Numerical analysis of PZT-Polymer composites using pb-3 Ritz method

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Abstract

An energy based formulation of piezocomposites and a general 3-dimensional Ritz method for the analysis of piezocomposite solids of arbitrary shape and arbitrary width to thickness ratio are developed. The displacement fields and the electric potential function are approximated using special base functions, which satisfy boundary conditions through pb-3 method. Furthermore, an innovative remedy will be given to treat the problem of the discontinuities in strain fields and in electric displacement across the interfaces. An important feature of the present method is that, it can be used to analyze arbitrary shaped piezoelectric plates with high accuracy without the need of mesh generations and hence eliminating its associated difficulties. The accuracy of the present analysis for some numerical experiments will be verified by comparison with the exact solutions. Effects of the amending terms accounting for the discontinuous nature of the strain fields and electric displacement across the interfaces, on the accuracy and convergence rate of the results are demonstrated.

1 Introduction

Piezoelectric composites have been used as ideal materials in some electromechanical devices in the last few decades (for example, see Pohanka and Smith [1] or Crawly [2]). Such usage are inspired by their excellent dual electromechanical behavior, where in their different applications they generate an electric field when subjected to stress (strain), and vice versa. When used as sensors, the most critical issue is formation of different shapes of faults and
micro defects [3] during the early stages of their service life as a result of their fragileness.

Many of the electromechanical devices are often constructed in the form of multilayer plates or shells. Hence, general solutions for solids consisting of piezoelectric and non-piezoelectric layers are of practical importance. Different analytical solutions of multi-layer elastic plates have been obtained by many researchers, e.g. see [4]. These solutions have revealed the weaknesses of the classic thick plate solutions and are used to assess the preciseness of the approximate multi-layer plate solutions. Recently, some of these methods have been used for multi-layer plates containing piezoelectric layers. The exact distribution of stresses, strains and electric field through the material are obtained in response to a static sinusoidal loading or voltaging of surfaces. A general solution for arbitrary loading will contain complicated processes of Fourier series transform and summing up of sinusoidal series ([5], [6] and [7]).

In this paper, pb-3 Ritz method is introduced, which is the classic Ritz method solution of deformations using pb-3 Ritz functions. These are 3-dimensional polynomials and are the product of a boundary base function (b) and a general 3-dimensional polynomial (p-3). Base polynomial is the product of powers 0, 1, or 2 of boundary geometry functions to indicate free, simply-supported, or clamped edges respectively. Employing the pb-3 Ritz functions and the minimum potential energy principal, the solution procedure can easily be casted in algorithmic form. This method has the advantage to the finite element method in the way that there is no need for mesh generation. Furthermore, the need to large memories due to large number of unknown variables is decreased. In this paper, we will prove the simplicity and applicability of this method to a rather wide range of problems.

2 Governing equations

The theory of Piezoelectricity consists of the simultaneous study of deformation and electric fields existing in anisotropic, non-conducting elastic media. The description of the piezoelectric effect is achieved by means of mechanical and electrical variables, namely strain and stress tensors, and the electric field and electric displacement vectors, which are denoted by \( \varepsilon_{ij} \), \( \sigma_{ij} \), \( E_i \), and \( D_i \) respectively. Consequently, there are two possible manners of describing electromechanical interaction. In theoretical analyses, it is customary to choose a representation in which the strain and electric field are the independent variables. However, in experimental analyses, constitutive relations bearing the stress and the electrical field as independent variables are preferred. In the end the choice is decided by the particular problem that one has in mind. The present study makes use of a form in which strains and electric field are the independent quantities, following Tiersten [8] we write

\[
\sigma_{ij} = C_{ijkl} \varepsilon_{kl} - \varepsilon_{kij} E_k, \quad i, j, k, l = 1,2,3, \quad (1a)
\]
where $C_{ijkl}$ is the elastic modulus tensor, $e_{ijk}$ is the piezoelectric tensor, and $k_{ij}$ is the dielectric tensor. There exists an electric potential function, $\Phi$ such that $E = -\nabla\Phi$. In the SI system the aforementioned variables are measured in the following units

$$
\begin{align*}
[\varepsilon] &= \text{Nm}^{-2}, [\sigma] = \text{Nm}^{-2}, [\mathbf{E}] = \text{Vm}^{-1} = \text{NC}^{-1}, \\
[D] &= C_m^{-2} = NV^{-1} m^{-1}, [C] = \text{Nm}^{-2}, \\
[e] &= Nm^{-1} V^{-1} = C_m^{-2}, [k] = C^2 N^{-1} m^{-2} = NV^{-2}, \\
[\Phi] &= V.
\end{align*}
$$

The governing field equations are:

$$
\sigma_{ij,j} = 0, \\
D_{i,i} = 0,
$$

and the boundary conditions may be written as:

$$
B_{mn} U_n = \begin{cases}
\sigma_{mj} (U_n) n_j - \tau_m, & 1 \leq m \leq 3, \\
D_j (U_n) n_j - \bar{D}, & m = 4, \\
U_m - \bar{U}_m & \text{on } \Gamma_U
\end{cases} \bigg|_{\text{on } \Gamma_U} = 0, 
$$

where $U_m$ is the generalized displacement given by:

$$
U_m = \begin{cases}
\mu_m, & 1 \leq m \leq 3, \\
\Phi, & m = 4
\end{cases}
$$

$B_{mn}$ is the generalized boundary condition operator, $\sigma_{mj} (U_n)$ and $D_j (U_n)$ are stress and electrical displacement, $n_j$ is the direction cosine, $\tau_m$ is the traction vector, and $\bar{D}$ is the prescribed normal electrical displacement to the boundary. $\Gamma_\Sigma$ and $\Gamma_U$ are the generalized traction and generalized displacement boundary conditions, and $\bar{U}_m$ is the prescribed generalized displacement vector on the boundary $\Gamma_U$.

The total energy functional is given by:

$$
F = \int_{\Omega} \left[ \frac{1}{2} (\varepsilon_{ij} \sigma_{ij}) - \frac{1}{2} (\mathbf{E}_i D_i) \right] d\Omega - \int_{\Gamma_\Sigma} \tau_m U_m d\Gamma.
$$
where

\[ i, j = 1, 2, \ldots, 9 \text{, and } m = 1, 2, \ldots 4 \]  

(7)

Using the weighted residual Galerkin method and selecting \( \delta U_m \) as weight functions, the following variational relation holds

\[ \delta F = 0 \]  

(9)

3 Ritz method strategies

Two main strategies are considered in this research. In the first strategy, continuous and adequately differentiable functions of the following form are considered as generalized displacement field

\[ U_m(x, y, z) = \sum_{q=0}^{p} \sum_{l=0}^{q} \sum_{\alpha=0}^{q-l} C_{m\beta} \phi_{m\beta}^{(R)}(x, y, z), \quad m = 1, 2, \ldots 4, \]  

(10)

in which

\[ \beta = \frac{q(q+1)(q+2)}{6} + \frac{(l+1)(l+2)}{2} - \alpha, \]  

(11)

\( p \) is the order of polynomial space, \( C_{m\beta} \) are the unknown coefficients, and the Ritz functions \( \phi_{m\beta}^{(R)} \) are taken as the product of the boundary functions \( \phi_{m}^{(B)} \), which serve as the basic and polynomial functions

\[ \phi_{m\beta}^{(R)}(x, y, z) = x^{q-l-\alpha} y^{\alpha} z^{l} \phi_{m}^{(B)}(x, y, z), \quad m = 1, 2, \ldots 4, \]  

(12)

\( \phi_{m}^{(B)} \) ensures that the Ritz function satisfies the kinematic boundary conditions, and is given by

\[ \phi_{m}^{(B)}(x, y, z) = \prod_{j=1}^{ne} \left[ \Gamma_j(x, y, z) \right]^{\Omega_j}, \]  

(13)

where \( ne \) is the number of boundaries, \( \Gamma_j \) is the equation of the \( j \)th boundary, and depending on the boundary conditions, \( \Omega_j \) takes on
\[ \Omega_j = \begin{cases} 0, & \text{if } j\text{th degree is free}, \\ 1, & \text{if } j\text{th degree is simply supported}, \\ 2, & \text{if } j\text{th degree is clamped}. \end{cases} \tag{14} \]

In lieu of Eqs. (7), and (10) the coefficients \( C_{\alpha \beta} \) are obtained by minimization of the total energy functional

\[ \frac{\partial F}{\partial C_{m\beta}} = 0. \tag{15} \]

In the second strategy Eq. (10) is modified to account for the discontinuities in the derivatives of the generalized displacement fields

\[ U_m^k(x, y, z) = \sum_{q=0}^{p_k} \sum_{l=0}^{q-l} \sum_{\alpha=0}^{q-l} C_{m\alpha} \phi^{(R)}_{m\alpha}(x, y, z) + \sum_{q=0}^{p_k} \sum_{l=0}^{q-l} \sum_{\alpha=0}^{q-l} C_{m\beta} \phi^{(R)}_{m\beta}(x, y, z), \tag{16} \]

where \( U_m^k(x, y, z) \) is the generalized displacement field of layer \( k \). The first term in the right hand side of Eq. (16) is defined as in (10). The second term consists of an amending polynomial of order \( p_k \) for layer \( k \), with unknown coefficients \( C_{m\beta} \). The functions \( \phi^{(R)}_{m\beta}(x, y, z) \) are defined as

\[ \phi^{(R)}_{m\beta}(x, y, z) = (x^{q-l-\alpha} y^{\alpha} z^{l}) \phi^{(B)}_{m}(x, y, z), \quad 1 \leq m \leq 4, \tag{17} \]

\[ \phi^{(B)}_{m}(x, y, z) = \varphi^{(B)}(x, y, z) \prod_{j=1}^{n_k} \Gamma_j(x, y, z), \tag{18} \]

where \( \beta \) and \( \varphi^{(B)} \) are given by Eqs. (11) and (13) respectively, \( n_k \) is the number of interfaces of the \( k \)th lamina with other laminates, and \( \Gamma_j \) is the equation of the surface of the inter-laminar. In this manner, the generalized displacement fields remain continuous, while their derivatives can have the required discontinuity up to a desired order. The consequent steps are the same as those of first strategy.

### 4 Numerical examples

To establish the accuracy and to verify the effect of several important parameters on convergence rate involved in the present theory such as the amending terms, two examples are considered. In subsection 4.1 a 2D problem
of a plate made of two different piezoceramic layers, and in subsection 4.2 a 3D problem of PZT-Polymer composite plate are considered. These problems are solved for trigonometric type loading and the results are compared with the exact solutions.

4.1 Analysis of a piezoelectric plate with different piezoceramic layers

The piezoelectric composite plate considered here is composed of two piezoceramic layers with total thickness of \( H = 0.01m \) and length \( L = 0.1m \) as shown in Fig. 1. The corresponding material properties for each layer are given in Table 1. The plate is assumed to be infinitely long in the \( x \)-direction, the applied mechanical loading on its upper face is:

\[
t_z = \cos \frac{\pi y}{L}.
\]  

The boundary functions corresponding to the displacements in the \( y \)-direction, \( v \), \( z \)-direction, \( w \) and electric potential function \( \Phi \) are taken as:

\[
\varphi_2^{(b)} = y.
\]
respectively. To account for the possible discontinuities in the derivatives of displacement fields and electric potential function, the following amending terms are used:

\[ \phi^{(B)}_m^{PZT-4} = \phi^{(B)}_m z, \quad m = 2,3,4, \]

where the superscript PZT-4 means that the terms correspond to that layer. The effects of amending terms are evident from Figs. 2 through 7. In the displayed Figures Ritz* refers to the cases where the amending terms are included, whereas Ritz corresponds to results when the amending terms are absent. The order of the polynomial for the amending terms was taken to be equal to the

Table 1. Electroelastic material properties.

<table>
<thead>
<tr>
<th>Property</th>
<th>PZT-4</th>
<th>(Pb_{0.38}Ca_{0.12})</th>
<th>(CO_3W_{0.4}Ti_{0.58})O_3</th>
<th>Elastic Polymer</th>
</tr>
</thead>
<tbody>
<tr>
<td>E_1 (GPa)</td>
<td>81.3</td>
<td>127</td>
<td>132.38</td>
<td></td>
</tr>
<tr>
<td>E_2</td>
<td>81.3</td>
<td>127</td>
<td>10.756</td>
<td></td>
</tr>
<tr>
<td>E_3</td>
<td>64.5</td>
<td>119</td>
<td>10.756</td>
<td></td>
</tr>
<tr>
<td>v_{12}</td>
<td>0.329</td>
<td>0.199</td>
<td>0.24</td>
<td></td>
</tr>
<tr>
<td>v_{13}</td>
<td>0.432</td>
<td>0.174</td>
<td>0.49</td>
<td></td>
</tr>
<tr>
<td>v_{23}</td>
<td>0.432</td>
<td>0.174</td>
<td></td>
<td></td>
</tr>
<tr>
<td>G_{33} (GPa)</td>
<td>25.6</td>
<td>53.5</td>
<td>3.606</td>
<td></td>
</tr>
<tr>
<td>G_{13}</td>
<td>25.6</td>
<td>53.5</td>
<td>5.654</td>
<td></td>
</tr>
<tr>
<td>G_{12}</td>
<td>30.6</td>
<td>53</td>
<td>5.654</td>
<td></td>
</tr>
<tr>
<td>e_{24} (C/m^2)</td>
<td>12.72</td>
<td>2.96</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>e_{15}</td>
<td>12.72</td>
<td>2.96</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>e_{31}</td>
<td>-5.2</td>
<td>0.8</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>e_{32}</td>
<td>-5.2</td>
<td>0.8</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>e_{33}</td>
<td>15.08</td>
<td>6.88</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>e_{11}/e_0</td>
<td>1475</td>
<td>202</td>
<td>3.5</td>
<td></td>
</tr>
<tr>
<td>e_{22}/e_0</td>
<td>1475</td>
<td>202</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>e_{33}/e_0</td>
<td>1300</td>
<td>181</td>
<td>3</td>
<td></td>
</tr>
</tbody>
</table>
Figure 2: Variation of electric potential along the z-axis

Figure 3: Distribution of normal stress along the z-axis.

Figure 4: Electric displacement along the z-axis.
Figure 5: Variation of electric potential along the z-axis.

Figure 6: Distribution of normal stress along the z-axis.

Figure 7: Electric displacement along the z-axis.
order of the main polynomial in the Ritz approximations, $p = p_k$. The results are compared with the exact solutions given by Heyliger and Brooks [5]. The Ritz solutions were obtained using 8th order polynomials, $p = p_k = 8$. Clearly, when the amending terms are excluded, then the results for the field variables that depend on the derivatives of displacement fields and potential function such as stress fields and electric displacement may be drastically inaccurate. This finding is demonstrated in Figs. (6) and (7). On the other hand, the displacement fields and electric potential are computed directly and independently of their derivatives. Therefore, their accuracy remain unaffected by the amending terms.

4.2 Analysis of a PZT-Polymer composite plate

The piezoelectric composite plate considered here is a $[0/90]$ cross ply composed of an elastic layer in the middle and two piezoelectric layers which are bonded to its upper and lower surfaces, as shown in Fig. 8. The rectangular plate is simply supported along all its edges and has dimensions $L_x$, $L_y$ and total thickness of $H$. The elastic layer and piezoelectric layers have thickness of $0.8H$ and $0.1H$, respectively. The material properties of the elastic and PZT-4 layers, which are both orthotropic materials, are given in Table 1.

$$t_z = \cos \left( \frac{\pi y}{L_y} \right) \cos \left( \frac{\pi x}{L_x} \right)$$

Figure 8: Schematic of the laminated piezoelectric plate pertinent to the example of subsection 4.2.
In order to compare the results with the exact results in literature, double sinusoidal loading on the upper surface with an amplitude equal to one is assumed. Taking the origin of the coordinate system at the center of the plate, $z$-axis perpendicular to the layers and $x$ and $y$ axes parallel to the main edges, the loading is given by

$$t_z = \cos \frac{\pi x}{L_x} \cos \frac{\pi y}{L_y}. \quad (24)$$

The aspect ratio is assumed to be $L_x/H = L_y/H = 4.0$ and the top and bottom laminate surfaces are fixed at zero potential. Under these conditions, the basic functions are as follows:

$$\phi_1^{(B)} = x(4y^2 - L_y^2), \quad \phi_2^{(B)} = y(4x^2 - L_x^2), \quad \phi_3^{(B)} = (4x^2 - L_x^2)(4y^2 - L_y^2), \quad \phi_4^{(B)} = (4x^2 - L_x^2)(4y^2 - L_y^2)(4z^2 - H^2). \quad (25-28)$$

The following amending terms for the elastic layer are considered:

$$\phi_m^{(B)\text{polymer}} = \phi_m^{(B)} \left[ z^2 - (0.4H)^2 \right], \quad m = 1,2,3,4, \quad (29)$$

where the values of these functions are equal to zero at the interfaces between the elastic and PZT-4 layers. These functions satisfy the continuity conditions for the displacement fields and the electric potential function. This problem has been solved with the amending terms. The order of the polynomial for the amending terms was taken to be equal to the order of the main polynomial in the Ritz approximations, $p = p_k$. The Ritz solutions obtained by the present methodology for $p = p_{\text{polymer}} = 9$ along with the exact solutions given by Heyliger [6] are given in Figs. 9 through 10. This comparison reveals that the results obtained by the present method are in excellent agreement with the exact solutions. The convergence rate of the proposed method for the vertical displacement and the electrical displacement at the midpoint of the plate, $x = 0, y = 0, z = H/2$ is demonstrated in Table 2. It is evident that the values of the displacement fields and the electric potential function converge to the exact solutions at a much higher rate than the values of stress fields and the electric displacement field. The low convergence rate of the values of stresses and electric displacement is due to their dependence on the derivatives of displacement and electric potential.
Figure 9: Electric displacement along the z-axis.

Figure 10: Distribution of shear stress along the z-axis.

Table 2. Convergence Rate for the vertical and electrical displacements.

<table>
<thead>
<tr>
<th>Order of Ritz's polynomials</th>
<th>$W(x=0,y=0,z=H/2) \times 1E11 (m)$</th>
<th>$Dz(x=0,y=0,z=H/2) \times 1E13 (c/m^2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>8.5535</td>
<td>-776.359</td>
</tr>
<tr>
<td>1</td>
<td>16.4294</td>
<td>-19971.567</td>
</tr>
<tr>
<td>2</td>
<td>18.2283</td>
<td>-1970.088</td>
</tr>
<tr>
<td>3</td>
<td>29.014</td>
<td>-351.38</td>
</tr>
<tr>
<td>4</td>
<td>29.0899</td>
<td>-179.1163</td>
</tr>
<tr>
<td>5</td>
<td>30.2991</td>
<td>-205.361</td>
</tr>
<tr>
<td>6</td>
<td>30.3167</td>
<td>-201.692</td>
</tr>
<tr>
<td>7</td>
<td>30.3922</td>
<td>-133.497</td>
</tr>
<tr>
<td>8</td>
<td>30.3922</td>
<td>-133.79</td>
</tr>
<tr>
<td>9</td>
<td>30.3951</td>
<td>-136.221</td>
</tr>
<tr>
<td>Exact solution</td>
<td>30.3962</td>
<td>-142.46</td>
</tr>
</tbody>
</table>
5 Conclusion

A general 3-dimensional pb-3 Ritz method incorporating amending terms was introduced for analyzing a general 3-dimensional piezoelectric solid. The amending terms accommodate the possible existence of any discontinuities in the derivatives of displacement fields and electric potential function across the interfaces. This method illustrated an excellent convergence to the exact solution. The inclusion of the amending terms increased the rate of convergence and lead to accurate solutions. When the amending terms were excluded, then the results for the field variables that depend on the derivatives of displacement fields and potential function such as stress fields and electric displacement became drastically inaccurate.

Acknowledgement

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References