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A data-driven process for estimating nonlinear material models

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Abstract. Driven by the wide range of new material properties offered by multi-material 3D printing, there is emerging need to create predictive material models for these materials. A data driven process for estimating nonlinear material model is presented in this paper. In contrast with classical methods which derive the engineering stress-strain relationship assuming constant cross-section area and fixed length of a specimen, the proposed approach takes full advantage of 3D geometry of the specimen to estimate the material models. Give a hypothetical material model, virtual tensile tests are performed using Finite Element Analysis (FEA) method, and the parameters of the material model are estimated by minimizing the discrepancies of the virtual responses and the experimental results. The detailed material models, numerical algorithms as well as the optimization approaches are presented and finally preliminary results are offered.

Introduction

Driven by the wide range of new material properties offered by multi-material 3D printing, there is emerging need to create predictive material models for these materials. Tensile tests are one of the most widely used mechanical tests to derive such material properties as Young's modulus and yield stress. The output of the tensile test is a force-elongation curve, which is usually converted to the stress-strain curve for estimation of material properties. In such a conversion, it is usually assumed that the cross-section area and the length of the specimen are constant in the entire tensile test. The derived stress/strain is referred to as *engineering* stress/strain. Because of its simplicity and satisfactory accuracy in modeling metallic materials, it has been widely used in the past.

For metallic materials, such engineering stress-strain based parameter estimation proves to be effective, since metals are significantly stiff and the change in the cross-section of the specimen is usually negligible. For polymer materials, such simplifications may introduce significant errors in the estimated parameters. In lieu of such classical approaches, there have been many targeted approaches that tries to get the *true stress-strain* from tensile tests. Arriaga *et al* [1] proposed empirical formulae to convert engineering stress-strain to true Cauchy stress. Grytten et al [2] used Digital Image Correlation (DIC) to measure local strain values in the tensile test of ductile thermoplastic materials.

In this paper, a different data-driven approach is proposed to estimate the material models. We propose different hypothetical material models, and for each material model, the parameters are estimated by minimizing an objective function which relates the model parameters to the discrepancies of the virtual and experimental tensile test data.

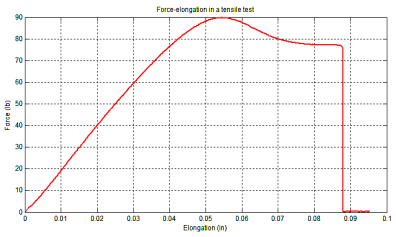
Problem Formulation

Fig.1 (a) shows a force-elongation curve derived from a tensile test on a resin-type material FullCure720 used by a rapid prototyping machine Objet PolyJet [3]. As is seen that there exists monotonically decreasing region in this curve where the elongation still increments even though the applied force decreases. In classical plasticity theory, such a phenomenon is generally referred to

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unstable behavior of a material [4]. As such, the region of interest in this research is confined in the stable range of this curve, as shown in Fig.1 (b).

(a) 

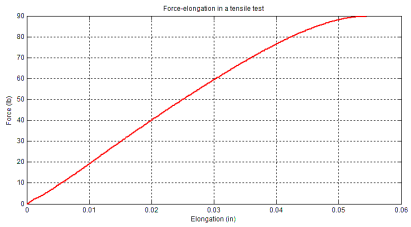
(b) 

Fig. 1 Nonlinear elastic behavior of polymer in a tensile test. (a) The entire *force-elongation* profile in a tensile test; (b) The data in stable range only.

In Fig.1 (b), it is clear that there is certain degree of nonlinearities which can hardly be explained using classical elastic model. To derive a material model for the FullCure720 material, we propose several hypothetical models. For each hypothetical material model, virtual tensile tests are performed using 3D Finite Element Analysis (FEA) method, and the results are compared against tensile test experiments. The parameters of the material model are then estimated by minimizing the discrepancies of the virtual responses and the experimental results.

Let the parameters of a material model be $p = [p_1, p_2, ..., p_m]$, where m is the total number of parameters, then the parameter estimation of a material model is formulated as an optimization problem:

$$\arg\min f(p) = f(p_1, p_2, ..., p_m) = \left| C_e - C_v \right| \quad (1)$$

where C_e and C_v are the experimental and virtual elongation-force curve, $|\bullet|$ is some metric describing the distance/consistency of the two curves.

Material Models and Specimen Geometries

In this paper, two hypothetical material models are proposed. The first *bilinear material model* is characterized with three parameters: the Young's modulus E_0 describes the elastic modulus in the elastic range where the stress is proportional to the strain; the yield stress defines the proportional limit; the tangent modulus E_{tan} is used for modeling the *plastic* hardening behavior. The second *strain-dependent plastic hardening model* is a generalized case of Model (I) in that the plastic hardening behavior is not represented with a constant tangent modulus, but with a general function of plastic strain. In this research, this function is represented by a spline-interpolation function using k interpolation points on the plastic strain-stress plane. For comparative reasons, the most widely used *linear elastic model* is also included as a reference to indicate the relative fitness of each model, as shown in Table 1.

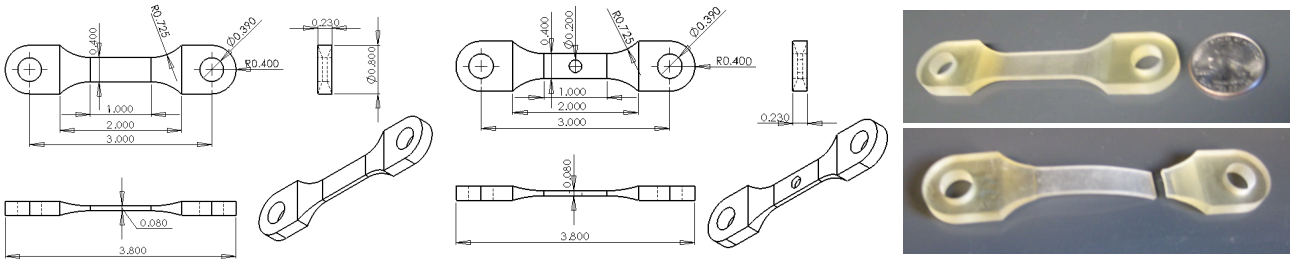
Two specimens with different geometries as shown in Fig. 2 are fabricated with Objet PolyJet 3D printer [3] using the FullCure720 material. Tensile tests are performed on these specimens using the same tensile test machine (MTS 858 Mini Bionix). For each specimen, six tensile tests are repeated with the same strain rate (0.0005 in/sec) applied in all tests.

Virtual Tensile Test and Parameter Estimation Algorithm

The virtual tensile tests are performed using commercial FEA package COMSOL Multiphysics [5]. To simulate the tensile test process, a number of points on the elongation-force plane must be determined. To accomplish this, prescribed displacements are imposed on given geometric faces, and the reaction forces are regarded as output, as shown in Fig. 3 (a). Given a specific set of parameter values (e.g. E_0 and E_{tan}) of the material model and a virtual elongation e, the responses (e.g. reaction forces and von-Mises stress) of the specimen can be evaluated using FEA method, as shown in Fig. 3

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(b). By sequentially inputting a collection of virtual elongations to the FEA module, the virtual force vectors can be calculated; by connecting these virtual (elongation, force) points, a virtual tensile test curve can be obtained.

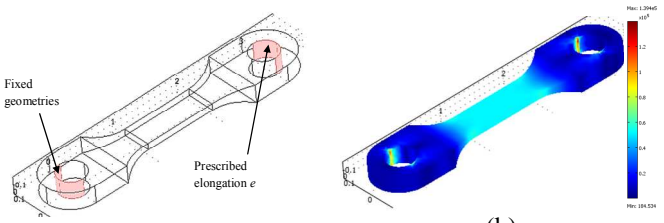


(a) Geometry (I) (b) Geometry (II) (c) Images of Specimen (I)

Fig. 2 Specimen geometries. (a) Specimen (I) with no hole; (b) Specimen (II) with a circular hole. (c) Specimens before and after tensile test.

Table 1 Material models and their parameters.

Material models		Model parameters
(I)	Bilinear material model	Young's modulus E_0; Yield stress σ_{ys} Tangent modulus E_{tan}
(II)	Strain-dependent plastic hardening model	Young's modulus E_0; Yield stress σ_{ys} Spline based plastic hardening function
(III)	Linear Elastic material model	Young's modulus E_0



(a) (b)

Fig. 3 Finite element analysis of the specimen with no holes in the middle. (a) Boundary and loading conditions of the finite element model; (b) von-Mises stress distribution of the specimen.

Let the *virtual* reaction force evaluated at the virtual elongation e_i be $f_{vir}(e_i)$, and the corresponding applied force in the *experimental* tensile test be $f_{exp}(e_i)$, then the discrepancies of the virtual and experimental tensile test curve can be calculated with Eq.(2):

$$\left|C_v - C_e\right| = \sqrt{\frac{\sum_{i=1}^{N}(f_{\exp}(e_i) - f_{vir}(e_i))^2}{N}} \tag{2}$$

Eq. (2) is essentially a Root Mean Squared (RMS) error representing the distance/consistency of the experimental and virtual tensile test curves. By substitution of Eq. (2) into Eq.(1), the objective function of the optimization problem can be then determined.

Fig. 4 shows a schematic flowchart of the proposed numerical optimization method using a *hill climbing* algorithm. Since the analytic gradient of the objective function is unavailable in this optimization, finite difference method is used instead.

Results

The optimization module is implemented with COMSOL Multiphysics with Matlab script. For each specimen geometry, the *averaged* elongation-force curve of six experiments is used as the final curve that a material model seeks to match. In this paper such averaged curves are called *training curves*. By changing the material model parameters iteratively as illustrated in Fig. 4 , the virtual elongation-force curve gradually converged to the training curve, as shown in Fig. 5 (a). Fig. 5 (b) plots the iterative update of objective function values. Here only the results of applying material model (I) on geometry

(I) are presented and similar curve convergence and objective function plots for other material models are omitted here.

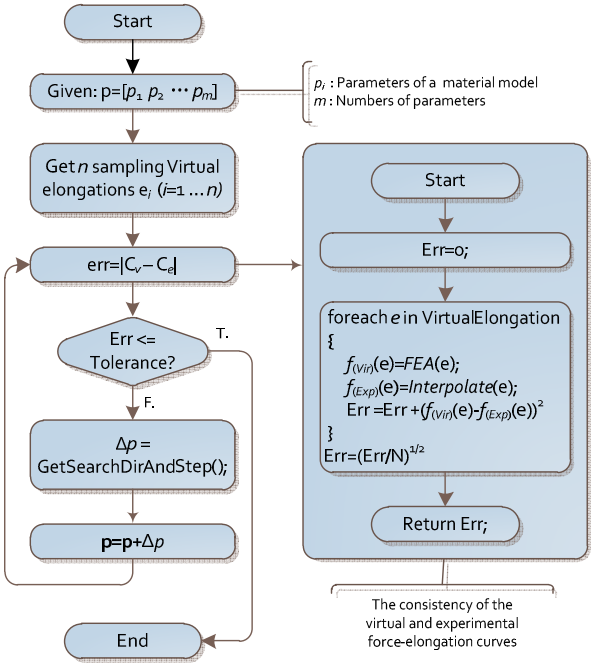


Fig. 4 Flowchart of the proposed numerical optimization algorithm

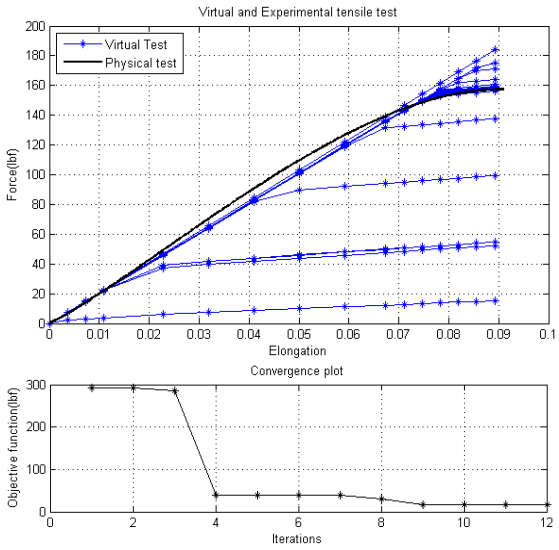


Fig. 5 (a) Iterative update of convergence plot of the virtual curve to the experimental elongation-force curve. (b) Iterative update of objective function values in the optimization process. The geometry of the specimen is shown in Fig. 2 (a).

Table 2 and Fig. 6 show the detailed material parameters derived from the proposed approach. Using the optimized material model parameters, the fitness of these models are further validated against experiment data. The results of using material model (I), (II) and (III) to evaluate the responses of specimen (I) are shown in Fig. 7 (a), (b) and (c) respectively. Due to limited space, the results for specimen (II) are not provided. For each experimental tensile test curve $C_e^{(i)}$, we calculate the RMS error $\Delta_{RMS}^{(i)}$ and maximum error $\Delta_{MAX}^{(i)}$ of the virtual and applied load evaluated at N elongations e_j using Eq. (3) and Eq. (4):

$$\Delta_{RMS}^{(i)} = \left| C_e^{(i)} - C_v \right| = \sqrt{\frac{\sum_{j=1}^{N} (f_{\exp}^{(i)}(e_j) - f_{vir}(e_j))^2}{N}}, 1 \le j \le N \tag{3}$$

$$\Delta_{MAX}^{(i)} = \max(f_{\exp}^{(i)}(e_1) - f_{vir}(e_1),\ f_{\exp}^{(i)}(e_2) - f_{vir}(e_2),\ \ldots,\ f_{\exp}^{(i)}(e_N) - f_{vir}(e_N)) \tag{4}$$

Table 2 Material models and the optimization parameter values.

Material Model	(I)	(II)	(III)
Iterations	12	16	10
Function evaluations	86	360	101
Time (Second)	4029.3	24240	399.3
Optimized parameters (psi)	E_0=130000.1 σ_{ys}=4109.9 E_{Tan}=10003.1	E_0=129998.4 σ_{ys}=3956.9	E_0= 117705

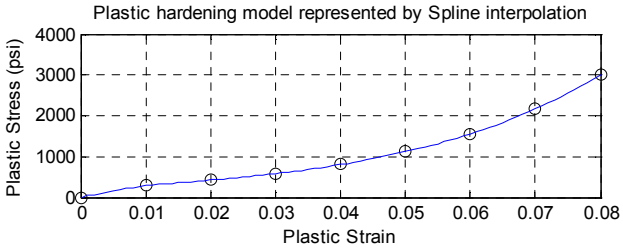
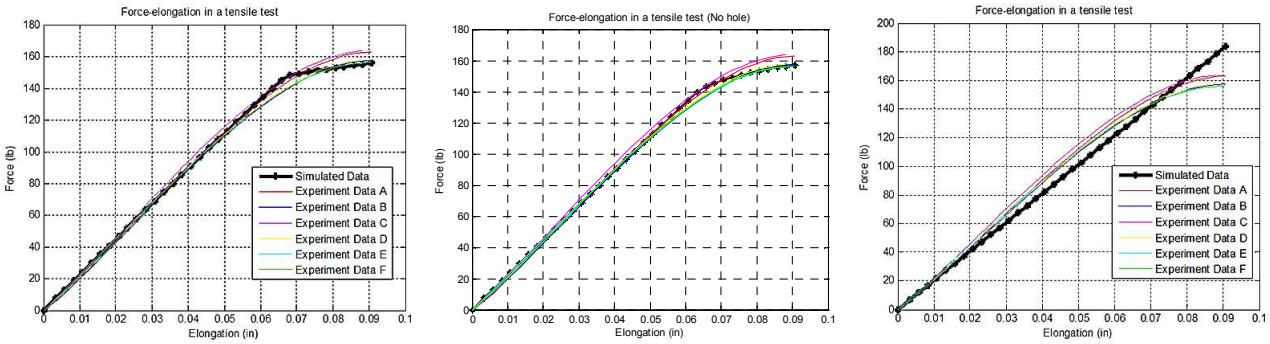


Fig. 6 Plastic hardening functions represented by spline interpolations. The 2nd to 8th ordinates of the data points are parts of the parameters of Material model (II).

For the six evaluated RMS error $\Delta_{RMS}^{(i)}$, the maximum of these errors are defined as the *RMS validation* errors of the material model, and the *maximum validation* errors can be similarly calculated. These validation errors are listed in Table 3.



(a) Material model (I) (b) Material model (II) (c) Material model (III)

Fig. 7 Validation of different material models.

Table 3 Validation errors of different material models.

	Specimen (I) shown in Fig. 2 (a)		Specimen (II) shown in Fig. 2 (b)	
Validation Error (lbf)	RMS	MAX	RMS	MAX
Material Model (I)	25.228	8.680	26.642	12.408
Material Model (II)	24.009	7.648	27.485	13.631
Material Model (III)	60.637	27.487	21.321	10.805

From Table 3, it can be seen that in terms of consistency with experiment results, material Model (II) demonstrated satisfactory performance for both specimens (I) and (II). Material model (III) though slightly outperforms Material (II) for specimen (II), however, the RMS and maximum errors for specimen (I) are much larger than those calculated from material model (II).

Conclusions

An new data driven approach based on virtual tensile tests and numerical optimization is proposed to estimate the parameters of a material model. In the virtual tensile test, 3D geometric information of the specimen is fully exploited, which differs from conventional approaches where only two dimensions (i.e. cross-section area and length of a specimen) were used. Experiments show that this is an effective approach for parameter estimation of a given material model.

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References

1. Arriaga, A., et al., *Finite-element analysis of quasi-static characterisation tests in thermoplastic materials: Experimental and numerical analysis results correlation with ANSYS.* Polymer Testing, 2007. **26**(3): p. 284-305.
2. Grytten, F., et al., *Use of digital image correlation to measure large-strain tensile properties of ductile thermoplastics.* Polymer Testing, 2009. **28**(6): p. 653-660.
3. *Objet PolyJet, http://www.interpro-rtc.com/objetPolyJet.html.*

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4. Kaliszky, S., *Plasticity: theory and engineering applications* 1990: Elsevier.
5. *COMSOL Multuphysics, http://www.comsol.com/*.

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