Correlation analysis of the elastic-ideal plastic material behavior of short fiber-reinforced composites

Natalie Rauter

Department of Mechanical and Civil Engineering, Helmut-Schmidt-University/University of the Federal Armed Forces Hamburg, Hamburg, Germany

Correspondence
Natalie Rauter, Department of Mechanical and Civil Engineering, Helmut-Schmidt-University/University of the Federal Armed Forces Hamburg, Holstenhofweg 85, 22043 Hamburg, Germany.
Email: natalie.rauter@hsu-hh.de

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Abstract
For the numerical simulation of short fiber-reinforced composites and the correct analysis of the deformation, information about the plastic behavior and its spatial distribution is essential. When using purely deterministic modeling approaches information of the probabilistic microstructure is not included in the simulation process. One possible approach for the integration of stochastic information is the use of random fields, which requires information about the correlation structure of all material input parameters. In this study the correlation structure for finite strain elasto-plastic material behavior of short fiber-reinforced composites is analyzed. This approach combines the use of already established procedures for linear-elastic material behavior with a homogenization method for plasticity. The obtained results reveal a complex correlation structure, which is approximated with triangle and exponential correlation functions influenced by the window size. Due to the dependence of the hyperelastic and plastic material parameters on the fiber mass fraction, the strain-energy density function coefficients are cross-correlated with the yield strength of the composite. With this knowledge at hand, in a subsequent work numerical simulations of tensile tests are conducted that cover the elastic and plastic domain and include spatially distributed material properties.

KEYWORDS
correlation analysis, plasticity, short fiber-reinforced composite

1 | INTRODUCTION

Short fiber-reinforced composites (SFRC) are thermoplastic materials that are reinforced by short fibers or other particles. In contrast to the reinforcing elements, which usually show a brittle behavior, the thermoplastic matrix materials are characterized by a distinctive plastic deformation when allowing finite deformations.1–3 Hence, the consideration of elasto-plastic material behavior is important for the modeling of SFRC to ensure an accurate prediction of the structural response under load. Furthermore, due to the spatial distribution and probabilistic characteristics of the reinforcing elements the material properties vary also over the spatial coordinates.4–7 Current modeling approaches address only one of these two aspects, either the local fluctuation of the material parameters of linear-elastic material behavior is investigated, or a modeling approach for the nonlinear material behavior is performed considering homogenization.
methods. A common approach for an elasto-plastic material model is the multiplicative decomposition of the deformation gradient as introduced by Lee and Mandel. Based on this approach, Simo et al. derived the framework of the finite strain elasto-plasticity by combining the multiplicative decomposition of the deformation gradient with hyperelastic strain-energy density functions. Since then, this approach has been used widely, for example by Reina et al. On the other hand, homogeneous second-order random fields are one possibility to model spatial distributed stochastic quantities like material properties of reinforced materials. Combining the finite strain elasto-plasticity with the use of random fields requires knowledge of the correlation structure of the strain-energy density function coefficients and the yield strength. When the correlation structure of the auto- and cross-correlation is established, random fields can be synthesized to represent the fluctuation of the nonlinear material properties on the component level without distinct modeling of the microstructure. Initial investigations of the correlation structure of material properties are provided by Sena et al., which is limited to a checkerboard pattern. A second analysis is provided by Rauter et al. focusing on the linear elastic domain.

Hence, the overall objective of this study is the numerical simulation of components made of SFRC including the spatial distribution of the plastic deformation described by the multiplicative decomposition of the deformation gradient in combination with hyperelastic material models for transversely isotropic symmetry. Therefore, the modeling approach presented in previous work by the author, which includes the spatial distribution of material properties but is limited to linear elasticity, will be extended to elasto-plastic material behavior. The work is divided into two parts. The first part, presented here, deals with the analysis of the correlation structure of the material properties. This knowledge is later used to generate second-order homogeneous random fields representing the spatial distribution of the material properties characterizing the elastic and plastic material behavior. Afterwards, these random fields are applied to a numerical model for the simulation of tensile tests covering the elastic and plastic domain. To validate the results, numerically obtained values are compared to experimental measurements in a subsequent work by the author.

Ensuing from this objective, the structure of the presented work is as follows. Section 2 holds the main aspects of the theoretical background including the fundamentals of the multi-scale and probabilistic modeling, finite strain elasto-plastic material behavior, and the homogenization of plastic material properties. In Section 3, the apparent overall material properties of the nonlinear material behavior are derived on the mesoscale by numerical simulations. The results of the correlation analysis are presented in Section 4. Finally, Section 5 gives a summary and conclusion.

2 | THEORETICAL BACKGROUND

This section comprises the basics concerning the stochastic framework, elasto-plastic material behavior, and a homogenization method for plastic material properties.

2.1 | Stochastic framework

2.1.1 | Apparent material properties

All materials and especially reinforced materials show different characteristics when observed at different scales. Reinforced materials are strongly heterogeneous on the microscale. However, for numerical simulations on the component level, usually, homogeneous material properties are assumed. Therefore, the component is characterized by effective material properties that replace the spatially distributed by homogeneous material properties that are independent of the location. This scale transition from the microscale to the macroscale is achieved by homogenization. The main concept behind this homogenization is the representative volume element (RVE), which was first introduced by Hill. The RVE is a volume that consists of a statistically sufficient number of inclusions, and therefore, represents the effective behavior of the material. This implies that the size \( l \) of the inclusion or a microstructural characteristic must be much smaller than the size \( d \) of the RVE. In addition, the RVE must be much smaller than the component with the dimension \( L \). This separation of scales can be formulated as

\[
l \ll d \ll L,
\]

where \( l \) is assigned to the microscale, \( L \) to the macroscale, and \( d \) to the edge length of the RVE.
To ensure the correct calculation of the effective material properties by numerical simulations Hill’s condition \(^2\) must be satisfied, given by

\[
\langle \sigma : e \rangle = \langle \sigma \rangle : \langle e \rangle.
\]

This condition expresses the equivalence between the local and global effective material properties of a heterogeneous material.\(^2\)\(^,\)\(^2\) The effective material properties for an RVE are written as

\[
\langle \sigma \rangle = C^{\text{eff}} : \langle e \rangle,
\]

and

\[
\langle e \rangle = S^{\text{eff}} : \langle \sigma \rangle,
\]

where \(\langle \cdot \rangle\) gives the volume average

\[
\langle \cdot \rangle = \frac{1}{V} \int_V \cdot dV.
\]

Hence, the strains \(e\) and stresses \(\sigma\) are microstructural quantities, whereas \(\langle e \rangle\) and \(\langle \sigma \rangle\) are related to the macroscopic scale. Furthermore, \(C^{\text{eff}}\) and \(S^{\text{eff}}\) are the effective stiffness and compliance tensor.\(^2\)\(^7\)

Suitable transformation of Equations (3) and (4) links the macroscopic quantities \(\langle e \rangle\) and \(\langle \sigma \rangle\) with the boundary values.\(^2\)\(^7\) For the resulting boundary value problem, different types of boundary conditions can be established. Applying the average strain theorem and the average stress theorem to Equations (3) and (4) gives kinematic uniform boundary conditions of the kind \(\sigma_0\) and static uniform boundary conditions of the kind \(e_0.\)\(^2\)\(^9\)

Applying the boundary value problem on an RVE with simultaneous fulfillment of Hill’s condition leads to three different kinds of boundary conditions:\(^3\)\(^0\)\(^,\)\(^3\)\(^1\)

\[
\mathbf{u} = e_0 \cdot \mathbf{x} \quad \forall \mathbf{x} \in \partial V,
\]

\[
\mathbf{t} = t_0 \cdot \mathbf{x} \quad \forall \mathbf{x} \in \partial V,
\]

and

\[
[\mathbf{t} - t_0 \cdot \mathbf{x}] \cdot [\mathbf{u} - e_0 \cdot \mathbf{x}] = 0 \quad \forall \mathbf{x} \in \partial V.
\]

In the context of continuum mechanics Equation (6) gives a boundary condition of Dirichlet type, since pure kinematic boundary conditions with the constant macroscopic strain \(e_0\) are defined on the complete surface, whereas Equation (7) is a boundary condition of Neumann type, because pure traction boundary conditions, with a constant macroscopic stress \(t_0\) are defined on the complete surface. A combination of these boundary condition types is given in Equation (8). For an RVE, the obtained material properties based on these boundary conditions are equal and hence, the material is assumed to be homogeneous. However, if the volume is smaller than the RVE one speaks of apparent overall properties.\(^2\)\(^9\)\(^-\)\(^3\)\(^1\) In this case the extraction on the mesoscale is referred to as a statistical volume element (SVE).\(^3\)\(^2\) To determine the material properties for an SVE, the same procedure is used as for the effective material properties. However, now the results depend on the size of the extracted volume and the boundary conditions.

2.1.2 Correlation

Combining the approach of apparent overall material properties with homogeneous second-order random fields on the component level enables one to model the structural behavior of inhomogeneous material properties induced by the probabilistic characteristics of the microstructure without the need of a scale transition.\(^2\)\(^6\) To synthesize these homogeneous second-order random fields, the correlation structure must be known, which describes the point-to-point information of
a stochastic quantity. For a continuous random field \( Z(\omega, x) \) this is described by the covariance defined as

\[
\text{Cov}[Z_1, Z_2] = \mathbb{E}[Z_1 Z_2] - \mu_1 \mu_2.
\]  

(9)

Here, \( Z_1 \) and \( Z_2 \) are observations of the random field at different locations \( x_i \), \( \mathbb{E} \) is the expectation operator, and \( \mu_1 \) and \( \mu_2 \) are the expected values of the random variables \( Z_1 \) and \( Z_2 \), respectively. Usually, the dimensionless correlation parameter \( \varphi_{12} \) is used, which is obtained by dividing Equation (9) by the standard deviations \( \sigma_i \) of the random variables. The standard deviation is defined as the square root of the variance, which is the second central moment

\[
\sigma_{Z(x)} = \sqrt{\text{Var}[Z(x)]}.
\]  

(10)

Hence, the dimensionless correlation parameter reads

\[
\rho_{12} = \rho_{Z_1 Z_2} = \frac{\text{Cov}[Z_1, Z_2]}{\sigma_1 \sigma_2}.
\]  

(11)

If the random variables \( Z_1 \) and \( Z_2 \) belong to the same random field Equations (9) and (11) give the auto-covariance and auto-correlation of the random field, otherwise it is referred to as the cross-covariance and cross-correlation, respectively. However, for most applications the random field is given by a discrete number of realizations \( \omega_i \), because the probability density function is unknown. In this case, instead of the expected value the spatial average is used

\[
\overline{Z(x)} = \frac{1}{N} \sum_{i=1}^{N} Z(\omega_i, x),
\]  

(12)

and rewriting the variance leads to

\[
s^2(x) = \overline{Z(x)^2} - \overline{Z(x)}^2.
\]  

(13)

Consequently, the dimensionless correlation parameter for a discrete number of realizations \( \omega_i \) is calculated by evaluating

\[
\rho_{12} = \rho_{Z_1 Z_2} = \frac{|Z_1 - Z_1||Z_2 - Z_2|}{s_1 s_2}.
\]  

(14)

For the synthesizing the random fields, the dimensionless correlation parameter is approximated by a correlation function. Examples for typically used correlation functions are the exponential correlation function

\[
\rho(\xi_1, \xi_2) = \exp \left( \frac{b_1 - |\xi_1|}{b_1} \right) \left( \frac{b_2 - |\xi_2|}{b_2} \right),
\]  

(15)

the triangle correlation function

\[
\rho(\xi_1, \xi_2) = \begin{cases} 
1 - \frac{|\xi_1|}{b_1} & \text{if } |\xi_1| \leq b_1, \ |\xi_2| \leq b_2 \\
1 - \frac{|\xi_2|}{b_2} & \text{else} \\
0 & \text{if } |\xi_1| > b_1, \ |\xi_2| > b_2 
\end{cases}
\]  

(16)

and the Gaussian correlation function

\[
\rho(\xi_1, \xi_2) = \exp \left( -\left( \frac{\xi_1}{b_1} \right)^2 - \left( \frac{\xi_2}{b_2} \right)^2 \right).
\]  

(17)

Here, \( b_1 \) and \( b_2 \) are the correlation lengths with respect to the coordinate \( \xi_1 \) and \( \xi_2 \), respectively. The functions given in Equations (15) and (16) have the advantage that they lead to analytical solutions for the eigenvalue problem, that needs to be solved when using the Karhunen–Loève expansion for the generation of random fields for a rectangular domain. 33,35,36 One technique to extract the relation between the information at different locations \( x_i \) is the moving window method. 37-39
Within this method a window of predefined size is used to extract segments of a larger microstructure. Since the material parameters of an SVE are assigned to the spatial coordinates and are no longer identical at each material point, the local fluctuation of the material properties can be derived.

### 2.2 Elasto-plastic material behavior

The modeling approach of plasticity in combination with finite deformation is based on the multiplicative decomposition of the deformation gradient, which is introduced by Lee\textsuperscript{12} and Mandel\textsuperscript{13}\n
\[ F = F_{el} \cdot F_{pl}. \]  

(18)

Here, $F_{el}$ holds the elastic and $F_{pl}$ the plastic deformation, respectively. Based on this approach, Simo et al. derived the framework of the finite strain elasto-plasticity by combining the multiplicative decomposition of the deformation gradient with hyperelastic strain-energy density functions\textsuperscript{14-16} Hence, for the material modeling of SFRC a strain-energy density function is required that considers transversely-isotropic material behavior. Usually these potentials are divided into two parts, one representing the isotropic response $\Psi_{iso}$ and a second part for the transversely-isotropic behavior $\Psi_{trn}$

\[ \Psi = \Psi_{iso} + \Psi_{trn}. \]  

(19)

In addition to the strain invariants for isotropic behavior $I_1$, $I_2$, and $I_3$, for the description of transversely-isotropic material behavior the pseudo-invariants $I_4$ and $I_5$ are required. For a symmetric second-order tensor $B$ these two are defined by

\[ I_4 = a \cdot B \cdot a \quad \text{and} \quad I_5 = a \cdot B^2 \cdot a, \]  

(20)

where the vector $a$ gives the fiber orientation of the material.

The isotropic behavior is mostly given by well-known potentials of Neo-Hooke or Mooney-Rivlin\textsuperscript{40-43} In this work, the Neo-Hooke potential in terms of the right Cauchy-Green tensor $C$ is used\textsuperscript{40}

\[ \Psi_{Neo}(C) = \frac{1}{2} \Lambda (J - 1)^2 - \mu \ln J + \frac{1}{2} \mu (\text{tr} C - 3). \]  

(21)

Here, $J$ is the Jacobian determinant and $\Lambda$ and $\mu$ are the Lamé coefficients. This potential already leads to a strain-dependent elasticity tensor and therefore, induces nonlinear material behavior. The corresponding elasticity tensor reads

\[ C_{Neo} = \Lambda J(2J - 1) C^{-1} \otimes C^{-1} + 2 [\mu - \Lambda J (J - 1)] G, \]  

(22)

with

\[ G_{ijkl} = (C^{-1})_{ik}(C^{-1})_{jl}. \]  

(23)

For the representation of transversely-isotropic material behavior there exist several strain-energy density functions\textsuperscript{44-47} However, most of these potentials are either not fully nonlinear, because the resulting stiffness tensor is independent of the deformation\textsuperscript{44,45} or include more than five independent material parameters\textsuperscript{46,47} Therefore, in this study the potential given by Bonet et al.\textsuperscript{48} is used, because it is fully nonlinear, but uses only five independent material parameters when combining the transversely-isotropic part with the isotropic potential given in Equation (21). The transversely-isotropic part of the potential reads

\[ \Psi_{trn}(C) = [\alpha + \beta (\text{tr} C - 3) + \gamma (I_4 - 1) (I_4 - 1) - \frac{1}{2} \alpha (I_5 - 1), \]  

(24)

where $\alpha$, $\beta$, and $\gamma$ are independent material parameters. The use of this strain-energy density function in combination with Equation (21) leads to a fully nonlinear representation of the material, since both parts of the potential result in a
strain-dependent elasticity tensor. Based on the full potential the elasticity tensor for the transversely-isotropic material as a function of the deformation is given by

\[
C_{\text{full}} = \Lambda J(2J - 1) C^{-1} \otimes C^{-1} + 2[\mu - \Lambda J(J - 1)] G
+ 8\gamma a \otimes a \otimes a \otimes a + 4\beta(a \otimes a \otimes C^{-1} + C^{-1} \otimes a \otimes a) - \alpha \dot{\epsilon}_a - 4\beta(I_4 - 1) G,
\]

where

\[
A_{ijkl} = a_i a_j \delta_{jk} + \delta_{ik} a_i a_l.
\]

To determine the five material parameters \(\Lambda, \mu, \alpha, \beta, \text{ and } \gamma\) of the strain-energy density function the elasticity tensor is linearized by evaluating at zero strain for a fiber orientation in \(x\)-direction. In matrix notation this leads to

\[
C_{\text{full}} =
\begin{bmatrix}
8(\gamma + \beta) + \Lambda + 2\mu - 2\alpha & 4\beta + \Lambda & 4\beta + \Lambda & 0 & 0 & 0 \\
4\beta + \Lambda & \Lambda + 2\mu & \Lambda & 0 & 0 & 0 \\
4\beta + \Lambda & \Lambda & \Lambda + 2\mu & 0 & 0 & 0 \\
0 & 0 & 0 & 2\mu - \alpha & 0 \\
0 & 0 & 0 & 0 & 2\mu - \alpha \\
0 & 0 & 0 & 0 & 0 & 2\mu - \alpha
\end{bmatrix}
\]

which holds the transversely-isotropic symmetry.

### 2.3 Homogenization of plastic material properties

To derive the apparent overall plastic material properties a homogenization method is used, that allows one to determine, the yield function and subsequently the yield strength of a reinforced composite.\(^49\) In this case the effective local potential of the phase \(r\) for a nonlinear composite is expressed as

\[
u^{(r)}(\mathbf{x}, \sigma) = \text{stat}_{\mu_0, k_0 \geq 0} \left\{ u_0(\mathbf{x}, \sigma) - V^{(r)}(\mathbf{x}, \mu_0, k_0) \right\}.
\]

Here, \(u_0\) is the local potential of a linear comparison composite,\(^50\) which has the same microstructure as the nonlinear composite, and \(\mu_0\) and \(k_0\) are the corresponding shear and bulk moduli, respectively. The functions \(V^{(r)}(\mu_0, k_0)\) are so called error functions given by\(^51\)

\[
V^{(r)}(\mathbf{x}, \mu_0, k_0) = \text{stat}_\sigma \left\{ u_0(\mathbf{x}, \sigma) - u^{(r)}(\mathbf{x}, \sigma) \right\}.
\]

In a next step the macroscopic potential of the composite is obtained by

\[
\bar{U}(\mathbf{\sigma}) = \min_{\sigma \in S} \langle u(\mathbf{x}, \sigma) \rangle = \text{stat}_{\sigma} \langle u(\mathbf{x}, \sigma) \rangle,
\]

where

\[
S = \{ \sigma, \text{div} \sigma = 0 \text{ in } \Omega, \langle \sigma \rangle = \bar{\sigma} \}.
\]

Introducing Equation (28) in Equation (30) and interchanging the stationary operators leads to the definition of the effective macroscopic potential of the nonlinear composite. Considering a composite consisting of two phases, with constant material properties and a volume fraction of \(c^{(r)}\) results in

\[
\bar{U}(\mathbf{\sigma}) = \text{stat}_{\mu_0, k_0 \geq 0} \left\{ U_0(\mathbf{\sigma}) - \sum_{r=1}^{2} c^{(r)} V^{(r)}(\mu_0, k_0) \right\},
\]

with \(U_0\) being the effective potential of the linear comparison composite.
Applying the procedure to SFRC both phases are assumed to be isotropic. Furthermore, the plastic deformation is exclusively assigned to the matrix material, since the reinforcing fibers show brittle fracture after linear elastic behavior. Therefore, first, the stress potential used for both phases, is given by

\[ U^{(r)}(\sigma) = \frac{1}{2k^{(r)}} \sigma_m^2 + \phi^{(r)}(\tau_e), \]  

where \( \sigma_m \) is the hydrostatic stress component and the function \( \phi^{(r)}(\tau_e) \) gives the distortional response of the corresponding phase, which depends on the equivalent shear stress \( \tau_e \). For the linear-elastic inclusion phase \( (r = 2) \) a linear distortional response is assumed

\[ \phi^{(2)}(\tau_e) = \frac{1}{2\mu^{(2)}} \tau_e^2. \]  

In contrast to this the matrix material \( (r = 1) \) is characterized by a plastic deformation for stresses above the yield strength in shear \( \tau_y^{(1)} \)

\[ \phi^{(1)}(\tau_e) = \frac{\tau_e^2}{2\mu^{(1)}} + \frac{(\tau_y^{(1)})^2}{2\mu^{(1)}} \left\{ \frac{2}{n + 1} \left[ \left( \frac{\tau_e}{\tau_y^{(1)}} \right)^{n+1} - 1 \right] - \left( \frac{\tau_e}{\tau_y^{(1)}} \right)^2 - 1 \right\} H(\tau_e - \tau_y^{(1)}). \]  

Here, \( H \) is the Heaviside function and \( n \) gives the hardening exponent. The dilational response for both phases is assumed to be linear. In conclusion, the SFRC is modeled as a two-phase composite consisting of an elasto-plastic matrix material with power-law hardening behavior and linear-elastic inclusions. For the hardening coefficient \( 1 \leq n \leq \infty \) holds, where \( n = 1 \) indicates linear-elastic and \( n = \infty \) rigid-ideally plastic behavior, respectively.52

Following the procedure introduced by Li et al.49 the error functions are bounded only in case \( k_0^{(1)} = k^{(1)} \), \( k_0^{(2)} = k^{(2)} \), and \( \mu_0^{(2)} = \mu^{(2)} \) hold, which is simultaneously the best choice considering Equation (32). Selecting these values the error functions reduces to

\[ V^{(1)}(x, \mu_0^{(1)}, k_0^{(1)}) = \text{stat}_{\tau_e > 0} \left\{ \frac{\tau_e^2}{2\mu_0^{(1)}} - \phi^{(1)}(\tau_e) \right\}, \]  

and

\[ V^{(2)} = 0, \]  

respectively, which enables one to rewrite the effective potential from Equation (32)

\[ \bar{U}(\sigma) = \text{stat}_{\mu_0^{(1)} \geq 0} \left\{ \bar{U}_0(\sigma) - c^{(1)}V^{(1)}(\mu_0^{(1)}) \right\}. \]  

At this stage not only the distortional response \( \phi^{(1)}(\tau_e) \) but also the error function \( V^{(1)} \) can be separated for the linear \( (\mu_0^{(1)} \geq \mu^{(1)}) \) and the nonlinear case \( (\mu_0^{(1)} < \mu^{(1)}) \). With this, the convexity of \( V^{(1)} \) in \( 1/\mu_0^{(1)} \), and the assumption of the monotone increasing behavior of \( \bar{U}_0 \) with \( 1/\mu_0^{(1)} \) it can be shown that the effective potential is quadratic. Subsequently, the composite shows a linear response if

\[ \frac{\partial \bar{U}_0}{\partial \mu_0^{(1)}} \bigg|_{\mu_0^{(1)} = \mu^{(1)}} + \frac{c^{(1)}}{2} \left( \frac{\tau_y^{(1)}}{\mu^{(1)}} \right)^2 > 0, \]  

is satisfied and in case

\[ \frac{\partial \bar{U}_0}{\partial \mu_0^{(1)}} \bigg|_{\mu_0^{(1)} = \mu^{(1)}} + \frac{c^{(1)}}{2} \left( \frac{\tau_y^{(1)}}{\mu^{(1)}} \right)^2 < 0, \]
holds the composite shows ductile deformation. Following these two conditions Li et al.\textsuperscript{49} proposed a yield function given by

$$
\Phi(\sigma) = -\left[ \frac{\partial \tilde{U}_0}{\partial \mu_{0}^{(1)}}(\sigma) \bigg|_{\mu_{0}^{(1)} = \mu^{(1)}} \right] + \frac{c^{(1)}}{2} \left( \frac{\tau_{y}^{(1)}}{\mu^{(1)}} \right)^2. \tag{41}
$$

Since the inclusions show linear-elastic material behavior, the yield function only depends on the material properties of the matrix material. Furthermore, it is independent of the hardening exponent. The initial yield strength is derived by solving $\Phi = 0$, which requires only linear-elastic simulations, because the derivative of the effective potential $\tilde{U}_0$ with respect to $\mu^{(1)}$ is based on the linear comparison composite. Beside this, the yield strength shows anisotropic behavior.

3 | DETERMINATION OF THE APPARENT MATERIAL PROPERTIES

3.1 | Methodology

To simulate the elasto-plastic behavior of a component made of SFRC the parameters of the strain-energy density function and the yield strength are required, since the matrix is assumed to show ideal-plastic behavior. Hence, the apparent values of these material properties are derived from artificial microstructures. This is done separately for the hyperelastic and plastic material properties. For the hyperelastic properties, the parameters of the strain-energy density function are determined based on numerically obtained stiffness matrices, which requires a linearization at zero strain. However, due to the reduction to a two-dimensional simulation, the stiffness matrix holds only four independent values. Therefore, an additional equation is required to receive unique solutions for all five independent coefficients of the strain-energy density function. Because of that, first, the engineering constants are calculated from the compliance matrix obtained by numerical simulation. Due to the plane strain assumption the elements of the compliance matrix are a function of all five independent engineering constants $E_1, E_2, \nu_{12}, \nu_{23}$, and $G_{12}$ of a transversely-isotropic material.

This problem is solved by utilizing the fiber volume fraction. Since, the artificial microstructures are based on a binary image\textsuperscript{7,20} the fiber volume fraction of each extraction is derived by dividing the number of pixels representing fibers by the number of all pixels of the extraction. With this information at hand the fiber volume fraction of the numerical model is known and the Poisson’s ratio $\nu_{23}$ can be approximated by using the Halpin–Tsai material model.\textsuperscript{53,54} Now it is possible to determine the remaining constants $E_1, E_2, \nu_{12}$, and $G_{12}$. With all this information at hand, the stiffness matrix of transversely isotropic material behavior is established before using its elements to compute the parameters of the strain-energy density function by evaluating Equation (27). A detailed summary of the used framework is provided in Appendix A.

For the determination of the yield strength, the homogenization procedure presented in Section 2.3 is used. To evaluate the yield condition

$$
\left[ \frac{\partial \tilde{U}_0}{\partial \mu_{0}^{(1)}}(\sigma) \bigg|_{\mu_{0}^{(1)} = \mu^{(1)}} \right] + \frac{c^{(1)}}{2} \left( \frac{\tau_{y}^{(1)}}{\mu^{(1)}} \right)^2 = 0, \tag{42}
$$

a linear-elastic numerical model of the linear comparison composite is solved for different values of $\mu^{(1)}$, characterizing the matrix material. Based on the obtained derivative of the effective potential $\tilde{U}_0$ the apparent yield strength of the microstructure can be calculated. It is equal to the stress for which Equation (42) is valid.

3.2 | Numerical model

In the work of Rauter et al.\textsuperscript{20} a modeling approach is introduced to determine the apparent material properties of SFRC for linear-elastic material behavior. This procedure is adapted to an elasto-plastic material response as shown below. As done
FIGURE 1 Moving window method applied to the artificial microstructure. All measures in μm.

TABLE 1 Material properties

| Component | $E$ (GPa) | $\nu$ (-) | $\rho$ (kg m$^{-3}$) |
|-----------|-----------|-----------|---------------------|
| Glass     | 72        | 0.22      | 2500                |
| PBT       | 2.6       | 0.41      | 1300                |

by Rauter et al.$^{7,20}$ based on the probabilistic information of the fiber length, fiber diameter, and fiber orientation distribution 500 artificial microstructures with a size of 2500 μm × 2500 μm are generated. The center coordinates of each fiber are provided by a Monte Carlo sampling, whereas the fiber properties are sampled with respect to their individual probability density function, which are taken from Günzel.$^{55}$ Next, for each microstructure 33 windows of the size 250 μm × 250 μm, 500 μm × 500 μm, and 750 μm × 750 μm are extracted in accordance with Figure 1, see also previous work by the author.$^{7,20}$ The distance between the windows is equal to a quarter of the window size in vertical and horizontal direction. Along the diagonal, the distance is $\sqrt{2}/4$ times the window size. This ensures the ability to determine the two-dimensional correlation function accurately. Next, the microstructures are translated into an array, which contains the material properties for every point. Finally, the material properties of the microstructure are passed to the integration points of the numerical model. For both constituents, only linear-elastic material behavior is required. The corresponding material parameters of polybutylene terephthalate (PBT) matrix material and of glass are given in Table 1. The fiber mass fraction is set to 30% (PBT GF 30).

The numerical model is generated in accordance with the findings in Rauter et al.$^{20}$ For the determination of the strain-energy density function coefficients and the yield strength, the same model is used. Since this two-dimensional model is a cross-section of a three-dimensional tensile test specimen, a plane strain state is assumed. This is reasonable, because the cross-section of SFRC manufactured by mold injection shows a layered structure.$^{56-58}$ In the middle is a core layer, which is characterized by an out-of-plane fiber orientation, that induces a resistance of the tensile test specimen against shrinking. To include this effect without an explicit modeling of this layer, the plane strain assumption is used. Therefore, only the shell layers are considered as shown by Rauter et al.$^{20}$

3.3 Results

In this section the results for the parameters of the strain-energy density function, the yield strength, and the correlation analysis are presented.
3.3.1  |  Hyperelasticity

In Table 2 the mean value and the standard deviation for each parameter of the strain-energy density function is given. Since the numerical simulations are performed by applying pure displacement boundary conditions the mean of the absolute values show a decreasing tendency with increasing window size. Furthermore, the standard deviation increases with an decreasing window size, as expected. These observations meet the expectation of simulations on the mesoscale. In addition, the Young’s modulus in horizontal direction is provided to validate the results with experimental investigations of tensile tests performed with specimens made of PBT GF 30. The experimentally obtained mean value based on 13 specimens is 9.75 GPa with a standard deviation of 0.27 GPa. A comparison with the numerically obtained values shows, that for all window sizes the numerical values cover the experimental results. Hence, the results for the parameters of the strain-energy density function appears to be reasonable.

3.3.2  |  Plasticity

In Table 3 the mean value and standard deviation of the obtained yield strength is given for each window size. For a validation of the results, Figure 2 gives the strain-stress curve for a tensile test specimen made of PBT GF 30, taken from the data sheet of the manufacturer. Assuming ideal plastic behavior, the experimentally obtained yield strength fits very well with the numerical results for the different window sizes.

Furthermore, in Figure 3 the spatial distribution of the yield strength is shown. First, Figure 3A gives an exemplary microstructure of the size 2500 μm × 2500 μm, where the center points of each extracted window with an edge length of 750 μm is indicated. In the context of SFRC the fiber mass fraction \( \varphi_m \) is commonly used. It can be computed from the fiber volume fraction by evaluating

\[
\varphi_m = \frac{\rho_m \varphi}{\rho_f \varphi + \rho_m (1 - \varphi)}.
\]  

Subsequently, in Figure 3B,C for each of these windows the fiber mass fraction and the resulting yield strength are provided, respectively. Since the reinforcing fibers are modeled with linear elastic material behavior and hence, they do not show any plastic deformation, it is expected that with an increasing amount of fibers in an extracted window the yield

| Table 2  | Mean values and standard deviations of the strain density function coefficients. |
|----------|-----------------------------------------------|
|          | Sample | \( \Lambda \) (GPa) | \( \mu \) (GPa) | \( \sigma \) (GPa) | \( \beta \) (GPa) | \( \gamma \) (GPa) | \( E_{11} \) (GPa) |
| Mean     | 250 μm | 5.62           | 1.34           | 1.16           | -0.20          | 1.35           | 11.9         |
|          | 500 μm | 5.43           | 1.24           | 1.13           | -0.14          | 1.19           | 10.5         |
|          | 750 μm | 5.38           | 1.20           | 1.10           | -0.13          | 1.13           | 10.0         |
| Standard- | Experiment | -              | -              | -              | -              | -              | 9.75         |
| deviation| 250 μm | 0.492          | 0.192          | 0.239          | 0.081          | 0.475          | 3.85         |
|          | 500 μm | 0.224          | 0.097          | 0.131          | 0.033          | 0.244          | 1.96         |
|          | 750 μm | 0.140          | 0.064          | 0.090          | 0.020          | 0.148          | 1.26         |
| Experiment | -              | -              | -              | -              | -              | -              | 0.27         |

| Table 3  | Results yield strength. |
|----------|-------------------------|
|          | Sample | Mean yield strength (MPa) | Standard deviation (MPa) |
|          | 250 μm | 151.7          | 57.1               |
|          | 500 μm | 130.3          | 24.2               |
|          | 750 μm | 125.7          | 14.7               |
FIGURE 2  Stress strain curve for PBT GF 30 under uniaxial loading in melt flow direction, values taken from the data sheet of the manufacturer.59

strength increases. This expectation can be validated by Figure 3B,C. Windows with a higher fiber mass fraction show a significantly increasing yield strength. Based on the comparison with experimental results as well as the correlation between the fiber mass fraction and the obtained yield strength, the homogenization procedure appears to be applicable to SFRC.

4  CORRELATION

4.1  Overall behavior

For the analysis of the correlation between the coefficients of the strain-energy density function and the yield strength first, in Figure 4 the parameters for a window size of 750 μm are plotted against each other. If the two parameters of a plot are not correlated, the realizations give a random cloud of points. On the other hand, the $\Lambda - \gamma$ parameter pair shows a distinct correlation, which is indicated by the alignment of the individual points on the diagonal. The stronger the correlation, the more pronounced is the concentration of the points, until they all lie on a straight line, as can be seen for the auto-correlations. One further example for a strong cross-correlation is the $\mu - \alpha$ parameter pair. This strong correlation meets the theoretical framework of the hyperelastic strain-energy density function. In Appendix A the relation
between the strain-energy density function coefficients and the components of the elasticity tensor is given. Following Equation (A5), the parameters $\mu$ and $\alpha$ are directly linked to each other. The same holds for the parameter group of $\gamma, \mu, \Lambda, \alpha,$ and $\beta$. Since $\gamma$ is a function of $\mu, \Lambda, \alpha,$ and $\beta$, these parameters should be significantly correlated to $\gamma$. This is confirmed in Figure 4. Finally, Figure 4 shows that the symmetry $\rho_{ij} = \rho_{ji}$ required by the definition is fulfilled and that the coefficients of the strain-energy density function and the yield strength are coupled by a complex correlation structure.

As already shown by Rauter et al.\textsuperscript{20} for the linear elastic material parameters, the correlation depends on the window size. First, due to the definition of the different correlation functions, as given in Equations (15) to (17), the correlation length is bounded to the window size. However, not only the correlation length $\rho_0$ but also the correlation strength given by the cross-correlation parameter $\rho$ is influenced by the window size. In Figure 5 three different scenarios are depicted,
that are obtained by evaluating Equation (11) for each window size. For better comparability, the coordinates $\xi_1$ and $\xi_2$ are normalized by the window size. The parameter pair $\gamma - \mu$ shows an independent cross-correlation strength with respect to the window size. Furthermore, the coefficient $a$ is close to one for completely overlapping windows, which indicates a very pronounced cross-correlation. This also meets the distribution of the realizations in Figure 4, where the points are strongly aligned on the diagonal.

In the middle, the coefficient pair $\alpha - \mu$ is given. Here, the cross-correlation shows a significant influence of the window size on the parameter $a$. With an increasing window size, the parameter $a$ also increases. In contrast to this, the parameter pair $\beta$ and $\sigma_y$ show the opposite behavior. With an increasing window size the parameter $a$ decreases, which leads to a reduction of the correlation. This behavior is also observed for linear-elastic material properties, as shown in

**Figure 5**  Dimensionless correlation parameters $\rho_{\gamma\mu}$, $\rho_{\alpha a}$, and $\rho_{\sigma_y}$ for each window size.

**Figure 6**  Cross-correlation coefficient $a$ for all window sizes.
Furthermore, in this case the value of the dimensionless correlation parameter is negative, which is induced by the different sign of the parameters $\beta$ and $\sigma_y$. As given in Table 2 the values of $\beta$ are negative, whereas the values of $\sigma_y$ are positive.

### 4.2 Correlation length

In a next step the correlation length is determined for each parameter pair. Therefore, first, the three different correlation functions given by Equations (15) to (17) are fitted with the calculated dimensionless correlation parameter. Based on the coefficient of determination $R^2$, the best fit is selected to analyze the correlation length in a second step. The results of $R^2$ for each window size and each correlation function are provided in Appendix B. The results of the curve fit for the

**FIGURE 7** Analysis of the correlation length for each auto- and cross-correlation.
auto-correlation indicate that the triangle correlation function is the best fit for the parameters \( \Lambda, \beta, \gamma, \) and \( \sigma_y \), whereas the exponential correlation function fits the parameters \( \mu \) and \( \alpha \) best. Consequently it is expected that the exponential correlation function is the best option for the cross-correlation of these two parameters. The remaining parameter pairs should be approximated best by triangle cross-correlation function, because the corresponding auto-correlation functions of these parameters are given by a triangle correlation function, which is confirmed by the \( R^2 \) values of the performed curve fits given in Appendix B.

For a detailed analysis of the auto- and cross-correlation, Figures 6 and 7 illustrate the results of the cross-correlation parameter \( a \) and the correlation lengths, respectively. The coefficient \( a \) describes the strength of the correlation between two parameters. Hence, for small absolute values of \( a \) the parameters are not correlated, which results in a random cloud of points in the corresponding diagram of Figure 4. For each window size and each parameter pair, the mean value and the 95% confidence interval is given. The dashed lines in Figure 6 indicate a cross correlation coefficient of \( |a| = 0.5 \). First, the dependence of \( a \) on the window size, as discussed before, is observable. Furthermore, the parameter pairs \( \Lambda - \alpha \) and \( \alpha - \beta \) are only very weakly cross-correlated, which is confirmed in Figure 4. For the remaining parameters, the correlation lengths \( b_1 \) and \( b_2 \) are calculated for both the auto- and cross-correlation, see Figure 7. Furthermore, dashed and dotted lines are added to indicate the window size \( l_w \) and a correlation length of 0.4\( l_w \). As done before, for each parameter pair the mean value and the 95% confidence interval are plotted. The results show, that with an increasing window size, the distance between \( b_1 \) and \( b_2 \) decreases. Furthermore, for an approximation with the triangle function the values converge to 0.4\( l_w \). However, it is important to note that this correlation analysis gives only the behavior of the correlation with respect to the window size and hence, is a qualitative statement. Since the correlation length can be interpreted as an additional independent material parameter its value, which is required to synthesize random fields for the representation of the spatial distributed material parameters, needs to be derived from experimental investigations.

## 5 SUMMARY AND CONCLUSION

In this work an approach is presented to extract the correlation structure of the finite strain elasto-plastic material properties of SFRC given by the five independent parameters of the transversely-isotropic strain-energy density function and the yield strength. Due to the linearization of the strain-energy density function at zero strain and the use of a homogenization procedure for the determination of the yield strength only linear-elastic simulations are required to obtain the apparent overall material properties for extractions of the microstructure at different locations. The obtained results are validated by experimental data, taken from literature. Furthermore, the expected link between the fiber mass fraction and the yield strength is confirmed.

With this data the dimensionless correlation parameter is calculated for the auto- and cross-correlation between the parameters of the strain-energy density function and the yield strength. It is shown, that the parameters are strongly correlated. Furthermore, the correlation shows a complex dependence on the window size. There are parameter pairs that are not influenced by the size of the microstructural extractions, others show a significant increasing and decreasing behavior, respectively. This is also supported by the results of the cross-correlation parameter \( a \).

Analyzing the development of the correlation function and the corresponding correlation lengths, reveals that most correlations are described best by a triangle function, only two auto-correlation functions and the corresponding cross-correlation are assigned to exponential correlation functions. This influences also the results of the correlation lengths due to the different function definitions. The results show, that for an increasing window size the correlation lengths \( b_1 \) converge to the window size \( l_w \) for a triangle function and to 0.4\( l_w \) for an exponential correlation function, respectively. Therefore, only one value needs to be determined based on experimental data to obtain the different correlation lengths for the generation of second-order random fields.

Summarizing, it can be concluded that the presented approach is suitable to derive the correlation structure for finite strain elasto-plastic material description of SFRC. The results of the correlation analysis are deployed in a subsequent study.\(^{21}\) With the information about the correlation structure at hand second-order random fields are synthesized to represent the spatial distribution of the hyperelastic and plastic material properties of tensile tests specimens made of SFRC and hence, incorporate the probabilistic nature of the microstructure on the component level.
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CONFLICT OF INTEREST
The author declares no conflict of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript, or in the decision to publish the results.

DATA AVAILABILITY STATEMENT
The data that support the findings of this study are available from the corresponding author upon reasonable request.

ORCID
Natalie Rauter https://orcid.org/0000-0003-1704-1426

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APPENDIX A. DETERMINATION OF THE APPARENT HYPERELASTIC MATERIAL PROPERTIES

Due to the five independent components of the elasticity tensor, a reduction of the material parameters automatically violates the symmetry properties induced by transversely isotropic behavior. Despite the fact, that the reduction of the elasticity tensor to a two-dimensional representation under plane strain assumption is independent of \( C_{44} \), it is still a function of all five independent engineering constants. The compliance matrix for plane strain assumption is calculated from the three-dimensional representation by

\[
S_{\text{strain}} = \begin{bmatrix}
S_{11} - \frac{S_{22}^2}{S_{11}} & S_{12} - \frac{S_{22}S_{33}}{S_{11}} & 0 \\
S_{12} - \frac{S_{22}S_{33}}{S_{11}} & S_{22} - \frac{S_{11}S_{33}}{S_{22}} & 0 \\
0 & 0 & S_{66}
\end{bmatrix}, \tag{A1}
\]

where the elements of the three-dimensional compliance matrix can be derived directly from the engineering constants. As mentioned before, due to the plane strain assumption all five independent engineering constants are required to obtain the compliance matrix for a plane strain assumption. The following relations hold

\[
S_{11} = \frac{1}{E_1}, \quad S_{12} = \frac{\nu_{21}}{E_2} = -\frac{\nu_{12}}{E_1},
\]

\[
S_{22} = \frac{1}{E_2}, \quad S_{23} = -\frac{\nu_{23}}{E_2}. \tag{A2}
\]

Since the two-dimensional modeling does not hold any information about the material properties in thickness direction, the out-of-plane Poisson’s ratio \( \nu_{23} \) is determined following the microstructural characteristics of the material by using the material model of Halpin–Tsai.\(^{53,54} \) If \( \nu_{23} \) is known the remaining engineering constants can be calculated by evaluating

\[
S_{\text{strain}}^{11} = \frac{1}{E_1} - \frac{\nu_{21}^2}{E_2}, \quad S_{\text{strain}}^{12} = -\frac{\nu_{21}}{E_1} - \frac{\nu_{21}\nu_{23}}{E_2},
\]

\[
S_{\text{strain}}^{22} = \frac{1}{E_2} - \frac{\nu_{23}^2}{E_2}, \quad S_{\text{strain}}^{66} = \frac{1}{G_{12}}, \tag{A3}
\]

which leads to

\[
E_1 = \frac{1}{S_{\text{strain}}^{11} + \frac{\nu_{21}^2}{E_2}}, \quad E_2 = \frac{1}{S_{\text{strain}}^{22}},
\]

\[
G_{12} = \frac{1}{S_{\text{strain}}^{66}}, \quad \nu_{21} = -\frac{S_{\text{strain}}^{12}E_2}{1 + \nu_{23}}. \tag{A4}
\]
To derive the coefficients of the strain-energy potential in a final step first the stiffness tensor for a three-dimensional representation is determined based on the known engineering constants. Afterwards the coefficients can be calculated by evaluating

\[
\Lambda = C_{23}, \quad \mu = \frac{1}{2}(C_{22} - \Lambda), \\
\alpha = C_{66} - 2\mu \quad \beta = \frac{1}{4}(C_{12} - \Lambda), \quad \gamma = \frac{C_{11} - 2\mu - \Lambda - 2\alpha}{8} - \beta.
\]

(A5)

**APPENDIX B. RESULTS OF THE COEFFICIENT OF DETERMINATION**

In Tables B1 and B2 the results of \(R^2\) for the auto-correlation and the cross-correlation curve fits are provided, respectively. There are no values of \(R^2\) given for the cross-correlation of the parameter pair \(\Lambda - \alpha\), because they are not connected by a cross-correlation.

**TABLE B1** Results \(R^2\) curve fit auto-correlation.

| Window size | Correlation function | \(\Lambda\) | \(\mu\) | \(\alpha\) | \(\beta\) | \(\gamma\) | \(\sigma_y\) |
|-------------|----------------------|-------------|---------|-------------|---------|-----------|----------|
| 250 \(\mu\)m | Exponential          | 0.89        | 0.90    | 0.90        | 0.90    | 0.90      | 0.90     |
|              | Triangle             | 0.96        | 0.76    | 0.45        | 0.96    | 0.98      | 0.97     |
|              | Gaussian             | 0.95        | 0.80    | 0.82        | 0.92    | 0.96      | 0.93     |
| 500 \(\mu\)m | Exponential          | 0.84        | 0.89    | 0.87        | 0.88    | 0.87      | 0.91     |
|              | Triangle             | 0.96        | 0.74    | 0.36        | 0.98    | 0.98      | 0.96     |
|              | Gaussian             | 0.96        | 0.81    | 0.79        | 0.94    | 0.96      | 0.94     |
| 750 \(\mu\)m | Exponential          | 0.79        | 0.89    | 0.81        | 0.85    | 0.86      | 0.91     |
|              | Triangle             | 0.92        | 0.72    | 0.37        | 0.95    | 0.97      | 0.95     |
|              | Gaussian             | 0.92        | 0.81    | 0.71        | 0.92    | 0.94      | 0.94     |

**TABLE B2** Results \(R^2\) curve fit cross-correlation.

| Parameter | 250 \(\mu\)m | 500 \(\mu\)m | 750 \(\mu\)m |
|-----------|--------------|--------------|--------------|
| \(\lambda\) | \(\mu\) | \(\alpha\) | \(\beta\) | \(\gamma\) | \(\sigma_y\) | \(\lambda\) | \(\mu\) | \(\alpha\) | \(\beta\) | \(\gamma\) | \(\sigma_y\) | \(\lambda\) | \(\mu\) | \(\alpha\) | \(\beta\) | \(\gamma\) | \(\sigma_y\) |
| \(\mu\) | 0.87 | 0.88 | 0.85 | 0.88 | 0.87 | 0.89 | 0.86 | 0.89 | 0.88 | 0.84 | 0.95 | 0.92 |
| \(\alpha\) | 0.91 | 0.97 | 0.97 | 0.88 | 0.98 | 0.96 | 0.85 | 0.95 | 0.93 | 0.83 | 0.93 | 0.92 |
| \(\gamma\) | 0.91 | 0.97 | 0.97 | 0.88 | 0.98 | 0.96 | 0.85 | 0.95 | 0.93 | 0.83 | 0.93 | 0.92 |
| \(\sigma_y\) | 0.84 | 0.92 | 0.93 | 0.86 | 0.94 | 0.93 | 0.83 | 0.93 | 0.92 | 0.83 | 0.93 | 0.92 |
| \(\beta\) | 0.60 | 0.67 | 0.63 | 0.82 | 0.75 | 0.83 | 0.82 | 0.75 | 0.75 | 0.83 | 0.93 | 0.89 |
| \(\gamma\) | 0.93 | 0.97 | 0.96 | 0.90 | 0.97 | 0.94 | 0.85 | 0.93 | 0.93 | 0.88 | 0.96 | 0.94 |
| \(\sigma_y\) | 0.89 | 0.97 | 0.96 | 0.88 | 0.97 | 0.95 | 0.88 | 0.96 | 0.95 | 0.88 | 0.96 | 0.95 |
| \(\gamma\) | 0.91 | 0.97 | 0.97 | 0.88 | 0.97 | 0.96 | 0.86 | 0.95 | 0.94 | 0.83 | 0.93 | 0.92 |
| \(\sigma_y\) | 0.85 | 0.92 | 0.93 | 0.85 | 0.93 | 0.92 | 0.83 | 0.93 | 0.92 | 0.83 | 0.93 | 0.92 |
| \(\delta\) | 0.92 | 0.97 | 0.96 | 0.92 | 0.97 | 0.96 | 0.88 | 0.97 | 0.96 | 0.88 | 0.97 | 0.96 |