Homogenization of plain weave Carbon-Carbon composites with imperfect microstructure

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Abstract

A two-layer statistically equivalent periodic unit cell is offered to predict a macroscopic response of plain weave multilayer carbon-carbon textile composites. Falling short in describing the most typical geometrical imperfections of these material systems the original formulation presented in [1] is substantially modified, now allowing for nesting and mutual shift of individual layers of textile fabric in all three directions. Yet, the most valuable asset of the present formulation is seen in the possibility of reflecting the influence of negligible meso-scale porosity through a system of oblate spheroidal voids introduced in between the two layers of the unit cell. Numerical predictions of both the effective thermal conductivities and elastic stiffnesses and their comparison with available laboratory data and the results derived using the Mori-Tanaka (MT) averaging scheme support credibility of the present approach, about as much as the reliability of local mechanical properties found from nanoindentation tests performed directly on the analyzed composite samples.

Key words: balanced woven composites, material imperfections, statistically equivalent periodic unit cell, image processing, X-ray microtomography, nanoindentation, soft computing, numerical homogenization, steady-state heat conduction

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1. Introduction

Despite a significant progress in theoretical and computational homogenization methods, material characterization techniques and computational resources, the determination of overall response of structural textile composites still remains an active research topic in engineering materials science [2]. From a myriad of modeling techniques developed in the last decades (see e.g. review papers [3, 4, 5]), it is generally accepted that detailed discretization techniques, and the Finite Element Method (FEM) in particular, remain the most powerful and flexible tools available. The major weakness of these methods, however, is the fact that their accuracy crucially depends on a detailed specification of the complex microstructure of a three-dimensional composite, usually based on two-dimensional micrographs of material samples, e.g. [6, 7, 8, 5, and reference therein]. Such a step is to a great extent complicated by random imperfections resulting from technological operations [9, 10], which are difficult to be incorporated to a computational model in a well-defined way. If only the overall, or macroscopic, response is the important physical variable, it is sufficient to introduce structural imperfections in a cumulative sense using available averaging schemes such as Voight/Reuss bounds [11] or the Mori-Tanaka method [12]. When, on the other hand, details of local stress and strain fields are required, it is convenient to characterize the mesoscopic material heterogeneity by introducing the concept of a Periodic Unit Cell (PUC).

While application of PUCs in problems of strictly periodic media has a rich history, their introduction in the field of random or imperfect microstructures is still very much on the frontier, despite the fact that the roots for incorporating basic features of random microstructures into the formulation of a PUC were planted already in mid 1990s in [13]. Additional extension presented in [14], see also our work [15] for an overview, gave then rise to what we now call the concept of Statistically Equivalent Periodic Unit Cell (SEPUC). In contrast with traditional approaches, where parameters of the unit cell model are directly measured from available material samples, the SEPUC approach is based on their statistical characterization. In particular, the procedure involves three basic steps [15]:

- To capture the essential features of the heterogeneity pattern, the microstructure is characterized using appropriate statistical descriptors. Such data are essentially the only input needed for the determination of a unit cell.

- A geometrical model of a unit cell is formulated and its key parameters are postulated. Definition of a suitable unit cell model is a modeling assumption made by a user, which sets the predictive capacities of SEPUC for an analyzed material system.

- Parameters of the unit cell model are determined by matching the statistics of the complex microstructure and an idealized model, respectively. Due to
multi-modal character of the objective function, soft-computing global optimization algorithms are usually employed to solve the associated problem.

It should be emphasized that the introduced concept is strictly based on geometrical description of random media and as such it is closely related to previous works on random media reconstruction, in particular to the Yeong-Torquato algorithm presented in [16, 17]. Such an approach is fully generic, i.e. independent of a physical theory used to model the material response. If needed, additional details related to the simulation goals can be incorporated into the procedure without major difficulties, e.g. [18, 19], but of course at the expense of computational complexity and the loss of its generality.

In the previous work [1], the authors studied the applicability of the SEPUC concept for the construction of a single-layer unit cell reflecting selected imperfections typical of textile composites. A detailed numerical studies, based on both microstructural criteria and homogenized properties, revealed that while a single-ply unit cell can take into account non-uniform layer widths and tow undulation, it fails to characterize inter-layer shift and nesting. Here, we propose an extension of the original model allowing us to address such imperfections, which have a strong influence on the overall response of textile composites [20, 21, 22]. A brief summary of the procedure for the determination of the two-ply SEPUC for woven composites is given in Section 3.

Such extensions, however, are hardly sufficient particularly in view of a relatively high intrinsic porosity of Carbon-Carbon (C/C) composites, which are in the center of our current research efforts. It has been demonstrated in our previous work [23] that unless this subject is properly addressed inadequate results are obtained, regardless of how “exact” the geometrical details of the meso-structure are represented by the computational model. Unfortunately, the complexity of the porous phase seen also in Figure 1 requires some approximations. While densely packed transverse cracks affect the homogenized properties of the fiber tow through a hierarchical application of the Mori-Tanaka averaging scheme [24], large inter-tow vacuoles (crimp voids), attributed to both insufficient impregnation and thermal treatment, are introduced directly into the originally void-free SEPUC in a discrete manner.

Not only microstructural details but also properties of individual composite constituents have a direct impact on the quality of numerical predictions. Information supplied by manufacturers are, however, often insufficient. Moreover, the carbon matrix of the composite has properties dependent on particular manufacturing parameters such as the magnitude and durations of the applied temperature and pressure. Experimental derivation of some of the parameters is therefore needed. In connection with the elastic properties of the fiber and matrix, the nanoindentation tests performed directly on the composite are discussed in Sec-
tion 2 together with the determination of the necessary microstructural parameters mentioned already in the previous paragraphs.

Still, most of the work presented in this paper is computational. In particular, a brief summary of the procedure for the determination of the two-ply SEPUC for woven composites is given in Section 3. Section 4 is then reserved for the validation of the extracted geometrical and material parameters. To that end, the heat conduction and classical elasticity homogenization problems are validated against available experimental measurements. The concluding remarks and future extensions are presented in Section 5.

2. Experimental program

As already stated in the introductory part, much of the considered here is primarily computational. However, no numerical predictions can be certified if not supported by proper experimental data [25]. The objective of the experimental program in the context of the present study is twofold. First, reliable geometrical data for the construction of the unit cell and material parameters of both the carbon fibers and carbon matrix for the prediction of effective properties are needed. Since still derived on the basis of various assumptions, these results must be next confirmed experimentally to acquire real predictive power.

Considering the mesoscopic complexity of C/C composites, the supportive role of experiments is assumed to have the following four components:

- Two-dimensional image analysis providing binary bitmaps of the composite further exploited in the derivation of two-layer SEPUC

- X-ray tomography yielding a three-dimensional map of distribution, shape and volume fraction of major pores to be introduced into a void-free SEPUC.

- Nanoindentation tests supplying the local material parameters which either depend on the manufacturing process or are not disclosed by the producer.

For the above purposes a carbon-polymer (C/P) laminated plate was first manufactured by molding together eight layers of carbon fabric Hexcel G 1169 composed of carbon multifilament Torayca T 800 HB and impregnated by phenolic
resin Umaform LE. A set of twenty specimens having dimensions $25 \times 2.5 \times 2.5$ mm were then cut out of the laminate and subjected to further treatment (carbonization $C$ at $1000^\circ C$, reimpregnation $I$, recarbonization, second reimpregnation and final graphitization $G$ at $2200^\circ C$ ($CICICG$)) to create the C/C composite, see Figure 2 for an illustration and [26] for more details. The reported specimens were then fixed into the epoxy resin and subject to curing procedure. In the last step, the specimen was subjected to final surface grounding and polishing using standard metallographic techniques.

![Image](a) ![Image](b) ![Image](c)

Figure 2: Examples of scanned microstructures; (a) Woven fabric, (b) carbonized composite, (c) graphitized composite

2.1. Two-dimensional image analysis

The actual image analysis device used for structural image acquisition and analysis consists of NIKON ECLIPSE E 600 microscope, M"arzhauser motorized scanning stage, digital monochrome camera VDC 1300C and image analysis software LUCIA G$^1$. Note that high reflectance of the woven fabric allows relatively good visual resolution of individual parts of a composite structure as demonstrated in Figure 2. Using the method of gradual abrasion, transverse sections of the composite laminate allowed us to generate a database of micro-images intended for further processing. Unfortunately, a low color contrast of the reinforcement (carbon fabric) and matrix is a major impediment to an automatic separation of individual objects. Therefore, a manual preprocessing of images by marking the borders of selected objects becomes often necessary, cf. Figure 3. Further image analysis and object measurement was, however, fully automatic providing an average thickness of carbon tows, shape and dimensions of fiber tow cross-section, size and shape of major voids, distribution of transverse and delamination cracks, etc.

Although, as demonstrated in Section 4, statistical consideration of the acquired results proved useful, the essential input for the preparation of physical

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models for computational analysis (SEPUC) is given by binary images of the composite. An illustrative example of the result of two-dimensional image processing is available in Figure 4 implicating that material porosity is neglected when treating only the geometrical imperfections of the fabric reinforcements. At this point, a direct comparison of the resulting mesoscopic predictions with experimental measurements would therefore be meaningless.

2.2. Three-dimensional X-ray microtomography

Porosity of C/C composites plays an important role in the derivation of effective material properties [27]. Most common approach to characterizing this property employs sectioning, recall Section 2.1. The influence of shape of pores, estimated from 2D images of real C/C composites [28], on the mechanical response has been addressed e.g. in [29, 27]. The X-Ray microtomography becomes a valuable tool rendering three-dimensional phase information [30, 31, 32]. In the present study, high resolution computer tomography images provided by the Interfaculty Laboratory for Micro- and Nanomechanics of Biological and Biomimetical Materials of the Institute of Lightweight Design and Structural Biomechanics were used to obtain the shape, size, location and volume fraction of inter-layer (crimp) voids. A particular example of the distribution of major porosity in C/C
multi-layered plane-weave composite is presented in Figure 5. While the basic characteristics of the porosity can be directly extracted from these images, a direct introduction of pores in their full complexity as seen in Figure 5(a) is impossible. Instead, a set of oblate spheroids approximating the shape and volume of actual pores is accommodated in between the two layers of the SEPUC fitting their true location as close as possible. The results of two- and three-dimensional image analysis appear in Table 1, quantifying the structural parameters of a single-layer textile composite, mutual shift of individual layers and the volume and shape of macroscopic pores.

![Figure 5: X-ray microtomography; (a) Interior distribution and shape of large vacuoles, (b) three-dimensional view of the porous composite structure](image)

| Parameter          | Average [µm] | Standard deviation [µm] |
|--------------------|--------------|-------------------------|
| Tow period         | 4500         | 300                     |
| Tow height         | 150          | 20                      |
| Inter-tow gap      | 400          | 105                     |
| Layer height       | 300          | 50                      |
| Horizontal shift   | 0            | 675                     |
| Vertical shift     | 0            | 110                     |
| Porosity           | 8            | 3.5                     |
| Pore aspect ratio  | 0.4          | 0.2                     |

Table 1: Parameters of the periodic unit cell [28]

2.3. Phase elastic moduli from nanoindentation

Prediction of complex macroscopic response of highly heterogeneous materials from local phase constitutive theories is an important aspect of micromechanical modeling. The reliability of these predictions, however, is considerably
influenced by available information on material data of individual constituents. Even though supplied by the producer, these information are often insufficient for three-dimensional analysis. It is also known that material properties of the matrix much depend on the fabrication of composite and may considerably deviate from those found experimentally for large unconstrained material samples [33].

Carbon matrix developed in the composite through a repeated process of impregnation, curing and carbonization of the phenolic resin is a solid example. This resin belongs to the non-graphitizing resins so that the final carbon matrix essentially complies, at least in terms of its structure, with the original cross-linked polymeric precursor. Therefore, the resulting material symmetry is more or less isotropic with material parameters corresponding to those of glassy carbon. Nevertheless, when constrained the assumed matrix isotropy may evolve into the one of the fibers particularly in their vicinity. Although the PAN (polyacrylonitril) based carbon fibers are known to have a relatively low orderliness of graphen planes on nano-scale, they still posses a transverse isotropy with the value of longitudinal tensile modulus (usually available) considerably exceeding the one in the transverse direction (often lacking). Additional experiments, preferably performed directly on the composite, are therefore often needed to either validate the available local data or to derive the missing ones.

At present, nanoindentation is the only experimental technique that can be used for direct measurement of mechanical properties at material micro-level. A successful application of nanoindentation to C/C composites has been reported in [34, 35, 36]. In the present study, our attention was limited to the evaluation of the matrix elastic modulus and the transverse elastic modulus of the fiber. The remaining data were estimated from those available in the literature for similar material systems.

Figure 6: Nanoindentation - location of indents; (a) Transverse direction, (b) longitudinal direction (compression)

Three locations, distinctly separated in optic microscope, were tested - matrix, parallel fibers Figure 6(a), perpendicular fibers Figure 6(b). The matrix was
therefore assumed isotropic and possible anisotropy, which may arise inside the fiber tow, was not considered. As seen in Figure 6 several measurements were recorded for each of the three locations. The measurements were performed using CSM Nanohardness tester equipped with a Berkovich tip allowing for 0.1-500 mN loading range. To ensure elastic response relatively low indentation forces up to 10mN were considered. The elastic moduli were extracted from an unloading part of the indentation curve using the well known Oliver-Pharr procedure [37]. In particular, the indentation elastic modulus is then provided by

\[ E_r = \frac{S \sqrt{\pi}}{2 \sqrt{A}}, \]

where \( A \) is the projected contact area at the peak load and \( S \) is the contact stiffness evaluated as the initial slope of the unloading curve. The following equation is then adopted to account for a finite elastic stiffness of the indenter

\[ \frac{1}{E_r} = \frac{1 - \nu^2}{E} + \frac{1 - \nu_i^2}{E_i}, \]

tested material and \( E_i \) and \( \nu_i \) are parameters of the indenter (for diamond: \( E_i=1141 \) GPa and \( \nu_i=0.07 \)). In this study, the matrix Poisson ratio was assumed equal to 0.2 while the fiber Poisson ration was set equal to 0.4. The complete set of parameters, both measured averages labeled by * and those adopted from the literature, is available in Table 2. Note that the matrix modulus agrees relatively well with the one found for the glassy carbon in [36].

| Material    | Young modulus [GPa] | Shear modulus [GPa] | Poisson ratio [-] |
|-------------|---------------------|---------------------|-------------------|
| fiber       |                     |                     |                   |
| longitudinal| 294                 | 11.8                | 0.24              |
| transverse  | 12.8*               | 4.6                 | 0.4               |
| matrix      | 23.6*               | 9.8                 | 0.2               |

Table 2: Material parameters of individual phases

The final note is concerned with heat treatment of the C/C composite during fabrication. It has been observed experimentally [38] that even for T800 based composites the tensile Young’s modulus increases for graphitized specimens (CICICG) when compared to only carbonized ones (CICIC). It is suggested that this phenomenon may be caused by further stiffening of carbon fibers. This, however, is difficult to address in the present study as the tensile modulus cannot be measured via nanoindentation. On the contrary, neither the matrix properties nor the porosity profile is expected to change considerably with graphitization. Therefore, the experimental data reported in [38] for the CICIC system rather
than those for CICICG system will be fostered for comparison with numerical predictions.

2.4. Laboratory evaluation of effective properties

Corroboration of a mechanics model by experimental data is still thought vital for the model to be accepted, inasmuch as there is simply nothing better, even though an experiment often comprises laboratory measurements and a theory for calculating not directly measurable parameters.

With regard to thermophysical parameters the pulse transient method [39] combined with a heat loss model for the calculation of temperature response, when lower currents are used for pulse generation, is adopted. The searched thermal conductivities are found subsequently using a general relation between thermal conductivity, specific heat and thermal diffusivity, the latter two given in terms of the maximum attained temperature, the elapsed time to reach this temperature, total amount of generated heat and a set of correction factors characterizing deviations of calculated thermal diffusivity and specific heat from those derived for an ideal system (ideal heat source placed in bundleless isotropic body). It is not the objective of this section to provide all details of this method, as these can be found, e.g. in [39, 40], but rather to suggest the complexity of deriving the effective thermal conductivities from an experiment, which in turn are to be used to question the quality of numerical predictions presented later in Section 4. In particular, the results presented in [40] (C/C laminate (EXP) row) are used to validate the numerical model. Averages of the measurements from six samples of an eight layer C/C laminate are available in Table 3.

| material                  | Thermal conductivities [Wm\(^{-1}\)K\(^{-1}\)] |
|---------------------------|-----------------------------------------------|
|                           | \(\chi_{11}\)   | \(\chi_{22}\)   | \(\chi_{33}\)   |
| air                       | 0.02            | 0.02            | 0.02            |
| fiber                     | 35              | 0.35            | 0.35            |
| matrix                    | 6.3             | 6.3             | 6.3             |
| porous tow (MT)           | 24.12           | 1.05            | 1.42            |
| C/C laminate (EXP)        | 10 (warp)       | 10 (weft)       | 1.6             |

Table 3: Phase [26], unidirectional (UD) C/C composite (porous fiber tow) and laminate effective thermal conductivities [40]

Similar difficulties arise when deriving the dynamic tensile and shear moduli from a resonant frequency method. This technique was employed in [38] to derive

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\(^{2}\)See Figure 7 for the definition of local \(x\) (fiber tow) and global \(X\) (textile ply) coordinate system. Note that the local \(x_1\) axis is aligned with the fiber direction and the global in-plane \(X_1\) and \(X_2\) axes represent warp and weft directions, respectively.
the homogenized tensile and shear moduli of a four layer T800 fiber fabric based plain weave C/C composite. As part of their study a unidirectional (UD) carbonized $CICIC$ composite was examined. The resulting moduli stored in Table 3 (porous tow (EXP) column) were utilized here to validate the Mori-Tanaka estimates of the homogenized properties of the porous fiber tow (porous tow (MT) column). Note also the corresponding MT predictions for the heat conduction problem listed in Table 3.

Contemplation of the MT micromechanics model on the level of fiber tow has two reasons. First, it provides the homogenized fiber tow conductivity and stiffness matrices needed in the mesoscopic study in Section 4 relatively easily. Second, the acquired predictions are sufficiently "reliable" when no microstructure information other than volume fractions of individual constituents are at hand. In the present study a relatively high volume fractions of fibers equal to 63.5\% and open porosity by water penetration of 6.6\% were taken from [38]. Comparing the predicted and measured longitudinal moduli in first two columns in Table 4 both verifies the local phase properties given in Table 2 and justifies the use of the MT method. It goes beyond the present scope, however, to give full details on this method. A few remarks are presented in Section 4.3, further details are available in [41, 12, 24, to cite a few].

| parameter | porous tow (MT) | porous tow (EXP) | C/C laminate (EXP) |
|-----------|----------------|-----------------|-------------------|
| $E_{11}$  | 193.8          | $\approx$ 200   | $\approx$ 65     |
| $G_{12}$  | 10.3           | $\approx$ 11.5  | $\approx$ 6      |
| $E_{22}$  | 8.0            | -               | -                 |
| $E_{33}$  | 14.3           | -               | -                 |
| $G_{13}$  | 7.4            | -               | -                 |
| $G_{23}$  | 4.0            | -               | -                 |
| $\nu_{12}$| 0.23           | -               | -                 |
| $\nu_{13}$| 0.23           | -               | -                 |
| $\nu_{23}$| 0.38           | -               | -                 |

Table 4: Effective elastic properties of UD C/C composite (porous fiber tow) and C/C laminate conductivities [38]. Young’s moduli are given in [GPa]

3. Statistically equivalent period unit cell

The concept of Statistically Equivalent Periodic Unit Cell for random or imperfect microstructures is now well established. Individual steps, enabling the substitution of real microstructures by their simplified artificial representatives - the SEPUCs - are described, e.g. in [14, 1, 15] and additional references given
3.1. Geometrical mesostructural model

The basic building block of the adopted SEPUC is provided by a single-ply model of plain weave composite geometry proposed by Kuhn and Charalambides in [42]. The model consists of two orthogonal warp and weft tows embedded in the matrix phase and it is parametrized by four basic quantities, directly measurable by two-dimensional image analysis (recall Table 1): the half-period of tow undulation $a$, the maximal tow thickness $b$, the width of the intra-tow gap $g$ and the overall height of the ply $h$, see Figure 7 (a). The three-dimensional woven composite SEPUC, shown in Figure 7 (b), is formed by two identical one-layer blocks, relatively shifted by distances $\Delta_1$, $\Delta_2$ and $\Delta_3$ in the direction of the corresponding coordinate axes. Finally, cutting a SEPUC by the plane $X_2 = a$ or $X_1 = a$ yields the warp or weft two-dimensional sections, used as the basis for the determination of the unit cell parameters.

Figure 7: Geometrical model of SEPUC; (a) Two-dimensional cut of a one-layer model, (b) two-layer model including periodic extension of upper layer, (c) two-dimensional cut
3.2. Quantification of random microstructure

Assuming a statistically homogeneous and ergodic binary material system, two basic statistical functions are available to capture essential characteristics of the analyzed tow-matrix material system. The first descriptor is a two-point probability function \( S(X) \) [43], which quantifies the probability of two points, separated by a vector \( X \), being both found in the domain occupied by the warp and weft tows. The alternative statistics, proposed by Lu and Torquato [44] to capture long-range effects, is the linear path function \( L(X) \) giving the probability that a randomly placed segment \( X \) is fully contained in the tow region. Both descriptors can be easily computed for digitized microstructures; in particular, the Fast Fourier transform library FFTW [45] is used to evaluate the \( S \) function and the sampling template consisting of \( N_d \) concentric rays discretized by \( N_\ell \) pixels (cf. Figure 8) is employed to determine the linear path function. The periodic boundary conditions were adopted for both descriptors to eliminate edge effects [46].

![Figure 8: Example of sample template for lineal path function](image)

3.3. Calibration of SEPUC parameters

In overall, the adopted model of the unit cell involves seven independent parameters

\[
y = [a, b, g, h, \Delta_1, \Delta_2, \Delta_3],
\]

to be determined from available microstructural data. For the sake of generality, we assume that the microstructure configuration is characterized by microstructural function associated with (at most) warp and weft directions; i.e. functions \( S_{\text{warp}} \) and \( L_{\text{warp}} \) for the warp cross-section and descriptors \( S_{\text{weft}} \) and \( L_{\text{weft}} \) for the
weft cross-section, recall Figure 7(b). In particular, see also [15, 16], the following quantities are introduced to measure the similarity between a SEPUC and the original microstructure:

\[
F_2^2 (y) = \frac{1}{i_{\text{max}}} \sum_{i=-i_{\text{max}}}^{i_{\text{max}}} \sum_{j=-j_{\text{max}}}^{j_{\text{max}}} (S_p(y, i, j) - \overline{S}_p(i, j))^2, \quad (2)
\]

\[
F_L^2 (y) = \frac{1}{N_d N_{\ell}} \sum_{p \in \{\text{warp, weft}\}} \sum_{i=1}^{N_d} \sum_{j=1}^{N_{\ell}} (L_p(y, i, j) - \overline{L}_p(i, j))^2, \quad (3)
\]

where, e.g. \( S_{\text{warp}}(y, i, j) \) denotes the two-point probability function determined for the warp cross-section of a SEPUC described by parameters \( y \) and the value of argument \( X = [i, j] \), \( L_{\text{wet}}(y, i, j) \) stores the value of the weft-section lineal path function for the \( j \)-th pixel of the \( i \)-th segment. \( \overline{S}_* \) and \( \overline{L}_* \) denote the statistics related to original media and the dimensions \( i_{\text{max}} \) and \( j_{\text{max}} \) are determined as half of the minimum height and width of the bitmaps representing a SEPUC and the reference image.

The two-dimensional data, obtained via image analysis in Section 2.1, can be complemented by independent experimental measurements of three-dimensional volume fractions of the tow phase, see [26] for further details. Such information is accounted for by an additional discrepancy measure

\[
F_\phi (y) = |\phi(y) - \overline{\phi}|, \quad (4)
\]

where \( \phi(y) \) denotes the SEPUC three-dimensional volume fraction and \( \overline{\phi} \) is the target value. The former quantity is determined from the analytical representation of the SEPUC geometry [42] using an adaptive Simpson quadrature [47, Chapter 4] with the relative accuracy set to \( 10^{-5} \).

Moreover, the multiple descriptors can be arbitrary combined in the form of a weighted sum. For example, if all available information is employed, the objective function attains the form

\[
F_{S+L+\phi}(y) = \alpha_S F_S(y) + \alpha_L F_L(y) + \alpha_\phi F_\phi(y) \quad (5)
\]

with \( \alpha_* \) denoting scale factors used to normalize the influence of each descriptor, determined from twenty randomly generated SEPUCs in the current study.

The final term is introduced into the objective function to eliminate the intersection of the upper-layer and lower-layer tows. To that end, we compute the

\[
\Delta_1 = \Delta_2.
\]
overlap δ as the minimum signed distance between the upper and lower tow surfaces and introduce the constraint δ ≥ 0 via a polynomial exterior penalty:

\[ f_D(y) = \left(1 + \frac{\delta_-(y)}{h}\right)^\beta F_D(y), \]  

where \( \delta_- \) denotes the negative part of \( \delta \), \( D \) refers to a particular combination of the descriptors and the value of exponent is set to \( \beta = 3 \). Note that this approach was inspired by a recent work of Collins et al. [48] related to high-density polydisperse particulate composites.

Now, the optimal values of the SEPUC parameters can be determined as the solution to a box-constrained global optimization problem

\[ y \in \operatorname{Argmin}_{l \leq z \leq u} f_D(z), \]  

where the lower and upper bounds \( l \) and \( u \) are directly based on the image analysis data acquired in Section 2.1. A closer inspection reveals that objective functions (6) are multi-modal and discontinuous due to the effect of limited bitmap resolution, cf. [49]. Based on our previous experience with evolutionary optimization, a stochastic optimization algorithm RASA [50, 51], based on a combination of a real-valued genetic algorithm and the Simulated Annealing method, is used to solve the optimization problem (7).

3.4. Verification of optimization procedure

Before applying the proposed methodology to the multi-layered C/C system, we first investigate the robustness of the stochastic optimization algorithm and the accuracy of the identified parameters. To that end, an artificial two-layer composite, with structural parameters corresponding to the average values in Table 1 (i.e. \( a = 2,250 \mu m, b = 150 \mu m, g = 400 \mu m \) and \( h = 300 \mu m \)) and the layer shifts \( \Delta_1 = \Delta_2 = 1,125 \mu m \) and \( \Delta_3 = -80 \mu m \), is selected as the target material. The unit cell cross-section is digitized into a \( 1,024 \times 140 \) pixel bitmap, which corresponds to horizontal and vertical resolutions of \( \approx 4.4 \mu m \) per pixel. A template with parameters \( N_d = 16 \) and \( N_\ell = 70 \) pixels is used to sample the values of the lineal path function. As the focus of this section is on the influence of the statistical descriptor on the accuracy of SEPUC parameters determined from planar statistics, only two-point probability and lineal path functions are employed in the current example.

Due to the stochastic nature of the optimization algorithm, we present the statistics of the results obtained from twenty independent executions. For each component of the vector \( y \), the lower and upper bounds were set to 50% and
200% of the target value, respectively. The algorithm was terminated once a solution with the value $f_D$ smaller than $10^{-6}$ was found. The setting of all parameters of the RASA algorithm are specified in detail in [49, page 65]. The results appear in Tables 5 and 6, storing average values and standard deviations of the number of the objective functions evaluations and of the geometrical parameters, respectively. Note that the standard deviations arise due to stopping criteria and due to the limited bitmap resolution.

| Objective | Success rate | Number of function calls |
|-----------|--------------|--------------------------|
|           |   Average   |   Standard deviation     |
| $f_S$     | 20/20       | 14,586                   | 13,115                   |
| $f_L$     | 20/20       | 3,698                    | 1,231                    |
| $f_{S+L}$ | 20/20       | 9,446                    | 1,614                    |

Table 5: Verification example: Success rate and statistics of the number of objective function evaluations

| Objective | $a$ [$\mu$m] | $b$ [$\mu$m] | $g$ [$\mu$m] | $h$ [$\mu$m] | $\Delta_1 = \Delta_2$ [$\mu$m] | $\Delta_3$ [$\mu$m] |
|-----------|--------------|--------------|--------------|--------------|-------------------------------|-------------------|
| $f_S$     | 2,245.9      | 149.7        | 394.5        | 299.8        | 1,125.9                      | -79.1             |
|           | (6.0)        | (0.2)        | (7.9)        | (0.6)        | (9.2)                        | (1.8)             |
| $f_L$     | 2,249.6      | 151.8        | 368.5        | 311.0        | 1,184.2                      | -107.0            |
|           | (44.4)       | (1.4)        | (37.5)       | (14.5)       | (152.5)                      | (34.4)            |
| $f_{S+L}$ | 2,249.9      | 150.0        | 399.9        | 302.7        | 1,127.2                      | -82.0             |
|           | (6.8)        | (0.1)        | (4.1)        | (2.0)        | (4.4)                        | (3.3)             |

Table 6: Verification example: Accuracy of identified parameters; numbers in parentheses correspond to standard deviations

For the two-point probability-based objective function $f_S$, we observe the parameters of the artificial target unit cell are back-identified with accuracy superior to the bitmap resolution 4.4 $\mu$m per pixel. From all the SEPUC parameters, the inter-tow gap $g$ and the horizontal shift $\Delta_1 = \Delta_2$ display the highest scatter; its value is, however, comparable again to the pixel size. The major difficulty with the $f_S$ objective function is a large scatter in the required number of function evaluations, cf. Table 5, which is the consequence of its highly multi-modal character. When the lineal path function is employed as the only objective, the optimization problem becomes easier to be solved; the average number of iterations considerably decreases to approximately 25% and the coefficient of variation reduces by about 60%, but it comes at the expense of substantially higher scatter in the optimal SEPUC parameters. Similarly to, e.g. [17, 52, 53], we observe the combination of both statistics results in pixel accuracy and scatter in all the parameters for a moderate number of objective function evaluations and therefore both
functions will be employed for to determine SEPUC parameters for disordered micrographs. It is also worth noting that, similarly to [1], the global optimization algorithm succeeded in locating the global optimum for every execution of the algorithm. This demonstrates the robustness of the RASA optimizer and further justifies the application of heuristic algorithms to the SEPUC determination.

3.5. SEPUC for multi-layered C/C composite

Having verified the optimization algorithm for the SEPUC calibration, we now proceed with the analysis of the eight-layer C/C composite represented by bitmap appearing in Figure 4(c). First, to keep the optimization process manageable, the original 2,261 × 861 bitmap was down-sampled to a 1,024 × 390 image, resulting again in the pixel size of 4.4 µm. In accordance with conclusions of the previous section, all available information was employed to determine SEPUC parameters, constrained to the range $\bar{y}_i \pm 3\sigma_i$, with $\bar{y}_i$ and $\sigma_i$ denoting the mean and the standard deviation of the $i$-th structural parameter taken from Table 1. Parameters of the algorithm were set to the identical values as previously and the termination criterion was set to 50,000 of $f_{S+L+}\phi$ function evaluations. Again, the optimization was executed independently twenty times to obtain reliable results.

The resulting two-point and lineal-path functions corresponding to the SEPUC and the original microstructure appear in Figure 9. In the $X_1$-axis direction, the original statistics is well-reproduced, particularly at the $X_3 = 0$ µm plane where the extreme values and the shape of the descriptors are in almost perfect agreement. The SEPUC also partially captures the local peaks appearing in the multilayer system for $X_3 \approx \pm 200$ µm, cf. Figure 9 (a). In the perpendicular direction, we observe that the SEPUC two-point probability function is influenced by periodic boundary conditions, leading to more oscillatory behavior and to a slight shift of the minimum values from 41% to 35%. The match between the lineal path functions in terms of extreme values and shape of the function is even closer, since this descriptor is non-periodic even for periodic microstructures. Finally note that the tree-dimensional volume fraction $\phi$ of the SEPUC is 51%, which coincides exactly with the reference value taken from [26]. Therefore, we conjecture that the idealized SEPUC captures the dominant geometrical features of the original system; the differences visible from Figure 9 arise mainly due to the periodic boundary conditions and idealized shape of SEPUC (see also Figure 10(b)).

In Table 7, we present the parameters of the SEPUC together with the standard deviations estimated from independent optimization runs. The scatter in the identified parameters is comparable to the values reported in the verification example and supports the claim that the SEPUC corresponds to the global minimum of the optimization problem. The values of the parameters demonstrate that SEPUC captures a moderate horizontal shift of individual layers and their mutual overlap. These conclusions are further supported by a three-dimensional representation.
Figure 9: Statistical descriptors for multi-layered C/C composite and SEPUC; (a) two-point probability function and (b) lineal path function determined for multi-layered composite, (c) two-point probability function and (d) lineal path function corresponding to SEPUC in Figure 10(b), showing that SEPUC reproduces the matrix rich regions together with the strong nesting of individual layers, of course within the constraints of the selected geometrical model and the tow impenetrability condition.

3.6. Computational model

The end goal of Section 3 is the formulation of a computational model intended for the finite element based homogenization. This implies the use of conforming finite element meshes enabling the implementation of periodic boundary conditions mentioned later in Section 4.1. This might seem daunting in that it requires not only incorporation of an arbitrary shift of the two layers of fabric reinforcement, but also an independent introduction of voids discussed in Section 2.2. An illustrative example of the geometry of such a model is presented.
In the present study this step is accomplished by combining the principles of CAD modeling [7] with the volumetric modeling capacities of the ANSYS® package4. In order to ensure the symmetry of the resulting FEM mesh, a primitive block of the tow is modeled first, see Figure 11(a). Subsequently, using mirroring, copying and merging operations, the whole volume of one reinforcement layer is generated, Figure 11(b). The second layer is derived analogously and then placed according to parameters $\Delta_1$, $\Delta_2$ and $\Delta_3$ as shown in Figure 11(c). The porous phase is introduced next being represented by four identical oblate spheroids, the volume of which is derived from X-ray microimages shown in Figure 5. These are then periodically extended over the entire model, Figure 11(d). Their location is assumed to mimic the distribution of large vacuoles that typically appear, as also seen in Figure 1, in the location of tow crossings. However, this is difficult to achieve in general, and this is also why the porous phase was excluded from the minimization problem presented in Section 3. Finally, the volume corresponding to the matrix is generated using the subtraction of the body of reinforcements and the $2a \times 2a \times (2h + \Delta_3)$ parallelepiped defining the SEPUC. The resulting geometrical model appears in Figure 10(b).

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| $a$ [\(\mu m\)] | $b$ [\(\mu m\)] | $g$ [\(\mu m\)] | $h$ [\(\mu m\)] | $\Delta_1 = \Delta_2$ [\(\mu m\)] | $\Delta_3$ [\(\mu m\)] |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 2, 181          | 118             | 394             | 251             | 288             | –47             |
| (10.0)          | (0.3)           | (0.1)           | (1.3)           | (10.5)          | (2.0)           |

Table 7: Optimal parameters of the two-layer periodic unit cell free of pores; numbers in parentheses correspond to standard deviations in Figure 10.

Figure 10: Computational model; (a) Two-dimensional cut of a two-layer model with voids (b) 3D view of the geometry of a two-layer UC model with voids
Now, the mapped meshing technique [6, 54] can be employed to ensure periodicity of the resulting finite element mesh. First, half of the external surfaces of the SEPUC are discretized and the mesh is then copied to the homologous surfaces. Next, the tetrahedral elements corresponding to tows, voids and matrix are generated based on the data created in the previous steps. The corresponding finite element mesh is shown for illustration in Figs. 11(e)–(f).

![Finite element mesh generation](image)

Figure 11: Finite element mesh generation; (a) primitive volume, (b) one layer of reinforcements, (c) two layers of reinforcements, (d) two layers of reinforcements with voids, (e) FEM mesh of tows and voids, (f) FEM mesh of SEPUC

4. Numerical evaluation of effective properties

Numerical evaluation of effective elastic moduli and thermal conductivities, the most classical subject in micromechanics, is described in this section. This selection of mechanical and heat conduction problem is promoted not only by available experimental measurements but also by their formal similarity, considerably simplifying the theoretical treatment as seen hereinafter.
4.1. Theoretical formulation of homogenization

First-order homogenization approaches are now well established and described in many papers [55, 56, to cite a few] to provide estimates of effective properties of material systems with periodic microstructures. Bearing in mind the analogy between basic quantities related to heat conduction problems (i.e. the local microscopic $h(x)$ and uniform macroscopic $H$ temperature gradients and fluxes $q(x)$ and $Q$ as their conjugate measures) and the corresponding quantities applied to mechanical problems (local $\varepsilon(x)$ and uniform $E$ strains and the conjugate stress measures $\sigma(x)$ and $\Sigma$), we consider a heterogeneous periodic unit cell $Y$ and variations of local temperature $\theta(x)$ and displacement $u(X)$ fields written in terms of the uniform macroscopic quantities $H$ and $E$ as

$$\theta(X) = H \cdot X + \theta^*(X), \quad u(X) = E \cdot X + u^*(X),$$

(8)

where $\theta^*$ and $u^*$ are $Y$-periodic temperature and displacements fluctuations, respectively and $\bullet(X)$ is introduced to represent a given quantity in the global coordinate system $X$, recall Figure 7. Next, denoting $\chi(x)$ the local conductivity matrix and similarly $L(x)$ the local stiffness matrix, the local microscopic constitutive equations in the local coordinate system $x$ become

$$q(x) = -\chi(x)h(x), \quad \sigma(x) = L(x)\varepsilon(x).$$

(9)

To complete the set of equations needed in the derivation of effective properties, we recall the Hill lemma for mechanical problem and the Fourier inequality [57] for an equivalent representation of steady state heat conduction problem together with Eqs. (9) and write the global-local variational principles, see e.g. [23, 58, for further details] in the forms

$$\left\langle \delta h(x)^T \chi(x) h(x) \right\rangle = 0, \quad \left\langle \delta \varepsilon(x)^T L(x) \varepsilon(x) \right\rangle = 0,$$

(10)

where $\langle a(x) \rangle$ represents the volume average of a given quantity, i.e. $\langle a(x) \rangle = \frac{1}{|\Omega|} \int_{\Omega} a(x) \, d\Omega$. In the framework of finite element approximation, the discrete forms of local gradients derived from Eqs. (8) read

$$h(X) = H + B^\theta(X)\theta_d, \quad \varepsilon(X) = E + B^\varepsilon(X)u_d,$$

(11)

where $B^*$ stores the derivatives of the element shape functions w.r.t. $X$ and $\theta_d$ and $u_d$ are the vectors of the fluctuation part of nodal temperatures and displacements, respectively. Substituting Eqs. (11) into Eqs. (10) gives

$$\delta \theta_d^T \left\langle B^\theta(X)^T \chi(X) B^\theta(X) \right\rangle \theta_d^* = -\delta \theta_d^T \left\langle \chi(X) \right\rangle H,$$

(12)

$$\delta u_d^T \left\langle B^\varepsilon(X)^T L(X) B^\varepsilon(X) \right\rangle u_d^* = -\delta u_d^T \left\langle L(X) \right\rangle E,$$

(13)
to be solved for nodal temperatures $\theta^*_j$ and nodal displacements $u^*_j$. Combining Eqs. (11) and Eqs. (9) now allows us to write the volume averages of local heat fluxes and local stresses as

$$Q = \left\langle T^\theta(X)^\top q(x) \right\rangle = \frac{1}{|\Omega|} \int_\Omega T^\theta(X)^\top \chi(x)T^\theta(x)h(X) \, d\Omega, \quad (14)$$

$$\Sigma = \left\langle T^E(X)^\top \sigma(x) \right\rangle = \frac{1}{|\Omega|} \int_\Omega T^E(X)^\top L(x)T^E(X)\varepsilon(X) \, d\Omega, \quad (15)$$

also showing the relationship between material matrices in the local and global coordinate systems in terms of transformation matrices $T^\theta$, $T^E$, see e.g. [59, 49, 23, 24],

$$\chi(X) = T^\theta(X)^\top \chi(x)T^\theta(X), \quad L(X) = T^E(X)^\top L(x)T^E(X). \quad (16)$$

The results of Eqs. (14) and (15) renders the macroscopic constitutive laws in the form

$$Q = -\chi^H H, \quad \Sigma = L^H E, \quad (17)$$

where $\chi^H$ and $L^H$ are the searched homogenized effective thermal conductivity and elastic stiffness matrices, respectively. In particular, for a three-dimensional SEPUC the components of the $3 \times 3$ conductivity matrix $\chi^H$ follow directly from the solution of three successive steady state heat conduction problems. To that end, the periodic unit cell is loaded, in turn, by each of the three components of $H$, while the other two vanish. The volume flux averages, Eq. (14), normalized with respect to $H$ then furnish individual columns of $\chi^H$. The components of the $6 \times 6$ elastic stiffness matrix $L^H$ are found analogously from the solution of six independent elasticity problems together with Eq. (15).

4.2. Numerical simulations

Section 3.6 introduced the computational model of a two-layer SEPUC on the basis of geometrical parameters derived in Section 3.5, see also Table 7. The mesoscopic porosity (large intertow vacuoles seen in Figs. 1 and 5) equal to 5.5% was subdivided, as suggested in Section 3.6, into four oblate spheroids ($\xi_1 = \xi_2 > \xi_3$) given the ratio of principal semi-axes as high as possible to fit in between the two layers. Note that this value corresponds to the volume of pores derived for the four-ply laminate in Figure 1 to make these results comparable with those presented in the next section, where the same laminate is analyzed using the Mori-Tanaka method. It is fair to mention that this value is slightly lower than the one provided by X-ray microtomography, which, on the other hand, is surely enhanced by an “artificial” open porosity in the vicinity of specimen edges caused by mechanical handling of the specimen before taking the measurements. Apart from that, the X-ray microimages still show a shape of pores similar to an
oblate spheroid and their alignment with layers of carbon tows as assumed in the present study.

Having the computational model the actual derivation of effective properties follows the steps outlined in the last paragraph of the previous section. The results pertinent to both heat conduction and elasticity problems are summarized in Table 8.

| Thermal conductivities [Wm⁻¹K⁻¹] | Elastic moduli [GPa] |
|-----------------------------------|----------------------|
| \(\chi_{\text{warp/weft}}\) | \(\chi_{\text{trans}}\) | \(E_{11}\) | \(G_{12}\) | \(E_{33}\) | \(G_{13}\) |
| 9.0 | 1.9 | 60.3 | 8.1 | 11.9 | 5.3 |

Table 8: The homogenized thermal conductivities and elastic moduli derived from the application of the two-layer SEPUC plotted in Figure 11(f) and FEM.

### 4.3. Mori-Tanaka approximations

The Mori-Tanaka method is known to provide quick and reliable estimates of the effective properties of heterogeneous materials albeit having only limited information about their microstructure. Although extensively used for several decades, it was only recently when this method was shown to provide reasonable results even for imperfect highly porous textile C/C composites. Inasmuch this method is used in the present study to supply, apart from laboratory measurements, additional results to compare with FEM simulations, we take the liberty of giving a brief summary of this method on the subject of meso-scale problem in Fig. 7 and refer the interested reader to [60, 12, 24]. We begin by writing the homogenized conductivity matrix of C/C composites, first in the absence of the porous phase, in terms of the partial temperature concentration factors (localization tensors) for the warp \(T_{\text{warp}}^\theta(0,\psi,0)\) and weft \(T_{\text{weft}}^\theta(\pi/2,\psi,0)\) directions as

\[
\chi_{\text{MT}}^m = \chi_1 + \frac{c_2}{2} \left[ \left\langle \chi_{\text{warp}} T_{\text{warp}}^\theta \right\rangle - \chi_1 \left\langle T_{\text{warp}}^\theta \right\rangle \right] + \left[ \left\langle \chi_{\text{weft}} T_{\text{weft}}^\theta \right\rangle - \chi_1 \left\langle T_{\text{weft}}^\theta \right\rangle \right] \times \left\{ c_1 I + \frac{c_2}{2} \left[ \left\langle T_{\text{warp}}^\theta \right\rangle + \left\langle T_{\text{weft}}^\theta \right\rangle \right] \right\}^{-1},
\]

where \(\chi_1\) is the 3×3 conductivity matrix of the matrix phase and the double brackets \(\left\langle \right\rangle\) denote averaging over all possible orientations depending on the adopted orientation distribution function \(g(\phi, \psi, \zeta)\) with \(\phi, \psi\) and \(\zeta\) being the Euler angles. This ushers in the issue of random distribution of orientation angle \(\psi\) (see also Fig. 7(a)) along the fiber tow path addressed already in [12, 24]. Providing the
histograms of inclination angle $\psi$ are available, consult e.g. [12] for that matter, the orientation average of, say $T_{\text{warp}}(0, \psi_i, 0)$, then reads

$$\langle T_{\text{warp}} \rangle = \sum_{i=1}^{m} p_i T_{\text{warp}}(0, \psi_i, 0),$$

(19)

where $m$ denotes the number of sampling values. The discrete angles $\psi_i$ and probabilities $p_i$ follow directly from the image analysis data [61].

Formal similarity between heat conduction and elasticity problems then provides the homogenized stiffness matrix in the form, recall Eq. (18),

$$L_{M}^{MT} = L_1 + \frac{c_2}{2} \left[ \langle L_{\text{warp}} T_{E}^{\theta} \rangle - L_1 \langle T_{E}^{\theta} \rangle \right] +
+ \left[ \langle L_{\text{weft}} T_{E}^{\theta} \rangle - L_1 \langle T_{E}^{\theta} \rangle \right] \times
\times \left[ c_1 I + \frac{c_2}{2} \left( \langle T_{E}^{\theta} \rangle + \langle T_{E}^{\theta} \rangle \right) \right]^{-1}.$$

(20)

The partial temperature $T_{\theta}^{\theta}$ and strain $T_{E}^{\theta}$, $r = \text{warp, weft}$, concentration factors are derived from the solution of the Eshelby equivalent inclusion problem, in which an isolated inclusion of an ellipsoidal shape is embedded into the matrix and subjected to either average temperature gradient $h_1$ or strain $\varepsilon_1$ found in the matrix. Bearing in mind certain randomness in the geometry of a single ply unit cell, Fig. 7(a), it is possible to derive a certain statistically equivalent ellipsoidal inclusion, for which the macroscopic estimates, Eqs. (18) and (20), are reasonably close to FE simulations for a certain range of parameters $a, b, g, h$. For the present material system, the three semi-axis $\xi_1 = 1, \xi_2 = 0.1, \xi_3 = 0.01$, characterizing the shape of the ellipsoidal inclusion, were found optimal regardless of the type of the homogenization problem. Further to this matter, searching for an optimal shape of the equivalent inclusion for various geometries permitted us to relate the values of $\xi_2, \xi_3$ axes, given $\xi_1 = 1$, to $g/a$ and $b/a$ ratios, respectively, see also discussions in [12, 24]. Therefore, knowing at least the averages of parameters $a, b$ and $g$ allows us to define the shape of the ellipsoid with a relative ease as

$$\xi_2 \approx \frac{1}{7} (1 - \frac{g}{a}), \quad \xi_3 \approx \frac{1}{60} (1 - \frac{4b}{a}).$$

(21)

The subscript $m$ in Eqs. (18), (20) identifying the mesoscopic effective properties of a pore-free textile ply was chosen purposely as these properties are assumed to play the role of matrix in the second homogenization step, in which the porous phase is introduced into the new homogeneous, but orthotropic, matrix. In this simple case the estimates of the effective properties of the homogeneous ply simplify as

$$X_{\theta}^{MT} = X_{m}^{MT} + c_2 (X_{\text{void}} - X_{m}^{MT}) A_{\text{void}}^{\theta},$$

(22)

$$L_{\theta}^{MT} = L_{m}^{MT} (I - c_2 A_{\text{void}}^{\theta}),$$

(23)
with
\[ L_{\text{void}} = 0 \quad \text{and} \quad A_{\text{void}}^e = T_{\text{void}}^e \left[ c_m I + c_{\text{void}} T_{\text{void}}^e \right]^{-1}, \quad s = \theta, \varepsilon. \quad (24) \]

Here, an optimal shape of the ellipsoidal inclusion (void) was found directly from 2D images of the composite, see e.g. Figure 1. Notice essentially three distinct plies with different porosity. While the most bottom ply is free of pores (I) with \( A_{m}^{MT}, L_{m}^{MT} \) properties, the middle (II) and top (III) ply effective properties are given by Eqs. (22), (23). Similar to FE simulations presented in the previous section, an oblate spheroid with \( \xi_1 = \xi_2 \) and \( \xi_3/\xi_1 = 0.33, c_{\text{void}} = 0.07 \) for the middle ply and \( \xi_3/\xi_1 = 0.66, c_{\text{void}} = 0.15 \) for the top ply was used.

Finally, the macroscopic properties of the homogeneous laminated plate are obtained applying standard averaging rules. While simple arithmetic and inverse rules of mixture are used for the components of effective conductivity matrix, the homogenized \( 6 \times 6 \) stiffness matrix can be determined as suggested in [62, page 163]. Final results are summarized in Table 9 adopting the material properties of individual phases from Tables 2–4.

| Thermal conductivities [Wm\(^{-1}\)K\(^{-1}\)] | Elastic moduli [GPa] |
|---------------------------------|--------------------------|
| \( \chi_{\text{warp/weft}} \) | \( \chi_{\text{trans}} \) | \( E_{11} \) | \( G_{12} \) | \( E_{33} \) | \( G_{13} \) |
| 8.63 | 2.25 | 55.7 | 7.8 | 16.3 | 6.5 |

Table 9: Mori Tanaka estimates of the homogenized thermal and elastic moduli of the four layer C/C composite laminate with I-II-III-I stacking sequence as seen in Figure 1

5. Conclusions

The present article summarizes recent developments in the study of imperfect carbon-carbon textile composites initiated already in [1]. To arrive at the present stage of understanding the complex structural response of these material systems, the machinery of homogenization tools has been fully exploited revealing both advantages and drawbacks of individual methods.

When introduced in the framework of hierarchical modeling, the Mori-Tanaka method yields reasonably accurate approximations of the effective properties yet at the fraction of time when compared to finite element based simulations.

In view of real material samples with a large amount of flaws (transverse and delamination cracks, large intertow vacuoles) even prior to loading, the modeling strategy based on the well known concept of periodic unit cell may become preferable, particularly if the response of the material exceeding its elastic limit becomes the primary interest. Presently, its potential is seen mainly in the formulation of statistically equivalent periodic unit cell that attempts to accommodate
the most severe imperfections of the real material. Supported by the results derived in the course of this work, the two-layer SEPUC enhanced by incorporating the porous phase appears to be a suitable candidate for the computational model of plain weave textile reinforcement based composites including, apart from the investigated C/C composites, a large group of textile reinforced ceramics with their anticipated application in bio-medicine.

To appreciate the concept of SEPUC we present, in addition, the results obtained from an independent stochastic analysis. There, a family of representative PUCs was generated assuming a random variation of individual geometrical parameters of the cell including the major porosity. Each variable was assigned the Gaussian probability distribution with the mean values and standard deviations taken from Table 1. Ten such unit cells were generated using the Latin hypercube sampling method. Details, including the assumed correlation between individual variables, are available in the doctoral thesis of the first author [63].

All results are presented in Figure 12 confirming the predictive superiority of the SEPUC over other methods employed in this study. The high computational cost must, however, be reminded to keep the two approaches (unit cell models against analytical micromechanics) on the same starting line.

![Figure 12: Comparison of the numerical and experimental results; (a) Coefficients of thermal conductivity, (b) elastic properties](image)

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