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Multiscale Modeling of Smart Materials under Static and Dynamic Thermo-mechanical Loading

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MULTISCALE MODELING OF SMART MATERIALS UNDER STATIC AND DYNAMIC THERMO-MECHANICAL LOADING

A Thesis

Submitted through the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College
in partial fulfillment of the requirements for the degree of Master of Science in Mechanical Engineering

in

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by

Soodabeh Sharafi
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ABSTRACT

Engineering material systems with tailored capabilities is a topic trend in plethora of research. Polymer based Artificial Muscle, PAM, and Shape memory polymer fiber, SMPF, enable structural engineers to incorporate smartness functionality into their design through programming cycles. Smartness functionality leads to the production of artificial muscles with different load carrying capability. SMPF is another category of smart materials, which are capable of being micro-structurally engineered to isolate vibration at different temperature and frequency conditions. The smartness functionality offers the adjustment between inherent properties of these materials with their industrial applications through modeling techniques. Mixture of phenomenological, numerical, mathematical models provides phenomenological Multiscale model to study effect of thermal fluctuation on mechanical response of polymer based artificial muscle. This model provides an insight to the nature of thermo mechanical response at macroscopic scale as well as the theory behind stress-strain evolution over working temperature. Multiscale modeling techniques is applied to study dynamic response through relating the damping and storage properties of a smart material, SMPF, to the stiffness and damping coefficient of a single degree of freedom system, SDOF. Damping coefficient, c, is related to the loss factor and natural frequency of the system; equivalent stiffness, k, is correlated to the storage modulus and geometry of the specimen.
CHAPTER 1   INTRODUCTION

1.1 Motivation

Modeling techniques become an essential part of analysis in order to minimize the experimental trial-and-errors efforts for finding the optimum range of design. Analytical and numerical models are highly desired in many scientific contexts. Multi scale models are established to relate a mechanical response of a system at different scales. There are two types of Multiscale modeling, one of which relies on quantum mechanics as a starting point and the other category is established on continuum mechanics. In quantum mechanics and molecular dynamic simulations, material is modeled as a discrete particle and continuum mechanics allows the analysis of the material as a continuous system. In fact, at Multiscale modeling, a material property is related hierarchically from atomistic level up to real world scale and vice versa; connecting the information from two or more scales, which is still a major challenge, provides a modeling framework; this technique can be used to relate mechanical property at discrete scale i.e. atomistic scale to continuum scale or vice versa. Difficult task is coupling length and time scale of different level of analysis.

One may generate a Multiscale model for polymeric materials, through force field theories, as well as applying the iterative Boltzmann theory in atomistic scale analysis. Then by way of applying primitive path [1] and affine deformations calculations are joined to the macroscopic scale and vice versa [2].

These types of atomistic calculations are initiated from quantum mechanics theories and related through application of force field analysis i.e. conformational analysis. Force field equation is extendable from atomistic to the molecular scale. This methodology and developed parameters provides a way to translate electron’s interactions to the bond vibration in Nano scale. Molecular dynamic simulation is a palatable technique for analyzing dynamic behavior,
mobility and α- and β-relaxations; it owns some drawbacks related to the high cost of computation and complexity of simulation. At Mesoscale analysis, tube models and random walk theories are described to translate the bond vibration to the chains snake like motion. In the tube model, a chains contains N monomeric segment is constrained by adjacent static chains. This tube-like configuration elucidates dynamic of chains using diffusion equations.

Molecular dynamic Multiscale modeling is expanded to the macroscopic scale using primitive path to scale up discrete formalism to micro scale. Then applying affine path lets scientist to obtain properties of polymer from atomistic level and vice versa.

However, in continuum formulations, the atomistic calculations are not considered and physical properties of material are illustrated by tensors. The body is considered to be a homogeneous material, in which the property is represented by internal state variables. Those variables represent the average amount of target property in the sample and evolve according to phenomenological formulations [3]. The main advantage of the continuum techniques is the low computational time required due to the fact that main analyses are handled in macro scale. Main disadvantage arise from dependence of this modeling on experimental results as a starting point of modeling; change in macroscopic response such as volume fraction of phases, direction of segments[4] enforce scientists to run new set of experiments to decipher microscopic evolution law.

Modification on this methodology is obtainable through understanding of the relation among the basic constituents of the polymers, chains and crystalline segments, and of the effects of their interactions in the response of the whole structure, artificial muscle or shape memory polymer fiber. Therefore, a model that can predict the evolution of a targeted property in the
form of micro scale evolution of chains in multiple length scales can be very useful as a tool to
design and analyze polymeric actuation mechanism [5].

In the Multiscale models, the analyses are performed separately in two different scales,
micro and macro, and it can be shown that the constitutive behavior of the macroscopic scale can
be obtained by the principles of homogenization as well as applying statistical mechanics
without significant loss of accuracy. Statistical mechanics is a methodology using probability
function to relate molecular level position and velocity to the macroscopic scale. This array of
mathematical tool is used to connect micro scale thermal actuation mechanisms to the
macroscopic actuation response through averaging technique.

However, it is important to notice that two important conditions should be satisfied in
order for validity of multi scale modeling in continuum mechanics: The two geometric length
scales should be widely separated; and, the micro scale should be statistically homogeneous,
represent accurately enough the macro scale behavior of the polymeric material.

In spite of extensive research effort, many questions regarding application of Multiscale
modeling for smart materials under static and dynamic thermo-mechanical loading are still to be
answered. These questions can be broadly divided as follows:

What type of modeling is suitable to describe nature of thermal actuation response of
smart structures i.e. atomistic or continuum, and if continuum based analysis then what kind of
models should be?

Whether conventional modeling techniques are extended to either static loaded system or
harmonically excited system?

How model’s parameters are related to the physics of the problems?
The first question is a major issue, and in the context of general Multiscale modeling technique, has been settled by choosing continuum based modeling techniques, although has been pointed out that in general this type of modeling will not be correct without having complete sets of experiment to verify microscopic response. The last two questions are related to each other in the sense that for pinpointing the response of smart material under different history of loading, knowledge of conventional modeling techniques same as SDOF or Gaussian model for polymers are also essential. Through this analogy, model parameters are obtained and associated error for modeling is reported. However, another relevant question in this context is what error margin is in our modeling terminology. These issues will be discussed in this dissertation. Following, the efforts involve in this dissertation is outlined briefly.

1.2 Outline of dissertation

A systematic study on Multiscale static and dynamic thermo-mechanical analysis of smart structures has been implemented in this dissertation to find solution to the existing questions and open problems identified in the last section. Proposed Multiscale modeling techniques provide a framework about the nature of the smart structures, which they stand for. Linear elasticity assumption in accordance with Gaussian chain application provide a fundamental line to obtain stress-strain response for the polymer based artificial muscle as well as descriptive path for modeling dynamic response of the shape memory polymer fiber. The dissertation is divided to the four chapters.

In Chapter 1, the concept of Multiscale modeling, well known for application in both continuum and discrete systems are elaborated. The major challenges and drawbacks of different types of Multiscale modeling are discussed.
Chapter 2 is aimed to illustrate a thermo-mechanical Multiscale modeling under static loading. In this study the nature of actuation response of a polymer based artificial muscle is analyzed by incorporating micro and macro scales evolution of Gaussian chains over working temperature. The statistical mechanic is applied to provide a theoretical background in order to pinpoint thermal actuation of the polymer based artificial muscle.

In Chapter 3 another application of Multiscale modeling for evaluating a dynamic thermo-mechanical problem is elucidated; the vibration damping response of SMPF material system is studied with a view to design damping response of smart structures that can mitigate severe vibrations; the proposed numerical approach is developed to tune up theoretical background of a SDOF system with a temperature and frequency dependent damping and stiffness parameters. The analogy between loss modulus with damping coefficient and storage modulus with material stiffness for a SDOF system is made to develop a Multiscale model for obtaining damping and stiffness property of the SMPF.

Finally, Chapter 4 presents the concluding remarks from this dissertation and provides few suggestions for future investigations.
CHAPTER 2 MULTISCALE MODELING OF STATIC RESPONSE OF PAM

This chapter describes a thermo-mechanical Multiscale modeling under static loading for smart artificial muscle. Artificial muscle is an emerging material in the field of smart materials with application in aerospace, robotic, and biomedical industries. Despite extensive experimental investigation in this field, there is a need for numerical modeling techniques that facilitate cutting edge research in this field. This work aims at studying an artificial muscle made of twisted Nylon 6.6 fibers that are highly cold-drawn. A computationally efficient phenomenological thermo-mechanical constitutive model is developed in which several physical properties of the artificial muscles are incorporated to minimize the trial-and-error numerical curve fitting processes. Two types of molecular chains are considered in micro-scale level that controls training and actuation processes viz. (a) helically oriented chains which are structural switches that store a twisted shape in their low temperature phase and restore their random configuration during thermal actuation process, and (b) entropic chains which are highly drawn chains that could actuate as soon as the muscle heats up, and saturates when coil contact temperature is reached. The thermal actuation response of the muscle over working temperatures has been elaborated in modeling section. The performance of the model is validated by available experiments in the literature. The model may provide a design platform for future artificial muscle developments.

2.1 Introduction

Man-made smart materials called artificial muscles are reversibly capable of extension, contraction or rotation, triggered by external stimuli such as chemical, electrical, pneumatic and thermal. Artificial muscles have become a popular topic of research in the past few years within the area of biomechanics, robotics, aerospace garment and many more. Pioneering designs comprise a vast category of materials based on four actuation mechanisms, including electric
field actuations, ion-based diffusions, pressurized mechanisms and thermal actuations [6-11] Bio inspired designs and their structural change have been studied comprehensively. Zhao et al. reviewed the recent methods for designing bio inspired materials in which the systematic procedure for design, analysis and producing new materials is categorized and elaborated for biological materials[12]. In another study by Qin et al., combination of theoretical and chemistry-based atomistic level model are utilized to study the effect of peptide length on the stability of alpha helix structure [13]. The study focuses on physical mechanism those results in maximum stability of alpha-helix critical length. The critical length and probability distribution are two key concepts for understanding the folding mechanism and stability of alpha helix structure formation. Liu et al. provides a macroscopic analysis for the effects of geometry of rod structures on actuation response, which is the number of twist and structural transition under tension[14].

Some limitations of the previous muscles include short life cycle and loss of stored energy due to dissipative mechanisms mainly rooted in hysteresis cycle and low work efficiency. The popularity of the subject motivates researchers to fabricate new category of muscles with almost zero structural loss. Haines et.al. introduced a new category of artificial muscles from low cost fishing lines or sewing threads. These muscles are working in a hysteresis-free actuation, which provide the highest efficiency compared to other kinds of artificial muscles[15]. The enhanced muscle response is sourced in its reversible contraction in the microscopic structure, which has large volumetric thermal expansion and inhomogeneous dimensional change due to thermal actuation. The thermal actuation occurs within temperature fluctuations from room temperature to above glass transition temperature ($T_g$) and *vice versa.*
Because of the varying actuation mechanisms for artificial muscles, a number of studies have been conducted in the literature. One may mention models proposed to study electrochemical driven artificial muscles that link the macro mechanical behavior to the change in chemical components [7, 16]. In the case of electrochemical muscles, the ion diffusion and some mechanical and chemical reordering should be controlled which may add more complexity to the model. In the case of pneumatic muscles, fluid dynamics models have been developed in which state variables are space and time dependent, and moreover, the boundary conditions are time dependent [17]. Control based design approaches have also been used to capture high nonlinearity of pneumatic artificial muscles [8]. A two-state model is also developed to study force deflection variations in shape memory alloy coiled spring actuator [18]. In the case of muscle made of shape memory Nitinol wire, a developed model works based on stress-strain-power relationship, which is applied to control underwater robotic movement [19].

While these models have been successful in modeling a specific category of muscles, they suffer from the large number of parameters that are needed to define the model behavior. Most importantly, the existing models do not address the newly developed polymer based artificial muscles, which is the subject of the current study.

In this work a phenomenological model has been developed based upon micro structural descriptions in which the muscle mainly comprises amorphous phase chains and the contribution by crystalline micro phases are negligible. Amorphous chains are subdivided into helically oriented chains and highly drawn chains. Specific types of deformation mechanisms are assumed for each helically oriented chain and highly drawn chain, to be responsible for actuation responses in various types of muscle structures.
This paper is arranged as follows. In section 2, namely physics behind polymeric artificial muscles, the effect of micro structural engineering process and training cycles on the formation of the muscles is elaborated. Then, principle for thermal actuation responses in artificial muscle is discussed and the microscopic and macroscopic responses are developed. In section 3, model description, phenomenological model and constitutive model are outlined and formulated. Modeling framework is defined in section 4 including mathematical modeling of actuation response of the muscle. Section 5 presents the numerical results.

2.2 Physical Characteristics

2.2.1 Microstructural Engineering and Training Cycles

Thermal actuation mechanism in polymeric artificial muscles is designed through a two-step engineering process, viz. microstructural engineering and training cycle. The microstructural engineering defines the shape of the muscle as well as the type of the actuation mechanisms, such as electro-chemical, etc. Different microstructures of polymer fibers have been examined by Haines et al.\cite{11} as a precursor to produce the muscle, such as nylon 6, nylon 6.6, etc. The microstructures of these fibers need to be engineered in order to add actuation capabilities to the fibers. The microstructural design process includes (1) cold drawn tension that results in the so-called precursor fibers, and (2) twisting the precursor fibers. The final product from these nylon fibers is capable of actuation in response to external stimuli; and it is called artificial muscle hereinafter. Details regarding the fabrication process of the artificial muscles by twist insertion can be found in [15], and is outlined herein for sake of completeness.

There are two types of muscle fabrication method, coiling muscle by extra twisting of the precursor fiber and annealed muscle by annealing the twisted fiber around a mandrel. In the coiling method, the coiling is inserted by over-twisting. In the annealing process, the size of a
mandrel defines the muscle’s final geometry. The precursor fiber is twisted around mandrel to build spiral structure named muscle. Then the annealing process is set to fix the muscle’s shape by raising the temperature to the melting point of the fiber. These methods result in different shape and load carrying response. The coiled muscle has lower stroke but higher load capability; the annealed muscle has higher stroke but lower load lifting capacity. From the microscopic point of view, the amount of helically oriented chains in the annealed muscle is less than that in the coiled muscle. Therefore, the annealing fabrication process produces muscles with lower load carrying ability and higher strain response.

The microstructure of the precursor fiber mostly consists of (a) amorphous phase, Gaussian chains that are highly oriented in the direction of cold strain, and (b) minor crystalline bridges, see Fig. 1a. These precursor fibers are famous for their high strength, enabling them to be used even as fishing lines. Fig. 1 schematically demonstrates the microstructural design process by microstructure engineering (Step 1). Both Fig. 1(a) and 1(b) show the first step in the micro structural engineering process. Fig. 1(a) shows the random distribution of the amorphous chains that are bridged by the crystalline phase before cold drawing. Fig. 1(b) illustrates the effect of cold drawing on the microstructure of the fiber in which highly drawn chains are produced in the direction of drawing. Fig. 1(c) depicts the effect of the twisting process in which helically oriented chains are produced due to the inelastic deformation mechanisms. The highly drawn and helically oriented polymer chains are capable of responding to external stimuli and the degree of stretch/twist governs the actuation efficiency of these smart muscles. In Step 2, training cycles are conducted. A muscle is trained in repetitive cycles to ensure a stable reversible actuation response with minimum hysteresis effects.
The helically oriented chains resulting from Step 1 are trained in the loading-unloading cycles. This process will ensure reversible response of the muscle by changing the temperature. This process of multiple heating and cooling cycles is designed to train thermally activated muscle until reversible actuation response is obtained. The heating process is initiated from room temperature with a very rapid cycle about 17 seconds up to above the glass transition temperature of the muscle. In each cycle the muscle shrinks when lifting loads by heating or expands while carrying load by cooling. In this step the reversible helical path of motion is established within the repetitive cycles. Training cycle between high (95°C) and low temperatures (25°C) as stated by [15] guarantees the actuation response of the polymeric artificial muscle (PAM).
2.2.2 Principle of Thermal Actuation Responses

From the thermodynamics point of view, amorphous phases are less energetically stable comparing to crystalline phases. Consequently upon applying thermo mechanical energies, amorphous chains undergo structural changes first while the crystalline phase remains intact.

Amorphous phase plays a dual role in thermal actuation responses in which the highly drawn chains behave like an entropic elastic chain that recovers their original shape upon unloading. For the helical chains, each helically oriented chain acts as a structural switch that twists or untwists over the actuation temperature range. Structural switches have two mechanisms that can be activated by temperature variation: relaxation mechanism that is activated during the cooling process and entropic mechanism that is turned on during the heating process. Fig. 2 shows the micro structural changes during the heating up process where the entropic mechanism enforces structural switches to move along the helical path; see Figs. 2(a) and 2(b).

The accumulations of these helical motions result in fluctuation in the form of contraction/expansion in the draw direction. Upon saturation of contraction, the helically oriented chains start to intervene with each other, as shown in Fig. 2(c). Fig. 2(c) shows two helically oriented chains, which are intervening with each other and shrinking in the helical path; this motion resulting in radial expansion because there is no room for motion in the longitudinal direction. In other words, the anisotropy in thermal expansion starts playing a role and the extra heat expands muscle radially while inter-coiling process continues. The resulting motion swells muscle radially; see Fig. 2(c).
Fig. 2  Schematic represents the change in the molecular unit of the muscle when temperature fluctuates. Three configurations of muscle's chains have been shown: (a) the low temperature structure in which chains are in their fully extended configuration shown by dashed blue extended chains, (b) activated chains, before Tc (coil contact temperature), twist in helical path in which overall motion leads to shrinking in longitudinal direction and (c) saturated structure, after Tc, starts expanding in radial direction, graphed as thick double lines for intervening chains. Reproduced from Ref. 5 with permission from The Royal Society of Chemistry.

During the cooling down process, relaxation mechanisms occur in which structural switches experience reverse motion along the helical path toward lower entropic levels. These relaxation mechanisms impel both structural switches and entropic chains (amorphous phase) to expand in the longitudinal direction upon regaining their low temperature configuration.

From macroscopic point of view, upon temperature rises, as shown in Fig. 3(b), the muscle contracts longitudinally. The red arrow is used to show the shrink initiation and propagation. At temperatures above coil’s contact temperature (Tc), at which there is no room for the longitudinal contraction, muscle starts to expand radially and stiffening simultaneously. The schematic of the process has been depicted in Fig. 3(c). Contrary, when temperature reduces, muscle shrinks along radial direction until coil contact temperature reaches and then further cooling result in expansion in longitudinal direction. When muscle reaches room temperature, all chains are at their relaxed and stress free status.
2.3 Model Description

In the sense of phenomenological formulation one may decompose the actuation response of the muscle into two elastic components that represent different thermal responses below and above the coil contact temperature $T_c$.

The actuation strain tensor $\varepsilon_{ij}^t$ is given by

$$
\varepsilon_{ij}^t = \varepsilon_{ij}^{(1)} \left( 1 - < T - T_c > \right) + \varepsilon_{ij}^{(2)} < T - T_c >
$$

(1)

where $<>$ denotes Macaulay bracket, $\varepsilon_{ij}^{(1)}$ denotes strain response below $T_c$, called activated state strain hereinafter, and $\varepsilon_{ij}^{(2)}$ shows strain in saturated state which represents the system above $T_c$ where coil contacts occur. Fig. 4 demonstrates schematics of the proposed phenomenological model where the actuation strain is correlated to the thermal actuation. The activated and saturated states are represented by two sets of elastic springs.
To model time dependent elastic deformation of the muscle system it is assumed that each state is constructed from a number of elastic springs that represent the individual molecular chains in each state. Below $T_c$ the molecular chains are free to have longitudinal motion and their deformation results in

$$\varepsilon_{ij}^{(1)} = \sum_{k=1}^{N} \varepsilon_{ij}^{(1)k}$$

where $N$ denotes the number of chains and $\varepsilon_{ij}^{(1)k}$ is the strain due to longitudinal deformation in the $k^{th}$ chain.

Once the temperature reaches to $T_c$, all molecular chains have reached to the full contact configuration, and they cannot have any longitudinal deformation. In this stage the active state must be switched to the saturated state in which the contacted coils undergo radial expansion that stiffens the muscle. Thus, in the saturated state, the *saturated chains* are responsible for deformation mechanisms and they are modeled with a gradual activation of the structural switches in the saturated state. Thus, the saturated state’s strain is given by

$$\varepsilon_{ij}^{(2)} = \sum_{k=1}^{N} \varepsilon_{ij}^{(2)k}$$

where $\varepsilon_{ij}^{(2)k}$ shows the strain components for the $k^{th}$ saturated chains. Two switches, shown in Fig. 4, are responsible to gradually exchange the muscle between activated and saturated states during heating or cooling processes.

In order to develop the constitutive model, it is assumed that the representative volume element (RVE) of the muscle is constructed from (a) $k$ units of helically oriented chains, denoted by superscript $h$, and (b) $l$ units of highly drawn chains, denoted by superscript $d$. The total number of chains in the unit volume of muscle is $N=k+l$. The volume fractions of helically oriented $\phi_h = k/N$ and highly drawn $\phi_d = l/N$ chains are linked together by the rule of mixture.

$$\phi_h + \phi_d = 1$$

(2)
Fig. 4 1D analogy of the model for artificial muscle made of fishing line which shows two series of springs (each spring is a symbol of individual polymer chain) with a thermal switch in which heat flux activates springs one by one; this process is a temperature dependent process. Before \( T_c \), both switches are open and the activated chains are responding to temperature change until muscle reach coil contact temperature (\( T_c \)). Coil contact temperature causes the activated chains to short circuit in a way that only saturated chains are responding to the temperature fluctuation. Reproduced from Ref. 5 with permission from The Royal Society of Chemistry.

To bridge the micro scale deformation mechanisms to the macroscopic deformation below \( T_c \), it is assumed that the strain response for each molecular unit of chain obeys the rule of mixture

\[
\varepsilon_{ij}^{(1)k} = \phi_h \varepsilon_{ij}^{(h)k} + \phi_d \varepsilon_{ij}^{(d)k}
\]

(3)

where \( \varepsilon_{ij}^{(h)k} \) and \( \varepsilon_{ij}^{(d)k} \) represent the microscale strain tensors in \( k^{th} \) molecular unit due to the twisting and drawing training processes, respectively. The macro scale strain tensor is then given by

\[
\varepsilon_{ij}^{(1)} = \sum_{1}^{N} \varepsilon_{ij}^{(1)k}
\]

(4)
Above \( T_c \), only helically oriented chains in the saturated state contribute to actuation response while highly drawn chains are no longer active. Thus, the micro scale strain tensor in each molecular unit is as follows:

\[
\varepsilon^{(2)k}_{ij} = \phi_h \varepsilon^{(h)k}_{ij}
\]

(5)

where \( \varepsilon^{(2)k}_{ij} \) denotes unit chain’s strain tensor above \( T_c \). The macroscopic strain above \( T_c \) is then given by

\[
\varepsilon^{(2)}_{ij} = \sum_{1}^{N} \varepsilon^{(2)k}_{ij}
\]

(6)

The switches in the model control the volume fractions and consequently the exchange between the two states occurs automatically. Fig. 5 shows the molecular unit, viz. microscopic RVE, and macroscopic RVE. The micro scale and macro scale strains are schematically shown in Fig. 5.

---

Fig. 5  (a) microscopic RVE below \( T_c \), (b) microscopic RVE above \( T_c \), and (c) Macroscopic RVE. Reproduced from Ref. 5 with permission from The Royal Society of Chemistry.

The total macroscopic actuation strain is then correlated to the two activated \( \varepsilon^{(1)}_{ij} \) and saturated \( \varepsilon^{(2)}_{ij} \) strains in Eq. (1). Total stress is based on the linear elastic assumption written per Hooke’s law as multiplications of effective stiffness \( L_{ijkl}^e \) and total strain \( \varepsilon_{ij}^t \).
\[ \sigma_{ij}^t = L_{ijkl}^e \varepsilon_{kl}^t \]  
with  
\[ L_{ijkl}^e = \phi_h L_{ijkl}^h + \phi_d L_{ijkl}^d \]  
where \( L_{ijkl}^h \) and \( L_{ijkl}^d \) are stiffness tensors for twisted and drawn trained chains, respectively. To obtain the constitutive modeling the relation between thermal actuation and microscale level strains must be developed. Thermal actuation functions are defined to relate the macroscopic response to inherent properties of microscopic components namely helically oriented chains and highly drawn chains. The microscopic actuation strains due to drawn and twisting processes are defined by  
\[ \varepsilon_{ij}^{(d)k} = \alpha^{(d)} \Delta T, \text{ and } \varepsilon_{ij}^{(h)k} = \alpha^{(h)} \Delta T, \]  
where \( \alpha^{(d)} \) and \( \alpha^{(h)} \) are thermal actuation functions below and above \( T_c \), respectively; and they are functions of molecular chains mechanical properties and also training cycles.

In other words, both fabrication and training processes have direct effect on moduli and actuation response of the molecular chains. This is in accordance with experimental observations in which muscles made of extra twisted insertion have higher load carrying capacity and higher actuation response. The effect of twist insertion has a direct correlation with stiffer helically oriented chains as a result of higher volume fraction of these chains, which leads to stiffer muscles. In order to formulate the dependence of the effective overall modulus on the drawn and twisted chains’ volume fraction, one may assume  
\[ L_{ijkl}^{(d)k} = \frac{1}{k} f(\varepsilon_{ij}^{(d)k}) \]  
\[ L_{ijkl}^{(h)k} = E g(\varepsilon_{ij}^{(h)k}) \]
where $L_{ijkl}^k$ is un-trained molecule stiffness tensor, for the $k^{th}$ chain, $L_{ijkl}^{(d)k}$ and $L_{ijkl}^{(h)k}$ are trained molecule stiffness tensors of $k^{th}$ chain after drawing and twisting, respectively; and $f$ and $g$ are two material functions. To simplify the formulation process, the rule of mixture is used to define the overall effective modulus of the $k^{th}$ chain as follows

$$L_{ijkl}^{(e)k} = \phi_h^k L_{ijkl}^{(h)k} + \phi_d^k L_{ijkl}^{(d)k}$$  \hspace{1cm} (11)$$

where volume fractions of twisted $\phi_h^k$ and drawn $\phi_d^k$ chains in microscale are defined as follows

$$\phi_h^k = \left(\frac{\epsilon^{(h)k}_1}{\epsilon^{(h)k}_{max}}\right)$$
$$\phi_d^k = \left(\frac{\epsilon^{(d)k}_1}{\epsilon^{(d)k}_{max}}\right)$$  \hspace{1cm} (12)$$

where $\epsilon^{(d)k}_1$ and $\epsilon^{(h)k}_1$ denote respectively applied drawing and twisting strains during training cycle, and $\epsilon^{(d)k}_{max}$ and $\epsilon^{(h)k}_{max}$ are the maximum allowable drawn and twisting strains for $k^{th}$ chain, respectively. $\epsilon^{(d)k}_{max}$ and $\epsilon^{(h)k}_{max}$ are two material parameters for the molecular chains that can be identified from experimental observations.

Statistical mechanics is utilized to model the physical behavior of the polymer chains. Gaussian distribution function has been used by Porter [20] and recently Shojaei and Li [21] to model the polymer mechanical responses. Following these works, two functions have been used to model physical behavior of the polymer chains during temperature variation (a) Gaussian distribution function, $G_g$, and (b) accumulative norm of $G_g$ which is denoted by $P_g$ [21].

$$G_g(T, T_\#, \sigma_\#) = \frac{1}{\sigma_g \sqrt{2\pi}} \exp \left( -\frac{T - T_\#}{2\sigma_\#^2} \right)$$  \hspace{1cm} (13)$$

$$P_g = \int_{T_1}^{T_2} (G_g(T, T_\#, \sigma_\#)) = -\frac{1}{2} \text{erf}_\# \left( \frac{T_\# - T}{\sqrt{2}\sigma_\#} \right) + \frac{1}{2}$$  \hspace{1cm} (14)$$
where ‘#’ is substituted by ‘g’ or ‘c’ to indicate glass transition and coil contact transition events, respectively; $T_g$ here is the glass transition temperature of the muscle or the initial fiber and erf is the error function [22]. The standard deviation $\sigma_g$ identifies half of the bandwidth for phase change during glass transition event. Based on a recent work by [21], the modulus has the following relation

$$E' = E'_0 \frac{1 - P_c}{1 + P_c}$$  \hspace{1cm} (15)$$

where $E'_0$ (MPa) is a reference elastic tensile moduli at the low temperature, e.g. 25 °C. $E'_0$ should be defined in the numerical model to produce the obtained reference moduli from the DMA testing machine. In order to include the effect of various manufacturing and training parameters on the overall stiffness of the muscle Eq. (15) is further refined as follows

$$E = E' - CT$$  \hspace{1cm} (16)$$

where $C$ is the muscle’s spring constant and $E'$ is the statistical elastic modulus, given in Eq. (15). In Eq. (16) the muscle’s stiffness is assumed to have a linear dependency on spring constant $C$ and also temperature $T$. It is shown that the proposed model correlated well with observed experimental data.

The actuation strain function is also temperature dependent and it is a function of muscle manufacturing and training cycle. The Gaussian distribution function has been used to formulate the actuation strain in which statistical mechanics provides a more physics based description for the chain actuation behavior. In order to include the manufacturing and training cycle in the actuation response, the effect of coiling has also been considered through material parameters $\alpha$, $\beta$ and $\gamma$. The actuation strain $\varepsilon$ reads

$$\varepsilon = \alpha - \gamma T - \beta. \text{erf} \left( \frac{(-T_g + T)}{\sigma_g \sqrt{2}} \right)$$  \hspace{1cm} (17)$$
Based on a parametric study, presented in the results and discussion section, it is concluded that $\alpha \cong \beta$ and $\gamma \cong 10^{-4}\alpha$. Also parameters ‘$\alpha$’ and ‘$\beta$’ are directly related to the coil spring constant in which $\alpha \approx 5C$ to $6C$ with the muscle’s spring index $C=1.7$. The linear elasticity assumption for stress - strain is then applied to calculate the stress

$$\sigma = E.\varepsilon$$  \hspace{1cm} (18)

Where $E$ and $\varepsilon$ are given by Eqs. (16) and (17), respectively.

2.4 Numerical Framework

The constitutive model is numerically solved in MATLAB. In this section, the numerical implementation steps are elaborated and shown by a flow chart in Fig. 6. An artificial muscle with the highest spring constant, $C = 1.7$, found in the literature, is considered during implementation, while parametric study is also carried out to evaluate the effect of various parameters on muscle responses.

Fig. 6 shows the flowchart for the numerical implementation together with equation numbers and parameters used in each step. In this schematic, the process starts by obtaining the material properties from experimental graphs, which are listed in the first six columns of the Table 1. Determining design parameters, which meet the stress and strain requirements at critical transition temperature and relative duration of their structural change, are the main objective of our model. The last three parameters are defined to reduce the discrepancy between numerical model and experimental data. The least square approach has been utilized to calculate the error. This process continues until the amount of error in the numerical model reaches to 5% of experimental results. The effect of deviation from each material parameter is parametrically studied. The simulations are compared with the experimental results presented in[15].
The error margin can be selected based upon the level of accuracy that is needed in a specific problem. In most engineering problems, 5% deviation provides an acceptable representation for the problem. In this work the least square method is used to find each of the three curve fitting parameters $\alpha$, $\beta$, and $\gamma$. Ranges of these numerical parameters for having error less than 5% are as follows, $10 < \alpha < 10.2$, and $0.000102 < \gamma < 0.00102$. Figures 7-9 in the next section show the simulation results based on the given ranges of the material parameters, $\alpha$, $\beta$, and $\gamma$, in which the deviation is less than 5%.

The numerical functions are defined and molded in a way to capture actual material response to temperature. In fact, these functions are applied to calculate the probability of activation of amorphous phase over working temperature and also estimate the saturation state of longitudinal motion at the coil contact temperature. They are defined based on probability density of the conformational evolution for the amorphous phase around critical temperatures ($T_g$ or $T_c$). Therefore the Gaussian distribution probability (statistical mechanics) is considered as a building block of the current modeling process. As a matter of fact, the produced function integrates the change of internal parameters such as the coil angles, the number of twists, and the micro structural engineering process over working temperature by considering the probability of change of structure based on its macro-mechanical response.

Consequently, the modulus of the coiled muscle has been modeled using integration method over Gaussian distribution function; meanwhile, the strain function has been reproduced in the same procedure. The strain, which is the actuation function per percentage of the length as reported in the experiments, is a mechanical response of the artificial muscle; it indirectly indicates the motion in the molecular length scale.
This temperature dependent function implies the probability of conformational rotation and also chain stretching processes as temperature increases. The modeled modulus and strain functions have been used to calculate the stress response. Then the nominal stress versus tensile actuation within the temperature range has been plotted and compared with the experimental data.

![Diagram](image)

*Error: least square of experimental and numerical actuation strains*

Fig. 6 Modeling process for artificial muscle made of fishing lines. Reproduced from Ref. 5 with permission from The Royal Society of Chemistry.
2.5 Results and Discussions

2.5.1 Determination of model parameters

In this section two types of material parameters have been introduced; the first type includes the first six parameters in Table 1; these parameters are indicated with asterisks in which they are directly imported from experimental results. The last three parameters indicating with Greek letters are determined from curve fitting efforts. Table 1 summarizes the material parameters used during the simulations.

<table>
<thead>
<tr>
<th>$T_g$(°C)*</th>
<th>$T_c$(°C)*</th>
<th>$E_0$(MPa)*</th>
<th>$\sigma_g$(°C)*</th>
<th>$\sigma_c$(°C)*</th>
<th>C*</th>
<th>$\alpha$</th>
<th>$\beta$</th>
<th>$\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>90</td>
<td>130</td>
<td>1000</td>
<td>10</td>
<td>40</td>
<td>1.7</td>
<td>10.2</td>
<td>10.2</td>
<td>$10.2 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

*Obtained from experiments (Haines et al. 2014)

Three curve fitting parameters ($\alpha, \beta, \gamma$) are introduced to mitigate deviation of numerical model. Consequently, the effect of these parameters on variation of the stress-strain numerical function has been studied. Variation in parameter ‘$\alpha$ ’results in change in terms of numerical stress-strain response as shown in Fig. 7. The numerical function is compared with the experimental data and this graph shows that the best estimation for this parameter, is $\alpha \cong 5C$ to $6C$, with C=1.7. In fact, Parameter ‘$\alpha$ ’ has dimension of $T^{-1}$, defines vertical movement of the model with respect to experimental results.

From modeling outcomes, one may infer that theses parameters are related to the microscopic strain tensors through following relations. $\alpha \cong f(\varepsilon_{ij}^1)$ and $\beta \cong f(\varepsilon_{ij}^2)$ and $\gamma \cong f(\varepsilon_{ij}^1)\& f(\varepsilon_{ij}^2)$. However, further experimental results are necessary to elaborate and extend modeling in order to provide a direct relation between microscopic strain tensors and proposed curve fitting parameters.
Parameter ‘α’ estimates the horizontal movement for the stress-strain numerical response versus experimental results. Fig. 8 shows that the parameter ‘β’ has the same value compared to parameter ‘α’. However, this parameter is used to study the probability of the variation of model in the horizontal direction. Parameter γ is defined to add accuracy in muscle’s stress-strain response. This parameter controls the span of the response. The optimal value for this parameter is $6 \times 10^{-4} C$, i.e., 0.000102, as shown in Fig. 9.

In order to verify the capability of the proposed framework, in this section parametric study has been conducted and the results show that the proposed model can predict different muscles as depicted in Fig. 13. Three artificial muscles with different spring constants $C=1.1$, 1.4 and 1.7 have been plotted at the end of this section. Same parameters are utilized to model different sizes of muscle.
Fig. 8  Depicts fluctuations in stress-strain response with parameter, $\beta$, compared with experimental results. Reproduced from Ref. 5 with permission from The Royal Society of Chemistry.

Fig. 9 Different stress-strain responses when parameter ($\gamma$) changes and these graphs are compared with experimental results. Reproduced from Ref. 5 with permission from The Royal Society of Chemistry.

2.5.2  Model validation and prediction

In this section the proposed formulation is numerically implemented and its performance is compared with the available experimental data from the literature. The numerical model is in a good agreement with experimental results. Fig. 10 shows the variation of the muscle’s modulus with respect to the temperature where Eq. (16) is used to plot this graph.
It is worth noting that the material parameters $T_c$ and $\sigma_c$ are directly obtained from the experimental data and no curve fitting is required to plot this graph. Nominal elastic modulus is introduced in experimental results to address application of simple elasticity theory to calculate nominal stress and strain. Nominal stress ($\sigma_N$) at each cross section can be calculated by simply dividing the applied force by the initial cross-section area of the muscle. Also, nominal strain ($\varepsilon_N$) is defined as the amount of deformation normalized by the length, $\varepsilon_N = \frac{\Delta L}{L}$. Therefore, the nominal modulus can be defined as a fraction of nominal stress over nominal strain.

Fig. 11 depicts the actuation strain versus temperature in which Eq. (17) is used to plot this graph. This graph can be obtained directly from the experimental parameters by only knowing the magnitude of the spring index input as parameter $\alpha$, however, the high degree of error resulted in definition of two other material parameters $\beta$, and $\gamma$. These parameters are numerically varied to achieve minimum deviation between simulation and experiment as it has been schematically presented in Fig. 6.

The calibrated model is then used to plot stress actuation in Fig. 12 along with the corresponding experimental results. The model has acceptable agreement with experimental results for the constrained actuation response of the muscle, including the existence of a low peak that arises from the glass transition of the coiled fiber. Though the muscle becomes saturated in longitudinal direction when the coils contact, the thermal expansion becomes positive and the muscle expands in radial direction in the range of 130°C to 175°C. Thorough scrutiny shows that the model can capture the trends and also the behavior of the experimental results for three different sizes of muscle.
Fig. 10 The temperature dependence of the Modulus for Nylon 6.6 has been modeled mathematically and compared to the experimental results. Reproduced from Ref. 5 with permission from The Royal Society of Chemistry.

Fig. 11 The strain-temperature response of the muscle with spring constant C=1.7 has been modeled and compared to the experimental results. Reproduced from Ref. 5 with permission from The Royal Society of Chemistry.
Fig. 12 The strain-stress recovery of the muscle with spring constant $C=1.7$ has been modeled and compared to the experimental results. Reproduced from Ref. 5 with permission from The Royal Society of Chemistry.

Fig. 13 Illustrations of the numerical simulation for three different muscles compared with their experimental results. Reproduced from Ref. 5 with permission from The Royal Society of Chemistry.

### 2.6 Conclusion

Skeletal muscles consist of bundles of twisted polymer fibers in which the integration of their motion enables us to lift loads in horizontal, vertical or even in twisted path. The current study may provide an interesting subject for further analysis in which mechanics of muscle structures can be incorporated into the modeling framework.
Artificial muscles are a new field of smart composite materials that are potentially applicable in different industries such as aerospace, robotic, biomedical, and self-healing [3, 23, 24]. In order to better design polymeric artificial muscles, it is highly desired to develop analytical and numerical models (21). In the current study, twisted and coiled Nylon 6.6 fibers are selected to fabricate an artificial muscle; these fibers are highly cold drawn before twisting. Micro-scale level of these muscles is controlled by engineering and training processes that provide two types of chains: (a) helically oriented chains that maintain a twisted shape in their training process and retrieve it during thermal actuation process; and (b) highly drawn chains that are able to actuate as soon as the muscle is heated up. However they saturate when coil contact temperature is reached.

Most previous modeling efforts in the case of artificial muscles concern different conceptual designs such as SMA or pneumatic muscles. Those models cannot simulate the twisting, coil contact, and transition events in twisted polymer based artificial muscles. The current modeling takes into account both polymer’s nature as well as fabricating and training procedure of the artificial muscle made of polymer fiber. The proposed multiscale model is based on statistical mechanics of polymer chains in which several physical mechanisms are considered to develop the modeling framework.

The actuation response of the muscle is correlated to two basic molecular level deformation mechanisms that are longitudinal shrinkage of polymer chains and radial swelling due to thermal expansion. These micro scale deformation mechanisms are linked to the macroscopic mechanical behavior through averaging techniques where a micro scale RVE is bridged to the macro scale RVE.
The thermal actuation response of the muscle over working temperatures has been scrutinized in the modeling section for both macro- and micro-scale response. Several design parameters such as manufacturing and training events are considered and their effects are coupled into the model.

Two categories of parameters are defined for estimation of the actuation response of the artificial muscle with temperature. Five parameters, viz. Tg, Tc, σc, σg, and C, are imported from experimental data to capture the effect of 1) critical temperature (Tg and Tc), 2) bandwidth for structural change during glass transition and coil contacts (σc and σg), and 3) macroscopic structure (spring index) of the muscle (C). The second categories of parameters, viz. α, β, and γ are numerically defined to estimate the molecular chain’s rotation and expansion above coil contact temperature.

Parameters α and β control the radial and angular deformation of the chains and parameter γ controls the deformation in the z direction. These three parameters, α, β, and γ, are interrelated and provide a good approximation to estimate the effect of temperature on the response of the artificial muscle. Their definition is basically commensurate to the training procedure for the artificial muscle. It is shown that the proposed model is in good agreement with experimental results found in the literature and it provides a design tool for further developments in polymeric artificial muscles. It is noted that the model is quite general. It may serve as a useful design tool for polymeric muscles with similar morphologies, such as Nylon, Polyethylene, shape memory Polyurethane fibers, etc., which are formed by coiling, and triggered by temperature rise.
CHAPTER 3  MULTISCALE MODELING OF DYNAMIC RESPONSE OF SMPF

In this chapter application of Multiscale modeling for evaluating a dynamic thermo-mechanical problem is elucidated. The importance of modeling lies in vast application of SMPF in many industries in which durability of component is a key point. In fact, Health of a structure under vibration loads is highly related to the damping characteristics of the system. This work explores the possibility of engineering a smart Shape Memory Polymer Fibers, SMPF, composite system that is capable of adjusting its damping capabilities based on applied load frequency and temperatures. A SMPF based structure with smart vibration/damping capability is of interest to many industries including aerospace, automotive and biomedical sectors. SMPFs enable structure engineers to incorporate smartness functionality into their design through programming cycles. While SMPF structural applications in the case of static loadings have been studied, the application of SMPFs in mitigating vibration responses of a structure has not been fully addressed in the research arena. The vibration damping response of SMPF material system is studied with a goal to design damping response of smart structures that can mitigate severe vibrations. In this work vibration damping response of a SMPF bundle is experimentally studied through Dynamic Mechanical Analyzer, DMA, machine, and a numerical model is developed to correlate the loss/storage moduli to the damping/stiffness characteristics of the SMPF system. The model is then applied to study forced vibration responses of SMPF. DMA data are utilized to verify the performance of the proposed model. The presented experimental data and the numerical model provide insight into vibration damping application of SMPFs in smart structures.
3.1 Introduction

Shape memory polymers are classified as smart materials that are able to respond to the external stimuli sources such as heat, sound, light, etc. [25-31]. Most recently, Li and co-workers have developed several Shape Memory Polymer Fiber (SMPF) based polymer matrix composite (PMC) systems with capabilities for crack self-healing [32-38]. Whilst most of the up to date studies concern quasi-static response of shape memory polymers, including shape memory polymer fibers and artificial muscles [5, 21, 39-59], there is currently a lack of modeling to addresses vibration analysis of SMPFs.

Vibration analysis enables designers to study stability of the structure when oscillation occurs. Unwanted noises or dissipative vibration mechanisms, resulted from lack of meticulous design of components, may lead to premature failure of structural components, and prognoses and elimination of severe oscillation loads become a cardinal point in structural design. For the past decades, the inception of new technologies such as space exploration programs has provided an increasing need for lightweight materials with high damping capabilities and tolerance to the harsh environments.

The nature of damping lies in microscopic response of material after initiation of vibration. Some media such as polymers have shown strong damping dependencies on temperatures. In fact, the highest level of damping can be obtained around glass transition temperature [60]. At this temperature the chains motions are released and this excessive motion provides a higher damping capability around glass transition temperature. Due to the long range molecular order associated with giant molecules, polymers exhibit rheological behavior between crystalline and liquid like states [61].
Stiffness and damping in polymers are frequency and temperature dependent. Crandall discussed the nature of some important damping mechanisms and an indication is given for how damping phenomenon depends on the amplitude and frequency of the cyclic motion [62].

The modeling techniques have become an essential part of the vibration damping design in order to minimize the experimental trial-and-error efforts for finding the optimum damping characteristics. In retrospect, many scientists have developed modeling approaches for simulating the damping phenomenon. Bagley and Torvik (1983) suggested that damping mechanism resulted from the frequency dependent modulus is a fractional power of frequency. The proposed model depends on five empirical parameters to form the equation of motion with derivative of the fractional order. A major limitation accompanied with this model is the cumbersome computation needed for modeling the viscoelastic behavior [63]. Raid’s non-linear model has been deployed by [64] to study linear hysteretic damping. The Golla-Huges-McTavish (GHM) method has been suggested to formulate the second-order matrix equations of motion. The material properties of viscoelastic materials were defined through mass, stiffness and damping matrices. An auxiliary coordinate was considered to manage the internal dissipation energy of these materials in the frequency domain analysis [62, 65]. The implementation of curve fitting parameters that requires modifications has been reported in the literature [66].

Methodology called augmenting thermodynamic fields (ATF) was basically in close relation to GHM method, in other words, it was a coupled equation of motion demanding the adaptability of the thermodynamic field at each element. Later development on ATF method resulted in application of anelastic displacement field (ADF) with emphasis on the effect on the displacement field. The ADF methodology provided a new approach to develop time-domain finite element models [67, 68].
Engineering material systems with higher damping capabilities is a topic trend in plethora of research. SMPF smart materials are capable of being micro-structurally engineered to damp vibration at different temperature and frequency conditions. This work aims at exploring the possibility of design and development of smart SMPF systems with capabilities of controlling the vibration damping properties. Both experimental tests and numerical modeling analysis are incorporated to fully understand the vibration damping response of SMPFs. Dynamic mechanical analyzer (DMA) tests are utilized to study the complex viscoelastic behavior of SMPFs in which frequency sweep tests are carried out to obtain the storage and loss moduli of SMPF bundles at various temperatures. A phenomenological Single Degree of Freedom (SDOF) model is developed that utilizes the DMA test data for calibration purposes. It is shown that the model can capture the forced vibration damping of SMPF system. The model is capable of correlating micro structural properties of polymer chains to macroscopic vibration/damping.

This work is organized as follows, first the theory behind the force vibration analysis is briefly discussed and then the Single degree of freedom model is described. The experimental setup and test results are presented; afterward multiscale modeling as well as the numerical implementation procedure is provided. The results and discussions are then presented.

### 3.2 Single Degree of Freedom (SDOF) Model for SMPF

The proposed SDOF model for SMPF system is discussed in this section and the performance of the developed model is examined in Section 6 where the reported experimental data, which concern with forced vibration of a SMPF sample under sinusoidal forces, together with the model performance are shown. It is assumed that the vibration response of the SMPF sample is described through a SDOF model. The steady state SDOF equation of motion reads
\[ m\ddot{x} + c\dot{x} + kx = F_0 e^{i\omega t} \]  

where \( m \) is the mass of a vibrating fiber, \( c \) is the coefficient of damping, \( k \) is the stiffness of SMPF sample, and \( F_0 \) is the amplitude of the applied force. Steady state response of the linear system to the harmonic force could be expressed through definition of a transfer function \( H(t) \) and a corresponding phase angle which is well-established in the literature and is given by [69].

\[ x(t) = \frac{F_0}{k} H(\omega) e^{i(\omega t - \phi)} \]  

where \( \omega \) is the frequency, \( H(\omega) \) is called transfer function or magnification factor, and \( \phi \) is the phase lag.

\[ \phi = \tan^{-1}\left(\frac{2\zeta r}{1 - r^2}\right) \]  

\[ H(\omega) = \frac{1}{\sqrt{(1-r^2)^2 + (2\zeta r)^2}} \]  

\[ \zeta = \left(\frac{c_s}{c_c}\right) \] is loss factor, \( c_c = 2m\omega_n \) is the critical damping, \( r = \frac{\omega}{\omega_n} \) is the ratio of the frequency over natural frequency.

The SMPF system differs from conventional materials in several aspects including (i) glass transition event can also change the stiffness and damping specs of the SMPF system, (ii) due to molecular chain rearrangements, the stiffness and damping properties of SMPF system vary with temperature and frequency, and (iii) SMPF system can be programmed to respond to external stimuli at specific temperature, i.e., strain or stress recovery at the transition temperature. Thus, upon transient recovery events of SMPF the stiffness and damping properties are changed and the SDOF solution should be able to take into account the programming history effect on stiffness and damping properties. In this paper the effect of glass transition event and temperature and frequency effects on the vibration damping of SMPF system is studied.
Although the proposed methodology can easily handle the programming history, due to lack of experimental data the effect of shape recovery on damping response of SMPF will be reported in a forthcoming paper by the authors where the DMA test data for programmed SMPF system will be utilized to verify the simulations. For studying the vibration damping of SMPF sample, it is assumed that the mass of the system is constant. In order to address the temperature and frequency dependence, the coefficient of damping $c$ and stiffness $k$ are formulated systematically in the following. It is trivial to relate the stiffness $k$ of the SMPF system to the storage modulus $E'$ and the damping coefficient $c$ to the fraction of the loss modulus $E''$ through experiments. Based on our simulation results, we have found that the classical stiffness-tensile modulus correlation provides a good relationship, if the dynamic storage modulus is used instead of Young modulus

$$k = \frac{E' A}{L}$$

(5)

where $A$ and $L$ are area and length of the SMPF sample. In the case of the underdamp systems with $\xi < 1$, the relationship between the damping coefficient $c$ and loss modulus $E''$ reads

$$c = c_c \times \frac{E'}{E}$$

(6)

Where $c_c = 2m\omega_n$ is critical damping which is a factor of natural frequency of a system, and $\omega_n = \sqrt{\frac{k}{m}}$ depends on stiffness and mass of an oscillatory system. The performance of Eqs.(5) and (6) are examined in Section 6, where these relations are utilized to study the forced vibration responses of SMPF system. The next step is to formulate the temperature and frequency dependent $k$ and $c$. In order to fulfill this task the temperature and frequency dependent $E'$ and $E''$ functions are formulated and Eqs. (5) and (6) are utilized to find the
temperature and frequency dependence of $k$ and $c$. With this strategy the frequency and temperature DMA sweep tests can be incorporated to calibrate the temperature and frequency effects.

One may note that $E'$ and $E''$ are strong functions of temperature and they change drastically near glass transition $T_g$. To include the temperature effect in the model the following linear relations are utilized

$$E_T' = \begin{cases} E_{EGT}' - m_1(T - (T_g + \sigma_g)) & \text{if } T < (T_g + \sigma_g) \\ E_{EGT}' - m_2(T - T_h) & \text{if } T > (T_g + \sigma_g) \end{cases}$$

(7)

$$m_1 = \frac{(E_{0T}' - E_{EGT}')}{\sigma_g}, m_2 = \frac{(E_{EGT}' - E_{hT}')}{(T_h - T_g)}$$

$$E_T'' = \begin{cases} E_{EGT}'' - n_1(T - (T_g + \sigma_g)) & \text{if } T < (T_g + \sigma_g) \\ E_{hT}'' - n_2(T - T_h) & \text{if } T > (T_g + \sigma_g) \end{cases}$$

(8)

$$n_1 = \frac{(E_{0T}'' - E_{EGT}'')}{\sigma_g}, \text{ and } n_2 = \frac{(E_{EGT}'' - E_{hT}'')}{(T_h - T_g)}$$

where $E_{0T}'$, and $E_{0T}''$, are respectively storage modulus and loss modulus at room temperature (below $T_g$), $E_{EGT}'$, and $E_{EGT}''$ are respectively storage modulus and loss modulus at the end of transition event and $E_{hT}'$, $E_{hT}''$ are storage modulus and loss modulus at high temperature (above $T_g$), respectively, and $T_g$ and $\sigma_g$ are respectively glass transition and half of bandwidth of the transition event. Coefficients $m_1$, $m_2$, $n_1$, and $n_2$, which are all obtained directly from DMA test data, correspond to the load carrying and damping capabilities of the SMPF sample. To include the frequency effects on the loss and storage moduli, the two following relations are developed to capture frequency dependent response

$$E'_f = E'_{1f} f^\beta$$

(9)

$$E'_f = E'_{0f} (f - f_E)' + E''_{0f} (f)' - E''_{0f}$$

(10)
where $E''_0$ is the loss modulus at low frequencies, $f_E$, is the upper limit of the frequency response and $\gamma$ corresponds to the loss factor, viz. $\tan\delta$, at the highest frequency available in a set of experiment; $E'_{1f}$ is the storage modulus at median frequency in a set of experiment, and $\beta$ is the corresponding loss factor at frequency $\beta$. It is worth noting that all parameters in Eqs. (7) - (10) are directly obtained from the DMA test results. Eventually, the temperature and frequency dependent storage and loss moduli of the SMPF system can be expressed as

$$E' = E'_f \times E'_T$$
$$E'' = E''_f \times E''_T$$

(11) (12)

3.3 Experimental Protocol and DMA procedure

The isothermal strain controlled frequency sweep tests were conducted, using DMA Q800 TA instruments, for two SMPF samples. Dynamic mechanical testing was used to characterize the dynamic responses of SMPF at controlled frequencies (0.01Hz-100Hz) for two temperatures, 25 and 50°C. Storage modulus, loss modulus, $\tan\delta$, displacement were measured at each frequency. The specimens were in the form of bundles of SMPF, and each bundle contained one hundred filaments and were fixed together by a fixture. The length of the specimen ranged from 10 mm to 11 mm. The cross-section is $2.25 \times 10^{-4}$ cm$^2$. The length and diameter of the samples were measured separately.

Step time is the time during a particular step at which the measurement was completely calculated. After passing this time, the macromolecule reach to a state of dynamic equilibrium in which output data are recorded. The step time depends upon temperature, composition and frequency of the applied loading. Oscillation force is an output parameter from DMA that indicates the maximum force due to the applied oscillation. A static force, preload, is applied at the beginning of the test to avoid fiber buckling during the tests.
3.4 Multiscale Analysis and Modeling Terminology

Polymers are materials made of very long intervened chains which are chemically or physically cross-linked at different points. In the case of Shape Memory Polymers, these points are called net points and some desired properties could be tailored to these materials through these points.

Chain segmental motion and side molecules rotation are dominant mechanisms of damping for polymers at glass transition temperature which provides maximum damping capability at this region. At glassy state chain conformational rotations are frozen; therefore, polymer molecules have high storage capabilities while the loss modulus is lower than that in the glass transition region. And slightly above this temperature, perturbation of random coils leads to the state of lower entropy, when stress relaxation mechanisms activate in order to absorb energy of vibration and damp vibration effects. The vibration produces dissipative heat in the structure in which the generated heat mainly activates two mechanisms 1) entropy driven force which impels chains to regain their original shape and 2) structural relaxation mechanism due to excessive absorption of heat. Furthermore, the increased mobility of chains may lead to fatigue initiation [70]. At these temperatures, dominant damping mechanism is accumulation of dissipative deformation mechanisms of chains.

The SMPF in the microscopic scale consist of soft and hard domains [23]. Soft phase is polybutylene adipate (PBA) and 4’4-diphenylmethane diisocyanate (MDI) and 1, 4-butanediol (BDO) as hard segment. The glass transition of soft phase is around -55oC and hard phase is observed around 110oC. However, Glass transition temperature of mix phases is 25°C which is basis of our analysis and half of the duration of this event is also 25°C.
Soft phase is made of a number of randomly distributed chains while hard phase consists of highly oriented polymer chains, semi-crystalline phase; this phase acts as a stiffener in the macromolecule which connects chains of soft phase and strengthens the SMPF. Amorphous chains respond elastically before glass transition event. At glass transition event, the mobility of chains is increased and their ability to absorb energy is elevated as well. Upon further heating, the mobility of chains keeps increasing and the applied heat is consumed by the structural relaxation mechanisms. At elevated frequencies and at higher molecular mobility the fatigue damage may happen between highly mobile soft chains and rigid hard phase as well as inside the hard phase that may result in chain break and melting.

3.5 Numerical Approach

To solve the equation of motion Runge-Kutta approach is adopted in this work. Runge-Kutta methodology provides higher degree of precision than typical Euler approach to solve second order differential equations. The fourth order Runge-Kutta is applied to obtain the time domain representation of the equation of motion. Typical algorithm for finding the solution for first order ODE’s contains four auxiliary quantities which should be calculated at each step and then the new value for the function should be updated based on these quantities [71]. The numerical procedure to obtain the stiffness and damping and to calculate the resulted displacement is given as follows

1- Input \( F, \omega \)

2- Calculate \( E' \) and \( E'' \) from Eqs. (7) and (8)

3- Calculate stiffness and damping from Eqs. (5) and (6)

4- Replace \( k \) and \( c \) to the Eq.(1)

5- Compute \( x(t) \) from Eqs. (2), (3) and (4)
6- Compute error, e, between $x(t)$ from Step (4) and experiments

7- Modify $k$ by $k_{i+1} = k_i \times (1 + e)$ where $k_i$ is the latest stiffness quantity

8- Go to the steps 4, 5, and then 6

9- If the error $e < 5\%$ then Go to Step12

10- If the error between modeling and experiment is higher than $5\%$ GO TO Step 11

11- Replace $c$ by $c_{i+1} = c_i \times (1 + e)$ where $c_i$ is the latest damping coefficient

12- Compute $x(t)$ and compare with experimental results

13- Display $c$ and $k$

The optimization process which is part of numerical steps is crucial specially for frequencies over 60 Hz. The importance of this step is to reduce the error associated with modeling the experimental results related to the storage moduluss and loss modulus in Fig.1 and Fig.2. Once viscous damping coefficient $c$, and stiffness are calculated from experiments and replaced to the equation of motion, the resulting displacement is obtained and shown in Fig.6 as square symbols; the results before optimization process provides an avarage error about 15% which majority of this discrepancy is related to the fact that model’s stiffness and damping coefficient carry errors at higher frequencies. However, through optimization process, step 7, stiffness is modified by incorporating error of calculations. The result of this modification shown in Fig.4 with circles. The corresponding result elucidates that at higher frequencies SMPF is in rubbery flow, i.e. in softenning event; however, model indicates continuous leathery response, i.e. stiffer structure at higher frequencies, which pronounce error in calculations. As a result of error mitigation process, the average error among actual results and simulation outcome reduced to 8%.
The acceptable error margin in majority of typical engineering designs is 5%. The further error is related to the effect of damping coefficient which in reality capability of specimen drops more drastically at high frequencies than calculations. Through step 11, the damping coefficient is modified and associated error is less than 2%.

3.6 Result and Discussion

Model parameters for computing the damping coefficient and stiffness are given in the Table 1. First $E'$ and $E''$ are modeled and their simulation together with the experimental results are plotted in Fig. 1 and Fig. 2 respectively. Then, the values of the damping coefficient, Fig. 4, and stiffness, Fig. 5, are calculated and optimized using displacement results obtained from the experiment. The equation of motion is solved and the displacement at different frequencies before and after parameter optimization is depicted in Fig. 6. Moreover, the natural frequency of the SMPF is estimated using Fig 3.

<table>
<thead>
<tr>
<th>Model’s parameter</th>
<th>$E_{0T}$ (MPa)</th>
<th>$E_{EGT}$ (MPa)</th>
<th>$E_{hT}$ (MPa)</th>
<th>$E_{1f}$ (MPa)</th>
<th>$\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k = \frac{EA}{L}$</td>
<td>3000</td>
<td>2100</td>
<td>20</td>
<td>1900</td>
<td>0.18</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Model’s parameter</th>
<th>$E_{0T}$ (MPa)</th>
<th>$E_{EGT}'$ (MPa)</th>
<th>$E_{hT}'$ (MPa)</th>
<th>$E_{0f}'$ (MPa)</th>
<th>$\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c = 2m \left( \sqrt{\frac{k}{m}} \right) \times \frac{E'}{E''}$</td>
<td>9000</td>
<td>3400</td>
<td>40</td>
<td>2720</td>
<td>0.08</td>
</tr>
</tbody>
</table>

Table 1 summarizes the parameters related to the Equations 5, 6, 7, and 8; they are introduced to calculate stiffness, $k$, and damping, $c$, for the SMPF. The glass transition of the SMPF is 25°C, which has been reported in the literature [23]. The modeling results for storage modulus and loss modulus are shown in Fig. 1 and Fig. 2, respectively.
The results provide an insight into defining the optimal vibration-damping range, which is 7Hz-70Hz. At this range, maximum energy absorption and damping capability are achieved; this energy activates all chains to dissipate energy through entropic elastic mechanism for obtaining random configuration. At frequencies beyond 70Hz, chains absorb energy of vibration to relax their structure. When the frequency of the vibration reaches to 80Hz, increased mobility of chains may lead to the fatigue initiation at the hard domain; illustrated drop in the amount of loss modulus at 100Hz, in particular for SMPF tested at temperature of 50°C, may be an outcome of this phenomena.

![Storage Modulus (E') changing by Frequency & Temperature](image)

Figure 10 Variation of the storage modulus vs. temperature and frequency. Damping capability of SMPFs can be tailored by changing the working temperature as well as cold strain and hot programming, which will be discussed in our next paper. Test at a higher temperature, 50°C, are also shown in Fig. 1 and Fig. 2. At this temperature, chains are more softened and they tend to relax faster. The overall 40% drop for storage capability as
depicted in Fig. 1 is its ramification. This implies that less than half of chains are saturated at higher temperatures. However, as illustrated in Fig. 2, SMPF shows 20% drop in loss modulus for frequencies lower than 1Hz. It shows pronounced effects at frequencies over 1Hz. This excessive drop is related to elevated step time in which chains are able to absorb heat and soften; as a result, the highest amounts of saturated chains are obtained.

For both samples at higher frequencies, relaxation time is shorter and chains are at stiffer state compared to the lower frequencies. However, the increased internal friction among them results in the initiation of rubbery flow state and may lead to the inception of fatigue in the hard domain as well. In other words, at higher frequencies chains should move faster in order to respond to the imposed frequency. Therefore, chains behave as if they are instigated at higher temperatures; hence, activation of structural relaxation phenomenon results in 40% increase in overall loss factor for sample at higher temperature which is depicted in Fig. 3.

Figure 11 Effect of temperature and frequency on loss modulus of SMPF
Loss factor vs. log frequency shown in Fig. 3 offers an interesting property related to the observed peak for this plot; the peak damping of tanδ occurs at natural frequency of the material which is a function of temperature [60]. Energy of vibration is usually dissipated in the form of heat. Loss factor is defined as the ratio of the imaginary part to the real part of modulus in the frequency domain analysis. However, this concept is equivalent to the energy dissipated per cycle to the energy stored in the material. When the loss factor, i.e., loss tangent plots logarithmically over the span of the frequency sweep test, it illustrates the rate of decay for the amplitude of vibration. At natural frequency, this rate is higher than other frequencies.

Every continuum matter has multiple modes of frequencies that can be a function of temperature and geometry of the specimen. SMPF is a continuum polymer solid which can vibrate at a series of distinct frequencies called natural modes, i.e., transition modes. At 50 °C, SMPF tends to damp energy of vibration strongly and therefore at least two major peaks is identified with which natural frequency of some segments of the polymer’s chain are met (0.063Hz and 6.3Hz). At these frequencies, most energy of vibration is damped by the chains; in fact, at higher temperatures, chains rearrangement, which translates the microstructure into a more ordered structure, i.e., crystallite, is triggered. Indication of this transition is shown as a pick in Fig. 3. There is no any evidence of transition event at the glass transition temperature.

In the free vibration analysis, the ratio of decay of amplitude of vibration is defined as logarithmic decrement, Δ, which is a measure of energy dissipation in the time domain analysis.

\[ \Delta = \frac{1}{n} \log \left( \frac{x_i}{x_{i+1}} \right) \]

where \( n \) is the number of cycles and \( T \) is period of vibration. The relation between loss factor i.e. \( \tan \delta \) and logarithmic decrement is given[72]:

\[ \tan \delta = \frac{\Delta}{\pi \left( 1 + \frac{\Delta^2}{4\pi^2} \right)} \]  \hspace{1cm} (13)
At lower vibration decay, $\Delta^2$ is negligible; therefore, one may conclude $\Delta = \pi \tan \delta$. As a result, the higher the tan delta, the greater the damping coefficient, the more efficient the material will be in effectively accomplishing energy absorption and dispersal. Consequently, the lower amplitude of vibration will be.

![Loss factor changing by Frequency & Temperature](image)

**Figure 12** Change of tan$\delta$ with temperature and frequency

The model parameters, damping coefficient and stiffness, have been obtained from the proposed model (shown in Fig. 1 and Fig. 2), and the equation of motion has been solved and their values have been calibrated using the displacement from the experiment. The corresponding error is obtained and incorporated to the model to modify the values of the stiffness and damping. Damping and stiffness quantities at different frequencies are calculated and reported. The results of the numerical optimization process as well as original simulation results are shown in Fig. 4 and Fig. 5. From them, it is seen that the modeling framework has minor errors for the whole range of frequencies.
Figure 13 Damping coefficient at different frequencies at 25 °C

Figure 14 Stiffness change with frequency at 25 °C
Stiffness and damping quantities obtained from Figs. 4 and 5 are used to solve the equation of the motion. The corresponding results are compared with experimental results. The displacement simulated with the parameter optimization tuned model, together with experimental results, is shown in Fig. 6. Clearly, the model can reproduce the test results with parameter optimizations. The least square methodology have been employed to evaluate the amount of associated error in the modeling technique.

Figure 15 Displacement with and without error mitigation
3.7 Conclusion

SMPF smart materials are capable of being micro-structurally engineered to isolate vibration at different temperature and frequency conditions. The smartness functionality offers the adjustment between inherent properties of these materials with their industrial applications through modeling techniques. Vibration analysis enables designers to study stability of the structure when oscillation occurs. Free vibration and forced vibration are two main categories of vibration analysis. The vibration testing provides a means to understand the real world’s response of the structure. The modeling techniques used in the vibration analysis introduce a simple way to evaluate and pinpoint faulty elements in structures.

The analogy between loss modulus with damping coefficient and storage modulus with material stiffness for a SDOF system is made to develop a numerical approach for obtaining damping and stiffness property of the SMPF theoretically.

The vibration damping mechanism of SMPF material system is studied with a view to design damping response of smart structures that can mitigate severe vibrations. The presented experimental data and the numerical model provide an insight into vibration damping application of SMPFs in smart structures. The damping capability changes with temperature and frequency. Higher frequencies activate more segments of polymer chains and increase the restoring force viz. entropic force; this force supports chains to obtain their random coil configuration. The higher entropic force results in higher storage modulus. And therefore, highest energy of vibration would be damped. At this optimum range both storage and loss moduli are at their apex which can be opted as a design range. For the present sample frequencies between (7Hz-70Hz) provides an optimum design region for a micro scale sample with mutual high damping and storage capability.
At the indicated range samples would have shown stability related to the coincidence of high intrinsic damping and storage capabilities. Moreover, at this region natural frequency of side branches for both samples are beyond. Glass transition temperature can change capability of SMPF to damp energy of vibration which has been shown. This investigation implies that programming of SMPF would result in higher damping capabilities. In fact, programming would result in translation of fundamental frequency of vibration to the higher frequencies as you may check in the response of sample at glass transition temperature with no evidence of meeting resonance frequency of side branches.

At elevated frequencies, when all segments of chains are activated, there is no room for further absorption of energy; at this stage all chains are fully coiled. After the so-called rubbery state, more energetic vibration result in the initiation of flow in soft phase and fatigue in the hard phase. Then, the storage modulus increases due to initiation of the fatigue phenomenon [70]. Main reason for higher capability to store energy is production of hysteresis energy. The main molecular process supporting these phenomena is viscous behavior of diol chains extenders at hard phase which leads to overall softening and losing capability to damp more energy of vibration. At this stage the amount of loss modulus drops noticeably which indicates that chains are softened and saturated.

The modeling technique provides a numerical approach to obtain damping property of SMPF from DMA results. Authors believe that damping coefficient and stiffness of every continuum system under dynamic loading can be obtained using DMA test results in combination with Eqs.(5) and (6). The proposed optimization steps are designed to control error associated in applying modeling techniques.
CHAPTER 4   CONCLUSION AND FUTURE WORK

The studies taken up in this dissertation have developed computationally efficient phenomenological Multiscale constitutive models for static and dynamic thermo-mechanical loadings. Summary and detailed discussions have been carried out at the end of relevant chapters. The purpose of this chapter is to reiterate the main findings, unifying them and to suggest some further research directions.

4.1 Conclusion

In the current study, the Multi scale modeling process initiates from investigating the experimental results in continuum scale and then a phenomenological based model is determined. Then proposed model applied to elicit multi-dimension, micro/macro mechanisms. From this step the knowledge about model translates to the knowledge about the smart materials through methodologies such as averaging method, statistical mechanics to related microscopic evolution principles to the macroscopic response. Two computationally efficient phenomenological Multiscale constitutive models are developed in which several physical properties of these smart materials are incorporated to minimize the trial-and error numerical curve fitting processes. Then proposed multi scale and theoretical models are utilized to build a numerical approach to reproduce the response of the systems.

The proposed Multiscale model is based on statistical mechanics of polymer chains in which several physical mechanisms are considered to develop the modeling framework. Micro scale deformation mechanisms are linked to the macroscopic mechanical behavior through averaging techniques where a micro scale RVE is bridged to the macro scale RVE.
The thermal actuation response of the muscle over working temperatures has been scrutinized in the modeling section for both macro- and micro-scale response. In micro-scale level two types of chains are introduced: (a) helically oriented chains that maintain a twisted shape in their training process and retrieve it during the thermal actuation process; and (b) highly drawn chains that are able to actuate as soon as the muscle is heated up. However they saturate when coil contact temperature is reached. Polymer’s nature as well as fabricating and also training procedure is considered in the multi scale modeling by utilizing statistical mechanics and homogenization concepts.

The Multiscale concept is applied to evaluate vibration-damping response of shape memory polymer fiber to relate experimental response to the microscopic phases, i.e. hard and soft phases. The analogy procedure is applied as a major modeling technique to translate material parameters of SMPF obtained from DMA results to the stiffness and damping coefficients in the equation of motion for a SDOF system. Through this analogy, a general numerical approach is proposed to apply DMA in order to find equivalent stiffness and damping coefficients for any continuum system. Vibration analysis for the SMPF shows that this micro scale fiber is capable of adapting its damping capabilities based on applied load, frequency and temperatures.

The answer to the question, whether conventional modeling techniques are extended to either static loaded system or harmonically excited system In this regard, statistical mechanics based assumption was proposed for polymer based systems. In this dissertation, the concept of Gaussian chain and probability density of its evolution around glass transition temperature is generalized for static thermo-mechanical loading. And classical SDOF dynamic model is solved using damping coefficient and stiffness of material obtain from solution to the conventional SDOF problem.
This result demonstrates that, contrary to the traditional beliefs, the damping property of material can be modeled using DMA results. To answer to the question regarding error associated in modeling, the numerical curve fitting parameters in the case of static modeling and optimization steps for dynamic modeling framework is suggested to reduce error of modeling.

In summary, the work conducted in this dissertation achieves the following:

- A Multiscale model which is implemented numerically using statistical mechanic to design polymer based artificial muscle (chapter 2)
- A Multiscale approach to analysis dynamic response through defining damping and stiffness used in SDOF model from DMA experimental data
- A optimization process to calibrate material parameters used in the dynamic model

4.2 Future Work

The proposed modeling techniques for the artificial muscle introduce 3 curve fitting parameters. The relation between these parameters and micro structure stiffness tensors is not made in the current study. However, these parameters are defined based on averaging technique to relate micro and macro structure; a new series of experiment is recommended to obtain their relation. The proposed modeling techniques can be used to model recovery behavior of the shape memory polymer fiber as well. This modeling technique can be used to simulate unloaded polymer based artificial muscle and a user defined subroutine in ABAQUS using the material parameter is needed to simulate thermal actuation response of the artificial muscle made of a polymer fiber. The proposed modeling technique for finding analogous stiffness and damping coefficients can be applied to any DMA results to obtain equivalent stiffness and damping used in SDOF model.
However, Gaussian distribution function is recommended to replace with a piece-wise temperature dependent function. Hamiltonian principle can be used to generalize the proposed modeling technique for a multiple degree of freedom system. Through this modeling technique, the optimum stability range of frequencies for industrial application is obtained. The outcome of the numerical approach can be imported to the commercial FEA software such as ANSYS or ABAQUS in order to find mode shapes of free vibration analysis. It is recommended to investigate the effect of cold drawing and hot programming in damping and stiffness coefficients of a SDOF model. Suggestion on optimum range for mutual damping and stiffness capability is essential. It is recommended to study the effect of combination of shape memory polymer fiber and artificial muscle in damping severe vibrations at different temperatures.
REFERENCES


VITA

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