Numerical homogenization and optimization of smart composite materials

Ulrich Gabbert, Sreedhar Kari, Niels Bohn and Harald Berger

Abstract The paper presents a numerical homogenisation approach to calculate the effective properties of fibre and particle reinforced materials including smart and multifunctional materials with a focus on piezoelectric fibre composites applied to control vibration and noise radiation of structures. This finite element based homogenisation is used to optimise the material distribution at the micro-scale by applying an evolutionary approach to receive a desired global behaviour of a structure at the macro-scale.

1 Introduction

Composite materials play a major role in meeting the increasing demand of the industry for lightweight and low-cost structures. Compared to classical monolithic engineering materials, composites offer higher specific strength and specific stiffness values.

Smart piezoelectric fiber and particle reinforced composites are a new class of materials, which are increasingly used to actively influence structures to reduce, e.g., the vibration and the noise radiation [10]. Recently, composite piezoelectric materials have been developed by combining piezoceramic fibers with passive non-piezoelectric polymers, such receiving active fibrous composites.

A number of methods have been developed to predict the homogenized material properties of composites, which are required to perform static and dynamic structural analysis. Analytical approaches ([1], [17]) are not capable of predicting the response to general loadings, i.e., they do not give the full set of overall material parameters. Semi analytical, Hashin/Shtrikman-type

Ulrich Gabbert, Sreedhar Kari, Niels Bohn and Harald Berger
Institute of Mechanics, Otto von Guericke University of Magdeburg, Universitätsplatz 2, D-391106 Magdeburg, Germany, e-mail: ulrich.gabbert@mb.uni-magdeburg.de

and other bounds for describing the complete overall behavior (i.e., providing all elements of the material tensors) have been developed (see [4], [7], [15], [16]), which are useful tools for theoretical considerations. However, the range between the bounds can be very wide for certain effective moduli. Mechanical mean field type methods have been extended to include electro-elastic and thermal effects based on an Eshelby-type solution [9], [14], [18]. The restrictions of the methods can be overcome by employing periodic micro field approaches where the fields are typically solved numerically with high resolution, e.g., by the finite element method [11]. Most of these methods are restricted to regular packings of fibers (rectangular and hexagonal). However, in practical situations the fibers are aligned in their longitudinal direction, while their arrangement in the matrix in transverse cross-section is usually distributed randomly. To the knowledge of the authors, there is not much development to handle the problem of transversely randomly distributed multi-field fiber composites properly. The aim of the present paper is to present a numerical finite element based approach to predict the full set of piezoelectric, dielectric, and mechanical effective material coefficients of such composites with complex geometrical reinforcements (for details see [5], [13]). This approach is used to optimize the microstructure (fiber distribution, fiber orientation, fiber-volume fraction etc.) with respect to an objective function defined at the macrostructure.

2 Numerical homogenization

Numerical finite element based micromechanical methods provide a powerful general tool to calculate the homogenized properties of fiber and particle reinforced and multi-field composite materials, such as piezoelectric fiber composites, through an analysis of a periodic representative volume element (RVE).

In piezoelectric fiber composites an electric potential gradient causes deformations (converse piezoelectric effect), while strains cause an electric potential gradient in the material (direct piezoelectric effect). The behavior of a piezoelectric medium in low electric and mechanical applications can be described by the following linear piezoelectric constitutive equations, which correlate stresses T, strains S, electric fields E, and electrical displacements D as follows (the superscript t for transpose)

$$\begin{bmatrix} T \\ D \end{bmatrix} = \begin{bmatrix} C & -e^t \\ e & \varepsilon \end{bmatrix} \begin{bmatrix} S \\ E \end{bmatrix}, \tag{1}$$

where C is the elasticity matrix, ε is the permittivity matrix, and e is the piezoelectric strain coupling matrix.

The numerical finite element based calculation of the mean values of a

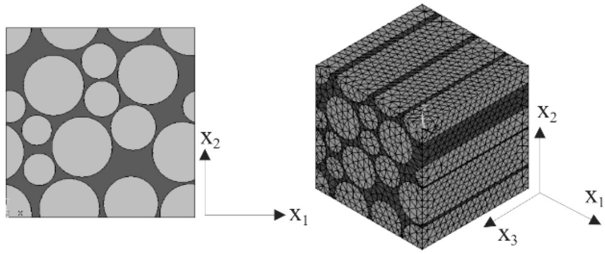

Fig. 1 Representative unit cell (left) and corresponding finite element mesh (right)

piezoelectric fiber composite is based on a representative volume element (RVE), which captures the global behaviour of the composite. If the fibers are randomly distributed the size of the RVE with respect to the diameter of the fibers is an important criterion. Our approach applies the random sequential absorption algorithm (RSA) [19] modified to provide a minimum distance between any two fibers and for periodicity between opposite boundary surfaces. In this algorithm the coordinates of the center of the fibers are generated randomly step by step. A new generated midpoint coordinate is checked for non-overlapping conditions with previously placed fibers. If there is no overlapping and the periodicity is satisfied, then the fiber will be placed on the plane. If a fiber cuts the boundary of the unite cell, then on the opposite site also a fiber has to be placed to grantee the periodicity. This process will be terminated when the desired volume fraction is achieved or when no more fibers can be added because of the jamming limit, which can occur at a volume fraction higher than 55%. For higher volume fractions, different diameters of fibers are used, and these are placed on the x_1-x_2 plane in a descending manner. With this approach the volume fraction achieved is about 80% with an adequate finite element meshing. Figure 1 shows an example of such a generated RVE with variable diameters of fibers, and their corresponding 3D finite element mesh.

Composite materials can be represented as a periodical array of the RVEs, where each RVE has the same deformation mode, and there is no separation or overlap between the neighboring RVEs after deformation. These periodic boundary conditions described in Cartesian coordinates are given by [17]

$$u_i = \bar{S}_{ij} x_j + v_i \tag{2}$$

$\bar{S}_{ij}$ denotes the average strains, and v_i is the periodic part of the displacement components (local fluctuation) on the boundary surfaces. The difference of the displacements of a pair of opposite boundary surfaces points (with their normal along the x_i axis) is

$$u_i^{K^+} - u_i^{K^-} = \bar{S}_{ij} \left(x_j^{K^+} - x_j^{K^-} \right), \tag{3}$$

where the index 'K^+' means along the positive x_i direction, and 'K^-' means along the negative x_i direction on the corresponding surfaces of the 3D RVE. The local fluctuations are identical on two opposing faces and disappear in the difference. Similarly, the periodic boundary conditions for the electrical potential are given as

$$\Phi^{K^+} - \Phi^{K^-} = \bar{E}_i \left(x_i^{K^+} - x_i^{K^-} \right), \tag{4}$$

where Φ represents the voltage and $\bar{E}_i$ represents the average electric field.

The average mechanical and electrical properties of a unit cell, calculated by

$$\begin{aligned} \bar{S}_{ij} &= \frac{1}{V}\int_V S_{ij} dV \quad , \quad \bar{T}_{ij} = \frac{1}{V}\int_V T_{ij} dV, \\ \bar{E}_i &= \frac{1}{V}\int_V E_i dV \quad , \quad \bar{D}_i = \frac{1}{V}\int_V D_i dV, \end{aligned} \tag{5}$$

are finally used to calculate the mean values of the material tensor with help of equation (1) (for details see [13]).

All finite element calculations are made with the commercial FE package ANSYS for fully coupled electromechanical analyses. An APDL-script allows performing all required calculations to evaluate finally the effective material properties automatically in a batch processing, which provides a powerful tool for a fast calculation of homogenized material properties for composites with a great variety of inclusion geometries.

3 Optimization of fiber reinforced composites

The optimization goal is the minimization of an appropriate objective function

$$\min_{\mathbf{x}\in S} f(\mathbf{x}) \ , \quad S = \left\{ \mathbf{x} \in \Re^N \left| h_i(\mathbf{x}) = 0 \, , \; g_j(\mathbf{x}) \leqslant 0 \right. \right\}, \tag{6}$$

where $\mathbf{x}$ is the N-dimensional vector of design variables, $h_i(\mathbf{x})\, , \; i = 1, ..., n$ and $g_j(\mathbf{x})\, , \; j = 1, ..., m$ are the equality constraints and the inequality constraints, respectively. To solve the optimization problem various methods have been developed [12], which require the computation of gradients. Their operability can only be guaranteed if the objective function is continuously differentiable and uni-modal. When composite materials are considered, the objective functions are more likely to be non-smooth, non-differentiable and multimodal [20]. In such cases we suggest direct methods, which apply principles of natural evolution (recombination, mutation and selection) to a set μ of feasible solutions, the individuals

$$\mathbf{w} = [x_1,\ x_2,\ \cdots\ x_N,\ \sigma_1,\ \sigma_2,\ \cdots\ \sigma_{N_\sigma}]\ ,\quad k = 1, ..., \mu \tag{7}$$

N stands for the problem dimension, x_i represent the design variables of the optimisation problem, and σ_i are the step-sizes for the mutation process. The generation of new solutions starts with recombination, where a number of $\lambda \geq \mu$ offspring individuals are created by exchanging or averaging the properties of randomly selected parents

$$w'_{ki} = \begin{cases} w_{pi} \text{ or } w_{qi} \\ (w_{pi} + w_{qi})/2 \end{cases} \quad k = 1, ..., \lambda, \quad i = 1, ..., N, \quad p, q \sim U(1, \mu). \tag{8}$$

For more recombination variants see [3]. A mutation is carried out by the application of small random changes in each component of an individual. The process starts with the variation of the mutation step-sizes as

$$\sigma''_{ki} = \sigma'_{ki} \cdot h\left(\bar{z}_k,\ \tau_1,\ \cdots\ \tau_r\right). \tag{9}$$

The function h depends on the standard normal distributed random variants $\bar{z} \sim N(1, 0)$ as well as on r heuristic factors τ_j, $j = 1, ..., r$ (see [2], [3], [6]). The object variables are then mutated according to

$$x''_{ki} = x'_{ki} + z_{ki}\ ,\quad k = 1, ..., \lambda, \tag{10}$$

where $z_{ki} \sim N(0, \sigma''_{ki})$ is a normal distributed random variant which depends on the individual mutation step-sizes. The population consists finally of λ offsprings

$$\mathbf{w}'' = \left[x''_1,\ x''_2,\ \cdots\ x''_N,\ \sigma''_1,\ \sigma''_2,\ \cdots\ \sigma''_{N_\sigma}\right]\ ,\quad k = 1, ..., \lambda. \tag{11}$$

After the evaluation of the objective function is performed for each individual, the μ best individuals are selected to become the parents for the next iteration.

The generation loop is repeated until a termination criterion, such as a lower limit for the mutation step-sizes, is fulfilled. A general software tool has been developed on the basis of evolution strategies with an interface to the commercial finite element code ANSYS. Our software possesses a modular structure, allowing for the implementation of various intermediate steps in the optimization process.

4 Results and Discussion

For the calculation of effective coefficients we consider a composite with circular piezoelectric (PZT-5) fibers uniformly polarized along the x_3 direction

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	e_{15}	e_{13}	e_{33}	ε_{11}	ε_{33}
PZT-5	12.1	7.54	7.52	11.1	2.11	2.28	12.3	5.4	15.8	8.11	7.35
Polymer	0.386	0.257	0.257	0.386	0.064	0.064	-	-	-	0.07965	0.07965

Table 1 Material properties of the composite constituents fiber (PZT-5) and matrix, (Polymer) ($C_{ij}\,[GPa]\,;\ e_{ij}\,[C/m^2]\,;\ \varepsilon_{ij}\,[nF/m]$)

50% volume fraction	C_{11}	C_{12}	C_{22}	C_{23}	C_{33}	C_{13}	C_{66}	C_{44}
Same diameter	9.40	4.93	9.07	5.47	31.96	5.58	1.87	1.99
Random diameter	9.23	4.93	9.13	5.49	31.91	5.52	1.87	2.0

50% volume fraction	e_{15}	e_{13}	e_{33}	ε_{11}	ε_{33}
Same diameter	0.0021	-0.224	9.81	0.273	3.86
Random diameter	0.0021	-0.219	9.80	0.266	3.85

Table 2 Comparison of piezoelectric fibers, ($C_{ij}\,[GPa]\,;\ e_{ij}\,[C/m^2]\,;\ \varepsilon_{ij}\,[nF/m]$)

and embedded randomly in a soft non-piezoelectric material (polymer) in the transverse cross section (Table 1).

4.1 Effect of the Fiber Diameter on Effective Material Properties

Investigations are performed to study the influence of the diameter of piezoelectric fibers on the effective material properties of these composites. The fluctuations (error) of effective material properties around the mean value, which are obtained from the ensemble averages of the effective material properties of five RVE samples, are negligible.

The numerical homogenization techniques are also applied to two different types of the RVE models, one with an identical diameter of all piezoelectric fibers and another with a random diameter of fibers between 0.32mm and 0.12mm at 50% volume fraction. In both cases, also five different RVE samples are considered, and the effective material properties are obtained from the ensemble average of the effective material properties. It is observed that the differences in the effective material properties are again negligible, and the differences between the random and identical diameter of piezoelectric fibers are at most 2% (see Table 2).

4.2 Influence of the fiber arrangement

The effective electrical and mechanical properties of transversely randomly distributed uni-directional piezoelectric fiber composites are evaluated for different volume fractions up to 80%. The effective material properties, which

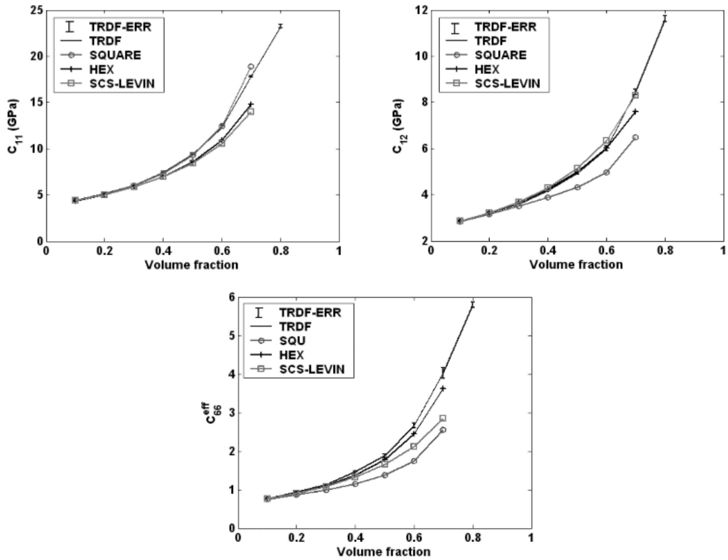

Fig. 2 Comparison of effective mechanical properties of transversely randomly distributed piezoelectric fiber composites (TRDF) with square (SQUARE) and hexagonal (HEX) array with the analytical self-consistent scheme by Levin [14] (SCS-Levin).

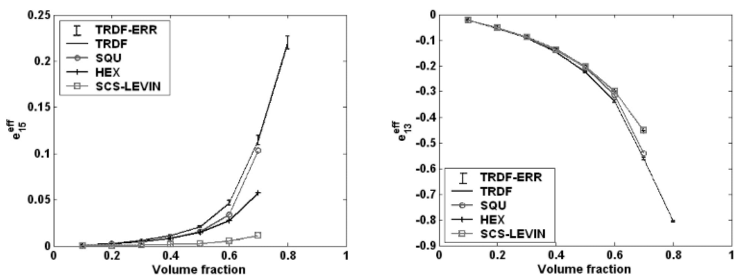

Fig. 3 Comparison of effective piezoelectric properties of transversely randomly distributed fiber composites (TRDF) with square (SQUARE) and hexagonal (HEX) array with the analytical self-consistent scheme by Levin [14] (SCS-Levin).

are obtained for these cases, are compared with a square arrangement and a hexagonal arrangement of the piezoelectric fibers. For the square arrangement the maximum theoretically achievable volume fraction is 78.54%. Due to the meshing limits with our finite element approach a maximum volume fraction of 70% can be generated only. Figs. 2 and 3 represent the effective mechanical and piezoelectric properties, respectively, calculated for different fiber arrangements in the composite. The figures compare the numerically calculated results based on different fiber arrangements, such as the transversely randomly distributed arrangement (TRDF), the square arrangement (SQUARE) and the hexagonal arrangement (HEX) with the results calculated by the self consistent schema (SCS-LEVIN) [14]. From Fig 2 it can be observed that the transverse mechanical properties are tending to increase for transversely randomly distributed composites when compared with regular array composites, especially for the hexagonal array, but not in all other cases. As a comparison between the square array and the hexagonal array, the hexagonal array has a 6-fold axis of symmetry along fiber direction, and results in a transverse isotropic behavior, i.e., $C_{11}^{\mathrm{eff}} - C_{22}^{\mathrm{eff}} = 2C_{66}^{\mathrm{eff}}$, whereas for the case of the square array, it has only 4-fold axis of symmetry, and it will give rise to a tetragonal behavior resulting in a higher transverse stiffness. For the transverse shear modulus C_{66}^{eff}, it is observed that the square array composite has a lower transverse shear modulus, and the hexagonal array composite has a higher value and satisfies the transverse isotropy.

In general, from our analysis it can be observed that the assumption of a transversely randomly distributed fiber composites results in higher transverse material properties when compared with a regular array of fiber arrangement. The longitudinal material properties are almost the same like for a regular array of composites. Also the numerical results of the effective material coefficients like C_{11}^{eff}, $\varepsilon_{11}^{\mathrm{eff}}$ along the transverse direction of a transversely randomly distributed fiber composites match well with the results of SCS at lower volume fractions in the considered fraction range between 10% and 40%. Beyond this volume fraction range, the effective coefficients of SCS are underestimated.

The transverse isotropy was checked for all generated RVE samples and for all effective material coefficients.

4.3 Optimization of a short fiber composite

We consider a quadratic plate with a hole in the middle consisting form a polysulfon matrix being reinforced by short aramid fibers and loaded in x-direction by a distributed load (for details see [8]). The amount of fibers in the plate is limited to a prescribed average fiber density. The purpose of the optimization is to distribute a fixed amount of fibres in the matrix material in such a way, that a maximal structural stiffness is obtained under restrictions concerning the maximal principal stress and the average fibre density in the plate. A (10, 70)-ES with discrete recombination and Schwefels mutation type is applied [6].

Fig. 4 shows the optimal fiber orientations and the directions of the principal stresses. The fibres concentrate in regions close to the upper side of the hole, where the maximal stresses occur. A similar result is published in [8]. The optimization algorithm converges after about 80 generations leading to

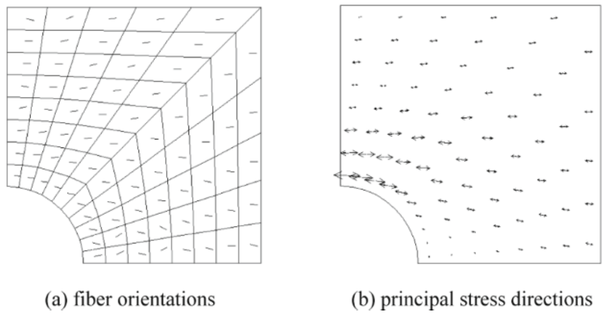

Fig. 4 Optimal short fibre orientations and principal stress directions

a decrease of 49% in the objective function when compared to the random initial design.

5 Conclusion

A finite element based numerical homogenization approach to evaluate the effective material properties of active piezoelectric fiber composites is presented. A generalized procedure has been developed to calculate all effective coefficients automatically for all volume fractions based on the ANSYS Parametric Design Language. It reduces the manual work and time and can be used as a template to evaluate the effective coefficients of piezoelectric fiber composites with arbitrary arrangement of fibers. It is shown that evolution strategies are a reliable and efficient method for the optimization of composite structures. The algorithm operates on a set of feasible solutions and requires no derivatives of the objective function. It has superior global search qualities and can be used even for non-differentiable, non-smooth and multimodal problems, which arise frequently in the context of the optimization of composite structures. The test example underlines the good research properties of evolution strategies.

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