ESTIMATING THERMOMECHANICAL RESIDUAL STRESSES IN FDM 3D PRINTED COMPOSITE PARTS

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Summary We implemented a two-step methodology to estimate the residual stresses induced by the FDM manufacturing process in 3D printed composite parts. The first step consisted in an analytical thermo-viscoelastic homogenization procedure to derive the effective behavior of the filament. The second step consisted in a coupled thermomechanical structural analysis of the part. The homogenization procedure was assessed by comparing its predictions to full-field FFT-based computations. The structural analysis was assessed by comparing its predictions to experimental results.

FRAMEWORK

We are interested in the capabilities and performances of 3D printed parts made of thermoplastic matrix reinforced by short (≈100 μm) to intermediate (≈1 mm) glass fibers. Our aim is to estimate the residual stresses induced by cooling these parts from extrusion to room temperatures, which is a critical requirement to design these parts, in particular their filament's deposition trajectory. This estimation is challenging because of the complexity of the material (thermo-visco-elastic composite) and that of the FDM process itself (Fig. 1).

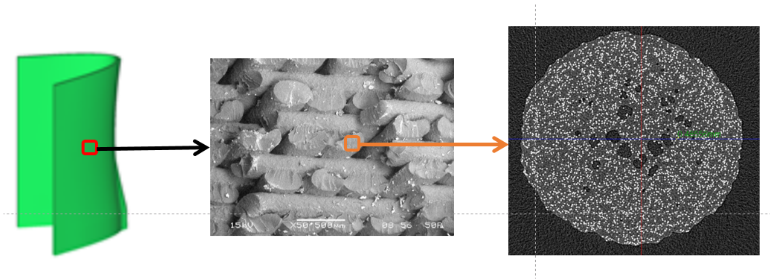

Figure 1: Three-scale configuration: printed part, fused filament structure and fiber-reinforced composite.

In the following, we provide some detail on each aspect of the methodology implemented.

HOMOGENIZATION OF REINFORCED POLYMER FILAMENTS

We estimated the FDM-induced residual stresses by using (i) a homogenization procedure to estimate the effective properties of the filament, and (ii) a coupled thermo-mechanical structural analysis. The homogenization procedure has two steps. The first step consisted in estimating the effective properties of the reinforced filament; the second step, in estimating the effective properties of the final 3D printed composite material.
The fibers of the filament were assumed to be elastic. Its matrix was assumed to be thermo-viscoelastic. Various mean-field methods were used to account for the fibers, and their predictions were compared with FFT-based full-field simulations. Finally, with these effective models at hand, the deflection and residual stresses in the whole part were estimated using an FEM code. Validation at the macroscale were then performed comparing FE simulations with experiments.

Thermo-viscoleastic modeling of the matrix The polymer matrix was assumed to be isotropic and its thermo-viscoelastic behavior to be described by an N-branch generalized Maxwell model, which is developed within the framework of generalized standard materials and characterized by the free energy $w(\boldsymbol{\varepsilon}, (\boldsymbol{\varepsilon}_v^i)_{i=1}^N, T)$ and the mechanical dissipation potential $\varphi((\dot{\boldsymbol{\varepsilon}}_v^i)_{i=1}^N, T)$, where $\boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon}_v^i$ are the strain and the viscous strain of branch i, respectively, and T is the temperature. For an N-branch model, these potentials can be written as

$$w(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}_v^i, T) = \sum_{i=1}^{N} \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_v^i) : \boldsymbol{L}^i : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_v^i) + \sum_{i=1}^{N} (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_v^i) : \boldsymbol{L}^i : \boldsymbol{\alpha}(T - T_0) + c_0 \left[(T - T_0) - T \ln \frac{T}{T_0} \right] - \eta_0 T + e_0,$$

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and

$$\varphi(\dot{\varepsilon}_v^i, T) = \sum_{i=1}^{N} \frac{1}{2} \dot{\varepsilon}_v^i : \boldsymbol{L}_v^i(T) : \dot{\varepsilon}_v^i,$$

where $\boldsymbol{L}^i$ and $\boldsymbol{L}_v^i$ are the elasticity and viscosity tensors of branch i, respectively, $\boldsymbol{\alpha}$ is the thermal expansion tensor, c_0 is the heat capacity at constant stress, and η_0 and e_0 are the initial entropy and internal energy, respectively. The number of branches and the tensors $\boldsymbol{L}^i$ and $\boldsymbol{L}_v^i$ were found using DMA and creep experiments at different temperatures.

Upscaling FEM calculations were used to solve the macroscopic coupled mechanical and thermal equilibrium equations for the macroscopic stress, strain and temperature. At each integration point, these quantities are the average over a representative volume element of their microscopic counterparts, which solve the local mechanical and thermal equilibrium equations given by:

$$\mathrm{div}\boldsymbol{\sigma}(\boldsymbol{x},t) = 0, \quad \boldsymbol{\sigma}(\boldsymbol{x},t) = \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{x}, \boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}_v^i, \overline{T}), \quad \frac{\partial w}{\partial \boldsymbol{\varepsilon}_v^i}(\boldsymbol{x}, \boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}_v^i, \overline{T}) + \frac{\partial \varphi}{\partial \dot{\boldsymbol{\varepsilon}}_v^i}(\boldsymbol{x}, \dot{\boldsymbol{\varepsilon}}_v^i, \overline{T}) = 0. \tag{1}$$

$$\mathrm{div}\boldsymbol{q}(\boldsymbol{x},t) = 0, \quad \boldsymbol{q}(\boldsymbol{x},t) = -\boldsymbol{k}(\boldsymbol{x}).\boldsymbol{\nabla} T(\boldsymbol{x},t), \tag{2}$$

where $\boldsymbol{q}$ and $\boldsymbol{k}$ are the heat flux and conductivity tensor respectively. It should be noted that the microscopic mechanical and thermal equations (1) and (2) are uncoupled because of the following: i) Only the average macroscopic, $\overline{T}$, is considered in the mechanical formulation (1). ii) The dissipated energy is taken into account at the macroscale, which simplifies the heat equation as shown in (2). The thermo-mechanical coupling is then achieved at the macroscopic scale. Equations (1) and (2) are supplemented with appropriate boundary conditions to enforce that $\overline{\varepsilon}$ and $\overline{T}$ are the respective averages of the local fields $\varepsilon(\boldsymbol{x})$, solution of (1), and $T(\boldsymbol{x})$, solution of (2).

Mean-field models to account for the fibers We used mean-field methods to estimate the average of the thermo-mechanical fields that solve the local equations (1) and (2). The used mean-field methods handle the complexity of the composite material (non-alignment of the fibers, thermo-viscoelasticity of the matrix, etc.).
Mean-field methods aim at determining closed-form approximations of the mean fields in each phase using simplifying assumptions (usually valid for low to medium densities of inclusions) and analytical results coming from Eshelby's equivalent inclusion method. We used several models to estimate the effective elasticity tensor of the filament, $\boldsymbol{L}_{\text{eff}}$, including the Interaction direct derivative model [4], which is characterized by the following equation:

$$\boldsymbol{L}_{\text{eff}} = \boldsymbol{L}_{\text{M}} + \left(\boldsymbol{I} - c_{\text{F}} \int_S f(\boldsymbol{n}) \Delta \boldsymbol{L}_{\text{F,M}}(\boldsymbol{n}) : \boldsymbol{A}_{\text{F,M}}(\boldsymbol{n}) : \boldsymbol{P}_{\text{F}}^{\text{D}}(\boldsymbol{n}) dS\right)^{-1} : \left(c_{\text{F}} \int_S f(\boldsymbol{n}) \Delta \boldsymbol{L}_{\text{F,M}}(\boldsymbol{n}) : \boldsymbol{A}_{\text{F,M}}(\boldsymbol{n}) dS\right) \tag{3}$$

where S is the unit sphere, c_{F} is the fibers' volume fraction, $\boldsymbol{n}$ is the fibers' orientation, f is the orientation probability density function, $\boldsymbol{A}_{\text{F,M}}$ is the localization tensor accounting for the fibers' shapes and material contrast, defined as $\Delta \boldsymbol{L}_{\text{F,M}}(\boldsymbol{n}) = \boldsymbol{L}_{\text{F}}(\boldsymbol{n}) - \boldsymbol{L}_{\text{M}}$, and $\boldsymbol{P}_{\text{F}}^{\text{D}}$ is Hill's tensor accounting for the fibers' spatial distribution.
In the case of linear viscoelastic constituents, Laplace-Carson transform is classically used which allows defining a linear symbolic elastic composite in the Laplace domain (the so-called correspondence principle [3]). This method cannot be used directly because of the temperature dependence of the viscous moduli of the matrix. To overcome this difficulty, we used an incremental formulation [1] that allows the Laplace-Carson transform to be used, provided that the moduli change slowly with the temperature.

VALIDATION

The proposed mean-field model was assessed by comparing its predictions in terms of effective moduli to those of FFT-based full-field simulations on representative volume elements (RVE). The proposed macroscopic structural analysis was assessed by comparing its predictions in terms of warping with the warping that develops within 3D printed asymmetric plates (plates with two deposition orientations: 0° and 90°).

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