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# IDENTIFICATION OF MATERIAL PARAMETERS USING HOMOGENIZATION APPROACH AND SFEPY SOFTWARE

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**Abstract:** The finite element solver SfePy and Python modules are used to identify the material parameters of the carbon fibers and the epoxy matrix which constitute a unidirectional long-fiber composite. The mathematical model of the heterogeneous structure is base on two-scale homogenization method using the linear material models. The computed responses are compared to the experimental data in an optimization loop in order to obtain the elastic modules and the Poisson's ratios of the composite constituents. The geometry of the unit cell representing the material microstructure is generated artificially using an event-driven algorithm.

**Keywords:** two-scale homogenization; material identification; finite element method; mesh generation

## Introduction

The material parameters of the constituents of industrially manufactured composites are usually not provided or are defined approximately. The numerical simulations of the mechanical behavior of heterogeneous structures are essential part of research and development of new modern mechanical components and appliances. To achieve an agreement between experiments and numerical simulations, the exact knowledge of the material parameters of the constituents is crucial.

This contribution is focused on the identification of the material parameters of composite structures consisting of unidirectional long fibers and a matrix. The volume fractions of structure components are determined with help of a scanning electron microscope. These values are used to generate equivalent artificial periodic reference cell representing the geometrical arrangement of the fibers at the microlevel of the structure. The reference cell is employed in the multi-scale model which is used to describe the mechanical behavior of a composite sample. The multi-scale analysis is embedded in an optimization loop in order to identify elastic modules and Poisson's ratios of the matrix and unidirectional fibers.

The multi-scale finite element analysis is implemented in the Python based package *SfePy*, see [1], and the identification procedure uses Python optimization functions from the *Scipy* module.

## Generating a unit cell

The volume fraction of the unidirectional fiber composite was determined using the images of the microstructure obtained with a scanning electron microscope. Based on the determined volume ratio, an artificial geometry representing the composite structure is built up with the event-driven algorithm described in [4]. The starting point for the algorithm is a square domain and a finite number of small circles. The circles are moving along straight lines, interfering with each other and growing until the required volume fraction is achieved. If any circle reaches the border of the square domain, it passes through that border and appears at the opposite side. This process results in the periodic structure with randomly distributed circles representing the composite fibers. The artificially generated periodic geometry is the input to the GMSH mesh generator, see [3], which creates the finite element mesh for the multi-scale numerical simulation.

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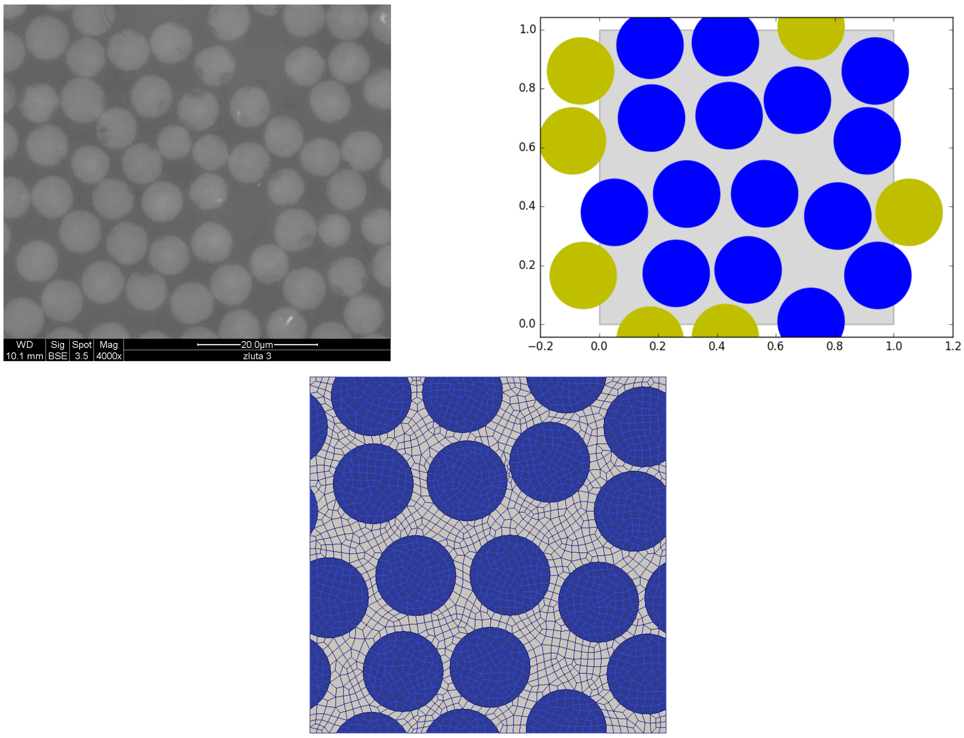


**Figure 1:** Top left – the electron microscope scan of the composite structure, the light parts are the fibers, the dark part is the matrix; Top right – the generated periodic geometry with the randomly distributed fibers; Bottom – the periodic finite element mesh representing the composite microstructure.

## Two-scale linear elastic model

We assume that the geometry of the composite structure can be characterize by a periodically repeated representative cell constituted by the carbon fibers and epoxy matrix. To describe the mechanical behavior of such a heterogeneous structure we use the two-scale homogenization method applied to the linear elastic problem. The method based on the two scale convergence or the unfolding operator techniques, see [2], can be used for the asymptotic analysis of the problem for $\varepsilon \longrightarrow 0$, where $\varepsilon$ is the scale parameter reflecting the size of a periodic unit. The homogenization procedure results in the decoupled local microscopic and the global macroscopic subproblems. At the microscopic level, the problem for the so-called characteristic responses is solved. The responses are used to evaluate the homogenized elastic coefficients that are employed in the homogenized problem to solve the macroscopic responses.

The heterogeneous linear elastic medium with a periodic lattice occupies an open bounded domain $\Omega \subset \mathbb{R}^3$ and its microstructure is represented by the periodic cell $Y$ which is decomposed into the fibers $Y_f$ and matrix $Y_m$, see Fig. 2. The microscopic problem is expressed in terms of the characteristic response $\boldsymbol{\chi}^{rs}$: find $\boldsymbol{\chi}^{rs} \in H_\#(Y)$ such that:

$$\int_Y D_{ijkl} e^y_{kl}(\boldsymbol{\chi}^{rs}) e^y_{ij}(\boldsymbol{\omega})\,\mathrm{dY} = \int_Y D_{ijkl} e^y_{kl}(\boldsymbol{\Pi}^{rs}) e^y_{ij}(\boldsymbol{\omega})\,\mathrm{dY}, \qquad \forall \boldsymbol{\omega} \in H_\#(Y), \tag{1}$$

where $\Pi^{rs}_i = y_s \delta_{ri}$, $\boldsymbol{y}$ is the microscopic coordinate, $\delta$ is the Kronecker delta symbol, $\boldsymbol{e}^y$ is the linear strain tensor, $\boldsymbol{D} = \boldsymbol{D}(\boldsymbol{y})$ is the elasticity tensor (with respect to $\boldsymbol{y}$ coordinate) and $H_\#(Y)$ is the Sobolev space of $Y$-periodic functions. Using the characteristic functions, the homogenized elasticity tensor $\boldsymbol{D}^H$ can be express as:

$$D^H_{ijkl} = \frac{1}{|Y|} \int_Y D_{pqrs} e^y_{rs}(\boldsymbol{\Pi}^{kl} - \boldsymbol{\chi}^{kl}) e^y_{pq}(\boldsymbol{\Pi}^{ij} - \boldsymbol{\chi}^{ij})\,\mathrm{dY}. \tag{2}$$

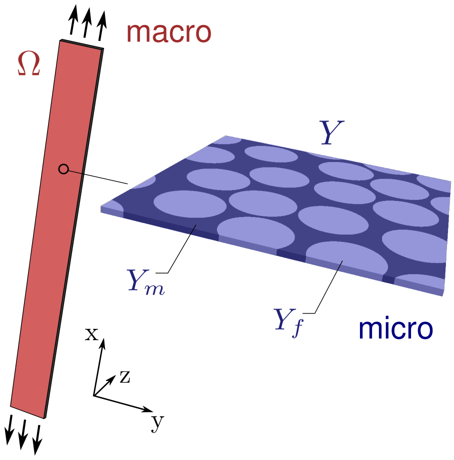


**Figure 2:** Domain $\Omega$ representing the macroscopic sample and the microscopic domain $Y$ (representative cell) decomposed into fibers $Y_f$ and matrix $Y_m$ subdomains.

The macroscopic problem is solved for the unknown macroscopic displacements $\boldsymbol{u}^0 \in H(\Omega)$:

$$\int_{\Omega} D^H_{ijkl} e^x_{kl}(\boldsymbol{u}^0) e^y_{ij}(\boldsymbol{v}) \, \mathrm{dV} = \int_{\Gamma_t} v_i t_i \, \mathrm{dS}, \qquad \forall \boldsymbol{v} \in H_0(\Omega), \tag{3}$$

where $\boldsymbol{e}^x$ is the macroscopic linear strain tensor and $H_0(\Omega)$ is the set of admissible displacements with a zero value at the Dirichlet boundary.

The two-scale mathematical model presented above is implemented in the Python based finite element solver *SfePy*, see [1].

## Identification of material parameters

We consider linear transversely isotropic material model for the carbon fibers. This model is described by five material parameters which are: Young's modulus $E_1^f$ in the fiber axis direction, Young's modulus $E_2^f$ in the radial direction, shear modulus $G_{12}^f$ in the planes parallel to the fiber axis, Poisson's ratio $\nu_{12}^f$ in the planes parallel to the fiber axis and Poisson's ratio $\nu_{23}^f$ in the planes perpendicular to the fiber axis. For the epoxy matrix, the linear isotropic model with only two material parameters, i.e. Young's modulus $E^m$ and Poisson's ratio $\nu^m$, is used.

Several composite specimens with different fiber orientations (0, 10, 20, 30, 40, 50, 60, 70, 80 and 90 degrees) were subjected to the tensile test in order to obtain force-elongation dependencies, see [5], [6] and Fig. 3. The slopes $k^i_{exp}$, $i \in \{0, 10, \dots 90\}$, of the linearized experimentally detected dependencies were used in the objective function of an optimization procedure. The identification algorithm is implemented in the Python language with help of *optimize.fmin_tnc()* function from the *Scipy* optimization module. The following objective function is minimized in the optimization process:

$$\phi(\mathbf{x}) = \sum_{i \in \{0,10,\dots 90\}} \left( 1 - \frac{k^i_{comp}(\mathbf{x})}{k^i_{exp}} \right)^2, \tag{4}$$

where $k^i_{comp}$ is the computed slope of the force-elongation tangent lines for a given fiber orientation and $\mathbf{x} = [E_1^f, E_2^f, \nu_{12}^f, G_{12}^f, E^m, \nu^m]$ is the vector of the unknown material parameters. The Poisson's ratio $\nu_{23}^f = 0.4$ is given by the manufacturer.

The each iteration step of the optimization loop includes the following operations: 1) solution of the microscopic subproblem, evaluation of the homogenized elasticity tensor; 2) solution of the macroscopic

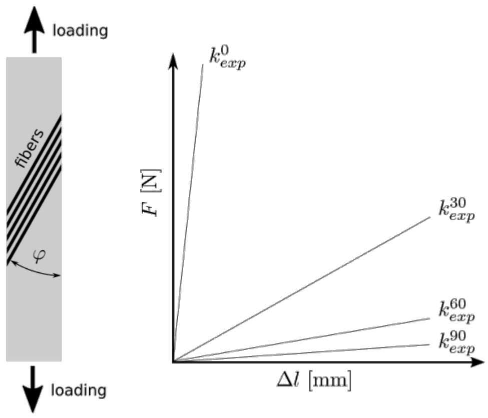


**Figure 3:** Left – loading of the composite sample; Right – linearized tensile dependencies for the different fiber orientations.

problems for different fiber orientations (this is done by rotation of the elasticity tensor); 3) evaluation of the objective function. The objective function values and the sought material parameters during the optimization process are depicted in Fig. 4. In Tab. 1, the initial and optimized parameters are presented.

| | $E_1^f$ [GPa] | $E_2^f$ [GPa] | $\nu_{12}^f$ [-] | $G_{12}^f$ [GPa] | $E^m$ [GPa] | $\nu^m$ [-] |
|---|---|---|---|---|---|---|
| initial | 150 | 50 | 0.2 | 50 | 50 | 0.4 |
| optimized | 164.29 | 18.95 | 0.197 | 50.10 | 3.23 | 0.369 |

**Table 1:** The initial and optimized material parameters.

## Conclusion

The presented approach and the employed software tools seem to be suitable for the identification of the material parameters of heterogeneous structures. The calculated elastic modules and Poisson's ratios of the carbon fibers and epoxy matrix are in expected ranges.

### Acknowledgement

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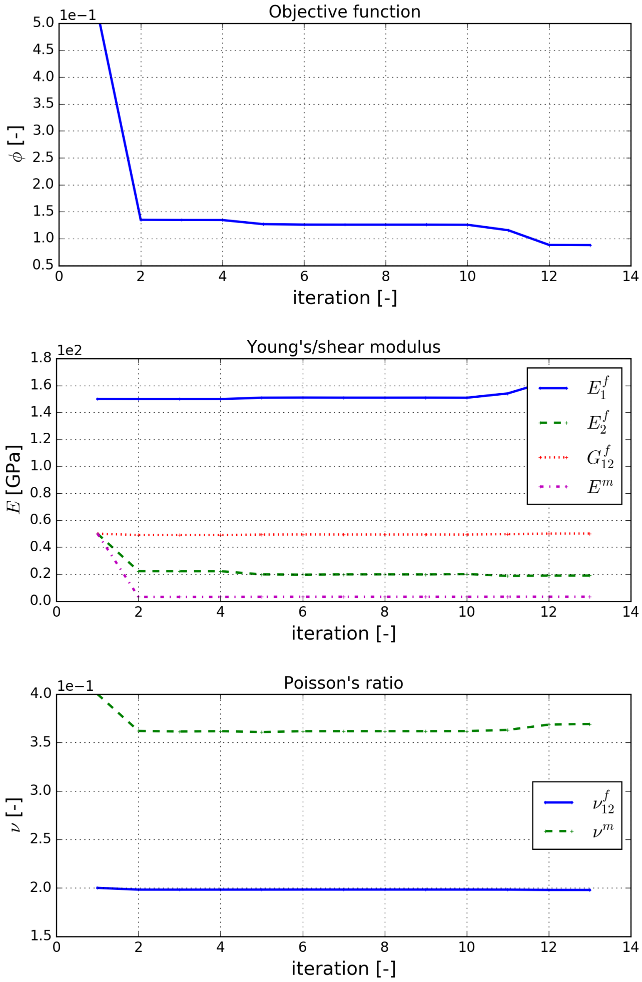


**Figure 4:** Evolution of the objective function values and the sought material parameters during the optimization process.

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