INFLUENCE OF BOUNDARY CONDITIONS ON THE DETERMINATION OF EFFECTIVE MATERIAL PROPERTIES FOR ACTIVE FIBER COMPOSITES

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Abstract. The study of Active Fiber Composites (AFC) in aerospace applications has increased due to the potential of manufacturing structures that satisfy high performance requirements needed in this area. Intelligent structures can be designed as sensors and actuators for applications such as structure health monitoring, vibration control or suppression, precision positioning and others. In this work, a model of AFC composed of lead zirconate titanate (PZT) and polymeric matrix is studied. Numerical simulations using finite element method are presented, considering the AFC with different fiber arrangements. Piezoelectric composites can be classified into 14 types, depending on the nature of fiber distribution in the matrix, and divided in 3 groups: unimodal-periodic, bimodal–periodic or aperiodic, concerning the periodicity of fiber distribution and size of fiber cross-sectional area. Simulations of relevant cases of the first group are presented. The AFC is modeled in a micro-mechanical view through Representative Volume Element (RVE - unit cell), appropriately chosen for each fiber arrangement with suitable boundary conditions applied to make the unit cell provide the entire behavior of the piezoelectric composite. The material properties of each component of the composite are known, which permits to estimate the effective properties of the AFC by applying different loading cases to the unit cell. The results are discussed and compared with previous results found in literature, investigating the influence of the applied boundary conditions.

Keywords: piezoelectric fiber composite, boundary conditions, effective material properties, finite element analysis, unit cell

1. INTRODUCTION

Several works have been developed, using analytical, numerical, experimental or hybrid approaches. A good review about these researches is presented by Berger et al. (2005) and Kar-Gupta et al. (2005, 2007a and 2007b) and it will not be discussed here. Some basic concepts are presented and researches related with this work are discussed along the text body. The connectivity between fiber and matrix is indicated by two numbers, the first indicating the number of directions of fiber continuity and the second the same for matrix phase (Bent, 1997). Kar-Gupta et al. (2007) studied and classified piezoelectric composites according to fiber arrangement for 1-3 composites. This classification divides the composites in 14 types, depending on the nature of fiber distribution in the matrix, and divided in three groups: unimodal-periodic, bimodal–periodic or aperiodic, concerning the periodicity of fiber distribution and size of fiber cross-sectional area. In this work cases of unimodal-periodic arrangement are presented. All fibers considered here have the same cross-sectional area (unimodal) and two different periodic fiber arrangement were studied, the square arrangement and hexagonal arrangement as also reported in the last paper developed by the authors (Moreno et al., 2009). The cases analyzed in this work refers to 1-3 composites. All numerical analysis are performed using the software ANSYS®, and the main goal of this paper consists on investigating the influence of applied boundary condition.

2. BASIC CONCEPTS

2.1. Representative Volume Element (RVE or unit cell)

Composites with unidirectional fibers arranged in periodic way can be modeled by a representative volume element (RVE or unit cell) and suitable boundary conditions that impose the periodicity condition to the model. According to the fiber arrangement and loading and boundary conditions needed, a more suitable unit cell can be chosen in order to save computational effort. In Figure 1(a) a unit cell for a square fiber arrangement is shown, including the system of coordinates adopted here (fibers aligned with z-axis) and designation adopted to the RVE faces. Figure 1(b) is the front view of the same unit cell after xy-shear loading. The points A, B, C and D are used to present the boundary conditions to represent the periodicity of the model. Considering the two opposite points, A and B and other set of opposite points, C and D, their displacements, \( u_n \), respecting the periodicity of the RVE can be written in terms of the average unit cell strain \( S_{ij} \) as (Berger et al., 2005):

\[
\begin{align*}
\Delta u_{A1} &= S_{11} a + S_{12} b + S_{13} c + S_{14} d \\
\Delta u_{B1} &= S_{11} a + S_{12} b + S_{13} c + S_{14} d \\
\Delta u_{C1} &= S_{21} a + S_{22} b + S_{23} c + S_{24} d \\
\Delta u_{D1} &= S_{21} a + S_{22} b + S_{23} c + S_{24} d
\end{align*}
\]
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\[
u_i^A = u_i^B + \overline{S}_{ij}(x_j^A - x_j^B)\]  
\[
u_i^C = u_i^D + \overline{S}_{ij}(x_j^C - x_j^D)\]  

(1)

(2)

The same relations are also valid to the electrical degrees of freedom. Subtracting both equations and keeping in mind that the average \( \overline{S}_{ij} \) is the same in both equations and \( x_j^A - x_j^B = x_j^C - x_j^D \) (as can be seen in Fig. 1(b)), the constraint equation can be rewritten as following, respectively to displacement and electrical potential degrees of freedom.

\[
u_i^A - \nu_i^C = u_i^B - u_i^D\]  
\[
\phi^A - \phi^C = \phi^B - \phi^D
\]  

(3)

(4)

Where \( \phi \) is the electrical potential correspondent to the node indicated by the superscript index. The last two equations represents a parallelism condition between the sides \( AC \) and \( BD \). This condition must be applied for each pair of nodes in opposite sides of the unit cell (in vertical and horizontal directions) and must be repeated along the depth of the cell. In the analysis presented it is not necessary to specify these conditions for all the analyzed cases because sometimes the displacement and electrical boundary conditions already ensures this parallelism restriction. It is interesting to avoid the direct application of this conditions because there is a large number of equations that must be input. Automatic procedures to search opposite nodes and applying restrictions must be used. In the loading cases involving shear forces this procedure cannot be avoided, and the constraint equations has to be used in the faces submitted to the shear loading.

2.2. Piezoelectric Composites

Piezoelectric composites are composites that have at least one phase made of piezoelectric material. In this work just the fiber is considered piezoelectric. Thus, the problem involves, besides the mechanical elastic coefficients, the dielectric coefficients and the mechanical-electrical coupling coefficients (or piezoelectric coefficients). The effective composite properties are written as a constitutive effective matrix, which includes elastic, electric and piezoelectric coefficients, being a homogenization of the properties of both constituents, fiber and matrix. This effective matrix relates the average values of stress, strain, electric potential and electrical displacements, evaluated at the whole composite according to Eq.(5).

\[
\{\overline{T}\} = \begin{bmatrix}
[C]^\text{eff} & [e]^\text{eff} \\
[e]^\text{eff} & [\varepsilon]^\text{eff}
\end{bmatrix} \{\overline{S}\} - \{E\}
\]  

(5)

Where \( \{T\} \) is the stress field, \( \{D\} \) is the electrical displacements field, \( \{S\} \) is the strain field and \( \{E\} \) is the electrical potential field; \( [C] \) is the elasticity matrix, \( [\varepsilon] \) the dielectric matrix, \( [e] \) is the piezoelectric matrix. Expanding the terms in Eq.(5) and applying symmetry conditions for 1-3 composites, the material coefficients matrix can be written in terms of eleven independent coefficients as shown in Eq.(6). In Eq.(5) and Eq.(6) the superscript \( \text{eff} \) means the effective value of the considered property and the bar over the field component means the average value evaluated over the unit cell volume as shown in Eq.(7).
The analysis procedure is based on six cases, summarized in Tab. 2. Each row of the Tab. 2 refers to one finite element analysis, showing the coefficients obtained by this analysis as well as prescribed loads, boundary conditions (BCs) and constraint equations. The coefficients are obtained through Eq.(6) and the applied conditions ensures that the

\[
\begin{bmatrix}
\mathbf{T}_{11} \\
\mathbf{T}_{22} \\
\mathbf{T}_{33} \\
\mathbf{T}_{12} \\
\mathbf{T}_{23} \\
\mathbf{T}_{31} \\
\mathbf{S}_{11} \\
\mathbf{S}_{22} \\
\mathbf{S}_{33} \\
\mathbf{S}_{12} \\
\mathbf{S}_{23} \\
\mathbf{E}_1 \\
\mathbf{E}_2 \\
\mathbf{E}_3
\end{bmatrix} = \begin{bmatrix}
C_{11}^{\text{eff}} & C_{12}^{\text{eff}} & C_{13}^{\text{eff}} \\
C_{12}^{\text{eff}} & C_{11}^{\text{eff}} & C_{13}^{\text{eff}} \\
C_{13}^{\text{eff}} & C_{13}^{\text{eff}} & C_{33}^{\text{eff}} \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix} \begin{bmatrix}
e_{11}^{\text{eff}} \\
e_{12}^{\text{eff}} \\
e_{13}^{\text{eff}} \\
e_{15}^{\text{eff}} \\
e_{15}^{\text{eff}} \\
e_{15}^{\text{eff}} \\
e_{33}^{\text{eff}} \\
e_{33}^{\text{eff}} \\
e_{33}^{\text{eff}} \\
e_{33}^{\text{eff}} \\
e_{33}^{\text{eff}} \\
e_{33}^{\text{eff}} \\
e_{33}^{\text{eff}}
\end{bmatrix} = \begin{bmatrix}
\mathbf{S}_{11} \\
\mathbf{S}_{22} \\
\mathbf{S}_{33} \\
\mathbf{S}_{12} \\
\mathbf{S}_{23} \\
\mathbf{E}_1 \\
\mathbf{E}_2 \\
\mathbf{E}_3
\end{bmatrix}
\]

(6)

\[
\mathbf{T}_{ij} = \frac{1}{V} \sum_{n=1}^{n\text{el}} T_{ij}^{(n)} V^{(n)}
\]

(7)

In the last equation, \( n\text{el} \) is the number of elements used to model the RVE, \( T^{(n)} \) is the average stress field at the \( n \)-th element, \( V^{(n)} \) is the volume of the \( n \)-th element and \( V \) is the RVE total volume. And \( T_{ij} \) can be replaced for any other field component present in Eq.(6) such as \( D, S \) or \( E \). Therefore the average values of these components, evaluated at the unit cell, can be easily post-processed in a standard finite element software.

3. MODELING

3.1. Material properties

Material properties of both, polymeric matrix and fiber are presented in Tab. 1. The simulated fiber material is ceramic PZT-5 and the the matrix uses typical polymeric values. Properties of both materials were obtained from Berger et al. (2005). For the analysis presented here a fiber volume fraction of 55.5% was adopted.

<table>
<thead>
<tr>
<th></th>
<th>( C_{11} )</th>
<th>( C_{12} )</th>
<th>( C_{13} )</th>
<th>( C_{33} )</th>
<th>( C_{44} )</th>
<th>( C_{66} )</th>
<th>( e_{11} )</th>
<th>( e_{12} )</th>
<th>( e_{13} )</th>
<th>( e_{33} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fiber</td>
<td>12.1</td>
<td>7.54</td>
<td>7.52</td>
<td>11.1</td>
<td>2.11</td>
<td>2.28</td>
<td>-5.4</td>
<td>12.3</td>
<td>15.8</td>
<td>8.11</td>
</tr>
<tr>
<td>Matrix</td>
<td>0.386</td>
<td>0.257</td>
<td>0.257</td>
<td>0.386</td>
<td>0.064</td>
<td>0.064</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.0797</td>
</tr>
</tbody>
</table>

Fiber volume fraction: 55.5%

3.2. Finite element models

The finite element models used in the numerical simulations are shown in Fig. 2. For square fiber arrangement case just one model was used for all proposed analysis, changing just the loading and boundary conditions, as shown in Figure 2(a). For the hexagonal fiber arrangement case three models were used. For the cases involving traction in one direction or electrical potential difference in one direction the model presented in Fig. 2(b) was used. This model has enough symmetry for these cases due to the nature of the loading condition, which does not ask for an explicit use of Eq.(3) and Eq.(4). For the cases involving shear loadings, it is necessary symmetry between nodes in opposite sides, therefore the model needs to be expanded according to the shearing plane considered. Figure 2(c) presents the model used for shear loading in plane \( x-y \) and Fig. 2(d) the model used for shear loading in plane \( y-z \). Actually the model in Fig. 2(c) does not need so many elements along \( z \) direction (fiber direction).

3.3. Analysis procedure: loading and boundary conditions

The analysis procedure is based on six cases, summarized in Tab. 2. Each row of the Tab. 2 refers to one finite element analysis, showing the coefficients obtained by this analysis as well as prescribed loads, boundary conditions (BCs) and constraint equations. The coefficients are obtained through Eq.(6) and the applied conditions ensures that the
terms not related with this coefficients are vanished. Table 2 also indicates which line of this system of equations is used to get the coefficient.

![Figure 2. FE models: (a) square; (b) hexagonal; (c) hexagonal shear 1-2; (d) hexagonal shear 2-3](image_url)

Table 2. Loading and boundary conditions

<table>
<thead>
<tr>
<th></th>
<th>Equation (a)</th>
<th>Prescribed displacement field [m]</th>
<th>Prescribed force field [N]</th>
<th>Prescribed electric potential field [V]</th>
<th>Displacement BCs [m]</th>
<th>Electric Potential BCs [V]</th>
<th>Additional constraint equations (b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>$C_{13}$ $C_{33}$</td>
<td>1st line 3rd line</td>
<td>positive $u_z$ / face $Z^+$</td>
<td>-</td>
<td>-</td>
<td>Zero normal displacements / faces $X^+$, $X^-$, $Y^+$, $Y^-$, $Z^+$, $Z^-$</td>
<td></td>
</tr>
<tr>
<td>2.</td>
<td>$\varepsilon_{13}$ $\varepsilon_{33}$ $\varepsilon_{13}$</td>
<td>1st line 3rd line 9th line</td>
<td>-</td>
<td>-</td>
<td>positive voltage / face $Z^+$</td>
<td>Zero normal displacements / all faces</td>
<td>Zero / face $Z^-$</td>
</tr>
<tr>
<td>3.</td>
<td>$C_{11}$ $C_{12}$</td>
<td>1st line 2nd line</td>
<td>positive $u_x$ / face $X^+$</td>
<td>-</td>
<td>-</td>
<td>Zero normal displacements / faces $X^-$, $Y^+$, $Y^-$, $Z^+$, $Z^-$</td>
<td>Zero / all faces</td>
</tr>
<tr>
<td>4.</td>
<td>$\varepsilon_{11}$</td>
<td>7th line</td>
<td>-</td>
<td>-</td>
<td>positive voltage / face $X^+$</td>
<td>Zero normal displacements / all faces</td>
<td>Zero / face $X^-$</td>
</tr>
<tr>
<td>5. (c)</td>
<td>$C_{66}$</td>
<td>4th line</td>
<td>-</td>
<td>$+F_z$ and $-F_z$ / faces $X^+$ and $X^-$ $+F_z$ and $-F_z$ / faces $Y^+$ and $Y^-$</td>
<td>-</td>
<td>Zero normal displacements / faces $Z^+$, $Z^-$</td>
<td>Zero / all faces between pairs of faces $X^+$, $X^-$ and $Y^+$, $Y^-$</td>
</tr>
<tr>
<td>6. (c)</td>
<td>$C_{44}$ $C_{45}$</td>
<td>5th line 8th line</td>
<td>-</td>
<td>$+F_z$ and $-F_z$ / faces $Z^+$ and $Z^-$ $+F_z$ and $-F_z$ / faces $Y^+$ and $Y^-$</td>
<td>-</td>
<td>Zero normal displacements / faces $X^+$, $X^-$</td>
<td>Zero / all faces between faces $Z^+$, $Z^-$ and $Y^+$, $Y^-$</td>
</tr>
</tbody>
</table>

(a): Lines number referred to Eq. (6);
(b): According to Eq. (3) and Eq. (4);
(c): Convenient restrictions to avoid rigid body movement are also added.

The first and second analysis involves the loading applied in $z$-direction (fiber direction), the first with mechanical loading and the second with electrical loading. The applied boundary conditions already ensure the conditions given by Eq.(3) and (4), so they do not need to be specified again by constraint equations. Third and fourth analysis are similar to the first set but the mechanical and electrical loadings are applied in $x$-direction. Once more the constraint equations are already ensured by the boundary conditions. The last two analysis related in Tab. 2 involves the RVE subjected to shear loading. In the 5th analysis the shear loading is performed in plane $x-y$ and in the 6th, plane $y-z$. Both cases require explicit implementation of constraining equations. The implementation was done using the ANSYS® Parametric Design Language (APDL) due the direct access to the model data. This procedure is easily implemented for the 5th analysis.
because the mesh is symmetric in all required directions (as shown in Fig. 3(a)): the nodes correspondence between opposite faces and repetition of the procedure along z-direction is regular for all nodes; nodes are arranged in a straight line along the depth. For the 6th analysis, there is the correspondence between nodes of opposite faces along x direction just with $Y^+$ and $Y^-$ faces. The coupling equations for $Z^+$ and $Z^-$ faces in this work were applied among the nodes belonging to the lines shown in green in Fig. 3(b).

It is necessary also include some notes about other procedures adopted to impose the analysis conditions in numerical simulations for the analysis number 5 and 6:

1. For boundary conditions to avoid rigid body movement it was avoided the application in nodes at the matrix. Fiber nodes were preferred instead because the higher stiffness in order to avoid the occurrence of eventual concentrated effects;

2. When applying constraint equations between opposite unit cell faces, nodes that belong to the unit cell edges perpendicular to the shearing plane should not be included. For example, in Fig. 3(a), for $xy$ shear loading, the edge nodes are ignored (green lines in Fig. 3(a)) and the first constraint equation for each direction uses the set of nodes in blue (pairs of nodes 1-2 and 3-4) and in red (pairs of nodes 5-6 and 7-8);

3. When applying the shear forces the loading was distributed among face nodes except those indicated by the green lines in Fig. 3(a) in a procedure similar to the adopted for the constraint equations. For the $yz$ shear case, the exceptions are the nodes at the edges aligned with $x$-axis.

![Figure 3. Boundary conditions: (a) plane x-y; (b) plane y-z](image)

4. RESULTS AND DISCUSSION

The results of numerical simulations for square and hexagonal fiber arrangement are presented in Tab. 3. For comparison purposes, the analytical and numerical results obtained by Berger et al. (2005) are also presented in Tab. 3. The analytical results provided by Berger et al. (2005) are used as reference for the error estimate.

In general, good results were achieved with the numerical simulations of both arrangements. As expected the results with hexagonal arrangement are, in general, closer of the analytical results. Berger et al. concluded that the difference between analytical and numerical analysis in their work could be explained by the fact that the square symmetry of fibers arrangement does not fulfill completely the transverse isotropy condition, hypothesis adopted in Eq. (5). According to this explanation, it was expected that a model with fibers in hexagonal arrangement provided results closer to analytical results than the obtained here.

Analyzing the relation between the applied loading / boundary conditions and the problems with convergence it can be concluded that the conditions where the loading is applied in fiber direction, such as the analysis to obtain $C_{13}$, $C_{33}$, $e_{13}$, $e_{31}$ and $e_{33}$ are the most reliable (see Tab. 3). So despite some of these coefficients ($C_{13}$ and $e_{13}$) can be obtained with other loading cases, it is highly recommended to avoid this procedure. The most difficult cases are those one where shear loading is involved. It is necessary to be careful when applying displacement constraint in these cases because if by one side they must avoid the rigid body movement, by other side they must allow the body distortion without over-constraint the model. The larger number of constraints conditions present in calculation of these parameters ($C_{66}$, $C_{44}$ and $e_{15}$) leads to a larger error when compared with analytical results. Particularly the coefficient $e_{15}$ presented high sensitivity to changes in constraint application methods. Coefficients calculated from $x$-direction loading presented, in general, an intermediate behavior, but better response in the case of fibers in square arrangement, probably consequence of the uniform symmetry between $x$ and $y$ directions.

5. CONCLUSION

The work presents a study analyzing the influence of two different fiber arrangements in the effective properties of a piezoelectric fiber composite. Analytical solutions are limited to take into account the fiber disposition and the hypothesis adopted are closer of an hexagonal arrangement. The numerical results presented here are in good agreement with investigations performed by other researchers.


Table 3. Analytical and numerical results comparison

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Units</th>
<th>(1)</th>
<th>(2)</th>
<th>(3)</th>
<th>(4)</th>
<th>Error <a href="a">%</a></th>
<th>Error <a href="b">%</a></th>
<th>Error <a href="c">%</a></th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{11}$</td>
<td>$x 10^{10}$ Pa</td>
<td>0.95</td>
<td>1.10</td>
<td>1.088</td>
<td>1.068</td>
<td>15.8</td>
<td>14.5</td>
<td>12.4</td>
</tr>
<tr>
<td>$C_{12}$</td>
<td></td>
<td>0.56</td>
<td>0.48</td>
<td>0.465</td>
<td>0.522</td>
<td>14.3</td>
<td>17.1</td>
<td>6.8</td>
</tr>
<tr>
<td>$C_{13}$</td>
<td></td>
<td>0.60</td>
<td>0.60</td>
<td>0.604</td>
<td>0.619</td>
<td>0.0</td>
<td>0.7</td>
<td>3.2</td>
</tr>
<tr>
<td>$C_{33}$</td>
<td></td>
<td>3.50</td>
<td>3.50</td>
<td>3.525</td>
<td>3.521</td>
<td>0.0</td>
<td>0.7</td>
<td>0.6</td>
</tr>
<tr>
<td>$C_{44}$</td>
<td></td>
<td>0.22</td>
<td>0.18</td>
<td>0.215</td>
<td>0.195</td>
<td>18.2</td>
<td>2.3</td>
<td>11.4</td>
</tr>
<tr>
<td>$C_{66}$</td>
<td></td>
<td>0.20</td>
<td>0.16</td>
<td>0.154</td>
<td>0.181</td>
<td>20.0</td>
<td>23.1</td>
<td>9.5</td>
</tr>
<tr>
<td>$\epsilon_{13}$</td>
<td>C / m²</td>
<td>-0.26</td>
<td>-0.26</td>
<td>-0.258</td>
<td>-0.269</td>
<td>0.0</td>
<td>0.7</td>
<td>3.5</td>
</tr>
<tr>
<td>$\epsilon_{15}$</td>
<td></td>
<td>0.02</td>
<td>0.018</td>
<td>0.0241</td>
<td>0.0164</td>
<td>10.0</td>
<td>20.5</td>
<td>18.0</td>
</tr>
<tr>
<td>$\epsilon_{33}$</td>
<td></td>
<td>11.0</td>
<td>11.0</td>
<td>10.86</td>
<td>10.86</td>
<td>0.0</td>
<td>1.3</td>
<td>1.3</td>
</tr>
<tr>
<td>$\epsilon_{32}$</td>
<td>$x 10^9$ F/m</td>
<td>0.28</td>
<td>0.29</td>
<td>0.284</td>
<td>0.303</td>
<td>3.6</td>
<td>1.4</td>
<td>8.2</td>
</tr>
<tr>
<td>$\epsilon_{33}$</td>
<td></td>
<td>4.20</td>
<td>4.20</td>
<td>4.27</td>
<td>4.27</td>
<td>0.0</td>
<td>1.6</td>
<td>1.6</td>
</tr>
</tbody>
</table>

(a): Comparing (1) and (2);  (b): Comparing (1) and (3);  (c): Comparing (1) and (4).

Practical problems and difficulties in the modeling process were presented and discussed and a final analysis procedure is suggested based in the experience acquired with the presented analysis and other preliminary results not discussed in this paper, but presented in Moreno et al (2009). The sensibility of the material coefficients to the boundary conditions is also discussed because there are some practical problems in implementing the necessary boundary condition in commercial available finite element codes, so results should be carefully analyzed, specially for the piezoelectric coefficient $\epsilon_{15}$, responsible for the largest errors in the presented results when compared to the analytical results. This work is part of the first step in a project to characterize active fiber composites by finite element method to further application in the design of complex aeronautic structures.

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7. REFERENCES


8. RESPONSIBILITY NOTICE

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