Mean-Field Approximations in Effective Thermo-viscoelastic Behavior for Composite Parts Obtained via Fused Deposition Modeling Technology

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Abstract. Aiming to estimate the effective behavior of the parts obtained by fused deposition modeling (FDM) in the case of short fiber composite materials, the Mean-field homogenization procedure, introduced in linear elasticity, is here extended to linear thermo-viscoelasticity. The variation of the parameters describing the state of the fibers inside the printing filament is represented by introducing appropriate distribution functions obtained through the statistical analysis of the microstructure. The validation of the procedure is achieved by comparing its predictions with calculations based on full-field Fast-Fourier-Transform homogenization and experiments results from samples treated in autoclave to remove layer-scale porosities from the printed filament.

INTRODUCTION

We are interested in the capabilities and performance of 3D printed parts, manufactured from a thermoplastic matrix reinforced with short (100 μm) or intermediate (1 mm) glass fibers. The goal is to estimate the residual stresses induced by the cooling of these parts from extrusion to room temperature, which is an essential requirement for the design of these parts, especially with respect to the filament deposition trajectory. This is difficult to estimate due to the complexity of the material (thermo-viscoelastic composite) and the complexity of the printing process itself (Fig. 1). This study therefore focuses on the influence of the topological and mechanical complexity of the microstructure of the printing filament.

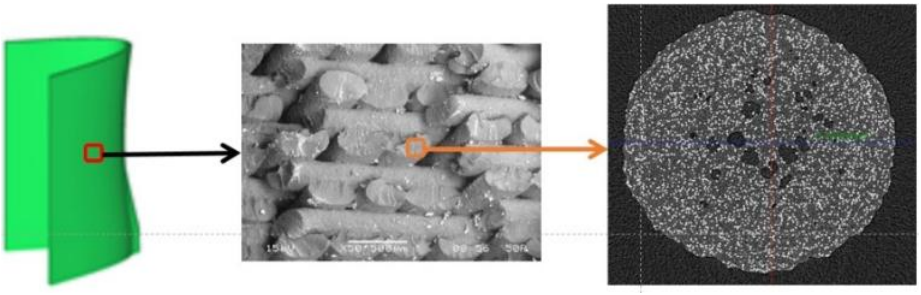

FIGURE 1. Three-scale configuration: printed part, printed filament structure and the short fiber reinforced composite filament.

HOMOGENIZATION OF REINFORCED POLYMER FILAMENTS

The homogenization procedure consists of the following two fundamental steps: the estimation of the effective properties of the reinforced filament and the estimation of the effective properties of the final composite material treated in the autoclave, which contains the particular arrangement of the filaments as a function of the printing path. In this modeling, the fibers of the filament are considered as linear elastic solids whereas the polymer matrix is described as a linear thermo-viscoelastic solid.

Thermo-viscoelastic modeling of the matrix

In general, linear viscoelastic materials behavior is characterized by a delayed response in a dual consideration of stress or deformations, this fact put in evidence the time dependency of the modulus relating these two physical quantities. The mathematical structure of the theory is defined via the Boltzman superposition principle [1] which in the case of a non-aging and homogeneous viscoelastic solid under isothermal conditions at equilibrium for $t \leq 0$, can be represented as follows:

$$\boldsymbol{\sigma}(t) = \int_0^t \boldsymbol{L}(t-\tau) d\boldsymbol{\varepsilon}(\tau) = \boldsymbol{L}(t) * \boldsymbol{\varepsilon}'(t) = \boldsymbol{L}(t) \otimes \boldsymbol{\varepsilon}(t) \tag{1}$$

where $\boldsymbol{\sigma}(t)$ and $\boldsymbol{\varepsilon}(t)$ are the stress and strain, respectively, and $\boldsymbol{L}(t)$ is the time dependent modulus known as the "relaxation modulus". The last expression in Eq. (1) is a symbolic form of the Stieltjes convolution product. In continuum mechanics the relaxation modulus is represented as an analogy of an assembly of elastic springs and viscous dashpots (e.g Maxwell and Kelvin-Voigt models) and its complexity depends on the material response observed from relaxation or creep experiments. In practice the material functions are defined for a fixed temperature. Operational calculus is presented as a mathematical tool in viscoelastic materials theory, allowing to avoid the computation of convolution products by using Laplace-Carson transform (Correspondence principle [1]), obtaining an equivalent problem that comes out as a symbolic analogy of linear elastic solids in the frequency domain, where the Laplace variable p is the complex circular velocity ($j\omega$).

In this study the matrix is considered as an isotropic and amorphous polymer; its linear viscoelastic behavior is described by a generalized N-branches Maxwell model. The consideration of thermally induced deformations is represented by a rheological model equivalent to the generalized N_T-branches Kelvin-Voigt model [2], to capture the information from delayed deformations as a function of temperature history, being the main source of residual stresses due to the nature of the manufacturing process. This model is similar to one presented in [3] in the case of shape memory alloys. An illustrative representation of the model is shown below.

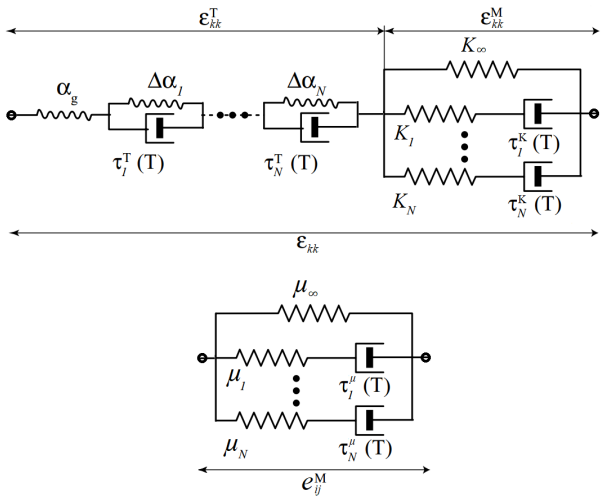

FIGURE 2. Rheological model of the polymer matrix

The difficulty in this step is the need to establish a form of the problem that is compatible with the correspondance principle in isothermal linear viscoelasticity. The nature of the printing process imposes continuous temperature variations, acting on the material properties. These variations in properties have been modelled based on the principle of time-temperature superposition of thermo-rheologically simple materials, with the introduction of a coefficient linking the observer's own time scale and that of the polymer, being a function of temperature [4]. According to this principle and taking into account the homogeneity of the temperature field in the formulation of the mean-field homogenization problem for the thermomechanical effective behavior, the problem is reduced to an equivalent form of the isothermal case in the "reduced" (or internal) time domain [5].

From the preceding considerations and the introduction of two types of internal variables [6], we obtain a simplified writing of the thermodynamic formulation of the thermo-viscoelastic problem. This formulation is developed within the framework of generalized standard materials and is characterized by the Helmholtz free energy, $\omega(\varepsilon,(\varepsilon_v^i)_{i=1}^N,(q^j)_{j=1}^{N_T},T)$, and by the mechanical dissipation potential, $\varphi((\dot{\varepsilon}_{v^i})_{i=1}^N,(\dot{q}^j)_{j=1}^{N_T},T)$, where $\varepsilon,\varepsilon_v^i,q^j$ are the deformation, the viscous strain in branch i, and the internal variable related to delayed thermal strain in branch j, respectively, and T, the temperature. Using this framework, these potentials can be written as follows:

$$\omega\left(\varepsilon,\varepsilon_v^i,T,q^j\right)=\sum_{i=1}^{N}\frac{1}{2}\left(\varepsilon-\varepsilon_v^i\right):L^i:\left(\varepsilon-\varepsilon_v^i\right)-\sum_{i=1}^{N}\left(\varepsilon-\varepsilon_v^i\right):L^i:\left(\alpha_g\theta+\sum_{j=1}^{N_T}\left(q^j\right)\right)+c_0\left[\theta-T\ln\frac{T}{T_0}\right]-\eta_0 T+e_0 \tag{2}$$

and,

$$\varphi\left(\dot{\varepsilon}_v^i,T,q^j\right)=\sum_{i=1}^{N}\frac{1}{2}\dot{\varepsilon}_v^i:\boldsymbol{L}_v^i(T):\dot{\varepsilon}_v^i+\sum_{i=1}^{N}\dot{\varepsilon}_v^i:\boldsymbol{L}_v^i(T):\sum_{j=1}^{N_T}\left(\dot{q}^j\right) \tag{3}$$

where $\boldsymbol{L^i}$ and $\boldsymbol{L_v^i}$ are the elasticity and viscosity tensors for the i-branch, respectively, $\boldsymbol{\alpha}_g$ is the instantaneous thermal expansion tensor, c_0 is the heat capacity at constant stress, η_0 and e_0 are the initial entropy and initial internal energy, respectively. The number of branches and the tensors $\boldsymbol{L^i}$ and $\boldsymbol{L_v^i}$ were found using dynamic-mechanical analysis (DMA) and creep experiments at different temperatures. The number of branches and the expansion coefficient tensors of the rheological model for thermal strains are obtained from isothermal recovery tests for step type thermal loading.

Upscaling

A finite element based calculations were used to solve the coupled mechanical and thermal equilibrium equations for macroscopic stress, strain, and temperature. At each integration point, these quantities are averaged over a representative elemental volume (REV) of their microscopic counterparts, solving the local mechanical and thermal equilibrium equations given by :

$$\begin{aligned}&\operatorname{div}\boldsymbol{\sigma}(\boldsymbol{x},t)=0,\boldsymbol{\sigma}(\boldsymbol{x},t)=\frac{\partial\omega}{\partial\varepsilon}\left(\boldsymbol{x},\varepsilon,\varepsilon_v^i,\bar{T},q^j\right)\\&\frac{\partial\omega}{\partial\varepsilon_v^i}\left(x,\varepsilon,\varepsilon_v^i,\bar{T},q^j\right)+\frac{\partial\omega}{\partial q^j}\left(x,\varepsilon,\varepsilon_v^i,\bar{T},q^j\right)+\frac{\partial\varphi}{\partial\dot{\varepsilon}_v^i}\left(x,\dot{\varepsilon}_v^i,\bar{T},\dot{q}^j\right)+\frac{\partial\varphi}{\partial\dot{q}^j}\left(x,\dot{\varepsilon}_v^i,\bar{T},\dot{q}^j\right)=0\end{aligned} \tag{4}$$

$$\operatorname{div}\boldsymbol{q}(\boldsymbol{x},t)=0,\boldsymbol{\sigma}(\boldsymbol{x},t)=-\boldsymbol{k}(\boldsymbol{x})\cdot\nabla T(\boldsymbol{x},t) \tag{5}$$

where $\boldsymbol{q}$ and $\boldsymbol{k}$ are the heat flux and the thermal conductivity tensor, respectively. It should be noted that the microscopic mechanical and thermal equations Eq. (4) and Eq. (5) are decoupled for the following reasons: (i) Only the macroscopic mean, $\bar{T}$, is considered in the mechanical formulation Eq. (4). (ii) The dissipated energy is considered at the macroscopic scale, which simplifies the thermal equation as shown in Eq. (5). The thermo-mechanical coupling is then carried out at the macroscopic scale. The equations Eq. (4) and Eq. (5) are supplemented by appropriate boundary conditions by noting $\bar{\varepsilon}$ and $\bar{T}$, the respective averages of the local fields $\bar{\varepsilon}$, solution of Eq. (4), and $\bar{T}$, solution of Eq. (5).

Mean-field models to account for the presence of fibers

Mean-field homogenization is a methodology used to approximate effective properties at the macroscopic scale based on the information at lower scales in heterogeneous media. this procedure is implemented on a characteristic region of the material known as the representative volume element (RVE) that must contains enough information about the physical quantities of interest and the morphological properties of the inhomogeneities coexisting in the predominant phase. Therefore the quality of the approximation depends on the way as one choose and use the information available. The existence of some effective property in proved from the Hill-Mandel lemma under the imposition of homogeneous stress or strain in the RVE, and its uniqueness proof comes from the convexity of the potentials related to the observable mechanical quantities. In this study Mean-field methods are intended to determine approximations of the mean fields ($\bar{\varepsilon}$ and $\bar{T}$) in each phase using simplifying assumptions (generally valid for at average volume fraction) and analytical results from methods equivalent to the well-known Eshelby's inclusion problem.

Analytical methods (Mori-Tanaka, Interaction Direct Derivative, Ponte-Castañeda-Willis, Lielens, etc.) were used to estimate and compare the mean of the thermomechanical fields that solve the local equations Eq. (4) and Eq. (5). The mean-field methods used, consider the high complexity of the composite material's microstructure (non-alignment of the fibers, thermo-viscoelasticity of the matrix, etc.). Several models were used to estimate the effective relaxation and creep thermal dilatation functions ($\boldsymbol{L}_{\text{eff}}$ and $\boldsymbol{\alpha}_{\text{eff}}$), including the Direct Derivative Interaction model (IDD) [7], which is characterized by the following equation :

$$L_{\text{eff}} = L_{\text{M}} + \left(I - c_{\text{F}} \int_S f(\boldsymbol{n}) \Delta \boldsymbol{L}_{F,M}(\boldsymbol{n}) : \boldsymbol{A}_{\boldsymbol{F},M}(\boldsymbol{n}) : \boldsymbol{P}^D_{\boldsymbol{F}}(\boldsymbol{n}) dS \right)^{-1} : \left(c_{\boldsymbol{F}} \int_S f(\boldsymbol{n}) \Delta \boldsymbol{L}_{\boldsymbol{F},M}(\boldsymbol{n}) : \boldsymbol{A}_{\boldsymbol{F},M}(\boldsymbol{n}) dS \right) \quad (6)$$

where S is the unit sphere, c_F is the volume fraction of the fibres, $\boldsymbol{n}$ is the unit vector describing the orientation of the fibres, f is the probability density function for the orientation distribution, $\boldsymbol{A}_{\boldsymbol{F},M}$, is the localization tensor, a function of the fiber geometry, the material contrast, defined as $\Delta \boldsymbol{L}_{F,M} = \boldsymbol{L}_F(\boldsymbol{n}) - \boldsymbol{L}_M$, and $\boldsymbol{P}^D_{\boldsymbol{F}}(\boldsymbol{n})$ is the Hill's tensor which takes into account the spatial distribution of the fibers inside the filament.

In the case of linear viscoelastic constituents, the Laplace-Carson transform is conventionally used to define a linear symbolic elastic composite in the Laplace domain (correspondence principle [1]). This method cannot be used directly because of the temperature dependence of the viscous modules of the matrix. To overcome this difficulty, we used an incremental formulation [8] for the equivalent form of the problem using as argument the "reduced time", an extension of the superposition principle for thermo-rheologically simple materials in the case of continuous temperature variations.

VALIDATION

The proposed mean-field model was evaluated by comparing its predictions in terms of effective moduli with those of full-field simulations based on Fast-Fourier-Transform approximations on representative volume elements (e.g. Fig. 3). The proposed macroscopic structural analysis was evaluated by comparing its predictions in terms of deformation with the deformation developed in asymmetrical 3D printed plates (plates with two deposition orientations: 0° and 90°), subjected to an additional heat treatment in the autoclave, thus limiting the degree of heterogeneity due to the presence of porosities that appear during the printing process and allowing to study the particular influence of the state of the fibers in the overall mechanical behavior of the part.

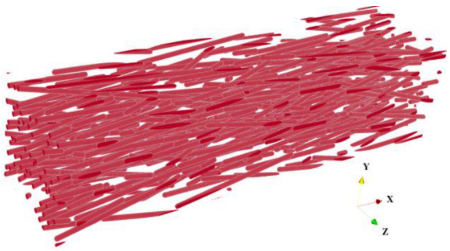

FIGURE 3. Representative element volume: Glass fibers in polymer matrix

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