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Fatigue Response and Constitutive Behavior Modeling of Poly(ethylene terephthalate) Unreinforced and Nanocomposite Fibers Using Genetic Neural Networks

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Abstract

The constitutive behavior of poly(ethylene terephthalate) (PET) unreinforced (control) and PET fibers reinforced with 5 wt% vapor-grown carbon nanofibers (VGCNFs) under uniaxial tension and subsequent to fatigue loading has been evaluated utilizing various analytical models. Two types of fatigue tests were performed: (1) Long cycle fatigue at 50 Hz (glassy fatigue) to evaluate fatigue resistance and (2) fatigue at 5 Hz (rubbery fatigue) to evaluate residual strength performance. The long cycle fatigue results at 50 Hz indicated that the PET-VGCNF sample exhibited an increased fatigue resistance of almost two orders of magnitude when compared to the PET unreinforced filament. The results of the fatigue tests at 5 Hz indicated that the constitutive response of both the PET control and PET-VGCNF samples changed subsequent to fatigue loading. The large deformation uniaxial constitutive response of the PET and PET-VGCNF fibers was modeled utilizing genetic-algorithm (GA) based training neural networks. The results showed that the large deformation uniaxial tension constitutive behavior of both PET unreinforced and PET-VGCNF samples with and without prior fatigue can be represented with good accuracy utilizing neural networks trained via genetic-based backpropagation algorithms, once the appropriate post-fatigue constitutive behavior is utilized. Experimental data of uniaxial tensile tests and experimental postfatigue constitutive data have been implemented into the networks for adequate training. The fatigue tests were conducted under tension-tension fatigue conditions with variations in the stress ratio (R), maximum stress ($\sigma_{\max}$), number of cycles (N), and the residual creep strain (ϵ_R).

INTRODUCTION

Polymer materials reinforced with nanosized particles such as carbon nanotubes and carbon nanofibers have drawn great interest from scientists and engineers recently due to the promise for enhancements in mechanical performance. Particularly, single filament fibers that are reinforced with nanoparticles could provide great benefits for applications in the automotive, medical, and civil engineering sectors. However, before these materials can be utilized as a replacement for conventional fiber materials, there needs to be a detailed and

systematic study of the fatigue and fracture behavior. Some authors have performed past microscopy investigations on single fibers to ascertain failure modes. Particularly, Hearle [1–3] has performed an extensive mechanical testing and SEM study on various polymeric fibers to determine modes of failure. In addition, the authors in [4–13,42–44] have performed extensive studies on the fracture performance and mechanical behavior of single polymeric filaments. These studies provide a basic understanding of the fatigue behavior of polymeric fibers subjected to fatigue loading.

In terms of quantitative mechanics studies conducted on single polymeric filaments, there has been limited research and investigations. Michielsen [14] has investigated the fracture behavior of larger nylon 66 fibers (900 μm wide and 250 μm depth), where the critical strain energy release rate (G_{Ic}) for highly oriented filaments was 17.8 kJ/m². As a comparison, the critical energy release rate for dry as molded (DAM) low-orientation bulk samples was 3.9 kJ/m², as described in [15]. Michielsen [16] also examined the effects of relative humidity (RH) on the strain energy release rate of nylon 66 fibers, where it was shown that increases in RH engendered a decrease in the initial modulus (E_i) and critical strain energy release rate (G_{Ic}) of the samples. In that study, G_{Ic} varied from 31.3 kJ/m² at 0% RH to 15.6 kJ/m² at 100% RH.

The aforementioned studies are of significant value for evaluation of the fracture behavior of polymeric fibers; however, they do not ascertain the direct effects of fatigue loading and underlying factors that affect the mechanical behavior of a polymeric filament during the fatigue process. The scientific and engineering community could benefit tremendously from a predictive constitutive model that evaluates the stress state of the materials when subjected to fatigue loading. In essence, the constitutive prediction results could be of great utility to researchers and manufacturers that wish to evaluate the effects of fatigue loading parameters on the mechanical behavior and the residual properties of the material subjected to fatigue loading. The genetic neural network evaluation method is rigorous in the sense that vital information about the mechanical testing parameters is correlated with the state of the material at certain points during the fatigue test. In addition, because the genetic algorithm (GA) searches the error space using a population of networks, rather than a single point, it is more efficient at finding an optimal solution to the constitutive law problem [41].

Specifically, in this research, uniaxial tensile experiments and stress controlled fatigue experiments were conducted on PET-VGCNF samples at room temperature to ascertain the effects of cycling on the mechanical behavior. It is understood from the fatigue experiments that cycling under stress-controlled conditions caused cyclic creep to occur in the samples with the retention of a permanent residual strain and a change to the mechanical behavior [16, 17]. Because of the retention of the strains, it is known from the literature on unreinforced PET samples that the molecular orientation changed [18]. Other studies have been conducted to assess the effects of drawing on the molecular orientation in PET samples [19]. The authors noticed that the PET samples retain the molecular orientation below T_g (glassy state), while above T_g , the molecular chains have sufficient energy for relaxation. The extent of drawing polyethylene terephthalate samples below T_g produced some crystallinity as observed from the DSC results. With the inclusion of VGCNFs, the problem of constitutive behavior prediction becomes more complicated. Based on the results from

this research, it was shown that cycling at a low frequency (5 Hz) in the rubbery regime changed the mechanical behavior (constitutive behavior) of the sample. Effects of the mechanical loading parameters and the residual creep strains have been used to assess how the mechanical properties changed based on the following input parameters: maximum stress ($\sigma_{\max}$), stress ratio (R), number of cycles (N), and residual strain (ε_r).

EXPERIMENTAL

Sample Preparation and Mechanical Testing

The PET-VGCNF specimens were prepared and processed at the Georgia Institute of Technology as described in [20] by the Kumar Group. The details of the specimen preparation for the mechanical testing paradigm are provided in [21]. The BOSE® ELectroForce® (ELF) 3200 tensile and fatigue testing machine (Enduratec) was used to conduct the mechanical experiments in uniaxial tension, uniaxial cyclic loading, and dynamic mechanical analysis (DMA). The uniaxial tensile tests were performed at an elongation rate of 10 mm/min and the fatigue tests were conducted at a frequency of 5 Hz. Using the ELF 3200, DMA tests were conducted at various frequencies to determine the response of the phase lag component ($\tan \delta$) and stiffness of the sample as a function of frequency in the range 0.1–100 Hz. The Enduratec has a maximum load of 225 N and a maximum frequency of 400 Hz. A set of low mass grips, Model GRP-TC-DMA450N from BOSE ELectroForce® (Eden Prairie, MN), were used to conduct the mechanical tests. The load cell had a maximum load rating of 2.5 N (250 g) and resolution of ± 10 mg. The ELF 3200 measures displacements via a Capacitec 100 μm displacement transducer (Model HPC-40/4101) used as a feedback for the control loop. All experiments were conducted at room temperature, laboratory air. The typical humidity of the laboratory air was about 50%.

The original diameter of the PET control filaments was $24 \pm 3 \mu\text{m}$ and the diameter of the PET-VGCNF filaments was $25 \pm 2 \mu\text{m}$. These diameters were obtained by laser diffraction using the protocol established according to [22]. For computation of the fracture strength, σ_f , an engineering stress based calculation was used, according to: $\sigma_f = \frac{P_f}{A_0}$. Here, P_f is the load at fracture and A_0 is the original diameter of the fiber.

Genetic Artificial Neural Networks: Background

Neural networks are mathematical models that contain elements similar to that of the human brain. One should refer to Abdi in [23] for a basic explanation of neural networks and their functionality. The concept of genetic training in neural networks extends that of basic training algorithms such that the training process is optimized through a method similar to evolution behavior that occurs in biological systems. Authors in [24–28] have investigated the employment of GA neural networks for mechanical behavior predictions in composite materials. Li et al. [24] have used genetic algorithms for modeling semisolid extrusion of composite tubes and bars, which involved solidification, heat transmission and large plastic deformation. The GA was applied in the optimization design of the technical parameters in the semisolid extrusion processes, where good agreement between the calculated data and the experimental results was achieved. Kemal et al. [25] used GAs to obtain optimal layer

sequences in symmetrically laminated square and rectangular plates. The GA and neural networks successfully predicted the natural frequencies of the composite plates and optimal layered sequences, as compared with results from a finite element model. Aijun et al. [26] utilized neural networks and genetic algorithms for the analysis and prediction of the correlation between CVI processing parameters and actual properties of carbon–carbon composite materials. The authors in [26] used GAs to optimize the input parameters of the model and select perfect combinations of CVI (chemical vapor infiltration) processing parameters. Suresh et al. [27] used particle swarm optimization and GAs to find the optimal geometry and stacking sequence of rotor blades. This system had elastic couplings and satisfied stiffness requirements. They found that both particle swarm optimization schemes and GAs provided close approximations to the experimental results. Abouhamze and Shakeri [28] used GAs for stacking sequence optimization in laminated composites and obtained good results as compared with the experimental results.

In regards to constitutive behavior prediction of materials, there have been researchers that have utilized GAs for the prediction of the mechanical behavior. Early studies by authors in [29, 30] were conducted using GAs for the prediction of the constitutive behavior of materials. Recently, Rao et al. [31] have utilized ANNs and GAs for simulation of the stress–strain response of whisker reinforced ceramic–matrix composite (CMC) materials. The training of the feedforward network was conducted for stress–strain paths of CMCs having various interfacial shear strengths and successful results were obtained, indicating the capability of the network to replicate the results from finite element analysis.

Genetic Artificial Neural Networks: Experimental Methods

Genetic training of an artificial neural network involves optimization of the neural network inputs and network parameters, such as step sizes, momentum values, and number of processing elements in the hidden layer [32]. The main goal of the optimization scheme is to search for the appropriate parameter settings that yield the lowest minimum error (lowest cost function). For GA training, a chromosome represents a solution to the problem of interest. This chromosome represents a collection of the parameters that are optimized, called genes. Because of the complexity of the constitutive law for this problem, a variable length chromosome was utilized to optimize both the input parameters and the network parameters. The genes that were optimized in this problem include the learning rate (for backpropagation problems), the number of elements in the hidden layer of the neural network, the step size, and the neural network inputs.

The process flow for the GA training scheme that was used in this research is shown in Fig. 1.

First, a random population of networks (chromosomes) was created. Each of the networks in this population contained different parameters (input parameters and network parameters). The networks were then trained using backpropagation with momentum or conjugate gradient and evaluated to determine their fitness (see Ref. 33 for description on backpropagation algorithms). In GA training, the fitness corresponds to the lowest mean-squared error (MSE) of all the networks within a corresponding generation. The network weights were saved into a database for later retrieval during testing and production of the

neural network. If the fitness of the networks did not meet the MSE requirement, they were not selected for mutation/reproduction. Proper fitness of the networks and selection can be performed using a variety of techniques, to include roulette, tournament, top percent, best, or random. In the current research, the roulette selection method was utilized. Roulette selection involved selection of networks based on the “survival of the fittest” methodology, in which selection was proportional to the fitness. In roulette selection, unfit networks were not selected for combination and mutation, while the most fit networks were selected for combination and mutation. In GA training, the combination of parameters is performed via crossover, which can either be one-point, two-point, three-point, or n-point crossover. For the current research, one-point crossover was performed. In one-point crossover, a crossover point is randomly selected within a chromosome and is then interchanged with two parent chromosomes at this point to produce two new offspring.

An example of the one-point crossover method using binary data is [32]: Parent 1: 11001|010, Parent 2: 00100|111. Subsequent to the exchange of the parent chromosomes at the crossover point, the following offspring are produced: Offspring 1: 11001|111, Offspring 2: 00100|010. After combination (crossover), mutation occurs in which one or more gene values in a chromosome is/are altered from its initial state. This operation results in new gene value creation, allowing the genetic algorithm to arrive at better solutions than previously possible. Mutation is an imperative step in the genetic search, because it decreases the chance of the network population stagnating at local optima. The mutation operation occurs during evolution according to a user-definable mutation probability. In this research, the mutation probability was set at a low value of 0.01 for optimal results. Other parameters that were optimized during the genetic computations relate to the network parameters themselves, to include the step size, momentum rate, and number of processing elements. Table 1 prescribes the upper and lower bound values for these parameters.

An idealized chromosome for the GA training is shown in Fig. 2, where the variable length was introduced via the network parameters (genes): learning rate, number of hidden PEs, and step size). The schematic in Fig. 2 indicates the two types of chromosomes that were utilized in this research.

The evolutionary process ended once the maximum number of generations was reached. The maximum number of generations was 50 for this research, with a population size of 25 networks (chromosomes) in each generation, which corresponded to 1,250 total networks (chromosomes) that were evaluated for each computational experiment. For each network, the training iterations evolved for 2,000 epochs. Subsequent to the evolution process, the network weights were saved to a *.bst file (best network weights) for later retrieval of the constitutive behavior prediction.

Artificial Neural Network Computations

Neural network simulations were performed on a standard PC with a Pentium M processor at 1.86GHz with 2.00GB of RAM. The Neurosolutions SW (NeuroDimension, Gainesville, FL) package was utilized to model the data. For the GA training, the *Train Genetic* function in Neurosolutions was implemented. For the samples with and without prior fatigue, a total of 43,825 data points were used for computation. From this, 70% were allocated for genetic

training (30,678 points), 15% were allocated for cross-validation (6,574 points), and 15% were allocated for testing the networks (6,574 points). The genes of the network for the constitutive behavior prediction consisted of the 5-input vector space, denoted as:

$$\tilde{X} = \{\sigma_{\max} \ R \ N \ \tilde{\epsilon} \ \epsilon_R\}^T$$

The output parameter was the stress (σ) from the neural network simulation. An example of the ANN architecture for prediction of the mechanical behavior of the fiber samples is shown in Fig. 3.

An initial 5-10-10-1 architecture was utilized, which corresponds to 5 input neurons, 10 hidden neurons in the first hidden layer, 10 hidden neurons in the second hidden layer, and one output variable. In Fig. 3, R represents the stress ratio, defined as:

$$R = \frac{\sigma_{\min}}{\sigma_{\max}}$$

Here, $\sigma_{\min}$ represents the minimum stress during fatigue loading and $\sigma_{\max}$ represents the maximum stress during fatigue loading. For PET control samples, stress ratios of $R = 0$ and $R = 0.333$ were utilized in this study and for the PET-VGCNF samples stress ratios of $R = 0$, $R = 0.333$, and $R = 0.667$ were utilized. Also, in the input vector space, N represents the number of fatigue cycles, ϵ represents the strain in the axial loading direction (ϵ_{zz}), and ϵ_R represents the residual creep strain from the fatigue loading history, and was computed as:

$$\epsilon_R = \xi \left\{ \frac{\sigma_0}{E} + \int_0^t K(t-t') \sigma \sin(\omega t' + \delta) dt' \right\} \quad (1)$$

The form of Eq. 1 is that of a Volterra function, which is normally used to describe the creep behavior of polymeric materials subjected to constant stress loading conditions [18]. In (1), $\sigma \sin(\omega t' + \delta)$ represents the sinusoidal stress (which varies between the min and max stress for this problem and leads the strain by an angle δ), E represents the initial elastic modulus, $K(t-t')$ represents the creep compliance function that evolves over time, and ξ is a factor that denotes the portion of the creep strain evolution that was retained subsequent to fatigue loading. All of the mechanical testing parameters, R , $\sigma_{\max}$, and N were prescribed directly into the Enduratec machine. The parameter ϵ (uniaxial strain) was the result of the uniaxial test and ϵ_R (residual strain) is the function described in (1) that is the result of the fatigue loading test. An example of the strain evolution and retention of residual strain is shown in Fig. 4.

RESULTS AND DISCUSSION

Results from Uniaxial Tensile Tests—No Prior Fatigue

Results from the uniaxial characterization tests indicate that the PET-VGCNF samples with 5 wt% were superior mechanically to the PET control samples. Shown in Figure 5 and Table

2 are results from the uniaxial tensile tests. Two methods were used to obtain the modulus of the samples: the 1% strain method according to [34] and the secant modulus method.

The results indicate that the modulus of the PET-VGCNF samples was more than twice the value of the PET control samples. The fracture strength of the PET-VGCNF samples was also twice the value of the PET control samples. Similar results indicating a superiority in strength from the employment of VGCNFs into polymeric matrices has been proven by the authors in [35]. These authors investigated the mechanical properties of VGCNFs employed in nylon and polypropylene composites and observed great improvements in tensile strength and elastic modulus. We have compared these results to the model by Cox [36]. The Cox model predicts the modulus value of the nanocomposite fiber for ideally oriented VGCNFs as:

$$E_c = V_m E_m + \left[1 - \frac{\tanh \beta}{\beta} \right] V_f E_f \quad (2)$$

Here, V_m represents the matrix volume fraction (96.4% in this case), E_m represents the matrix modulus (6.6 GPa from the experimental results), V_f represents the fiber volume fraction (which is 3.6% based on 5 wt% VGCNFs according to Ref. 37), and E_f represent the VGCNF modulus (240 GPa according to Ref. 38). The factor β is estimated according to the following expression:

$$\beta = \frac{l}{d} \sqrt{\frac{E_m}{(1 + \nu) E_f \times \ln(\pi/4 V_f)}} \quad (3)$$

Here, l represents the VGCNF length, d represents the VGCNF diameter, and ν represents Poisson's ratio of the matrix (taken as 0.37) [39]. According to the Cox model, the matrix modulus is highly dependent upon the aspect ratio (l/d). The authors in [20] have investigated the effect of nanocomposite fiber modulus on the aspect ratio and noticed that the modulus increases with increasing aspect ratio, and then plateaus off to a steady state value. Based on the values stated above, and based on the Cox model results utilizing an aspect ratio greater than 50 (indicates approximate steady state value according to Ref. 20), the nanocomposite fiber modulus was estimated and is shown in Fig. 6. The results in Fig. 6 show the prediction of the modulus as a function of VGCNF aspect ratio (l/d), as well as the average result of the experimental modulus calculated using the 1% strain calculation [34] and the secant modulus calculation. The graph in Fig. 6 shows that the experimental results from the 1% strain modulus and secant modulus of the PET-VGCNF fibers were in the range of values for that predicted by the Cox model for fibers. Nanocomposite moduli predictions were computed for PET matrices containing VGCNF with moduli in the range 150–240 GPa. This range of values was utilized because there was more than likely a statistical distribution of aspect ratios (l/d) for VGCNFs that existed in the samples. The authors in [38] have reported that the modulus of VGCNFs is 240 GPa, and this modulus curve has been displayed as well. The overall goal of Fig. 6 is to indicate that the experimental results

obtained from this study agree well with results predicted from the Cox model when typical values for the modulus of the VGCNFs are implemented into the model.

Results from Fatigue—Fatigue in the Viscoelastic/Glassy Regime

Fatigue tests were conducted on the PET control and PET-VGCNF fibers at 50 Hz to determine the fatigue resistance above the rubbery threshold. These fatigue tests were conducted at 60% of the maximum fatigue stress of the respective samples, with $R = 0$.

The results in Fig. 7 indicate that the PET-VGCNF 5 wt% samples outperformed their respective unreinforced counterparts for almost two orders of magnitude more cycles at 50 Hz. There was significantly more scatter in the number of cycles to failure data for the PET control samples, as shown in Fig. 7. These data represent the results from 7 samples tested under uniaxial fatigue conditions at 50 Hz. Four PET samples and three PET-VGCNF samples were tested to determine the average number of cycles to failure (N_f) value. These were lengthy experiments that took several weeks to complete due to the millions of cyclic iterations required for testing (i.e. 50E6 cycles @ 50 Hz requires 11.6 days of testing). These results are significant in the fact that one notices that PET-VGCNF fibers tested above the glass transition frequency were noticeably more resistant to failure than their PET unreinforced counterparts, even when tested at a higher stress ($\sigma_{\max} = 300$ MPa for PET-VGCNF samples and $\sigma_{\max} = 170$ MPa for the PET control samples).

Results from Fatigue—ANN Training and Testing Results

The computational training procedures were run two times and the results were averaged to obtain the stress–strain response of the materials with and without prior fatigue (these two trials required several hours of computation each). The two training procedures represent different randomized data trials. The results from the conjugate gradient, GA training procedure are shown in Table 3. Results of the mean-squared error (MSE) were fairly low, with an average value of 0.00863 for the two runs. On average, the minimum MSE was reached between 3 and 4 generations. The testing results, which were obtained on stress values not previously exposed to the neural network set, displayed mixed results, where the average correlation coefficient (r) for the two trials was 0.9269. To delineate the agreement of the testing results, the experimental stress values (actual) vs. the computational (predicted) stress values are shown in Figs. 8 and 9. The R^2 value for Trial 1 was 0.8895 and the R^2 value for Trial 2 was 0.8297. The results from Fig. 8 show a very good correlation to the predicted stress output signal; however, from Fig. 9 one observes that the model exhibits a poor correlation of the experimental stress vs. the predicted stress.

In addition to the results from the testing and training procedures, a sensitivity analysis was performed on the networks in Trials 1 and 2 to determine the effect of each input variable on the output (stress) signal. The results of this sensitivity analysis are shown in Fig. 10. To conduct the sensitivity analysis, each individual input signal was varied while the other inputs remained constant. This was done in an effort to determine the change in the output signal (“sensitivity”) with respect to the variation of the input signal. It is seen from Fig. 10 that the number of cycles (N) was the least important parameter in affecting the stress output. Intuitively, the strain (ϵ) showed the strongest correlation to the output stress signal.

Surprisingly, the residual creep strain parameter (ϵ_R) exhibited the second lowest sensitivity. However, it is known from the experimental results and residual property predictions [16, 17] that the postfatigue mechanical behavior of both PET and PET-VGCNF fiber samples is a strong function of ϵ_R . The graphical results in Fig. 11 that illustrate example stress–strain responses of the samples before and subsequent to fatigue loading exhibit results that correlate with the results in Figs. 8 and 9. From Fig. 11, it is shown that the GA-based ANN trained via conjugate gradient procedures was somewhat efficient at representing the unfatigued response of the materials. In contrast, the GA based ANN trained via backpropagation was not successful at representing the unfatigued constitutive behavior of the samples, as it displayed a distinct overshoot of the yield point. Neither procedure (conjugate gradient or backpropagation) was effective at capturing the postfatigue constitutive response of the materials. Thus it was decided that the network should be modified to accommodate for the exclusion of the input variable N from the input vector set, and implement a new constitutive law to accurately reflect the postfatigue linear elastic strain hardening constitutive behavior, which will be discussed in the next section. From Fig. 11, one can see the gradual decreases in the hardening behavior with the further accretion of residual strain, as well as an abrupt change in slope subsequent to yield. This has been quantified and discussed in Refs. 39, 40.

Results for Prediction of Postfatigue Constitutive Response—Piecewise Linear Elastic Strain Hardening Law

The testing results from Section 3.3 indicate that a different approach was necessary for the successful modeling of the constitutive response of the materials subsequent to fatigue loading. From the experimental results, it is known that the postfatigue stress–strain response of the materials is linear-elastic, strain hardening with a clearly defined yield point. Thus it can be stated that the postfatigue constitutive response is non-differentiable at ϵ_Y . The mathematical statement that expresses this discontinuity in the constitutive response at the yield point (ϵ_Y) is:

$$f'(x) = \lim_{h \rightarrow 0} \frac{f(\epsilon_Y + h) - f(\epsilon_Y)}{h} \text{ is nonexistent}$$

is nonexistent Because of this discontinuity, an open-form solution was utilized to capture the stress–strain response, and the GA neural network was retrained to determine the correct response. The open-form mathematical relationship that appositely describes this piecewise constitutive behavior is:

$$\begin{aligned} \tilde{\sigma} &= \tilde{\sigma}(\tilde{X}) \\ &= \begin{cases} E(\tilde{X})\epsilon & \epsilon < \epsilon_Y \\ E(\tilde{X})\epsilon_Y(\tilde{X}) + H(\tilde{X})[\epsilon - \epsilon_Y(\tilde{X})] & \epsilon \geq \epsilon_Y \end{cases} \end{aligned} \quad (3)$$

In (3), $E(\tilde{X})$, $\varepsilon_Y(\tilde{X})$, and $H(\tilde{X})$ represent the modulus, yield strain, and hardening modulus as a function of the input mechanical testing parameters. Thus, the task was to determine the three functions (modulus, yield strain, and hardening modulus) as a function of the input vector space using the GA neural networks.

The ANNs were retrained using a GA backpropagation with momentum procedure. Figures 12–14 indicate the capability of the network to minimize the MSE cost function over the number of network generations. In total, nine trials were run to determine the mechanical properties stated in Eq. 3 (three trials for $E(\tilde{X})$, three trials for $\varepsilon_Y(\tilde{X})$, and three trials for $H(\tilde{X})$). After the networks were trained using the GA procedure, the best network weights were saved into a database and used to predict the specified mechanical properties. Figures 15–17 indicate the good capability of the GA-based procedure in estimating the mechanical properties specified in Eq. 3. From the figures, it is observed that good correlation was obtained for prediction of $H(\tilde{X})$, $\varepsilon_Y(\tilde{X})$, and $E(\tilde{X})$, where R^2 values of 0.856, 0.851, and 0.956 were obtained, respectively.

Once the models were obtained for prediction of the mechanical properties using the linear elastic, strain hardening constitutive law of Equation 3, the material behavior of the materials was again plotted to illustrate the effectiveness of the new approach. These results are displayed in Fig. 18.

The results in Fig. 18 indicate that the GA neural network procedure was efficient at capturing the constitutive response, indicating the applicability of the open-form constitutive law outlined in Eq. 3. The predicted parameters $H(\tilde{X})$, $\varepsilon_Y(\tilde{X})$, and $E(\tilde{X})$ were used as inputs into the equation and plotted against the experimental results. Because of the piecewise behavior of the post-fatigue response of both PET and PET-VGCNF samples, the open-form law was efficient at capturing the material behavior. From Fig. 18, some of the samples show a slight overshoot at the yield point of the material ($\varepsilon_Y(\tilde{X})$); however, the model was not efficient at capturing this behavior. This load drop behavior at the yield point has been qualitatively associated with an intrinsic yield process and/or decrease in the cross-sectional area of the specimen (necking) [40]. Thus an improvement to the model would be to ascertain and quantify the overshoot and dip at the yield point, $\varepsilon_Y(\tilde{X})$, and include in the GA based neural network model.

CONCLUSIONS

Fatigue experiments were conducted on PET control and PET-VGCNF samples to determine the response of the materials. For both PET control and PET-VGCNF samples conducted at 50 Hz, the results indicate that the fatigue resistance of the PET-VGCNF samples is ~2 orders of magnitude higher than their unreinforced counterparts, indicating superiority of the PET-VGCNF fatigue properties in the glassy regime. For tests conducted at 5 Hz, residual strength tests were performed to ascertain the change in material properties and constitutive behavior subsequent to fatigue loading. GA-based artificial neural networks (ANNs) were used to model the constitutive response of both PET control and PET-VGCNF samples with and without prior fatigue. The GA-based ANNs were successful at replicating the constitutive behavior of samples without prior fatigue, due to the nonlinearity and continuity

of the stress–strain curve. Since the ANNs tended to generate continuous and differentiable functions, their applicability to the prediction of the large deformation constitutive behavior of both PET and PET-VGCNF samples under uniaxial loading conditions is sufficient. However, for samples with prior fatigue, an open-form solution was necessary to capture the stress–strain response of the materials, due to the nondifferentiable behavior at ϵ_y . On the basis of the neural network testing results, the GA-based ANNs were not successful at representing the postfatigue response of the materials. A piecewise linear elastic strain hardening model was implemented for the material behavior, where the GA-based ANN was utilized to predict the key parameters: elastic modulus, yield strain, hardening modulus. Utilizing this method, good results were achieved for the model of the postfatigue stress–strain response. This work is significant in the sense that both computational researchers and experimental scientists and engineers can benefit from understanding the employment of neural networks applied to unreinforced polymeric and nanocomposite material behavior. In addition, the work is of great utility to researchers in the area of health monitoring of unreinforced and nanocomposite materials subjected to fatigue loading where instantaneous and vital material information is relayed to the system.

References

1. Hearle JWS, Prakash R, Wilding MA. *Polymer*. 1987; 28:441.
2. Hearle JWS, Simmens SC. *Polymer*. 1973; 14:273.
3. Hearle, JWS., Lomas, B., Cooke, WD. *Atlas of Fibre Fracture and Damage to Textiles*. 2. CRC Press; Boca Raton: 1998.
4. Lechat C, Bunsell AR, Davies P, Piant A. *J Mater Sci*. 2006; 41:1745.
5. Colomban P, Marcellan A, Bunsell AR, Piques R. *J Mater Sci*. 2003; 38:2123.
6. Nasri L, Lallam A, Bunsell AR. Fatigue failure in technical polyamide 66 fibers. *Textile Research Journal*. May; 2001 71(5):459–466.
7. Oudet C, Bunsell AR. *J Mater Sci*. 1987; 22(12):4292.
8. Veve JC, Bunsell AR, Baillie C, Hagege R. *Kautschuk und Gummi Kunststoffe*. 1987; 40(10):941.
9. Bunsell AR, Oudet C, Veve JC. *J Mater Sci Lett*. 1986; 5(11):1101.
10. Bunsell AR, Oudet C, Veve JC, Hagege R, Sotton M. *Plast Rubber Inst*. 1985; 63:1.
11. Oudet C Ecole des Mines de Paris, Cent des Materiaux, Evry, Fr, Bunsell AR, Hagege R, Sotton M. *J Appl Polym Sci*. 1984; 29(12):4363.
12. Fuwa M, Bunsell AR, Harris B. *J Mater Sci*. 1975; 10(12):2062.
13. Bunsell AR, Hearle JWS. *J Appl Polym Sci*. 1974; 18(1):267.
14. Michielsen S. *J Mater Sci Lett*. 1992; 11:982.
15. Adams GC, Bender RG, Crouch BA, Williams JG. *Polym Eng Sci*. 1990; 30(4):241.
16. Averett R, Realff ML, Jacob K, Kumar S. *Compos Part A: Appl Sci Manufact*. 2009; 40(6–7):709.
17. Averett R, Realff ML, Jacob K. *Compos: Part A*. 2010; 41:331.
18. Ward, I., Hadley, DW. *An Introduction to the Mechanical Properties of Solid Polymers*. Wiley; West Sussex: 1993. p. 348
19. Lu XF, Hay JN. *Polymer*. 2001; 42:8055.
20. Ma H, et al. *Compos Sci Technol*. 2003; 63(11):1617.
21. Averett RD, et al. *Compos Sci Technol*. 2006; 66(11–12):1671.
22. Perry AJ, Ineichen B, Eliasson B. *J Mater Sci*. 1974; 9(8):376.
23. Herve A. *J Biol Syst*. 1994; 2(3):247.
24. Li HJ, Qi LH, Han HM, Guo LJ. *J Mater Proc Technol*. 2004; 151:126.
25. Kemal Apalak M, Yildirim M. *Compos Sci Technol*. 2008; 68(2):537.

26. Aijun L, Hejun L, Kezhi L, Zhengbing G. *Acta Materialia*. 2004; 52(2):299.
27. Suresh S, Sujit PB, Rao AK. *Compos Struct*. 2007; 81(4):598.
28. Abouhamze M, Shakeri M. *Compos Struct*. 2007; 81(2):253.
29. Feng XT, Yang C. *Comput Methods Appl Mech Eng*. 2001; 190(45):5957.
30. Pal S, Wathugala GW, Kundu S. *Comput Geotechnics*. 1996; 19(4):325.
31. Sudarsana Rao H, Ghorpade VG, Mukherjee A. *Comput Struct*. 2006; 84(5–6):330.
32. NeuroSolutions Software. Copyright 2006. NeuroDimension, Inc; Available at: <http://www.neurosolutions.com/products/ns/>
33. Werbos, PJ. PhD Dissertation. Applied Mathematics, Harvard University; Boston, MA: 1974. Beyond regression: new tools for prediction and analysis in the behavioral sciences.
34. Dowling, NE. *Mechanical Behavior of Materials: Engineering Methods for Deformation, Fracture, and Fatigue*, 2/E. Upper Saddle River, New Jersey: Prentice Hall; 1999.
35. Tibbetts GG, McHugh JJ. *J Mater Res*. 7; 14:1999.
36. Cox HL. *Brit J Appl Phys*. 1982; 3:72.
37. Ma H, et al. *Compos Sci Technol*. 2003; 63(11):1617.
38. Tibbetts, GG. *Carbon Fibers Filaments and Composites*. Vol. 73. The Netherlands: Kluwer Academic Publishers; 1990.
39. Ward IM. *J Macromol Sci Phys*. 1967; 1(4):667.
40. Brown N, Ward IM. *J Polym Sci A2*. 1968; 6:607.
41. Byungjoo Y, Holmes DJ, Langholz G, Kandel A. *Inform Sci*. 1994; 76(1–2):67.
42. Raju, IS., Newman, JC. Stress intensity factors for circumferential cracks in pipes and rods under tension and bending loads. In: Underwood, JH, Chait, R, Smith, CW, Wilhelm, DP, Andrews, WA., Newman, JC., editors. *Fracture Mechanics*. Vol. 17. Philadelphia: American Society for Testing and Materials (ASTM STP 905); 1986. p. 789
43. Griffith AA. *Philos Transact, Series A*. 1920; 221:163.
44. Michielsen S. *J Appl Polym Sci*. 1994; 52:1081.

FIG. 1.
Process flow for genetic algorithm (GA) training.

FIG. 2. Depiction of chromosome length for GA training to predict constitutive behavior: (a) postfatigue (b) no prior fatigue. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 3. Schematic of ANN architecture used in this study for prediction of constitutive behavior of the PET-VGCNF samples subsequent to fatigue.

FIG. 4.

Example strain amplitude vs. time for specimen that underwent 5,000 cycles illustrating the creep evolution and retention of strain [39]. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 5.

Stress–strain curve results from uniaxial tensile tests on PET control and PET-VGCNF samples. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 6.

Cox model prediction of the elastic modulus as a function of aspect ratio. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 7. Results from fatigue tests at 50 Hz indicating the superior fatigue properties of the PET-VGCNF samples in the viscoelastic/glassy state. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 8.

Randomized trial 1: Experimental stress (actual) vs. predicted stress from GA ANN for constitutive behavior prediction of samples representing good correlation. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 9.

Randomized trial 2: Experimental stress vs. predicted stress from GA ANN for constitutive behavior prediction of samples representing overestimation of the predicted stress (poor correlation). [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 10. ANN genetic sensitivity analysis of the input parameters for prediction of the constitutive behavior of PET-VGCNF samples. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 11.

Results from Trials 1 and 2 from ANN genetic neural networks used to predict unfatigued and postfatigue constitutive response of PET and PET-VGCNF fibers. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 12. MSE vs. generation for three genetic ANN trials: hardening modulus ($H(X)$) prediction. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 13. MSE vs. generation for three genetic ANN trials: yield strain ($\Sigma y(X)$) prediction of PET and PET-VGCNF fibers. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 14.

MSE vs. generation for three genetic ANN trials: elastic modulus ($E(X)$) prediction of PET and PET-VGCNF fibers. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 15. Actual vs. genetic ANN predicted hardening modulus ($H(X)$) of PET and PET-VGCNF fibers. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 16. Actual vs. genetic ANN predicted yield strain ($\Sigma y(X)$) of PET and PET-VGCNF fibers. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 17.

Actual vs. genetic ANN predicted elastic modulus ($E(X)$) of PET and PET-VGCNF fibers.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 18.

Representative normalized stress–strain curves of PET control and PET-VGCNF samples (experimental and GA ANN predictions utilizing piecewise linear elastic strain hardening constitutive law) subsequent to fatigue loading. (The data to the left of the curve prescribe the testing conditions of the sample). [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

TABLE 1

Upper and lower bound properties of step size, momentum, and PE element optimization parameters for GA training.

	Constitutive behavior prediction (no prior fatigue)		Constitutive behavior prediction (post-fatigue)	
	Lower bound	Upper bound	Lower bound	Upper bound
Step size optimization	0	1	0	1
Momentum optimization	0	1	0	1
PE element optimization	10	20	1	10

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TABLE 2

Properties of PET/VGCNF filaments at elongation rate of 10 mm/min under uniaxial stress conditions without prior fatigue.

	<i>E</i> (GPa) 1% strain	<i>E</i> (GPa) secant	σ_f (MPa)	ϵ_f	Energy (μ J)
<i>PET control</i>					
Average	6.6	4.2	250	0.45	1.1 E +03
Std. Dev.	1.1	1.1	33	0.019	1.5 E +02
95% Interval	1.1	1.0	31	0.017	1.4 E +02
<i>PET-VGCNF</i>					
Average	15.8	11.1	526	0.28	1.5 E +03
Std. Dev.	0.38	0.47	23	0.050	3.5 E +02
95% Interval	0.47	0.58	29	0.062	4.4 E +02

TABLE 3

Optimization summary results for GA neural networks-conjugate gradient (5-10-10-1 architecture) for PET-VGCNF samples.

	Training results		Testing results
	Min MSE	Generation	<i>R</i>
Trial 1	0.00655	4	0.943
Trial 2	0.0107	3	0.910
Average	0.00863	3.5	0.926