl}, f_{ijklmn}, g_{ijklmn} coefficient tensors of electric enthalpy density
a_0, a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2, b_3, c_1, c_2, c_3, f_1, f_2, f_3, f_4, f_5, f_6, g_1, g_2, g_3 special coefficients of electric enthalpy density for tetragonal crystals
$A^{\mathrm{I}}_{\mathrm{fix}}$, $A^{\mathrm{II}}_{\mathrm{fix}}$ small fixed regions around the crack tip before the crack extends
$A^{\mathrm{I}}_{\mathrm{move}}$, $A^{\mathrm{II}}_{\mathrm{move}}$ small moving regions at the crack tip after the crack extends
D_i, E_i the electric displacement and the electric field
G energy release rate of the crack extension
h_{I}, h_{II} thickness of ferroelectric layer
h electric enthalpy density of ferroelectrics
$\tilde{h}$ electric enthalpy of the ferroelectric body
H electric enthalpy per unit thickness
$\tilde{J}_i$-vector revised *J*-integral vector for ferroelectrics
l length of crack extension
l_0 characteristic thickness of a domain wall
L crack length
$M_{i\bar{i}}$ coordinate transformation tensor
n_i normal vector to boundary surface
P_i $P_{i,j}$ electric polarization vector and its gradient
$\tilde{S}_{ik}$ energy-momentum tensor for ferroelectrics
r_Γ radius of integral contour
t normal tensile force
t_i surface traction vector
u_i mechanical displacement vector
(x_1, x_2, x_3) global Cartesian coordinate system
$(x_{\bar{1}}, x_{\bar{2}}, x_{\bar{3}})$ local Cartesian coordinate system
(X_1, X_2) a moving Cartesian coordinate system fixed at the crack tip
$(\theta, \varphi, \gamma)$ Euler angles
ψ Helmholtz free energy density for ferroelectrics
ϕ electric potential
σ_{ij}, ε_{ij} stress tensor and strain tensor
ξ_{ij}, η_i micro-forces
χ_i internal micro-force vector
ω electric surface charge density
ω_0 constant surface charge density to balance the normal component of the initial spontaneous polarization
ω_A electric surface charge increment
κ_0 dielectric permittivity of free space
Γ_ε,Γ'_ε the outward boundaries of $A^{\mathrm{I}}_{\mathrm{fix}} + A^{\mathrm{II}}_{\mathrm{fix}}$ and $A^{\mathrm{I}}_{\mathrm{move}} + A^{\mathrm{II}}_{\mathrm{move}}$
Φ_α,$\Sigma_{\alpha j}$ generalized displacement vector and generalized stress tensor
^{T} superscript denoting the transposition of a tensor
$^+$, $^-$ superscripts denoting the upper and the lower interfaces of the crack
$o(\,)$ higher order infinitesimal
$'$ superscript denoting the state after infinitesimal transformation

elastodynamics through a more general group of transformations. Olver [10] outlined general conditions for the existence of generalized symmetries in homogeneous elastostatic variational problems. Shi and Kuang [11] obtained conservation integrals for linear electro-magneto-elastic solids relying on similar manipulations.

(ii) The second type is from the energy–momentum tensor proposed by Eshelby [12] for linear or nonlinear elasticity, analogous to the Maxwell's stress tensor in electrostatics. Eischen and Herrmann [13] established conservation integrals by subjecting the Lagrangaian density to the gradient, curl, and divergence operations in space coordinates. Wang and Shen [14] derived conservation integrals and energy release rates in linear electro-magneto-elastostatics.

(iii) The third type is using Betti's reciprocal theorem. Bueckner [15] proposed a work conjugate integral based on Betti's reciprocal theorem, which are used to construct weight functions for calculating crack dominant parameters. *J*-integral and *M*-integral are merely two special cases of the work conjugate integral [16].

Conservation integrals for interfacial cracks in bimaterial and layered composites have also been widely studied. Specifically, *J*-integral constitutes a robust approach to determine critical parameters of interfacial crack problems. Atkinson [17] applied the *J*-integral to plane and anti-plane crack problems of quasi-static elastic layers through a specific integral contour. Using the two state integral [18] that is an important variant of *J*-integral, Yau and Wang [19] obtained the stress intensity