THREE-DIMENSIONAL CRACK ANALYSIS IN FERROELECTRICS USING CONFIGURATIONAL FORCES CONCEPT

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Summary The following paper presents the application of the configurational forces concept to the fracture mechanics analysis of ferroelectric ceramics. The underlying electromechanical boundary value problem is solved using finite element method. A micromechanical material model is implemented to simulate the non-linear ferroelectric and ferroelastic material behavior.

MICROMECHANICAL MATERIAL MODEL

The material model employed here is mainly based on works of Huber *et al* [1] and Pathak, McMeeking [2]. The idea of the model is to consider the ferroelectric polycrystal as an assembly of single crystals with specific lattice orientations. Each of the crystals consists of several domains with different spontaneous polarization directions. Assuming tetragonal material, as e.g. $BaTiO_3$ or PZT, eight domain variants are possible in three-dimensional space. The volume fractions of these domains can change if an electric field or mechanical stress is applied. This change is caused by domain switching and is determined in the model by an energy-based switching criterion. Due to switching the average polarization vector, the remanent strain and the average mechanical, electrical and piezoelectrical material properties of the crystal change, resulting in nonlinear macroscopic response. The material model is implemented in the commercial finite element software ABAQUS by means of a three-dimensional user element and a user material routine. The non-linear system of equations is solved in the usual way by Newton's iteration scheme.

CONFIGURATIONAL FORCES

The theory of configurational forces is based on ideas of Eshelby [3] and represents a very useful tool for analysing the thermodynamic driving energy on all kinds of defects in a material, such as voids, dislocations or cracks. The configurational force g_k can be derived as the negative divergence of the configurational stress tensor Σ_{kj}:

$$g_k = -\Sigma_{kj,j}. \tag{1}$$

The latter is given as:

$$\Sigma_{kj} = h\delta_{kj} - \sigma_{ij} u_{i,k} - D_j \varphi_{,k} \tag{2}$$

with the stresses σ_{ij}, the displacment vector u_i, the dielectric displacement D_i and the electric potential φ. Following [4] the electric enthalphy h is defined by:

$$h = \frac{1}{2}\sigma_{ij}\left(\varepsilon_{ij} - \varepsilon_{ij}^R\right) - \frac{1}{2}(D_i + P_i^R)E_i \tag{3}$$

considering the remanent strain ε_{ij}^R and polarization P_k^R. To calculate the configurational forces numerically within the finite element method, Eq. (1) is multiplied with a vectorial test function η_i and integrated over the domain B [5]:

$$\int_B \left(\Sigma_{kj,j} + g_k\right)\eta_i dV = 0. \tag{4}$$

Discretising the test function with nodal values and shape functions N^I leads to the definition of the discrete configurational forces at the nodes I of a finite element:

$$G_i^{eI} = \int_{V^e} N^I g_i dV = \int_{V^e} \Sigma_{ij} N_{,j}^I dV \tag{5}$$

with the volume of the finite element V^e. The second integral in Eq.(5) can be easily calculated using Eqs.(2) and (3). The total discrete configurational force at a node I consists of the contributions of all adjacent elements:

$$G_i^I = \bigcup_{e=1}^{n^{el}} G_i^{eI}. \tag{6}$$

APPLICATION TO FRACTURE MECHANICS

It is well known that the configurational forces and the J-integral of fracture mechanics are related. If the classical electromechanical line integral J is computed along an arbitrary contour Γ around the crack tip in a ferroelectric material

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it is found that J is not independent of the chosen path. This is obvious, since J includes not only the effect of the crack tip singularity but also the non-linear remanent strains and polarizations due to domain switching in the enclosed region. To separate both effects the integration contour is shrunk to the crack tip [6] yielding the near tip J-integral $\tilde{J}_k$:

$$\tilde{J}_k = \lim_{\varepsilon \to 0} \int_{\Gamma_\varepsilon} \Sigma_{kj} n_j ds. \tag{7}$$

It can be easily shown that $\tilde{J}_k$ corresponds to the configurational force acting at the very crack tip node. Considering a three-dimensional crack front it is finally found:

$$J_{tip} = \tilde{J}_k^I m_k = -\frac{G_k^{tipI}}{l_c^I} m_k \tag{8}$$

with the unit vector m_k lying in the crack plane and perpendicular to the crack front and l_c^I being the length of a crack front segment assigned to the crack front node I. By these considerations the dissipative processes in the switching domain are separated from the real crack driving force.

NUMERICAL EXAMPLE

The configurational forces are used to calculate the J-integral of a part-through crack in a finite plate under cyclic loading by a perpendicular electric field. The results of two nodes at the crack front are shown in Fig.1. Applying the electrical load, the J-integral becomes negativ first. When the coercive field strength E_c is reached domain switching occurs, which has a strong influence on the J-integral. After unloading the remanent strain and polarization remain in the body, leading to a positive value of J. This means the residual fields yield a positive crack driving force. The behavior is qualitatively the same for both considered nodes. However, the domain switching processes are different in the regions at the two nodes due to the random distribution of lattice orientations in the model, influencing the crack driving force along the crack tip.

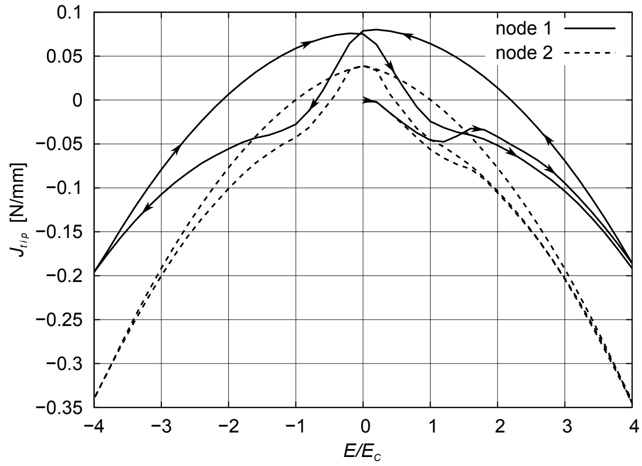

Figure 1. J-integral of a 3D part-through crack under cyclic electrical loading

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