A NUMERICAL HOMOGENIZATION TECHNIQUE FOR PIEZOELECTRIC COMPOSITES WITH ARBITRARY FIBER DISTRIBUTION

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Abstract. In this paper a numerical technique for calculating effective properties of piezoelectric fiber composites with arbitrary fiber distribution is introduced. The method is based on finite element modeling of a unit cell. Due to the involved systematic scheme of appropriate boundary conditions and loads for ensuring periodicity this technique can be applied to composites with various fiber volume fractions and fiber distributions, from square over hexagonal and rhombic to random arrangements. That means in contrast to many published approaches the developed technique allows the extension to composites with arbitrary geometrical inclusion configurations and provides a powerful tool for fast calculation of their effective material properties.

The geometrical generation of random distribution of fibers in the three dimensional unit cell is based on a modified random sequential adsorption (RSA) algorithm. By using the finite element code ANSYS with its included ANSYS Parametric Design Language (APDL) a high automation can be achieved for generating the model, applying the boundary conditions and calculating the full set of elastic, piezoelectric and dielectric effective material coefficients. For some test cases the results are compared and verified with analytical and other numerical solutions.

Keywords: Homogenization, Unit cell, Piezoelectric composite, Finite Element Method

1. INTRODUCTION

Piezoelectric materials have the property of converting electrical energy into mechanical energy, and vice versa. But bulk piezoelectric materials have several drawbacks, hence composite materials are often a better technological solution in the case of a lot of applications such as ultrasonic transducers, medical imaging, sensors, actuators and damping. Recently, due to miniaturization of the piezocomposites and the use of PZT fibers instead of piezoelectric bars, new applications toward electromechanical sensors and actuators have become possible. To design such structures it is of interest to know the overall electro-mechanical behavior of the composite. Different homogenization techniques have been developed to predict effective material constants of piezocomposites.

Several analytical methods allow the prediction of overall moduli for composites with regular fiber arrangements (Dunn and Taya, 1993, Guinovart-Díaz et al., 2001). However, numerical methods give the basis for treatment of more complex fiber configurations (Li, 2000, Pettermann and Suresh, 2000, Kari et al., 2007). Based on a unit cell model with appropriate periodic boundary conditions and load cases the finite element method can be used to calculate the full set of effective coefficients of the composite. In this paper a general numerical homogenization concept is introduced which can be used to composites with arbitrary piezoelectric fiber inclusions.

2. CONSTITUTIVE EQUATIONS AND UNIT CELL MODEL

For a transversely isotropic 1-3 piezoelectric composite the material behavior is based on only eleven independent constants. But this is only ensured for a regular hexagonal fiber arrangement. In this paper arbitrary fiber distributions are considered which result in an anisotropic material behavior for the composite. Using effective coefficients \( C^{\text{eff}}_{ij} \) - elastic, \( e^{\text{eff}}_{ij} \) - piezoelectric, \( \varepsilon^{\text{eff}}_{ij} \) - dielectric) and averaged values \( \bar{T}_{ij} \) - stresses, \( \bar{S}_{ij} \) - strains, \( \bar{D}_{i} \) - electrical displacements, \( \bar{E}_{i} \) - electric fields) the constitutive equations for the homogenized composite can be expressed in matrix form by
Under the assumption of periodicity of the fiber arrangement in the infinite composite a unit cell can be used for calculation of effective coefficients by applying appropriate periodic boundary conditions. Figure 1 shows such unit cells for different types of fiber arrangements.

The main idea of the method is to find a globally homogeneous medium equivalent to the original composite, where the strain energy stored in both systems is approximately the same. To find the effective coefficients special load cases with different boundary conditions must be constructed in such a way that for a particular load case only one value in the strain/electric field vector (see Eq. (1)) is non-zero and all others become zero. Then from one column in Eq. (1) the corresponding effective coefficients can be evaluated using the calculated averaged non-zero value in the strain/electric field vector and the calculated averaged values in the stress/electrical displacement vector.

\[
\mathbf{T} = \begin{bmatrix}
T_{11} & T_{12} & T_{13} \\
T_{21} & T_{22} & T_{23} \\
T_{31} & T_{32} & T_{33}
\end{bmatrix},
\]

\[
\mathbf{S} = \begin{bmatrix}
S_{11} & S_{12} & S_{13} \\
S_{21} & S_{22} & S_{23} \\
S_{31} & S_{32} & S_{33}
\end{bmatrix}.
\]

(1)

Under the assumption of periodicity of the fiber arrangement in the infinite composite a unit cell can be used for calculation of effective coefficients by applying appropriate periodic boundary conditions. Figure 1 shows such unit cells for different types of fiber arrangements.

The periodic boundary conditions on two opposite surfaces \( K^- \) and \( K^+ \) (\( A^-/A^+ \), \( B^-/B^+ \) and \( C^-/C^+ \) in Fig. 2) of the unit cell can be defined by the differences

\[
\mathbf{u}_i^{K^-} - \mathbf{u}_i^{K^+} = \mathbf{S}_i \left( x_i^{K^-} - x_i^{K^+} \right), \quad \mathbf{F}^{K^-} - \mathbf{F}^{K^+} = \mathbf{E}_i \left( x_i^{K^-} - x_i^{K^+} \right)
\]

for displacement components \( \mathbf{u}_i \) and electric potential \( \mathbf{F}_i \), which are caused by averaged strains \( \mathbf{S}_i \) and electric fields \( \mathbf{E}_i \), respectively. The averaged values are calculated by integration over unit cell volume \( V \)

\[
\bar{S}_i = \frac{1}{V} \int_S S_i dV, \quad \bar{E}_i = \frac{1}{V} \int_E E_i dV, \quad \bar{T}_i = \frac{1}{V} \int_T T_i dV, \quad \bar{D}_i = \frac{1}{V} \int_D D_i dV.
\]

(3)

For applying the periodic boundary conditions to the finite element model of the unit cell identical meshes on opposite surfaces must be ensured. Furthermore for every pair of opposite nodes appropriate constraint equations must be defined.

Figure 1. Unit cells for square, hexagonal, rhombic and random arrangement of fibers

Figure 2. Notations for surfaces of the unit cell
3. FINITE ELEMENT MODELING

For finite element calculations three-dimensional multi-field elements from FE package ANSYS were used. Furthermore for modeling and applying the constraint equations the advantages of the ANSYS Parametric Design Language (APDL) could be used. This provides a comprehensive tool for highly automated generation of unit cell FE models based on certain input parameters.

Special algorithms were developed for geometric modeling of cells with randomly distributed uni-directional piezoelectric fibers. The calculation of the random fiber distribution is based on a modified random sequential adsorption (RSA) algorithm (Wang, 1998). In a separate program this algorithm is used to create a random distribution of circles in $x_1$-$x_2$ plane. The results are prepared as input data for ANSYS where the further generation of the FE model is done. This includes also extrusion of circles in $x_3$ direction and cutting fibers at surfaces of the cell by Boolean operations.

The RSA algorithm starts with random center coordinates of the first circle with a prescribed radius. Then a next circle is randomly generated. It is checked for non-overlapping with previously deposited circle. If there is no overlap between the current circle and actual circle then it is placed on the plane. Otherwise it is rejected. A second check is made for intersection with the boundary of the cell. In case of intersection it is copied to the opposite edge with the distance of the cell width to ensure periodicity. So more and more circles are created at random positions. This process will be terminated when a desired volume fraction is achieved or when no more circles can be added because of the jamming limit. For circles with equal diameters a volume fraction of around 55% is possible. The algorithm was extended to fibers with different diameters. When no more circles can be placed the diameter is reduced by a certain amount and further circles can be generated. With this modification a volume fraction up to around 80% can be reached.

Figure 3 show the typical steps of the generation process. In Fig. 4 the cutting process is demonstrated for cells with equal fiber diameter and with different fiber diameters.

The generation process can be controlled by some input parameters like size of cell, starting fiber diameter and desired volume fraction. Furthermore a certain minimal distance between the fibers must be ensured to generate a suitable finite element mesh.

For applying the periodic boundary conditions to the finite element model the unit cell must have identical meshes on opposite surfaces. This is necessary to define constraint equations between opposite nodes. To achieve identical mesh configurations in a first step surface meshes are generated on surfaces $A^-$ and $B^-$. Then these meshes are copied to $A^+$ and $B^+$ and in a second step the volume mesh is generated based on the pre-meshed surfaces. Figure 5 show meshed models for different cell types. Because of the transverse behavior one element in $x_3$ direction is sufficient.
4. CALCULATION OF EFFECTIVE COEFFICIENTS

With nine load cases it is possible to predict the full set of anisotropic effective coefficients. To demonstrate the algorithm the calculation of effective coefficients $C_{13}^{\text{eff}}$, $C_{23}^{\text{eff}}$, $C_{33}^{\text{eff}}$, … is explained in detail. For this case the boundary conditions have to be applied to the unit cell in such a way that, except the strain in $x_3$ direction ($\varepsilon_{33}$), all other mechanical strains and electrical fields ($E_i$) become zero. This can be achieved by applying appropriate constraint equations between opposite nodal pairs. The constraint equations must be defined so that all displacement differences are zero except the displacement differences between $u_3^C$ and $u_3^C$. Here a unit value is used for the difference. To avoid rigid body motion the corner point ($A$, $B$, $C$) is fixed in all directions. To make electric field $E_3$ zero, the constraint equations for all nodal pairs are defined with zero electric potential difference and the above mentioned corner node is set to zero electric potential.

For the calculation of the total average values $\bar{S}_{33}$, $\bar{T}_{11}$, $\bar{T}_{22}$, $\bar{T}_{33}$, … according to Eq. (3), the integral is replaced by a sum over averaged element values multiplied by the respective element volume. Using these total average values the coefficients $C_{13}^{\text{eff}}$, $C_{23}^{\text{eff}}$, $C_{33}^{\text{eff}}$, … can be calculated from the matrix Eq. (1). Due to zero strains and electric fields, except $\bar{S}_{33}$, the first row becomes $\bar{T}_{11} = C_{13}^{\text{eff}} \bar{S}_{33}$. Then $C_{13}^{\text{eff}}$ can be calculated as the ratio of $\bar{T}_{11}/\bar{S}_{33}$. Similarly $C_{23}^{\text{eff}}$ can be evaluated as the ratio of $\bar{T}_{22}/\bar{S}_{33}$ from the second row of matrix Eq. (1) and so on.

Analogously all other coefficients whose formulae are based on average normal strain, can be evaluated applying the appropriate boundary conditions.

Special attention must be given to the coefficients, which are based on averaged shear strains, i.e. $C_{44}^{\text{eff}}$, $C_{55}^{\text{eff}}$, $C_{66}^{\text{eff}}$, $C_{15}^{\text{eff}}$ and $\varepsilon_{24}^{\text{eff}}$. Here a displacement differences must be set for opposite tangential displacements. Similar for calculation of piezoelectric and dielectric coefficients appropriate constraint equations with electric potential differences must be defined.

5. RESULTS AND DISCUSSION

Various investigations were made for evaluation of the developed algorithm and the different unit cell types. In this paper only a selection can be presented.

Square and hexagonal cells have been treated in many publications. The rhombic cell includes these types as special cases with skew angles of 90 and 60 degrees. The proposed general algorithm allows modeling of rhombic cells with arbitrary skew angles and arbitrary volume fractions in the range of geometrical limits.

For skew angles of 40 and 80 degrees the calculated effective coefficients shall be compared with analytical results. For the out-of-plane coefficients such results are available from asymptotic homogenization method (AHM) (Guinovart-Díaz et al., 2001). Material values are taken from Pastor (1997) with PZT-5 for fiber and epoxy for matrix.

Figure 6 show the comparisons between the presented FEM model and AHM. A good agreement can be observed. A comparison between $C_{44}^{\text{eff}}$ and $C_{55}^{\text{eff}}$ as well as $\varepsilon_{24}^{\text{eff}}$ and $\varepsilon_{15}^{\text{eff}}$ show obviously the violation of transverse isotropy for rhombic cells.

In Fig. 7 results are shown for a cell with random fiber distribution in comparison with other models and analytical self-consistent scheme by Levin (1999). In the second plot $C_{11}^{\text{eff}}$ and $C_{22}^{\text{eff}}$ are compared which shows that for random fiber distribution nearly a transverse isotropy is existent.
Figure 6. FEM and AHM results for selected elastic and piezoelectric effective coefficients for rhombic cells with two different angles

In Fig. 8 the behavior of selected piezoelectric and dielectric coefficients against other models can be observed. The composite with random distribution of fibers provides in general slightly higher values.
Figure 7. $C_{11}^{\text{eff}}$ for cell with random fiber distribution and comparison between $C_{11}^{\text{eff}}$ and $C_{22}^{\text{eff}}$

Figure 8. Piezolectric coefficient $\varepsilon_{15}^{\text{eff}}$ and dielectric coefficient $\varepsilon_{11}^{\text{eff}}$ for cell with random fiber distribution

6. CONCLUSIONS

A powerful algorithm for calculation of effective mechanical, piezoelectric and dielectric coefficients is presented which can be used to composites with arbitrary fiber arrangements. The focus is set to rhombic cells and cells with random fiber distribution. Especially for these cells it is possible to calculate anisotropic material constants. Automated tools for generation of the cells provide convenient possibilities for practical use. Some presented results give an impression of the capability of the developed algorithm.

7. REFERENCES


8. RESPONSIBILITY NOTICE

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