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**Numerical/Experimental Assessment of 3D Printed Shape Memory Polymeric Beams**  
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**Response**  
Dear Dr. Stefan Spiegel, Editor-in-Chief  
We would like to submit a revised manuscript entitled "Numerical/Experimental Assessment of 3D Printed Shape Memory Polymeric Beams" to the Journal of Applied Polymer Science.  
We would like to thank you and the respected reviewers for the time and comments. We do our best to share our views and address the reviewers’ comments. The manuscript has been revised accordingly and detailed revisions or responses have been provided. The changes in the revised manuscript have been highlighted by turquoise and yellow colors. We hope that you and reviewers will find this revised manuscript together with our replies satisfactory, for publication in Journal of Applied Polymer Science.  
Thank you very much for your attention and kind help.  
Best regards,  
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Numerical/Experimental Assessment of 3D Printed Shape Memory Polymeric Beams

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A B S T R A C T

The main objective of this paper is to present different computational tools to replicate thermo-mechanical shape memory responses of beam-like structures fabricated by 3D printing technology. To simulate thermo-mechanical behaviors of shape memory polymer (SMP) beams, 1D finite element model (FEM) building with MATLAB and 3D FEM by means of COMSOL Multiphysics are established. All governing equations are developed based on a 3D thermo-mechanical SMP constitutive model. 1D FEM is derived on the basis of the Euler-Bernoulli beam theory and linear geometrical assumption. The 3D SMP constitutive model is implemented into geometrically nonlinear COMSOL Multiphysics software through a user-defined material subroutine to provide a powerful 3D simulation tool. Comparative studies on FEMs of MATLAB and COMSOL Multiphysics reveal that geometrically linear assumption is appropriate for models in large/small deformation under tension/bending. 1D analytical solution for deflection of an SMP beam employing Euler-Bernoulli beam theory is also developed. An experiment is conducted to demonstrate a full shape memory cycle of SMPs. It is experimentally shown that a 3D printed beam recovers the deformation incurred by external loads upon heating over the transition temperature. The accuracy of the 3D FEM in COMSOL Multiphysics is checked with analytical solutions and experimental data. It is found that simulation results of the program are in good agreement with characteristics observed in the experiment and analytical solutions. The developed computational tools are expected to be instrumental in the design of simple/complicated SMP structures.

Keywords:
shape memory polymer, thermo-mechanical response, analytical solution, finite element model, experimental validation

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I. INTRODUCTION

Shape memory materials are a class of intelligent materials, which are capable of returning original shapes from deformed ones by external stimuli, such as heat, chemicals, light, moisture, and PH. Among different types of shape memory materials, shape memory polymers (SMPs) as thermal responsive polymers have gained much attention. SMPs can recover from deformed shapes to original ones by heating over the glassy transition temperature, $T_g$. SMPs possess several advantages, including low cost, simple manufacturing, 3D-printability and highly dimensional deformability. In comparison with other shape memory materials, linear mechanical behavior of the SMPs lowers threshold for programming, which further promotes its applications in industries. With their unique thermo-mechanical characteristics, potential applications of the SMPs are sketched out as medical devices, temperature sensors and actuators, self-assembly robots and self-deployable structures. Among SMP applications, diverse structures are deeply involved, e.g., in origami robots where multi-layer bodies, components with complex shapes and sophisticated joints under coupled loads are commonly used.

To realize pre-set functions of SMP structures, the first step is to find out their thermo-mechanical properties and then proceed with modelling based on the properties. To this end, numerous constitutive models of SMPs have been developed in past decades. Tobushi et al. proposed viscoelastic constitutive models for SMPs to characterize time and temperature dependent property parameters. Their model is able to reliably express thermomechanical properties of SMPs. A thermo-viscoelastic constitutive model combined with nonlinear Adam-Gibbs model and a modified Eyring model was presented by Nguyen et al. The model replicates the evolution of the structural transformation of SMPs with temperature in experiments. To provide simpler and more practical prediction for SMPs, some researchers developed viscoelastic models incorporating the glass transition. Compared with viscoelastic models, the phase transition model relates shape memory effects to glass transition. The model was widely adopted to predict the thermo-mechanic behavior of SMPs in the work of Baghani et al., Li et at., Kim et at. and Liu et at.. In these research works, the continuum constitutive
model is commonly described as a mixture of the rubber phase and the glass phase. With internal state variables employed, the phase transition model is able to reasonably reproduce the shape memory effects of SMPs. Recently, with technological advancement in 3D printing, Mao et al.\textsuperscript{25}, Ding et al.\textsuperscript{26} and Bodaghi et al.\textsuperscript{8,27} Liu et al.\textsuperscript{28} utilized 3D printing approaches to fabricate and program SMP objects simultaneously based on the developed SMP models mentioned above. It is known as 4D printing technology where a capability for movement is latent within the 3D printed materials. For instance, Ding et al.\textsuperscript{26} fabricated self-folding SMP/elastomer composites with compressive strains built in through photo-polymerization of PolyJet procedure. They simulated experiments by using ABAQUS finite element method (FEM) commercial software. Bodaghi et al.\textsuperscript{27} programmed SMP beams by fused deposition modeling (FDM). They developed 3D FEM in-house code to replicate experimental results with an acceptable accuracy. Liu et al.\textsuperscript{28} presented a self-folding hinge printable by carbon fiber/SMP composites, whose deployment part consists of two symmetrical arc-shaped laminates. Their FE simulation with ABAQUS reliably predicted the behavior of the hinge in experiments.

SMP structures can be designed based on the theoretical understanding of their thermo-mechanics. Researchers have mostly developed their own FEM codes or used FEM commercial softwares. This research work develops different digital tools like analytical solutions and in-house and commercial FEMs and assesses their capabilities to replicate experiments conducted on 3D printed beam-like structures. In particular, we concentrate on the effects of geometric nonlinearity on SMP modelling and establishment of 3D FEM utilizing COMSOL Multiphysics that is suitable for analyzing 3D complicated SMP structures.

This paper is organized as follows. We first introduce a full shape memory cycle, including deformation at high temperature and recovery upon heating beyond the transition temperature. All governing equations are then derived based on a 3D SMP constitutive equation model. In the aspect of 1D FEM building with MATLAB, the constitutive model is dimensionally reduced into a 1D one. The Euler-Bernoulli beam theory and linear geometrical assumption are adopted. Gauss numerical integration rules are employed to evaluate volumetric
integral of discretizing inelastic strain. The 3D SMP constitutive model with geometric nonlinearity is enforced and then implemented into COMSOL Multiphysics through a user-defined material subroutine. Material Jacobian matrix is computed based on the 3D SMP unified constitutive equation. To investigate the effects of deformation range on the accuracy of FEM, simulations on the responses of a cantilever SMP beam for tensile test and bending test are subsequently carried out by MATLAB and COMSOL Multiphysics. Comparative studies reveal that geometrically linear assumption is only suited to small-deformation models under bending.

Next, analytical expressions for inelastic strain are developed on the basis of Euler-Bernoulli beam theory. Then, an experiment on examining thermo-mechanical behavior of a clamped-clamped SMP beam through a full memory cycle is conducted. It is experimentally observed that the shape of the SMP beam is fixed through cooling process and recovers its initial shape by heating. Finally, reliability of SMP programming by the way of COMSOL Multiphysics is demonstrated via validation with analytical solutions and experimental data. The program in COMSOL Multiphysics is expected to serve as a digital tool in optimization of complicated SMP structural designs in future work.

II. SMP CONCEPT

The shape memory cycle is composed of elastic deformation at high-temperature followed by a shape recovery by heating. Figure 1 depicts schematic diagram of temperature, strain and stress relations of SMPs. (1) the material starts at a low temperature, \( T_I \), and then is heated above the transition temperature, \( T = T_h > T_g (1 \rightarrow 2) \). (2) it next experiences loading, reaching the maximum strain, \( \epsilon_m (2 \rightarrow 3) \). (3) subsequently, the SMP is fixed to the deformed shape followed by cooling treatment until the temperature drops down to \( T_I (3 \rightarrow 4) \). (4) constraint suspension leads to disappearance of thermo-elastic strain while a pre-strain remains, \( \epsilon_5 (4 \rightarrow 5) \). (5) the pre-strain is eliminated by heating SMP over \( T_g, (5 \rightarrow 2) \). (6) finally, thermal strain is removed by cooling the material down to \( T_I (2 \rightarrow 1) \).
III. SMP CONSTITUTIVE MODEL

A. General form of SMP constitutive model

A constitutive model basically introduced in Ref. [8] is described here for phase transformation, between glassy phase and rubbery phase, of SMPs based on the continuum thermodynamics of irreversible process.

Adopting a general assumption of additivity of strains, the total strain, $\varepsilon$, is decomposed into four parts:

$$\varepsilon = \xi_g \varepsilon_g + (1 - \xi_g) \varepsilon_r + \varepsilon_t + \varepsilon_i = \varepsilon_m + \varepsilon_t$$  \hspace{1cm} (1)

where $\xi_g$ is volume fraction of glassy phase. $\varepsilon_g$ and $\varepsilon_r$ stand for elastic strains of glassy and rubbery phases, respectively. In this study, subscripts $g$ and $r$ represent the glassy and rubbery phases, respectively. $\varepsilon_t$ is thermal strain induced by temperature difference, $\varepsilon_i$ denotes inelastic strain and $\varepsilon_m$ stands for mechanical strain.

Introducing Helmholtz free energy density functions, $\psi$, for the glassy and rubbery phases and applying the second law of thermodynamics in the sense of the Clausius-Duhem inequality, stress vector, $\sigma$, is expressed as:

$$\sigma = \frac{\partial \psi_r}{\partial \varepsilon_r} = \frac{\partial \psi_g}{\partial \varepsilon_g} = C_r : \varepsilon_r = C_g : \varepsilon_g$$  \hspace{1cm} (2)

where $C_r$ and $C_g$ represent a fourth-order elasticity tensor of rubber and the glass phases, respectively.

By substituting Eq. (1) into Eq. (2) and considering a vectorial notation, the stress-strain relationship can be derived as:

$$\sigma = C_e (\varepsilon - \varepsilon_t - \varepsilon_i)$$  \hspace{1cm} (3)

where $C_e$ denotes an overall equivalent stiffness defined as:

$$C_e = \left( S_r + \xi_g (S_g - S_r) \right)^{-1}.$$  \hspace{1cm} (4)

in which $S_g$ and $S_r$ denote the compliance matrix of glassy and rubbery phases, respectively. $S_i = C_i^{-1}$ can be expressed as:
\[ s_i = \begin{pmatrix} \frac{1}{E_i} & -v_i/E_i & -v_i/E_i & 0 & 0 & 0 \\ -v_i/E_i & 1/E_i & -v_i/E_i & 0 & 0 & 0 \\ -v_i/E_i & -v_i/E_i & 1/E_i & 0 & 0 & 0 \\ 0 & 0 & 0 & 2(1 + v_i)/E_i & 0 & 0 \\ 0 & 0 & 0 & 0 & 2(1 + v_i)/E_i & 0 \end{pmatrix} \]  

(5)

with respect to Poisson’s ratio, \( v_i \), and Young’s modulus, \( E_i \), whose values are presented in Table 1. The subscript \( i \) in Eq. (5) can be either \( g \) or \( r \).

Several interpolation methods have been proposed in literature to define \( \xi_g \). In this work, we consider the trigonometric function to fit DMA test as follows:

\[ \xi_g = -\frac{\tanh(aT_g - bT_h) - \tanh(aT_g - bT_l)}{\tanh(aT_g - bT_h) - \tanh(aT_g - bT_l)} \]  

(6)

where \( T \) stands for the temperature of SMPs. The material parameters of \( a, b, T_l, T_g \) and \( T_h \) as listed in Table 2 can be calibrated from DMA tests.

1) Thermal strain

To quantify the thermal expansion of the SMP, thermal strain, \( \varepsilon_t \), is introduced and formulated as:

\[ \varepsilon_t = \int_{T_r}^{T} \alpha_e(T) dT, \]  

(7)

in which \( \alpha_e \) denotes effective thermal expansion, following mixture rules,

\[ \alpha_e = \alpha_r + (\alpha_g - \alpha_r) \xi_g(T) \]  

(8)

where \( \alpha_r \) and \( \alpha_g \) are thermal expansion coefficients of the rubber phase and glass phase, respectively, whose values are listed in Table 1.

Since \( \alpha_r = \alpha_g \), \( ^{27} \) Eq. (8) is simplified to

\[ \alpha_e = \alpha_r. \]  

(9)

Substituting Eq. (9) into Eq. (7) yields

\[ \varepsilon_t = \alpha_r(T - T_r). \]  

(10)
where $T_r$ is reference temperature whose value can be found in Table 2. Eq. (10) reveals that thermal expansion of SMPs is dependent on material temperature alone.

2) Inelastic strain

In the cooling process, rubbery phase transforms to glassy phase leading to a strain stored in material. The stored strain is eliminated on the condition that SMPs are heated over the glassy transition temperature. This stored strain is so-called inelastic strain, expressed as:

$$
\dot{\varepsilon}_i = \begin{cases} 
\dot{\xi}_g \varepsilon_i & \dot{T} > 0 \\
\dot{\xi}_g \varepsilon_r & \dot{T} < 0 
\end{cases}
$$

(11)

As inelastic strain is in a rate form, current inelastic strain during heating is derived after implementation of implicit backward Euler integration technique, which is derived as:

$$
\varepsilon_{i,h}^t = \frac{\dot{\xi}_g}{\xi_g^{t-1}} \varepsilon_{i,h}^{t-1},
$$

(12)

where superscript $t$ means the current step and $t-1$ denotes the previous step. $\dot{\xi}_g$ is a function of temperature from Eq. (6); therefore, $\varepsilon_{i,h}^t$ is obtained, provided that $\varepsilon_{i,h}^{t-1}$ and temperature gradient are known.

$\varepsilon_i^t$ in cooling process can be formulated as:

$$
\varepsilon_{i,c}^t = \left(I + \Delta\xi_g S_r C_e\right)^{-1} \left(\varepsilon_{i,c}^{t-1} + \Delta\xi_g S_r C_e (\varepsilon^t - \varepsilon_i^t)\right)
$$

(13)

in which $\Delta\xi_g = \xi_g^t - \xi_g^{t-1}$ and $I$ is an identity matrix.

Substituting Eqs. (12) and (13) into Eq. (3) yields a unified constitutive equation during cooling and heating as:

$$
\sigma = C_{ei}(\varepsilon - \varepsilon_i - \mu \varepsilon_i^{t-1}),
$$

(14)

where

$$
\begin{cases} 
C_{ei} = C_e \left(I - \Delta\xi_g \left(\Delta\xi_g I + (S_r C_e)^{-1}\right)^{-1}\right), & \dot{T} < 0 \\
C_{ei} = C_e, & \mu = 1, \quad \dot{T} < 0 \\
C_{ei} = C_e \frac{\dot{\xi}_g}{\xi_g^{t-1}}, & \dot{T} > 0
\end{cases}
$$

(15)
Equation (15) shows that the SMP constitutive model for the rubbery phase reduces to a linear thermoelastic stress–strain model. It is worthwhile to mention that kinematic strain-displacement relationship can be chosen to be geometrically either linear or non-linear.

B. Constitutive equations in different steps of a shape memory cycle

1) Heating (1 → 2)

In this step, stress $\sigma = 0$ as no constraint is imposed. The state of inelastic strain at $T_l$ is enforced on the inelastic strain through Eq. (12). In this regard, we have the constitutive equation Eq. (3) simplified as:

$$\varepsilon = \varepsilon_i(T).$$

(16)

It reveals that $\varepsilon$ is positively proportional to $T$ in this step.

2) Loading (2 → 3)

Likewise, $\varepsilon_i = 0$ and $T = T_h$, leading $C_e$ and $\varepsilon_t$ to be constant. Accordingly, Eq. (3) is recast as:

$$\sigma = C_e(\varepsilon - \varepsilon_i).$$

(17)

In this case, strain and stress are directly proportional, exhibiting linear material behavior.

3) Cooling (3 → 4)

During cooling, $\varepsilon$ stays at maximum value, $\varepsilon_{max}$, because the material is fixed. As temperature gradient is user-defined, $T$ at each update step is known. Initial inelastic strain in cooling, $\varepsilon_i^0$, evolves from zero. Accordingly, $\varepsilon_i$ can be updated by Eq. (13) evolutionarily.

With $\varepsilon_i$ known, $\sigma$ can be deduced by Eq. (3).

4) Unloading (4 → 5)

With constraints released, $\sigma$ vanishes, and temperature remains at $T_l$ in this step. Eq. (3) is simplified as:

$$\varepsilon = \varepsilon_i + \varepsilon_t.$$

(18)

5) Reheating (5 → 2)
τ_1 in this step starts with the final value of inelastic strain during cooling and temperature at each update step that is known. Therefore, τ_1 can be updated by Eq. (12) and σ is derived from Eq. (3).

IV. COMSOL SIMULATION

The model by means of MATLAB is suitable for beam-like structures in small deformation; however, when it comes to complicated structures and/or large deformation regime, geometrically linear MATLAB FE model cannot work accurately. To resolve these confines, geometrically nonlinear COMSOL Multiphysics is employed in modeling SMP structures.

Shape memory effect and SMP constitutive equations are not taken into consideration in the framework of the software. Therefore, compiling a user-defined subroutine becomes an inevitable way to go. In the current mechanism of COMSOL, there are two methods to establish an external material. The first one is to use the General stress-strain relation socket, in which we need to code the entire constitutive equation, including thermal strain and inelastic strain. For this socket, we would be faced with two tasks:

- Computation of second Piola-Kirchhoff stress tensor
- Computation of material Jacobian matrix

The other way is about inelastic residual strain socket where only inelastic strain is considered. In this case, two quantities need be computed:

- Computation of inelastic strain
- Computation of Jacobian matrix τ_1 with respect to τ.

No matter which socket is considered in the user material subroutine, Jacobian matrix is required to perform a global Newton-Raphson root search. The relation between elastic strain and inelastic strain is implicit from Eq. (1), which increases difficulty to build up Jacobian matrix τ_1 with respect to τ. On contrast, τ_1 and C_τ_1 are the functions of T, and τ_1^{t-1} is constant in the unified constitutive equation Eq. (14). Taking derivative of both
sides of Eq. (14) with respect to $\epsilon$ yields material Jacobian, $\frac{\partial \sigma}{\partial \epsilon} = C_{ei}$. Therefore, general stress-strain relation socket is adopted to compile the subroutine.

Another task is to implement $\epsilon_i$ update. Heating and cooling processes are discretized into some steps. Within each step, Eq. (14) is firstly used to compute stress $\sigma$ and then Eq. (12) and Eq. (13) are employed to update $\epsilon_i$. Details are demonstrated in the flow chart Figure 2. Regarding equation $T = T_0 \pm p \cdot \Delta T$ in Figure 2, $T_0$ means the initial temperature of cooling or heating and $\Delta T$ refers to temperature gradient. $p$ denotes update times. Minus sign is in place during cooling while plus sign is chosen over heating. $T_m$ is the material temperature.

The subroutine is compiled in C programming; however, matrix computations are much more difficult to realize in C programming than in MATLAB. Therefore, we compute Jacobian matrices in MATLAB at first and then export them to C programming to enhance code efficiency. To activate the user material subroutine in the model, the physical condition of External Stress-Strain Relation is required. According to system settings, the use of External Stress-Strain Relation will force the study to be geometrically nonlinear.

V. 1D FEM MATLAB

In this section, we aim to establish a 1D FE program by means of MATLAB specified for beam-like structures. Two types of loadings on a cantilever SMP beam are studied: tension and bending. In this section, we assume temperature distribution across the material domain is uniform. Additionally, $C_{ei}$, $\sigma$, $\epsilon$, $\epsilon_t$ and $\epsilon_i$ are dimensionally reduced to 1D.

A. Governing equations

The geometric linearity in 1D is considered as:

$$\epsilon = u'$$

(19)

where $u$ stands for longitudinal displacement. Prime denotes the derivative with respect to $x$ coordinate.

The geometry of the cantilever SMP beam and configurations of loadings are demonstrated in Figure 3.
To derive governing equations, the principle of minimum of total potential energy is implemented as:

\[ \delta U = \delta W , \]  

(20)

where \( \delta \) represents the variation symbol. \( \delta U \) and \( \delta W \) stand for the variation of strain energy and virtual work, respectively.

After integration over the material domain, the virtual strain energy is written as:

\[ \delta U = \iiint_V \delta \varepsilon^T \sigma dV, \]  

(21)

where \( V \) is the volume of the SMP. Substituting Eq. (14) into Eq. (21), the virtual strain energy is rewritten as:

\[ \delta U = \iiint_V \delta \varepsilon^T C_{ei} (\varepsilon - \varepsilon_t - \mu \varepsilon_i t^{-1}) dV. \]  

(22)

The virtual work done by concentrated force \( F \) is formulated as:

\[ \delta W = \delta d^T F \]  

(23)

where displacement field is \( d = \{ u \}_{\omega} \), and \( F = \{ F_x \} \). \( \omega \) refers to the deflection of the beam and \( F_x \) and \( F_y \) represent the applied forces in horizontal and vertical directions, respectively.

**B. FEM formulation**

1) **Tension on a cantilever beam**

Substituting Eq. (19) into Eq. (22) results in:

\[ \delta U = \iiint_V (\delta u')^T C_{ei} (u' - \varepsilon_t - \mu \varepsilon_i t^{-1}) dV. \]  

(24)

The virtual work by external load can be expressed as:

\[ \delta W = \delta u^T F_x. \]  

(25)

The governing equation of the cantilever beam under tension is derived via Eqs. (24), (25) and (20) as:

\[ \iiint_V (\delta u')^T C_{ei} (u' - \varepsilon_t - \mu \varepsilon_i t^{-1}) dV = \delta u^T F_x. \]  

(26)

Boundary conditions under the configuration of tensile test are listed in Table 3.
The cantilever beam has one degree of freedom and the constitutive equation acts linearly from Eq. (14). In this respect, two-node linear element is employed to discretize the beam domain. Lagrangian function, $N(x)$, is adopted in evaluation of displacement, $u$, and its variation, $\delta u$, expressed as:

$$u = Nu,$$

$$\delta u = N\delta u,$$  \hspace{1cm} (27)

where $u$ and $\delta u$ are generalized nodal displacement and its variation. The shape function vector, $N$, is defined as:

$$N = \sum_{e=1}^{n} N^e L^e.$$  \hspace{1cm} (28)

in which $N^e$ and $L^e$ are elemental shape function and gather matrix. In this study, superscript $e$ indicates the function for a particular element $e$. $n$ means the number of elements.

Let $B = \frac{\partial N(x)}{\partial x} = N'$, then Eq. (26) can be collected into three terms:

$$\delta u^T Ku - \delta u^T K_1 \varepsilon_i - \delta u^T K_2 \mu \varepsilon_i^{t-1} = \delta u^T F_x$$  \hspace{1cm} (29)

where stiffness matrix, $K$, is

$$K = C_{el} A \sum_{e=1}^{n} L^e T \int_{x_e}^{x_{e+1}} B^e T B^e dx L^e,$$  \hspace{1cm} (30)

thermal stiffness vector, $K_1$, is

$$K_1 = C_{el} A \sum_{e=1}^{n} L^e T \int_{x_e}^{x_{e+1}} B^e T dx,$$  \hspace{1cm} (31)

and inelastic stiffness vector, $K_2$, is

$$K_2 = C_{el} A \sum_{e=1}^{n} L^e T \int_{x_e}^{x_{e+1}} B^e T dx.$$  \hspace{1cm} (32)

where $A$ stands for the area of cross section. $x_e$ and $x_{e+1}$ represent the first and end nodes in $x$ coordinate within element domain.

In extensional mode, $\varepsilon$ is evenly distributed along $y$ axis, so, $\varepsilon_i$ can be considered constant along $y$ coordinate. Accordingly, $\varepsilon_i^{t-1}$ can be extracted out of volumetric integration, as shown in Eq. (29).

2) Bending on a cantilever beam
In flexural mode, Bernoulli-Euler beam theory is adopted to describe the displacement filed of the beam as:

\[ u(x, y) = -y\sin(\omega'(x)) \approx -y\omega'(x). \] (33)

Substitution of Eqs. (19) and (33) into Eq. (22) gives

\[ \delta U = \iint_{V} (-y\delta \omega')^T C_{el} \left( -y\omega' - \varepsilon_t - \mu \varepsilon_t^{-1} \right) dV. \] (34)

Expanding and recasting Eq. (34), we obtain:

\[ \delta U = C_{el} \left( I_0 \int_{x_1}^{x_2} \omega' \, \omega' \, dx + t_b \int_{-h/2}^{h/2} (\mu y \varepsilon_t^{-1} + \varepsilon_t y) dy \int_{x_1}^{x_2} \omega' \, \omega' \, dx \right). \] (35)

in which \( t_b \) is the width, \( I_0 \) means the inertia moment and \( h \) stands for the thickness of the beam. Based on the assumption of uniform temperature distribution, \( \varepsilon_t \) is not a function of space, which leads to\( \int_{-h/2}^{h/2} \varepsilon_t \, y \, dy = 0 \).

For virtual work by external load, Eq. (23) is rewritten as:

\[ \delta W = \delta \omega^T F_y. \] (36)

Combination Eq. (35) with Eq. (36) yields the governing equation as:

\[ C_{el} \left( I_0 \int_{x_1}^{x_2} \omega' \, \omega' \, dx + \mu t_b \int_{-h/2}^{h/2} y \varepsilon_t^{-1} dy \int_{x_1}^{x_2} \omega' \, \omega' \, dx \right) = \omega^T F_y, \] (37)

Boundary conditions are listed in Table 4.

In bending situation, the beam has two degrees of freedom, one vertical displacement \( \omega \), the other rotational angle of neutral axis \( \omega' \). In this respect, Hermite function \( N(x) \) is employed in approximation of displacement field.

Similarly, let \( D = \frac{\partial B(x)}{\partial x} = N' \), then the governing equation under bending can be written as:

\[ \delta \omega^T K \omega - \delta \omega^T \mu K_{2} t_b \int_{-h/2}^{h/2} y \varepsilon_t^{-1} dy = \delta \omega^T F_y \] (38)

where stiffness matrix is

\[ K = C_{el} I_0 \sum_{e=1}^{n} L^e \int_{x_e_1}^{x_e_2} D^e \, D^e \, dx L^e, \] (39)
and inelastic stiffness vector is given by

$$K_2 = C_0 \sum_{e=1}^{n} L e^T \int_{x_i}^{x_{i+1}} D e^T dx.$$ (40)

In flexural mode, $\varepsilon$ varies not only in $x$ direction but in $y$ direction as well. Accordingly, $\varepsilon_i$ is not constant along $y$ direction any more. In this respect, Gauss numerical integration rule is employed to evaluate the integral

$$\int_{-h/2}^{h/2} y \varepsilon_i t^{-1} dy.$$

We define function $f(y) = y \varepsilon_i t^{-1}(y)$ and take five Gauss points to evaluate the integral

$$\int_{-h/2}^{h/2} y \varepsilon_i t^{-1}(y) dy = J \sum_{i=1}^{5} w_i f(\varepsilon_i)$$ (41)

where $\varepsilon_i$ and $w_i$ are Gauss point location in physical domain and weight of the point, respectively. Jacobian $J = h/2$. Table 5 records values of $\varepsilon_i$ and $w_i$.

3) Results and discussions

In extensional and flexural modes, we consider a cantilever beam with geometry of 1m (length) × 5cm (width) × 5cm (thickness), as depicted in Figure 3. Material parameters of the SMP beam are reported in Tables 1 and 2 adopted from [27].

At first step, the cantilever beam is heated up to $T_h$ and then different types of loads are imposed on the beam corresponding to each mode. To investigate the effects of deformation range on the accuracy of the model with geometric linearity, we compare simulation results between MATLAB and geometrically nonlinear COMSOL Multiphysics.

Displacement fields of the cantilever beam on various boundary conditions are presented in Figs. 4 and 5. In extensional mode, axial forces, $F_x = 100$ N and $F_x = 1$ kN, are applied on the free end of the cantilever beam, respectively. In flexural mode, vertical loads, $F_y = 0.1$ N and $F_y = 1$ N, are exerted vertically on the free side of the beam. For MATLAB modelling, 20 elements along axial direction are meshed in both tensile and flexural modes. Boundary conditions for each mode are listed in Table 3 and Table 4, respectively. While in COMSOL Multiphysics simulation, a 20×15 mesh (20 elements along $x$ direction and 15 elements in $y$
direction) is established to obtain results converged up to two significant digits. The boundary conditions of COMSOL Multiphysics model are the same as those of MATLAB that the beam is loaded incrementally on the beam right side while keeping the left one fixed axially and transversely.

From Figure 4, it is concluded that results of MATLAB and COMSOL Multiphysics are in good agreement under tensile force of 100 N and 1 kN. This reveals that geometrically linear FEM is not significantly affected by deformation range under tension.

Figure 5 reveals excellent consistency between MATLAB simulation and COMSOL Multiphysics simulation under bending load of 0.1 N, whereas the maximum deformation of the cantilever beam calculated by MATLAB is 18.3% greater than the estimation of COMSOL Multiphysics under bending load of 1 N. It means the FE program with geometrically linear assumption is only able to accurately simulate small deformation range under bending.

In the large deformation regime of the flexural mode, material points on the neutral axis do not only deflect perpendicularly, as Euler-Bernoulli beam theory assumes, but have longitudinal movement as well. These results reflect that axial and vertical displacements of the beam decouple in small deformation, but they would interact with each other when it comes to large deformation.

It should be noted that in tensile simulation, it is assumed that elongations of each axial layer of the beam are the same, based on the FE results in MATLAB plotted in 2D. As for the case of bending, with Euler Bernoulli beam hypothesis that cross-sections of the beam remain plane and perpendicular to the neutral plane during deflection, we could visualize 1D FE results of MATLAB to a 2D plot.

VI. ANALYTICAL SOLUTION

It is difficult to measure $\varepsilon_i$ distribution across the material through experiments. To check whether or not $\varepsilon_i$ computed by COMSOL Multiphysics is correct, 1D analytical expressions for $\varepsilon_i$ of an SMP beam under bending basically presented in Ref. [30] are developed here.

Applying Euler-Bernoulli beam theory in characterizing deflection gives the geometrical expression as:
\[ \varepsilon_m = -ky \]  

(42)

where \( k \) is beam neutral axis curvature.

\[ \varepsilon_m' = \left( 1 - \xi_g \right) \frac{E}{E_r} + \frac{E_g}{E_g} \sigma ' \]  

(43)

\[ \xi_g = \frac{-k_y}{(42)} \]

where prime signifies derivative with respect to temperature.

A. Cooling from 3 to 4

Taking derivative of Eq. (1) with respect to the temperature and substituting Eq. (2) and Eq. (11) yields

\[ \sigma' = \left( 1 - \xi_g \right) \frac{E}{E_r} \varepsilon_m' + \frac{E_g}{E_g} \sigma \]  

where \( \xi_g \) is beam neutral axis curvature.

The stress in cooling, \( \sigma \), can be solved by integrating Eq. (43) resulting:

\[ \sigma = e^{-\int (\psi E/E_g) dT} \left[ \int_{T_h}^{T} C_0 \varepsilon_m e^{\int (\psi E/E_g) dT} dT + C \right] \]  

(44)

where \( C \) is a temperature-independent parameter and \( E \) represents a 1D equivalent stiffness.

Since stress at \( T_h \), the last state of stress in loading process, is

\[ \sigma = \frac{-M_{0y}}{I_0}, \quad T = T_h \]  

(45)

where \( M_0 \) is moment distribution at \( T_h \). Substituting Eq. (45) into Eq. (44) and recasting Eq. (44) result in:

\[ \sigma = \psi_c^{-1} \left[ \int_{T_h}^{T} -E \varepsilon_m' \psi_c dT - \frac{M_{0y}}{I_0} \right] \]  

(46)

in which \( \psi_c(\xi_g) = [\xi_g \left( E_r/E_g - 1 \right) + 1]^{E/E_r - E_g} \). Combining Eq. (42) and equilibrium conditions with Eq. (46) gives

\[ M = -\int_A \psi_c^{-1} \left[ \int_{T_h}^{T} -E k' y \psi_c dT - \frac{M_{0y}}{I_0} \right] ydA \]  

(47)

where \( M = -\int_A \sigma y dA \). Since external moment in cooling is fixed, \( M = M_0 \), it gives:

\[ \int_{T_h}^{T} E k' \psi_c dT = \frac{M}{I_0} (1 + \psi_c) \]  

(48)

By substituting Eq. (48) into Eq. (46), we derive the stress in the cooling process as:

\[ \sigma = -\frac{M_{0y}}{I_0} \psi_c^{-1} (1 + \psi_c - 1) = -\frac{M_{0y}}{I_0} \]  

(49)
Since $\sigma = E_r \varepsilon_r$, integrating both sides of Eq. (11) gives

$$\varepsilon_{i,c} = -\frac{M_y}{E_r I_0} \xi g$$

(50)

**B. Reheating from 5 to 2**

For inelastic strain released in heating treatment, it is written as:

$$\varepsilon_{i,h} = \varepsilon_{i,c}^f \xi g$$

(51)

in which $\varepsilon_{i,c}^f$ is the final value of inelastic strain at $T_l$ in the cooling process.

**C. Results and discussion**

To coordinate simulation of COMSOL Multiphysics and analytical solutions with the experiment to be conducted, a clamped-clamped SMP beam with initial dimensions (40 mm (length) $\times$ 5 mm (width) $\times$ 1 mm (thickness)) is adopted with a concentrated force applied in the middle of the beam. Material parameters reported in Table 1 and Table 2 are adopted from Ref. [17] and used for both analytical solutions and simulation by COMSOL Multiphysics.

In cooling, a concentrated force of 0.1N, equivalent to the weight put on the beam in the experiment, is applied. The beam is load free in reheating.

In COMSOL Multiphysics modelling, numerical simulations are carried out by considering 4-node quadrilateral elements. A 20 $\times$ 36 mesh (20 and 36 elements along axial and transverse directions) are assumed to achieve accurate results converged up to two significant digits. For the double clamped beam, the boundary conditions of the beam are assumed to be clamped. It means both end edges are fixed in axial and transverse directions. Since strain concentrates on $x$-$y$ plane, plane strain assumption is adopted in the software in 2D FEM modelling.

Figure 6 and Figure 7 demonstrate $\varepsilon_i$ distribution in $x$-$y$ plane of the clamped-clamped SMP beam in the process of cooling and reheating. In particularly, $\varepsilon_i$ experiences rapid changes near the transition temperature, $T_g$. The obtained results between simulation and analytical solutions are qualitatively in agreement.
VII. EXPERIMENT

In this section, the objective is to validate COMSOL Multiphysics model with experimental data in a full shape memory cycle. A 3D printed clamped-clamped SMP beam is selected as an experiment subject to test its thermal-mechanical features in high-temperature programming and in the shape recovery upon heating.

A. Experimental setup

- A 3D printed SMP specimen, 60 mm (length) ×5 mm (width) ×1 mm (thickness)
- Two supports are used to fix the ends of the specimen. The distance between them is 40 mm.
- An electric heat chamber with a temperature range from 25 °C to 100 °C.
- A nut and a segment of wire, 10.519 g in total.

B. Specimen Preparation

In this study, polyurethane-based SMP filaments with diameter of 1.75 mm are employed, whose glass transition temperature reaches 60 °C. The specimen with 60 mm (length) ×5 mm (width) ×1 mm (thickness) is fabricated by a New Creator Pro desktop 3D printer developed by FlashForge. Equipped with a nozzle of 0.4 mm diameter, this desktop printer extrudes SMP filaments at low cost. In this work, Craft-Ware software is in control of the procedure parameters of liquefier temperature and printing speed. By default, liquefier temperature is set at 230 °C while temperatures of chamber and build platform remain as 24 °C. The printing speed and layer height are set as 20 mm/s and 0.2 mm, respectively.27

C. Procedure

An SMP specimen with 60 mm (length) ×5 mm (width) ×1 mm (thickness) is printed and fixed on two supports, as shown in Figure 8. The effective beam length between two supports is 40 mm. A nut is then hung on the specimen center. Upon equilibrium, the specimen is heated by the heat chamber set at 100 °C until the shape of the specimen does no longer change. The specimen is cooled down to room temperature, followed by
load removal. Finally, the specimen is reheated with the same conditions until the shape of the beam is recovered.

D. Results and discussions

First of all, it should be mentioned that the specimen in the experiment is identical to the one used in analytical solution and simulation of COMSOL Multiphysics in terms of geometry and material parameters. In particular, the settings of the finite element model of COMSOL Multiphysics remain the same as the ones in the comparative study of analytical solution and COMSOL model.

In the experiment, due to difficulty of measuring deflection happening on the beam, we calculate it by reading pixels on the photographs. The distance between two supports is fixed with 40 mm, serving as a reference. By comparing pixels of the distance between two supports, red line in Figure 8 II, and the deflection, yellow line in Figure 8 II, the deflection incurred are calculated. Images used for deflection measurement are 4961 ×3508 px. The distance between two clamps, 40 mm, corresponds to 3851 px in the images, so we could calculate the resolution of deflection measurement, which is $40 \text{ mm} \div 3851 \text{ px} \approx 0.01 \text{ mm/px}$. Admittedly, values of deflections by this method may suffer certain errors; however, it is acceptable to take them as reference.

The computational COMSOL Multiphysics tool is used to simulate the changes in the shape of the specimen, including loading at low and high temperatures, cooling, unloading at low temperature and reheating beyond the transition temperature. As it can be seen in Figs. 8 and 9, the FEM can well replicate the shape programming process via loading-heating-cooling-unloading. It is seen that the largest deflection occurs at loading at high temperature. For example, it is computed 5.19 mm, by the FEM that is 5.9% larger than the experimental result (4.90 mm). It is overserved that the beam recovers low elastic deformation by unloading at low temperature. The shape during unloading is almost fixed to the deformed one. For example, computed by FEM, the central deflection changes slightly from 5.19 mm to 5.17 mm by releasing central point force on the beam that is 6.2% larger than experiment. Finally, it is seen that the 3D printed beam recovers the initial shape upon heating to
high temperature while infinitesimal strain exists because of thermal strain. From the topological point of view, simulation results by means of COMSOL Multiphysics are in good agreement with experimental data.

In the experiment, the ratio of length to thickness \((L/T)\) of the beam equals 40, which means shear deformation is inconsiderable in this \(L/T\) range. Furthermore, it is worth mentioning that COMSOL Multiphysics model is able to evaluate the effect of shear deformation with built-in physics of Solid Mechanics and 4-node quadrilateral elements adopted in this study.

Finally, it should be mentioned that the present formulation based on the small strains and large rotations are able to accurately replicate large experimental deflections in the rubbery phase. It is due to the fact that the 3D printed beam in the rubbery phase experiences strains around 0.04 with large deflections. It justifies considering a linear elastic model for the rubbery phase.

VIII. CONCLUSION

The main aim of this research was to come up with different computational tools to implement simulation on varieties of SMP structures. In order to realize programming mechanism, 1D FEM in MATLAB and 3D FEM by means of COMSOL Multiphysics were established. All governing equations were developed based on a 3D thermo-mechanical SMP constitutive model. A 1D FE formulation coupled with geometric linearity was developed in MATLAB. The 3D SMP constitutive model was implemented into geometrically nonlinear COMSOL Multiphysics through a user-defined material subroutine. To investigate effects of geometric linearity on FEM results, comparative studies of FEMs in MATLAB and COMSOL Multiphysics were conducted. It was shown that the model with geometrically linear assumption was able to estimate shape changes of SMP beams under tension/bending in large/small deformation regime with an acceptable accuracy but performed low reliability in the large deformation range under bending due to the coupling of multidirectional motions. 1D analytical solution based on Euler-Bernoulli beam theory was also derived. An experiment on thermo-mechanical response of a 3D printed SMP beam under a full shape memory cycle was conducted to validate the model building with COMSOL Multiphysics. It was experimentally shown that the
3D printed SMP specimen was capable of recovering the initial shape from the temporary one upon heating over the transition temperature. The accuracy of the 3D FE program in COMSOL Multiphysics was validated with both analytical solution and experiment. It was found that this computational method can replicate the main characteristics observed in the experiment and analytical solutions with an acceptable accuracy. The model developed in COMSOL Multiphysics is expected to serve in optimization of complicated SMP structural designs.

IX. ACKNOWLEDGEMENT

The work described in this paper was supported by the Research Grants Council of the Hong Kong Special Administrative Region, China (Project No. CUHK 14202016).

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Figure 7. $\varepsilon_i$ released during reheating process of the clamped-clamped SMP beam. Results of COMSOL (left) analytical solutions (right).

Figure 8. SMP beam profiles in different steps of a memory cycle in the experiment.

Figure 9. SMP beam profiles in different steps of a memory cycle in simulation by COMSOL Multiphysics.
Figure 1. Temperature-strain-stress diagram.
Initialize $p$, $\varepsilon_i^{p-1}$

$T = T_0 \pm p \ast \Delta T$

Update $\xi_i, \varepsilon_t, C_e$

Compute $\Delta \xi_i, C_{ei}, \mu$

Input $\varepsilon$

Compute $\sigma$ by Eq. (14)

Update $\varepsilon_i$ by Eq. (12) or Eq. (13)

Yes

Output $\sigma, C_{ei}$ and $T = T_m$

No

$? ? ?$

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Table 1. Material properties of SMP

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Rubbery Phase ($i = r$)</th>
<th>Glassy Phase ($i = g$)</th>
<th>Description</th>
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<td>$\alpha_i$ ($10^{-4}$ K$^{-1}$)</td>
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<td>1</td>
<td>Thermal expansion coefficient</td>
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<td>Young’s Modulus</td>
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<td>$\nu_i$</td>
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Table 2. SMP phase transformation coefficients

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<th>Parameter</th>
<th>Value</th>
<th>Description</th>
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</tr>
<tr>
<td>$b$</td>
<td>0.145</td>
<td>Coefficient</td>
</tr>
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<td>Low temperature</td>
</tr>
<tr>
<td>$T_g$</td>
<td>60 °C</td>
<td>Glassy transition temperature</td>
</tr>
<tr>
<td>$T_h$</td>
<td>100 °C</td>
<td>High temperature</td>
</tr>
<tr>
<td>$T_r$</td>
<td>24 °C</td>
<td>Reference or room temperature</td>
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Table 3. Boundary conditions for different steps of a shape memory cycle under tension

<table>
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<tr>
<th>Process</th>
<th>Boundary condition</th>
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<td>heating, releasing and reheating</td>
<td>$u(0) = 0$</td>
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<td>(1 → 2) &amp; (6 → 2) &amp; (6 → 2)</td>
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<tr>
<td>loading (2 → 3)</td>
<td>$u(0) = 0$</td>
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<tr>
<td>$EAu'(L) = F_x$</td>
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<tr>
<td>cooling (3 → 4)</td>
<td>$u(0) = 0$</td>
</tr>
<tr>
<td></td>
<td>$u(L) = u_0$</td>
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</table>
Table 4. Boundary conditions for different steps of a shape memory cycle under bending

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<th>Process</th>
<th>Boundary conditions</th>
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<tr>
<td>heating, releasing and reheating</td>
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<tr>
<td>((1 \rightarrow 2) &amp; (6 \rightarrow 2) &amp; (6 \rightarrow 2))</td>
<td>( \omega'(0) = 0 )</td>
</tr>
<tr>
<td>loading ((2 \rightarrow 3))</td>
<td>( \omega(0) = \omega'(0) = 0 )</td>
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<tr>
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<td>( E\omega^{(3)}(L) = F_y )</td>
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<tr>
<td>cooling ((3 \rightarrow 4))</td>
<td>( \omega(L) = \omega(L)^f )</td>
</tr>
<tr>
<td></td>
<td>( \omega'(L) = \omega'(L)^f )</td>
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Table 5. Gauss point location and weight

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<th>Location ( \epsilon_i )</th>
<th>Weight ( w_i )</th>
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<td>0.0</td>
<td>0.568 888 8889</td>
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Graphical Abstract Image

Loading at $T_l$

Loading at $T_h$

Reheating to $T_h$

Cooling and unloading
Detailed Responses to the Reviews

Authors:

The authors would like to express our sincere appreciation to the reviewers who made valuable comments and suggestions to improve the paper. The manuscript has been modified accordingly and highlighted in turquoise and yellow colors in response to the comments by the reviewers # 1 and 2, respectively. The corrections are also listed below point by point.

******************************************************************************

Reviewer # 1

The paper presents a numerical/experimental study of shape memory polymers (SMP). The Authors discuss the model adopted to study SMP, present the results of their analysis and compare it with Finite Elements analysis, and briefly compare their numerical results with a set of experiments. I would recommend publication after some revisions.

Authors:

Thanks for the comments and recommendation.

******************************************************************************

Comment No. 1:

Authors should report a complete account of the literature in the field of SMP modelling. Only few references are cited and they are mostly from the same Authors.

Response:

We have updated the literature survey section and added some new references.

Location of modification: on pages 2 and 3; added Refs. [15-24, 28].

******************************************************************************
Comment No. 2:

Figure 1, please add arrows to the cycle.

Response:

Arrows have been added in Figure 1.

Location of modification: Figure 1.

Comment No. 3:

Figure 2, Euler Bernoulli beam cross-sections remain plane and parallel during deflection.

Response:

We have modified the mentioned figure.

Location of modification: Figure 3.

Comment No. 4:

On page 5, equation 5, please report both $S_g$ and $S_r$ separately, the matrix $S$ is not defined/used anywhere else in the paper.

Response:

We have added subscript $i$ in Eq. (5) that can be $g$ or $r$. $C_e$ includes both $S_g$ and $S_r$ and is applied in all 1D and 3D formulations.

Location of modification: on page 6.
Comment No. 5:

Please justify how a linear elastic model can be used to model a rubber phase at moderate to large deformations. Why is not a more accurate hyperelastic model adopted?

Response:

As it can be seen from figures that strain in the rubbery phase is mostly around 0.04 while the beam experiences large deflections. It fact, we deal with small strains and large rotations. For the case in hand, considering a linear elastic model for the rubbery phase is accurate enough to calculate the structural deformation with a good correlation with experiments. We have mentioned this fact in the revised manuscript.

Location of modification: on page 20.

Comment No. 6:

Please describe in details the Finite Elements (Comsol) model employed. Please report the number of elements/nodes, materials models, boundary conditions, convergence analysis, etc.

Response:

We have provided more details on the FEM with Comsol.

Location of modification: on pages 14, 15, 17 and 19.

Comment No. 7:

Same objection as before, the Authors employ a geometrically nonlinear Comsol model for the kinematic but they assume an elastic linear constitutive relation for the material (rubber-like).
*How they justify their choice?*

**Response:**

Equation (15) shows that the SMP constitutive model for the rubbery phase is reduced to a linear thermo-elastic stress-strain model. It is worthwhile to mention that kinematic strain-displacement relationship can be chosen to be geometrically either linear or non-linear. In Comsol simulation, we chose geometrical nonlinearity that is suitable for small strains and large rotations. We have added these explanations to the manuscript.

**Location of modification:** on page 8.

******************************************************************************

**Comment No. 8:**

In results and discussion, traditionally beam models can be employed when the Length/Diameter > 10 (L/D) but the ratio is less than 8 for the experiment discussed. How the Authors justify the validity of their modeling approach?

**Response:**

Sorry for unclear notation in dimensions of the beam in the experiment. With dimensions of 40 mm (length) × 5 mm (width) × 1 mm (thickness), the length/thickness = 40 where shear deformation is inconsiderable. Furthermore, COMSOL Multiphysics model considers the effect of shear deformation with built-in physics of Solid Mechanics and 4-node quadrilateral elements adopted in this study. We have clarified the matter.

**Location of modification:** on page 20.
Comment No. 9:

Please discuss the preparation of the SMP beam. Which materials are employed? How the beam is prepared? Experiments should be reproducible by other groups.

Response:

The detailed information regarding specimen preparation has been added into the manuscript.

Location of modification: on page 18.

**************************************************

Comment No. 10:

Which is the size of the image employed to measure deflection? How many pixels? Which is the resolution of the deflection measurement?

Response:

The image used for deflection measurement is 4961 ×3508 px. The distance between two clamps, 40 mm, corresponds to 3851 px, so we could calculate the resolution of deflection measurement, which is 40 mm/3851 px ≈ 0.01 mm/px. Admittedly, deflection values may suffer certain errors; however, it is acceptable to take them as reference. We have added this information in the revised manuscript.

Location of modification: on page 19.

**************************************************
Reviewer # 2

The authors present 1D and 3D finite element methods to investigate the thermo-mechanical shape memory responses of beam-like structures fabricated by 3D printing technology. Furthermore, this work formulates a 1D analytical solution for deflection of an SMP beam by Euler-Bernoulli beam theory and conducts an experiment to illustrate a full shape memory cycle of SMPs. The comparative studies of 1D and 3D modeling and experimental demonstration for the SMP beams are interesting and the manuscript is well written. Therefore, I am glad to recommend its publication after some minor revisions as listed below.

Authors:

Thanks for the comments and recommendation.

***************************************************************

Comment No. 1:

Page 5, line 59, alpha_r and alpha_g in Eq(8) were not defined.

Response:

We have defined them in the revised manuscript.

Location of modification: on page 6 and Table 1.

***************************************************************

Comment No. 2:

Page 7, line 44, "sigma can be deducted by Eq(30)" : please check "deducted".

Response:

It has been corrected.
Comment No. 3:

Page 8, line 44, "Substituting Eq. (3) into Eq. (21)", it seems that Eq.(3) should be Eq.(14).

Response:

We have corrected it.

Location of modification: on page 11.

Comment No. 4:

Page 11, line 51, "value" should be "values".

Response:

It has been corrected.

Location of modification: on page 14.

Comment No. 5:

Section 4: The comparative study of MATLAB and COMSOL modelling is conducted in this section, but the implementation details of COMSOL modelling is given in Sec. 5, therefore, it is better to place the comparative results of MATLAB and COMSOL computations behind the Sec. 5.
Response:

We have swapped section 4 with section 5.

Location of modification: on pages 9 and 10.

Comment No. 6:

Page 14, line 56-57: \( M_0 \) in Eq(45) was not defined.

Response:

The mentioned parameter has been added in the revised manuscript.

Location of modification: on page 16.

Comment No. 7:

Page 14, line 42, please check it is \( T_l \) or \( T_h \).

Response:

Having double checked that position, it is \( T_l \). But, the notation of \( \varepsilon_{f_{lh}} \) may be confusing, so it has been corrected.

Location of modification: on page 17.

Comment No. 8:

In Sec.4, this work develops a 1D FE program in MATLAB, however, from the computed contours in Figs.3 and 4, it seems like the FE models both in COMSOL and MATLAB are 2D. Please clarify.


**Response:**

In the tensile simulation of MATLAB, it is assumed that elongations of each axial layer of the beam are the same, based on the FE results plotted in 2D. As for the case of bending, with Euler Bernoulli beam hypothesis that cross-sections of the beam remain plane and perpendicular to the neutral plane during deflection, we could visualize 1D FE results of MATLAB to a 2D plot. We have clarified the matter in the revised manuscript.

**Location of modification:** on page 15.

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Authors:

We hope the revised manuscript together with replies are satisfactory so as to fulfill the expectation of the respected reviewers.