

# A New Finite Element Formulation for Electromechanics

Chad M. Landis\*

Rice University, Department of Mechanical Engineering and Materials Science

## ABSTRACT

A new finite element formulation for the solution of electromechanical boundary value problems is presented. As opposed to the standard formulation that utilizes a scalar electric potential as nodal variables, this new formulation implements a vector potential from which components of electric displacement are derived. For linear piezoelectric materials with positive definite material moduli, the resulting finite element stiffness matrix from the vector potential formulation is also positive definite. If the material is nonlinear in a fashion characteristic of ferroelectric materials, it is demonstrated that a straightforward iterative solution procedure is unstable for the standard scalar potential formulation, but stable for the new vector potential formulation. Finally, the method is used to compute fields around a crack tip in an idealized non-linear ferroelectric material, and results are compared to an analytical solution.

Keywords: finite element method, vector potential, piezoelectricity, ferroelectricity

## 1. INTRODUCTION

Since the original work of Allik and Hughes [1] in 1970, a rather larger literature has developed on finite element methods for linear piezoelectric materials and structures [2]. However, much less attention has focused on problems involving non-linear electromechanical constitutive response, with the exception of the work of Ghandi and Hagood [3]. It will be demonstrated in Section 4 of this paper, that difficulties arise in the solution of electrically non-linear problems when the standard, scalar potential, finite element formulation developed in [1] is used. In order to overcome these difficulties, Ghandi and Hagood [3] developed a hybrid finite element formulation that employs the standard displacement and electric potential nodal degrees of freedom along with additional electric displacement degrees of freedom within the element. In this work, an alternative approach that implements a vector potential formulation is developed.

As opposed to the standard scalar potential formulation, where the electric potential is interpolated from nodal quantities and the electric field derived from the electric potential; the vector potential formulation derives the *electric displacement* from the components of the vector potential which are the interpolated nodal quantities. Advantages of the vector potential formulation include a positive definite stiffness matrix and stability for non-linear electrical material behavior characteristic of ferroelectric ceramics. The disadvantages of the method include an increase in the number of nodal degrees of freedom for three-dimensional problems and the inability of the method to account for a free charge density within the material volume.

The body of the paper is concerned with comparing the scalar and vector potential formulations. Section 2 is devoted to introducing the equations governing a dynamic electromechanical boundary value problem. Section 3 develops the scalar and vector potential formulations, and then compares features of the stiffness matrices and system sizes. Section 4 presents a simple numerical stability analysis of the two formulations for a one-dimensional electrical system with non-linear material behavior. Section 5 implements the vector potential formulation to solve for the electrical fields around a crack tip in an idealized ferroelectric material, and compares the numerical results to a known analytical solution. Finally, Section 6 summarizes the merits of the new vector potential formulation for the solution of non-linear electromechanical boundary value problems.

## 2. GOVERNING EQUATIONS

In this section the equations governing a small deformation, small electric field, mechanically dynamic but electrically quasi-static, isothermal electromechanical boundary value problem will be reviewed. Throughout this section standard Einstein notation is utilized with summation implied over repeated indices.

Consider a volume of material,  $V$ , bounded by the surface,  $S$ . Newton's second law is given by

$$\sigma_{ji,j} + b_i = \rho \ddot{u}_i \text{ in } V \quad (2.1)$$

and

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\* landis@rice.edu, phone 713-348-3609, fax 713-348-5423,

MEMS MS 321, Rice University PO Box 1892, Houston, TX 77251-1892

$$\sigma_{ji}n_j = t_i \text{ on } S. \quad (2.2)$$

Where  $\sigma_{ij}$  is the symmetric Cauchy stress tensor,  $b_i$  is the body force in the volume,  $\rho$  is the mass density of the material,  $u_i$  are the components of the material displacement,  $n_i$  is a unit vector normal to the surface directed outward from the volume, and  $t_i$  is the traction applied to the surface. The superposed double dot represents a second derivative with respect to time.

The infinitesimal strain-displacement compatibility conditions are

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}), \quad (2.3)$$

where  $\varepsilon_{ij}$  is the infinitesimal strain tensor.

Gauss' law is written as

$$D_{i,i} = q^v \text{ in } V \quad (2.4)$$

and

$$D_i n_i = -q^s \text{ on } S. \quad (2.5)$$

Where  $D_i$  is the electric displacement,  $q^v$  is the free charge per unit volume in  $V$  and  $q^s$  is the free charge per unit area (also accounting for the effective charge due to material outside of  $V$ ) residing on  $S$ .

Under quasi-static conditions the electric field,  $E_i$ , can be written as the gradient of a potential,  $\phi$ , such that

$$E_i = -\phi_{,i}. \quad (2.6)$$

Finally, the four forms of the linear piezoelectric constitutive law about a fixed remanent strain and polarization state are given by

$$\varepsilon_{ij} - \varepsilon_{ij}^r = s_{ijkl}^E \sigma_{kl} + d_{kij} E_k, \quad D_i - P_i^r = d_{ikl} \sigma_{kl} + \kappa_{ij}^\sigma E_j \quad (2.7)$$

$$\sigma_{ij} = c_{ijkl}^E (\varepsilon_{kl} - \varepsilon_{kl}^r) - e_{kij} E_k, \quad D_i - P_i^r = e_{ikl} (\varepsilon_{kl} - \varepsilon_{kl}^r) + \kappa_{ij}^\varepsilon E_j \quad (2.8)$$

$$\sigma_{ij} = c_{ijkl}^D (\varepsilon_{kl} - \varepsilon_{kl}^r) - h_{kij} (D_k - P_k^r), \quad E_i = -h_{ikl} (\varepsilon_{kl} - \varepsilon_{kl}^r) + \beta_{ij}^\varepsilon (D_j - P_j^r) \quad (2.9)$$

$$\varepsilon_{ij} - \varepsilon_{ij}^r = s_{ijkl}^D \sigma_{kl} + g_{kij} (D_k - P_k^r), \quad E_i = -g_{ikl} \sigma_{kl} + \beta_{ij}^\sigma (D_j - P_j^r), \quad (2.10)$$

where  $\varepsilon_{ij}^r$  and  $P_i^r$  are the remanent strain and polarization,  $s_{ijkl}^E$ ,  $s_{ijkl}^D$ ,  $c_{ijkl}^E$  and  $c_{ijkl}^D$  are fourth order tensors of elasticity,  $d_{kij}$ ,  $e_{kij}$ ,  $h_{kij}$  and  $g_{kij}$  are third order tensors of piezoelectricity and  $\kappa_{ij}^\sigma$ ,  $\kappa_{ij}^\varepsilon$ ,  $\beta_{ij}^\sigma$  and  $\beta_{ij}^\varepsilon$  are second order dielectric tensors. Note that any set of moduli can be manipulated algebraically to yield any other set. The constitutive form of Eqn. (2.7) is commonly used to report experimentally measured moduli, that of Eqn. (2.8) is required for the standard scalar potential finite element formulation, and the form in Eqn. (2.9) will be used in the vector potential finite element formulation.

Finally, Eqns. (2.1) – (2.6) can be written in the following two weak forms as

$$\int_V \rho \ddot{u}_i \delta u_i dV + \int_V \sigma_{ij} \delta \varepsilon_{ij} - D_i \delta E_i dV = \int_V b_i \delta u_i - q^v \delta \phi dV + \int_S t_i \delta u_i - q^s \delta \phi dS \quad (2.11)$$

or

$$\int_V \rho \ddot{u}_i \delta u_i dV + \int_V \sigma_{ij} \delta \varepsilon_{ij} + E_i \delta D_i dV = \int_V b_i \delta u_i + \phi \delta q^v dV + \int_S t_i \delta u_i + \phi \delta q^s dS. \quad (2.12)$$

### 3. FINITE ELEMENT FORMULATIONS

In the following formulations vector-matrix notation will be used where the field quantities are given as

$$\begin{aligned} \{\mathbf{u}\} &= \{u_x \quad u_y \quad u_z\}^T, \quad \{\mathbf{E}\} = \{E_x \quad E_y \quad E_z\}^T, \quad \{\mathbf{D}\} = \{D_x \quad D_y \quad D_z\}^T, \\ \{\boldsymbol{\varepsilon}\} &= \{\varepsilon_{xx} \quad \varepsilon_{yy} \quad \varepsilon_{zz} \quad 2\varepsilon_{yz} \quad 2\varepsilon_{xz} \quad 2\varepsilon_{xy}\}^T, \quad \{\boldsymbol{\sigma}\} = \{\sigma_{xx} \quad \sigma_{yy} \quad \sigma_{zz} \quad \sigma_{yz} \quad \sigma_{xz} \quad \sigma_{xy}\}^T, \end{aligned} \quad (3.1)$$

et cetera, and the nodal quantities will be represented by  $\{\mathbf{u}^n\}$  and  $\{\boldsymbol{\phi}^n\}$ . Eqns. (2.8) and (2.9) are then written in matrix form as

$$\{\boldsymbol{\sigma}\} = [\mathbf{c}^E] (\{\boldsymbol{\varepsilon}\} - \{\boldsymbol{\varepsilon}^r\}) - [\mathbf{e}] \{\mathbf{E}\}, \quad \{\mathbf{D}\} = [\mathbf{e}]^T (\{\boldsymbol{\varepsilon}\} - \{\boldsymbol{\varepsilon}^r\}) + [\boldsymbol{\kappa}^E] \{\mathbf{E}\} + \{\mathbf{P}^r\} \quad (3.2)$$

and

$$\{\boldsymbol{\sigma}\} = [\mathbf{c}^D] (\{\boldsymbol{\varepsilon}\} - \{\boldsymbol{\varepsilon}^r\}) - [\mathbf{h}] (\{\mathbf{D}\} - \{\mathbf{P}^r\}), \quad \{\mathbf{E}\} = -[\mathbf{h}]^T (\{\boldsymbol{\varepsilon}\} - \{\boldsymbol{\varepsilon}^r\}) + [\boldsymbol{\beta}^E] (\{\mathbf{D}\} - \{\mathbf{P}^r\}). \quad (3.3)$$

#### THE STANDARD SCALAR POTENTIAL FORMULATION

As noted by Alik and Hughes [1] the standard formulation exploits the similarities in the mathematical structure, Eqns. (2.1) – (2.6), governing the distributions of electrical and mechanical fields. In the standard scalar potential formulation the displacements and the electric potential are interpolated from the associated nodal quantities as

$$\{\mathbf{u}\} = [\mathbf{N}^u] \{\mathbf{u}^n\} \quad \text{and} \quad \phi = [\mathbf{N}^\phi] \{\boldsymbol{\phi}^n\}. \quad (3.4)$$

The strains and electric field components can then be derived from the nodal variables as

$$\{\boldsymbol{\varepsilon}\} = [\mathbf{B}^u] \{\mathbf{u}^n\} \quad \text{and} \quad \{\mathbf{E}\} = -[\mathbf{B}^\phi] \{\boldsymbol{\phi}^n\}. \quad (3.5)$$

The matrices  $[\mathbf{B}^u]$  and  $[\mathbf{B}^\phi]$  are given as

$$[\mathbf{B}^u] = \begin{bmatrix} \partial_x & 0 & 0 \\ 0 & \partial_y & 0 \\ 0 & 0 & \partial_z \\ 0 & \partial_z & \partial_y \\ \partial_z & 0 & \partial_x \\ \partial_y & \partial_x & 0 \end{bmatrix} [\mathbf{N}^u] \quad \text{and} \quad [\mathbf{B}^\phi] = \begin{bmatrix} \partial_x \\ \partial_y \\ \partial_z \end{bmatrix} [\mathbf{N}^\phi], \quad (3.6)$$

where  $\partial_i$  represents partial differentiation with respect to the  $i$  coordinate direction. Eqn. (2.11) then yields the finite element equations

$$\begin{aligned} [\mathbf{m}] \{\ddot{\mathbf{u}}^n\} + [\mathbf{K}^{uu}] \{\mathbf{u}^n\} + [\mathbf{K}^{u\phi}] \{\boldsymbol{\phi}^n\} &= \int_V [\mathbf{B}^u]^T \{\boldsymbol{\sigma}^r\} dV + \int_V [\mathbf{N}^u]^T \{\mathbf{b}\} dV + \int_S [\mathbf{N}^u]^T \{\mathbf{t}\} dS \\ [\mathbf{K}^{\phi u}] \{\mathbf{u}^n\} + [\mathbf{K}^{\phi\phi}] \{\boldsymbol{\phi}^n\} &= -\int_V [\mathbf{B}^\phi]^T \{\mathbf{D}^r\} dV - \int_V [\mathbf{N}^\phi]^T q^v dV - \int_S [\mathbf{N}^\phi]^T q^s dS \end{aligned} \quad (3.7)$$

where

$$\begin{aligned} [\mathbf{K}^{uu}] &= \int_V [\mathbf{B}^u]^T [\mathbf{c}^E] [\mathbf{B}^u] dV, \quad [\mathbf{K}^{u\phi}] = \int_V [\mathbf{B}^u]^T [\mathbf{e}] [\mathbf{B}^\phi] dV, \\ [\mathbf{K}^{\phi u}] &= \int_V [\mathbf{B}^\phi]^T [\mathbf{e}]^T [\mathbf{B}^u] dV, \quad [\mathbf{K}^{\phi\phi}] = -\int_V [\mathbf{B}^\phi]^T [\boldsymbol{\kappa}^E] [\mathbf{B}^\phi] dV, \\ [\mathbf{m}] &= \int_V [\mathbf{N}^u]^T \rho [\mathbf{N}^u] dV, \end{aligned} \quad (3.8)$$

and

$$\begin{aligned} \{\boldsymbol{\sigma}^r\} &= [\mathbf{c}^E] \{\boldsymbol{\epsilon}^r\} \\ \{\mathbf{D}^r\} &= -[\mathbf{e}]^T \{\boldsymbol{\epsilon}^r\} + \{\mathbf{P}^r\} \end{aligned} \quad (3.9)$$

Eqns. (3.7) represent the standard finite element formulation for piezoelectric solids. Note that usually the first terms associated with the remanent state on the right-hand sides of Eqns. (3.7) are taken to be zero. It is physically reasonable to assume that the remanent strain is equal to zero as long as it does not change. However, a similar treatment of the remanent polarization is not suitable unless the electrical boundary conditions are adjusted appropriately.

### VECTOR POTENTIAL FORMULATION

As opposed to the scalar potential formulation, the vector potential formulation exploits the similarities in the constitutive (i.e. thermodynamic) structure, Eqn. (2.9), between the electrical and mechanical variables. The vector potential formulation is restricted to problems where the free charge density in the volume is equal to zero. In other words Eqn. (2.4) is re-written as

$$D_{i,i} = 0 \text{ in } V. \quad (3.10)$$

Then Eqn. (3.10) can automatically be satisfied by the vector potential,  $\psi_i$ , if

$$D_i = \epsilon_{ijk} \psi_{j,k}, \quad (3.11)$$

where  $\epsilon_{ijk}$  is the permutation tensor. Now, the nodal degrees of freedom consist of the three displacements and the three components of the vector potential. The vector potential field will be represented by  $\{\boldsymbol{\psi}\}$  and the associated nodal quantities by  $\{\boldsymbol{\psi}^n\}$ . Along with the weak form of Eqn. (2.12), the following interpolations are the foundation of the formulation,

$$\{\mathbf{u}\} = [\mathbf{N}^u] \{\mathbf{u}^n\} \text{ and } \{\boldsymbol{\psi}\} = [\mathbf{N}^\psi] \{\boldsymbol{\psi}^n\}. \quad (3.12)$$

Then the strains and electric displacement components are derived from the displacements and the vector potential as

$$\{\boldsymbol{\epsilon}\} = [\mathbf{B}^u] \{\mathbf{u}^n\} \text{ and } \{\mathbf{D}\} = [\mathbf{B}^\psi] \{\boldsymbol{\psi}^n\}. \quad (3.13)$$

The matrix  $[\mathbf{B}^u]$  was defined in Eqn. (3.6) and  $[\mathbf{B}^\psi]$  is given as

$$[\mathbf{B}^\psi] = \begin{bmatrix} 0 & \partial_z & -\partial_y \\ -\partial_z & 0 & \partial_x \\ \partial_y & -\partial_x & 0 \end{bmatrix} [\mathbf{N}^\psi]. \quad (3.14)$$

Eqn. (2.12) then yields the finite element equations

$$\begin{aligned} [\mathbf{m}] \{\ddot{\mathbf{u}}^n\} + [\mathbf{K}^{uu}] \{\mathbf{u}^n\} + [\mathbf{K}^{u\psi}] \{\boldsymbol{\psi}^n\} &= \int_V [\mathbf{B}^u]^T \{\boldsymbol{\sigma}^r\} dV + \int_V [\mathbf{N}^u]^T \{\mathbf{b}\} dV + \int_S [\mathbf{N}^u]^T \{\mathbf{t}\} dS \\ [\mathbf{K}^{\psi u}] \{\mathbf{u}^n\} + [\mathbf{K}^{\psi\psi}] \{\boldsymbol{\psi}^n\} &= \int_V [\mathbf{B}^\psi]^T \{\mathbf{E}^r\} dV - \int_S [\mathbf{B}^\psi]^T \phi \{\mathbf{n}\} dS \end{aligned} \quad (3.15)$$

where

$$\begin{aligned}
[\mathbf{K}^{uu}] &= \int_V [\mathbf{B}^u]^T [\mathbf{c}^D] [\mathbf{B}^u] dV, \quad [\mathbf{K}^{u\psi}] = -\int_V [\mathbf{B}^u]^T [\mathbf{h}] [\mathbf{B}^\psi] dV, \\
[\mathbf{K}^{\psi u}] &= -\int_V [\mathbf{B}^\psi]^T [\mathbf{h}]^T [\mathbf{B}^u] dV, \quad [\mathbf{K}^{\psi\psi}] = \int_V [\mathbf{B}^\psi]^T [\boldsymbol{\beta}^\epsilon] [\mathbf{B}^\psi] dV, \\
[\mathbf{m}] &= \int_V [\mathbf{N}^u]^T \rho [\mathbf{N}^u] dV,
\end{aligned} \tag{3.16}$$

and

$$\begin{aligned}
\{\boldsymbol{\sigma}^r\} &= [\mathbf{c}^D] \{\boldsymbol{\epsilon}^r\} - [\mathbf{h}] \{\mathbf{P}^r\} \\
\{\mathbf{E}^r\} &= -[\mathbf{h}]^T \{\boldsymbol{\epsilon}^r\} + [\boldsymbol{\beta}^\epsilon] \{\mathbf{P}^r\}.
\end{aligned} \tag{3.17}$$

Note that  $\{\mathbf{n}\}$  represents the unit vector normal to the surface  $S$ . Also note that  $[\mathbf{K}^{uu}]$  and  $\{\boldsymbol{\sigma}^r\}$  defined in Eqns. (3.16) and (3.17) are different from those defined in Eqns. (3.8) and (3.9). Any possible confusion can be avoided by noting the other matrices and vectors that  $[\mathbf{K}^{uu}]$  and  $\{\boldsymbol{\sigma}^r\}$  are grouped with.

### STIFFNESS MATRIX CHARACTERISTICS

For the solution of Eqns. (3.7) or (3.16) it is useful to know if the stiffness matrix is symmetric and if it is positive definite or non-definite. First note that the total stiffness matrices,  $\begin{bmatrix} [\mathbf{K}^{uu}] & [\mathbf{K}^{u\phi}] \\ [\mathbf{K}^{\phi u}] & [\mathbf{K}^{\phi\phi}] \end{bmatrix}$  from the standard formulation and

$\begin{bmatrix} [\mathbf{K}^{uu}] & [\mathbf{K}^{u\psi}] \\ [\mathbf{K}^{\psi u}] & [\mathbf{K}^{\psi\psi}] \end{bmatrix}$  from the vector potential formulation, are both symmetric. Note that the symmetry of the stiffness matrix

for the scalar potential formulation is dependent upon the minus sign appearing in front of the  $D_i \delta E_i$  term in the weak form of Eqn. (2.11).

Now let us define a stable piezoelectric material as one in which the material stiffness matrix  $\begin{bmatrix} [\mathbf{c}^D] & -[\mathbf{h}] \\ -[\mathbf{h}]^T & [\boldsymbol{\beta}^\epsilon] \end{bmatrix}$  is positive

definite. A material with positive definite stiffness requires a positive amount of work to be done on it in order to change the strain or electric displacement from the stress and electric field free state. In other words, the stored internal energy density of the material

$$\begin{aligned}
U &= \frac{1}{2} \left( \{\boldsymbol{\epsilon}\}^T - \{\boldsymbol{\epsilon}^r\}^T \right) [\mathbf{c}^D] \left( \{\boldsymbol{\epsilon}\} - \{\boldsymbol{\epsilon}^r\} \right) \\
&\quad - \left( \{\boldsymbol{\epsilon}\}^T - \{\boldsymbol{\epsilon}^r\}^T \right) [\mathbf{h}] \left( \{\mathbf{D}\} - \{\mathbf{P}^r\} \right) \\
&\quad + \frac{1}{2} \left( \{\mathbf{D}\}^T - \{\mathbf{P}^r\}^T \right) [\boldsymbol{\beta}^\epsilon] \left( \{\mathbf{D}\} - \{\mathbf{P}^r\} \right)
\end{aligned} \tag{3.18}$$

is greater than zero for any strain and electric displacement combination not equal to the remanent state. Hence, when the material stiffness is positive definite, it can be readily shown that the stiffness matrix for the vector potential formulation,

$\begin{bmatrix} [\mathbf{K}^{uu}] & [\mathbf{K}^{u\psi}] \\ [\mathbf{K}^{\psi u}] & [\mathbf{K}^{\psi\psi}] \end{bmatrix}$ , is also positive definite. However,  $\begin{bmatrix} [\mathbf{K}^{uu}] & [\mathbf{K}^{u\phi}] \\ [\mathbf{K}^{\phi u}] & [\mathbf{K}^{\phi\phi}] \end{bmatrix}$ , the stiffness matrix for the scalar potential

formulation, is non-definite. Therefore, solutions to boundary value problems using the vector potential formulation exist at a global minimum in nodal degree of freedom space, while solutions for the scalar potential formulation lie on a saddle point. Furthermore, the positive definiteness of the stiffness matrix for the vector potential formulation lends itself to efficient iterative solution techniques like the conjugate gradient method [4].

## SYSTEM SIZE

It is of interest to note that for the full three-dimensional case, the standard scalar potential formulation requires four degrees of freedom per node, three displacements and the electric potential. Unfortunately, the vector potential formulation requires six degrees of freedom per node, three displacements and three components of the vector potential. Hence, an increase in the size of the matrix system to be solved, by twice the number of nodes, is required for three-dimensional problems with the vector potential formulation.

Fortunately, the increase in system size from the scalar to the vector potential formulations in three dimensions does not exist in two dimensions. The nodal degrees of freedom required for in-plane, two-dimensional problems with the scalar and vector potential formulations are  $\{u_x \ u_y \ \phi\}$  and  $\{u_x \ u_y \ \psi_z\}$  respectively. Hence, the system sizes for two-dimensional problems are the same for both formulations.

## 4. NUMERICAL STABILITY FOR NON-LINEAR ELECTRICAL PROBLEMS

To this point it has been assumed that the remanent strain and polarization states remain fixed, and the problem is linear. However, the primary reason for introducing the vector potential formulation is due to its stability for solving non-linear problems. Specifically, the vector potential formulation is most useful when the electric field versus electric displacement relationship is characteristic of ferroelectric ceramics. To investigate the effectiveness of the scalar and vector potential formulations for solving non-linear electrical problems, the stability of a simple, fixed-point, iterative solution scheme for a single degree of freedom electrical system will be determined. The non-linear constitutive law used for this problem is highly simplified, but it does contain the essential feature of ferroelectric behavior required to understand the stability of the two numerical methods.

Consider the non-linear electrical constitutive relationship given by

$$\begin{aligned} D &= \kappa E, \quad P^r = 0 \quad \text{if } E \leq E_0 \\ D &= \kappa E + P^r, \quad P^r = (H - \kappa)(E - E_0) \quad \text{if } E \geq E_0 \end{aligned} \quad (4.1)$$

where  $E_0$  is the coercive field, and the hardening modulus,  $H$ , is greater than the initial dielectric permittivity  $\kappa$  for ferroelectric materials. For the scalar potential formulation, the single degree of freedom system considered is a one-dimensional capacitor with the electric displacement fixed across it. The proposed iterative solution procedure is given by,

$$E^{i+1} = \frac{1}{\kappa} (D - P^{r,i}), \quad (4.2)$$

where  $D$  is the fixed electric displacement,  $E^{i+1}$  is the electric field computed at the  $i+1$ th iteration, and  $P^{r,i}$  is the remanent polarization computed from Eqn. (4.1) after the  $i$ th solution step. Then, for levels of electric field greater than the coercive field, Eqn. (4.1) can be used in (4.2) to yield

$$E^{i+1} = \left(1 - \frac{H}{\kappa}\right) E^i + \frac{1}{\kappa} D - \left(1 - \frac{H}{\kappa}\right) E_0. \quad (4.3)$$

From Eqn. (4.3) it can be readily seen that this iterative method is unstable if  $H/\kappa > 2$ , and the solution for  $E$  oscillates if  $H/\kappa > 1$ . For most ferroelectric materials of technological interest  $H/\kappa > 2$ , and this solution method will be unstable.

The analogous single degree of freedom system for the vector potential formulation has the applied electric field fixed across the one-dimensional capacitor. The iterative scheme analogous to Eqn. (4.2) is

$$D^{i+1} = \kappa E + P^{r,i}, \quad (4.4)$$

implying that

$$D^{i+1} = \kappa E_0 + H(E - E_0). \quad (4.5)$$

Notice that Eqn. (4.5) will converge to the exact solution after two iterations, i.e. the first iteration will predict that  $D^1 = \kappa E$  and then the second will reach the exact solution given by Eqn. (4.5).

It is true that a more sophisticated iterative solution scheme, such as a Newton-Raphson method, could provide a solution for the scalar potential formulation. However, for certain problems, the scheme represented by Eqn. (4.3) is the only one available. For example, many authors have relied on this procedure to solve for the fields around a steadily growing crack in a material with a path dependent constitutive behavior, see for example [5]. Furthermore, this simple iterative solution procedure requires only one inversion of the system stiffness matrix, while Newton-Raphson methods require an inversion at each step. Hence, for some problems this solution method is the only scheme available, and for some problems this method can provide a savings in computational time.

## 5. COMPARISON OF A CALCULATED CRACK TIP FIELD TO AN ANALYTICAL SOLUTION

In this section the vector potential formulation is demonstrated for a non-linear electrical problem with a known analytical solution. The physical problem is to determine the distributions of electric field and electric displacement very close to a crack tip with an electrically conducting medium in the space between the crack faces. A simple semi-circular radial mesh is used for this problem. The mesh contains 1926 nodes and 625 8-noded isoparametric elements with 4 integration stations each. Every node has one degree of freedom,  $\psi_z$ , associated with it. The mesh and the boundary conditions are shown in Figure 1.

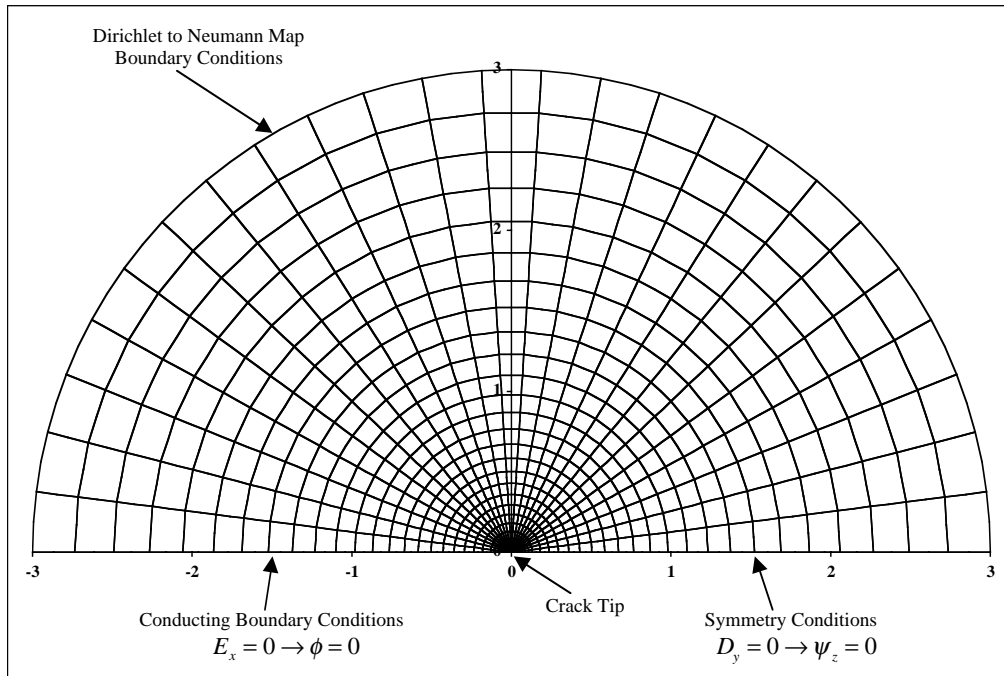


Figure 1. The finite element mesh used for the solution of the electrical fields around a crack tip. The mesh consists of 1926 nodes and 625 8-noded isoparametric elements. Conducting boundary conditions are applied to the crack surface and symmetry conditions are applied ahead of the crack tip. A so-called Dirichlet to Neumann map is applied to the outer circular boundary to account for material outside of the mesh and the far field loading conditions. The coordinate axes are normalized by the size of the non-linear switching region  $R_s$ .

The coordinate axes are normalized by the size of the non-linear switching zone,  $R_s$ . Note that a Dirichlet to Neumann map [6] is applied to the outer circular boundary in order to simulate the appropriate asymptotic crack tip conditions and the response of the material outside of the mesh. The far field solution and the size of the switching zone are given by

$$\psi_z \rightarrow \kappa K_E \sqrt{\frac{2}{\pi}} \operatorname{Im}[(x + iy)^{1/2}] \quad \text{as } |x + iy| \rightarrow \infty \quad (5.1)$$

and

$$R_s = \frac{1}{2\pi} \left( \frac{K_E}{E_0} \right)^2, \quad (5.2)$$

where  $\kappa$  is the dielectric permittivity,  $K_E$  is an electrical intensity factor, and  $E_0$  is the coercive field.

A simple constitutive law is assumed where the electric displacement is always aligned with the electric field. The relationship between the magnitude of the electric field,  $E$ , and the magnitude of the electric displacement,  $D$ , is specified by

$$E = \begin{cases} D/\kappa & \text{if } D < D_0 \\ E_0 & \text{if } D_0 \leq D \leq D_L, \\ E_0 + (D - D_L)/\kappa & \text{if } D > D_L \end{cases}, \quad (5.3)$$

where  $D_0 = \kappa E_0$ . This constitutive law is shown schematically on the inset in Figure 2. The variational form of the procedure used to solve this non-linear problem, analogous to Eqn. (3.15), is given by

$$\int_V \frac{1}{\kappa} D_i \delta D_i dV = \int_V \frac{1}{\kappa} P_i^r \delta D_i dV - \int_S \phi n_i \delta D_i dS. \quad (5.4)$$

The left-hand side yields the stiffness matrix dotted with the vector of unknown nodal degrees of freedom. The second term on the right hand side produces a nodal driving potential vector along with contributions to the stiffness arising from the Dirichlet to Neumann map. Finally, the first term on the right-hand side accounts for the material non-linearity, with the remanent polarization evaluated from the solution to the previous iteration. Note that the remanent polarization is in the direction of the applied electric field, and its magnitude can be derived from Eqn. (5.3) as

$$P^r = \begin{cases} 0 & \text{if } D < D_0 \\ D - D_0 & \text{if } D_0 \leq D \leq D_L. \\ D_L - D_0 & \text{if } D > D_L \end{cases}. \quad (5.5)$$

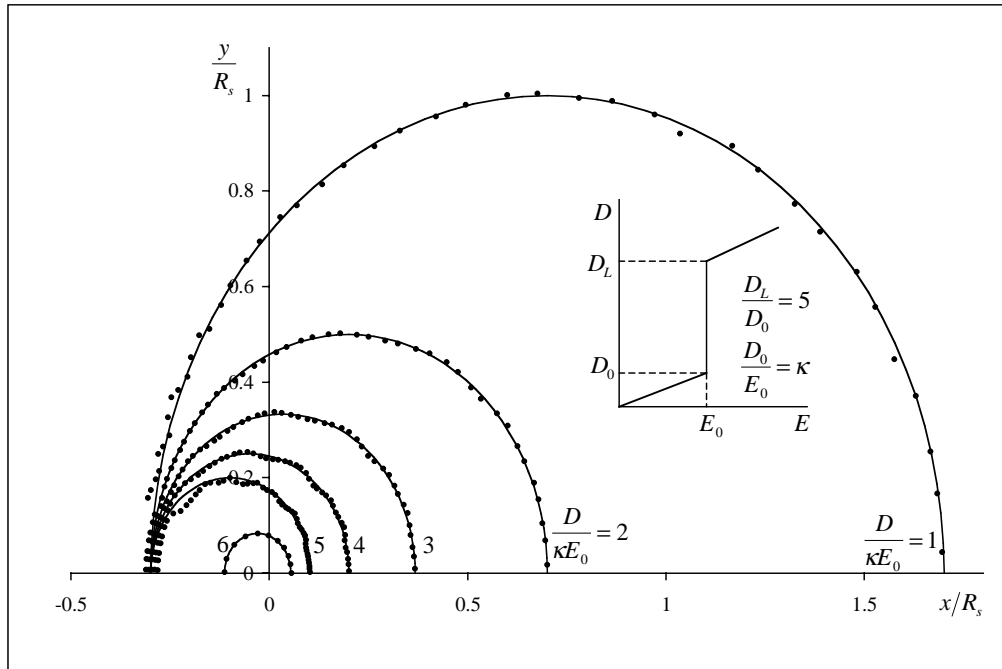


Figure 2. Contours of constant electric displacement magnitude near the crack tip. The dots represent the numerical finite element results and the curves are the analytical solution from [7]. The inset is a schematic of the non-linear material constitutive law used for the calculation. Notice that very large gradients of electric displacement occur at the left edge of the switching zone.

For the example shown in Figure 2 the ratio of  $D_L/D_0$  was taken to be equal to 5. The iterative procedure was allowed to proceed for 2000 steps, with the entire calculation taking approximately 5 minutes on a Silicon Graphics O2000 workstation. Figure 2 plots contours of constant electric displacement magnitude from the results of the numerical calculation (dots interpolated from the nearest integration stations) against the analytical solution (lines) obtained by Landis [7]. To monitor the convergence of the solution scheme, the sum over all nodes, of the square of the difference between  $\psi_z$  at the current step and  $\psi_z$  at the previous iteration was computed. This quantity obtained values of  $10^{-3}$ ,  $10^{-6}$ ,  $10^{-9}$ ,  $10^{-12}$ , and  $10^{-14}$  after 13, 50, 168, 654 and 1857 iterations respectively. Note that a similar solution procedure was attempted for this problem with a scalar potential formulation; however, convergence was not achieved, as predicted by the analysis of Section 4.

## 6. CONCLUDING REMARKS

A new finite element formulation for the solution of electromechanical boundary value problems, based on an electrical vector potential has been developed. The method requires 2 extra degrees of freedom per node over the standard formulation for three-dimensional problems, and it cannot be used for problems where a volumetric free charge density must be considered. However, the method yields a positive definite stiffness matrix for stable electromechanical materials, and it exhibits superior numerical stability over the standard formulation for non-linear electrical problems. Furthermore, for two-dimensional problems, the vector potential formulation yields the same number of degrees of freedom per node as the scalar potential formulation.

The formulations presented in Section 3 are sufficiently general. Specific forms for the interpolation functions in Eqns. (3.4) and (3.12) and for the non-linear description of the remanent state of the material were not given. Appropriate forms of the interpolation functions required to ensure spatial convergence of the solution can be found in many texts, e.g. [8], and forms for the constitutive law describing the evolution of the remanent state are given in [9]. Lastly, the new vector potential formulation provides a numerical tool for the investigation of electromechanical fields in structures like the piezoelectric stack actuator, and around structural features like electrodes and crack tips.

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