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Predictability of mechanical behavior of additively manufactured particulate composites using machine learning and data-driven approaches



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ABSTRACT

Additive manufacturing and data analytics are independently flourishing research areas, where the latter can be leveraged to gain a great insight into the former. In this paper, the mechanical responses of additively manufactured samples using vat polymerization process with different weight ratios of magnetic micro-particles were used to develop, train, and validate a neural network model. Samples with six different compositions, ranging from neat photopolymer to a composite of photopolymer with 4 wt.% of magnetic particles, were manufactured and mechanically tested at quasi-static strain rate and ambient environmental conditions. The experimental data were also synthesized using a data-driven approach based on shape-preserving piecewise interpolations while leveraging the concept of simple micromechanics rule of mixture. The overarching objective is to forecast the mechanical behavior of new compositions to eliminate or reduce the need for exhaustive post-manufacturing testing, resulting in an accelerated product development cycle. The ML model predictions were found to be in excellent agreement with the experimental data for prognostication of the mechanical behavior of physically tested samples with near-unity correlation coefficients. Furthermore, the ML model performed reasonably well in predicting the mechanical response of untested, newly formulated compositions of photopolymers and magnetic particles. On the other hand, the data-driven approach predictions suffered from processing artifacts, demonstrating the superiority of ML algorithms in handling this type of data. Overall, this analysis approach holds great potential in advancing the prospects of additive manufacturing and model-less mechanics of material analyses. A by-product of the ML approach is using the results for quality assurance, accelerating the acceptance of additively manufactured parts into industrial deployments.

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1. Introduction

Recent advances in manufacturing processes and unprecedented progress in data analytics have nurtured important innovation in materials and design, and fueled the fourth industrial revolution. On the one hand, advanced manufacturing has engulfed every aspect of the supply chain in every industrial sector, ranging from consumer goods to space and defense applications (Goh et al., 2020). For

example, additively manufactured (3D printed) running shoes and protective helmets are now available in the open market at relatively competitive prices, revolutionizing many aspects of the conventional supply chains such as leading to skilled labors, shorting time-to-market (i.e., logistics), and eliminating or reducing material waste (Tan et al., 2020). The latter is an inherent aspect of additive manufacturing, where the part or component is fabricated from the ground up by adding one layer of material at a time, in contrast to conventional subtractive manufacturing. On the other hand, the industrial tracking and scientific testing of the additively manufactured parts using a plethora of materials and methods results in a wealth of experimental data that can be mined in real-time for ways

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to improve the manufacturing processes and the material performance simultaneously. These combined advances present a unique opportunity for the process-structure-property-nexus at the foundation of the mechanics of materials discipline (Youssef, 2021). The progress in 3D printing, including new processes, materials, and design approaches, must be continuous to meet the rigorous requirements of trans-disciplinary fields such as medicine and engineering (Ngo et al., 2018; Beaman et al., 2020). There are a few recent review papers holistically dedicated to the state-of-the-art, to which the reader is referred to (Goh et al., 2020; Tan et al., 2020; Beaman et al., 2020; Bikas et al., 2016; Alshahrani, 2021).

Of specific interest to this study is the liquid-crystal display (LCD) 3D printing process based on photo-curable polymer resin. In LCD, the part is additively printed one entire layer at a time, accelerating the print time in comparison to the infamous fused filament fabrication (FFF), where each layer is deposited one bead at the time (Huynh et al., 2020; Youssef et al., 2021). Recently, Malley et al. demonstrated the fabrication of particulate magnetoelectric composites, discussed next, using the LCD process, overcoming significant challenges such as particle agglomeration, premature curing, and pre-fabrication gelation (Malley et al., 2021). Malley et al. fabricated samples with different geometries for mechanical, electrical, and magnetic testing, evidencing the persistence of multifunctionality of the samples (Malley et al., 2021). Additionally, Lantean et al. performed comprehensive experimental investigations on the suspension of magnetic particles in a photo-curable resin used in 3D printing while concurrently controlling the strength and direction of an applied magnetic field (Lantean et al., 2021, 2018, 2019), an aspect that Malley et al. study proposed as future work (Malley et al., 2021). They studied the conditions leading to the self-assembly of the magnetic particles during the 3D printing process and the physical attributes of the self-assembled particles. It was also demonstrated that an off-the-shelf digital light project (DLP) printer could be readily modified to align the magnetic particles along or away from the printing direction by manipulating the magnetic field during printing (Lantean et al., 2021, 2018). These recent studies add to the burgeoning efforts of multifunctional structures using advanced additive manufacturing approaches (Ngo et al., 2018; Youssef et al., 2021; Malley et al., 2021; Lantean et al., 2021, 2018).

Magnetoelectric composite materials constitute a scientifically and technologically viable alternative to materials with intrinsic coupling between the magnetic field and electrical polarization. However, the intrinsic counterpart is scarce, resulting in suboptimal coupling at room temperature, while a greater coupling efficacy exists at cryogenic temperatures (Spaldin and Ramesh, 2019). On the other hand, magnetoelectric composites can be developed using a broad range of magnetic and electrical materials constituents in different geometries and configurations, including laminated plates, stacked cylinders, or particulate composites (Bichurin et al., 2020). Compliant particulate composites, consisting of magnetic particles suspended in an electroactive polymer matrix, are of specific interest to flexible and wearable electronics due to their low mechanical stiffness and multifunctional coupling between electric and magnetic energies (Newacheck et al., 2021; Newacheck and Youssef, 2021, 2019). While superior magnetoelectric coupling is theoretically predicted, two overarching challenges prevent the broad industrial adaptations of the aforementioned multifunctional composites, namely, manufacturability and performance. The latter challenge is due to the discrepancy between theoretically predicted coupling coefficients and their experimentally measured values. This challenge is sometimes manifested by the laboratory values showing inferior efficacy (Newacheck et al., 2021). Moreover, it has been reported that the samples breakdown prematurely during testing and characterization. Newacheck et al. pinpointed the source of the breakdown, attributing it to the viscosity of the polymer matrix that results in particle mobility and attraction to the testing electrodes

(Newacheck et al., 2021; Newacheck and Youssef, 2021). They demonstrated particle mobility, even after fully curing the composite samples, using experimental and theoretical models (Newacheck et al., 2021; Newacheck and Youssef, 2021). Furthermore, Newacheck and collaborators explained the difference between predicted and measured coupling coefficients based on the geometry and distribution of magnetic particles as a function of the applied magnetic field (Newacheck et al., 2021). The second challenge of manufacturability stems from the disparity in the physical properties between the magnetic particles and the surrounding polymer matrix. This challenge represents the primary motivation leading to the present research. Here, the manufacturability challenge is overcome using the digital light projection additive manufacturing approach, as discussed later.

The advents in data analytics using machine-learning algorithms have invigorated new research directions in mechanics and materials at different spatial and temporal scales in a broad range of material systems (Miyazawa et al., 2019; Yang et al., 2020; Murugesan et al., 2019; Weng et al., 2020; Stendal et al., 2019; Jordan et al., 2020; DebRoy et al., 2021). Data-driven modeling and scientific discovery have led to a paradigm change on how many problems, both in science and engineering, are addressed. The addition of physics in machine-learning models has created new excitements due to combining physical constitutive equations with the power of artificial intelligence, accelerating the scientific discovery cycle. For instance, machine learning algorithms have been used to predict the stress-strain behavior of elastic and elastoplastic material systems after modeling, training, and tuning a neural network using experimental data (Murugesan et al., 2019). These algorithms have also been leveraged to classify whether the material behavior represents a brittle or ductile response. The continuous advancement in data analytics using artificial intelligence is conducive to alleviating the experimental burden by reducing the number of samples and testing conditions (e.g., volume or weight percentages of reinforcement fillers in composite materials). In this work, we demonstrate the ability of a machine-learning algorithm to forecast the stress-strain behavior of composite materials with different magnetic particles, followed by exemplifying the utility of these algorithms in forecasting the mechanical response of new compositions. That is, the application of machine-learning algorithm to predicting the mechanical response of tested and untested compositions (i.e., different volume fractions of the constituents) represents the primary novelty of this research. However, other approaches are also available to alleviate the experimental burdens at lower computational effort, the prime of which are data-driven approaches, where the experimental data of known material compositions are used to forecast the response of other untested conditions. This was recently demonstrated by Uddin et al. (2020). Therefore, we will compare the predictive ability of machine learning algorithms with those of data-driven approaches.

This research aims to combine the capabilities of 3D printing of multifunctional composite materials with the power of data analytics using machine learning to predict the mechanical performance of fabricated parts. In doing so, samples with different magnetic filler contents were fabricated using digital light projection additive manufacturing. These samples were then mechanically characterized using a standard load frame in tension at quasi-static strain rate conditions. The experimental data was exploited using machine-learning and data-driven approaches to forecast the mechanical performance of 3D printed materials that were not printed or characterized.

2. Sample preparation and testing

Six sets of samples were fabricated and tested in this research. Each set consisted of five specimens printed in dog-bone geometry

according to ASTM D638 Type IV in two batches (*i.e.*, three dog-bones per printing batch) (International, 2014). The first set of samples was 3D printed using an unaltered neat photopolymer (PP, Monoprice Rapid UV Printer Resin). The remaining sets included magnetic iron oxide particles (Fe_3O_4 , 44 μm (mesh size 325) average size powder). As-received Fe_3O_4 particles with different weight ratios (0.5 wt.%, 1 wt.%, 2 wt.%, 3 wt.%, and 4 wt.%) were suspended in the photopolymer while sonicating for 20 min.

The samples were additively manufactured using a vat polymerization 3D printer (Crealty LD002R LCD Resin 3D Printer) with 0.02 mm layer height. Additional details regarding the fabrication method included an exposure time of 10 s for ten bottom layers, 80 s bottom exposure time, 5 mm bottom lift and lifting distance, and 65 mm/min bottom lift and lifting speed (Malley et al., 2021). The specimens were post-cured in an ultraviolet enclosure (built in-house) with a radiation dose of $\sim 18 \text{ mJ}/\text{cm}^2$ for two 10 min dosages. In the first 10 min, one surface of the specimen was directly facing the ultraviolet source, while in the second dose, the other surface was set to face the UV light. All printing and curing artifacts were removed before starting mechanical testing, including excess material on the surface close to the print bed. The specimens were then allowed to rest for one week before mechanical testing commenced. The stress-strain responses of the additively manufactured composites were characterized using a standard load frame (Instron Series 5843) equipped with a $\pm 1 \text{ kN}$ load cell and a long travel extensometer (Instron Long Travel XL Extensometer 2603-084XL) at a quasi-static strain rate of $\sim 0.03 \text{ s}^{-1}$. Malley et al. compared several mechanical attributes of these samples, including the elastic modulus and the yield strength (Malley et al., 2021), to which the reader is referred for more information. Here, the stress-strain data were used as inputs for analytics using machine-learning and data-driven approaches. Fig. 1 summarizes the mixing of constituents, 3D printing using a LCD printer, and mechanical testing of 3D printed dog-bone composite samples.

3. Modeling approaches

In the area of mechanics of materials, constitutive equations (*i.e.*, a mathematical description of stress-strain behavior and its correlations with material properties) have been and continue to be a topic of research, especially with new material subclasses springing into existence. However, these relatively restrictive models require exhaustive numerical and computational efforts to process the mechanical testing data and to facilitate the extraction of the model parameters. Moreover, any changes in the material composition, *e.g.*, heterogeneity due to the addition of a reinforcement phase in composites, necessitate the repetition of the attributes extraction process. Furthermore, given the applicability of several of these parametric models, additional efforts must be made to fit the

experimentally measured values with prescribed (and often overly simplified) mathematical expressions. In the case of novel material systems with unknown behaviors, the latter challenge may lead to significant errors due to the parametric fitting process. Alternatively, data-driven and machine-learning algorithms utilize the unprocessed testing data to predict the behavior without constraining assumptions beyond those imposed during the data collection phase. This includes the potential of predicting the mechanical behavior of new compositions, as demonstrated later. Here, we leverage the analytical power of these algorithms to investigate the mechanical behavior (*i.e.*, stress-strain curves) of 3D printed neat photopolymers and a composite of magnetic microparticles embedded in the same polymer matrix. It is imperative to note that the overarching limitation of the machine-learning algorithm used herein is the absence of physics and mechanics in the model; a limitation that can be mitigated using physics-informed neural networks by combining the advantages of physical and mechanical constitutive models with the power of artificial intelligence (Miyazawa et al., 2019; Yang et al., 2020; Murugesan et al., 2019; Karniadakis et al. 2021; Wang et al., 2017; Fuhg, 2021).

3.1. Machine-learning approach

A supervised machine-learning algorithm was constructed and trained in this research to predict the entire stress-strain curves of 3D printed particulate composite samples, consisting of photocurable polymer resin and magnetic microparticles. Here, the inputs and the outputs were known to the algorithm *a priori* based on the experimental data collected during the tensile testing, as discussed in the previous section. We used an artificial neural network (ANN) in the Deep Learning Toolbox in MATLAB® to construct, train, and test the machine-learning model. Given the importance of data structures on the performance of the ANN, the inputs and outputs were carefully paired. The inputs consisted of two attributes, including the strain values and their corresponding coded compositions (listed in Table 1), where the strains were sequentially stacked from all the samples data in one column and their compositions in a companion column.

The stresses were also stacked similarly and fed into the neural network as the output. It is worth noting that the input and output values were normalized with respect to their respective global maxima, resulting in accelerated optimization and better overall performance. In general, we used a fully connected cascade feed-forward neural network (similar to feedforward networks with additional connections between the input and previous layers to following layers, see the right panel in Fig. 2). Several hyper-parameters were adjusted during the network optimization process based on the Levenberg-Marquardt backpropagation optimization algorithm, a ubiquitous nonlinear least-squares fitting algorithm widely used in machine-learning models. It was found that initialization of the hidden and output layers before training had a profound effect on the overall performance of the ANN. The optimized ANN model consisted of two hidden layers with 2 and 1 interconnected artificial neurons. The transfer function prescribed to all the hidden and output layers neurons was the hyperbolic tangent, resulting in the best performance based on the mean squared error (*mse*) cost function

$$mse = \frac{1}{n} \sum_{i=1}^n (T_i - Y_i)^2 \quad (1)$$

where, T_i is the known output stress values (*i.e.*, the target), Y_i is the predicted output stresses using the neural network, and n is the number of data points. The latter was 11,700 stress data points for the current research collected during physical testing. The number of iterations was set to 2000 epochs; however, the best performance of

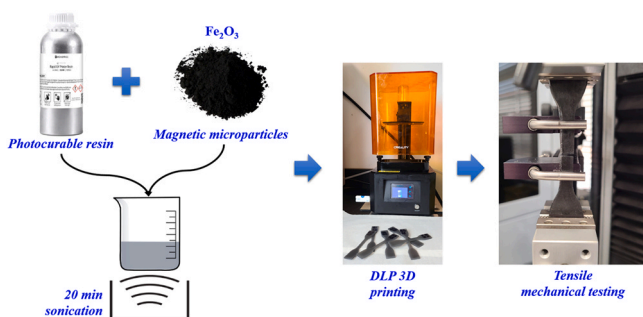


Fig. 1. Synthesis, fabrication, and testing of 3D printed dog-bone composite samples, consisting of magnetite microparticles suspended in photocurable resin. The samples were manufactured using LCD 3D printing approach and tensile tested in standard load frame at quasi-static loading rate.

Table 1
List of the 3D printed compositions using LCD printer and their corresponding code used in codifying the inputs.

Composition	Code	Description
PP	0	Pure (neat) photopolymer resin samples
PP/0.5 wt.% Fe ₃ O ₄	0.5	A composite of PP and 0.5 wt. % of iron oxide microparticles
PP/1 wt.% Fe ₃ O ₄	1	A composite of PP and 1 wt. % of iron oxide microparticles
PP/2 wt.% Fe ₃ O ₄	2	A composite of PP and 2 wt. % of iron oxide microparticles
PP/3 wt.% Fe ₃ O ₄	3	A composite of PP and 3 wt. % of iron oxide microparticles
PP/4 wt.% Fe ₃ O ₄	4	A composite of PP and 4 wt. % of iron oxide microparticles

$mse \approx 4.3 \times 10^{-4}$ was attained with less than 1000 epochs. The learning rate and the Marquardt adjustment parameter were taken to be 0.01 and 0.005, respectively. The entire dataset (organized as described above) was fed to the ANN, divided randomly and internally into 70% for training, 15% for validation, and 15% for testing. Fig. 2 is a schematic representation of the framework used herein to develop a deep machine-learning model using a cascade feedforward neural network, with the aforementioned configuration and parameterization. It is worth noting that other neural network architectures were explored but the selected cascade feedforward neural network outperformed the others.

3.2. Data driven approach

The mechanistic foundation of this data-driven approach is the concept of the rule of mixtures, broadly used to estimate the properties of composite materials. The essence of the rule of mixtures is that the resulting attribute of a mixture is the scaled contributions of the constituents based on their weight or volume fractions. However, the exact contribution of adjusting the content of the magnetic particles to the holistic mechanical behavior (in contrast to just one property) is convoluted due to smeared influence of the particle-matrix interface, the conditions surrounding the manufacturing process (e.g., the influence of the 3D printing parameters on the mechanical performance), the particle agglomeration and size distributions, and the geometry of the particles. Even sophisticated continuative mechanics models commonly assume a spherical particle geometry, resulting in response mispredictions (Newacheck

et al., 2021; Newacheck and Youssef, 2021), while experiments have shown that platonic geometries are more suitable to achieve accurate predictions but challenging to account for analytically. To this point, Newacheck et al. recently demonstrated the effect of particle geometries on the magnetoelectric particulate composites using computational multi-physics simulations, delineating the dependence of the coupling coefficient on the particle geometry and its orientation within the matrix (Newacheck et al., 2021; Newacheck and Youssef, 2021, 2019). Therefore, we opted to treat each sample configuration as a standalone composition that contributes equally to predicting the mechanical behavior of new compositions. For example, the experimental stress-strain curves of neat photopolymer and PP/0.5 wt.% Fe₃O₄ are interpolated to forecast the mechanical response of PP/0.25 wt.% Fe₃O₄. It is worth noting that the latter was neither fabricated nor tested; instead, it was used to demonstrate the predictive ability of the reported data-driven approach, which is then compared to similar predictions using the ANN approach discussed above. The approach is oblivious to any mechanics constitutive models (even the simple micromechanics rule of mixtures); it solely relies on the data, hence terming it data-driven.

The proposed data-driven approach is faced with two symbiotic challenges, which also constitute its limitations. First, the ultimate strength and strain-to-failure for each sample, even from the exact composition of photopolymer and magnetic filler, are not consistent, resulting in considerably different dataset lengths from one sample to another and from one composition to another (see left panel of Fig. 3). The variance in the mechanical behavior, including the terminal stresses and strains, is attributed to the manufacturing

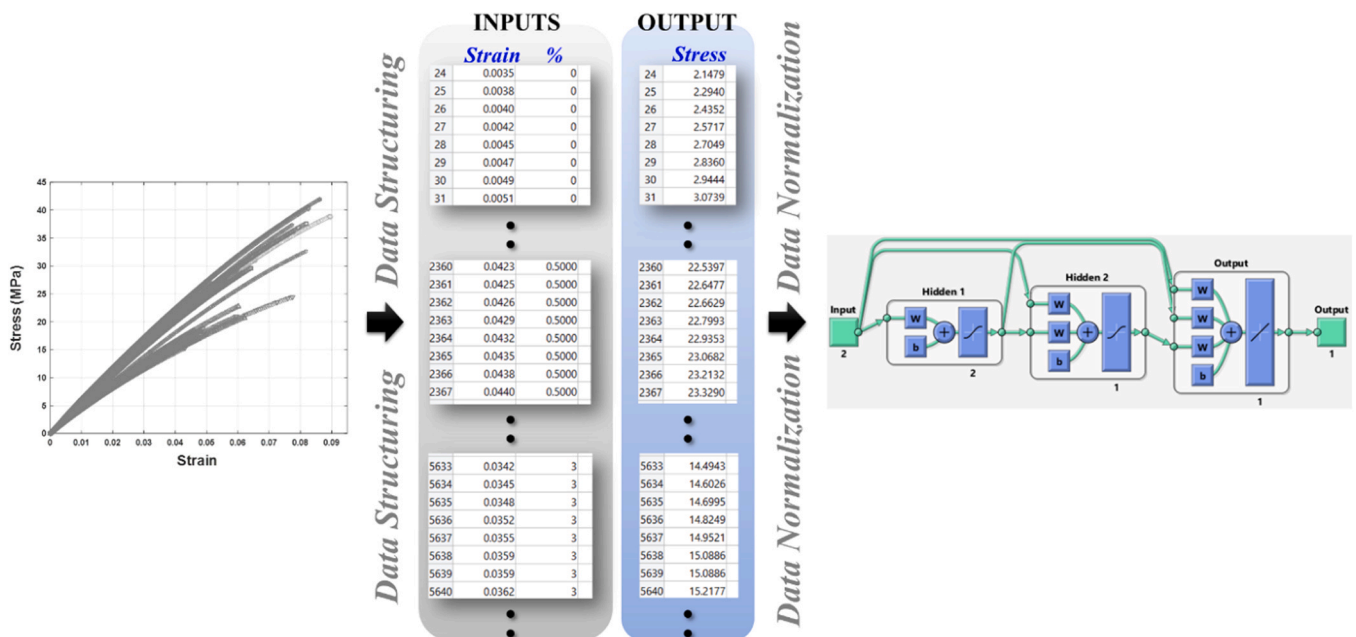


Fig. 2. Schematic of the utilized deep learning framework to predict the stress-strain behavior of 3D printed particulate composites, where all the stress-strain histories (left panel) were collated and organized as two attribute inputs and an output (middle panel) then fed into a cascade feedforward neural network (right panel) that was optimized using the Levenberg-Marquardt backpropagation algorithm.

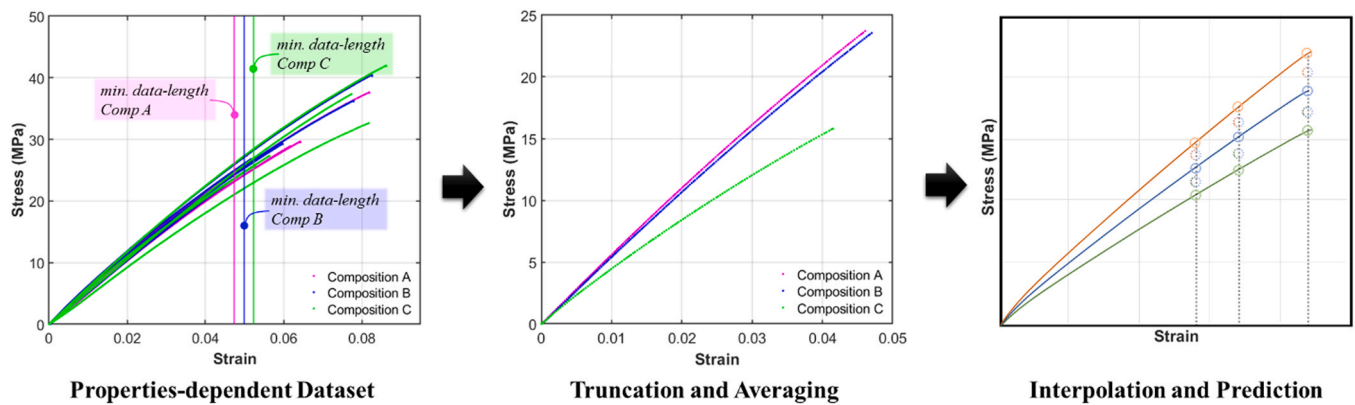


Fig. 3. Schematics of the data-driven approach processing the stress-strain curves of 3D printed samples, demonstrating the variability of the dataset length (left panel), truncation based on the minimum data length and averaging (middle panel), and interpolation and prediction (right panel).

process, implying material anisotropy, which is conformal with the primary characters of composite and 3D printed materials (Tan et al., 2020; Ngo et al., 2018; Alshahrani, 2021; Malley et al., 2021; Lantean et al., 2018; Yang et al., 2020). Secondly, the variable data length is not conducive for calculating the average or interpolating between the stress-strain curves, resulting in unintended artifacts, as demonstrated in the results in the next section. Therefore, we truncated the dataset of each configuration to the minimum size within the set, *i.e.*, averaging the stress-strain curves up to the smallest dataset length, limiting the predictions of the mechanical behavior to nearly half of that possible using the ANN approach discussed in the previous section.

The data-driven approach used herein is succinctly summarized in Fig. 3, which is divided into three steps:

1. The dataset for each sample composition is compared, and the minimum data length is calculated. This was done to eliminate the inevitable biasing of the averaging process at the end of the mechanical response due to the variance in the terminal stresses.
2. The datasets were truncated based on the calculated minimum size from the previous step. The average of nonzero stress and strain values was then calculated, accounting for all data from the five samples.
3. At each strain value, all the stresses were shape-preserving piecewise cubic interpolated with C^1 continuity as a function of the compositions to generate the stresses of new compositions with several magnetic particle volume fractions bounded between the volume fractions of their fabricated and tested counterparts. The new predicted compositions included PP/0.75 wt.% Fe_3O_4 , PP/1.5 wt.% Fe_3O_4 , PP/2.5 wt.% Fe_3O_4 , and PP/3.5 wt.% Fe_3O_4 .

4. Results and discussion

Fig. 4 is a collage of plots comparing experimental data (displaying the stress-strain curves from all five samples) and the ANN predictions for all six compositions listed in Table 1. Overall, the ANN performed very well in prognosticating the mechanical behavior of neat and composite 3D printed materials. In Fig. 4, the predictions are shown to be in excellent agreement with the experimental data, exemplifying the correct behavior and forecasting accurate values. Furthermore, the correlation coefficient between all targets (*i.e.*, experimental stress initially fed to the model) and the ANN predicted stress values were calculated to be 0.9959, quantitatively affirming the excellent agreement between the measured and predicted values irrespective of the composition. In all, there are three noteworthy observations based on the results presented in Fig. 4: (1) the mechanical behavior of the 3D printed samples, (2) the

statistical demeanor of the experimental data, and (3) the accuracy of the ANN predictions. These observations are further substantiated based on the recent work by Malley et al. (2021).

First, the stress-strain data in Fig. 4a indicates that the neat photopolymer exhibits a brittle behavior with an average elastic modulus of 621 ± 79 MPa and ultimate strength of 35.7 ± 5.1 MPa with strain-to-failure of 0.08 ± 0.01 . The rest of the compositions investigated herein, *i.e.*, the composite materials with different magnetic particle content, inherited the brittleness of the neat photopolymer given the large weight percentage of the resin matrix. It is worth noting that the maximum stress and strain values in Fig. 4a-d are approximately the same despite the change in the magnetic filler content. For samples with relatively low Fe_3O_4 weight ratio (*i.e.*, 0.5, 1, and 2 wt.%), the mechanical behavior closely mimicked that of the pure polymer, with an average elastic modulus of 563 ± 40 MPa, 603 ± 47 MPa, and 512 ± 99 MPa, respectively, evidencing only an average reduction of $\sim 10\%$ in the material stiffness. Malley et al. discussed the source of the reduction using a simplified mechanics model, treating the stiffer particles (that may have agglomerated during the printing process) as sample porosity due to the inability to transfer stress between the matrix and the particles seemingly (Malley et al., 2021). Nonetheless, such reduction is expected since the magnetic particles affected the polymerization process and weakened the cohesion strength of the neat polymer due to the introduced discontinuities from the Fe_3O_4 particles, *i.e.*, particle-matrix interface. Moreover, the magnetic particles obscured the ultraviolet light path used in printing, given the disparity in the refractive index between the resin and the particles, resulting in a potential difference between the quality and mechanics of the particle-matrix interfaces of the areas facing towards and away from the light projection screen. That is to say, the shadow of the particles may affect the photocuring process during 3D printing, a topic of future research. While the ultimate strength displayed a close resemblance to the behavior of the elastic modulus, the yield strength exhibited the most significant difference, changing from 13.2 ± 4.5 MPa for the pure photopolymer samples to $\sim 18 \pm 4.5$ MPa for PP/2 wt.% Fe_3O_4 . The drastic change in the yield point can be attributed to the light-particle interactions discussed above, where the polymer chains can sustain higher stresses due to the relative motion of the particles with respect to the surrounding macromolecules. Similar behavior was recently reported when Terfenol-D magnetic particles were suspended in an electroactive polymer matrix (Newacheck and Youssef, 2019). On the other hand, the stress-strain behavior is penalized when the weight ratio of the magnetic microparticles increases, reaching 3 and 4 wt. %, where the stress respectively reaches a maximum of 19.2 ± 2.6 MPa and 18.3 ± 2.0 MPa, while the maximum strain was limited to 0.05 ± 0.01

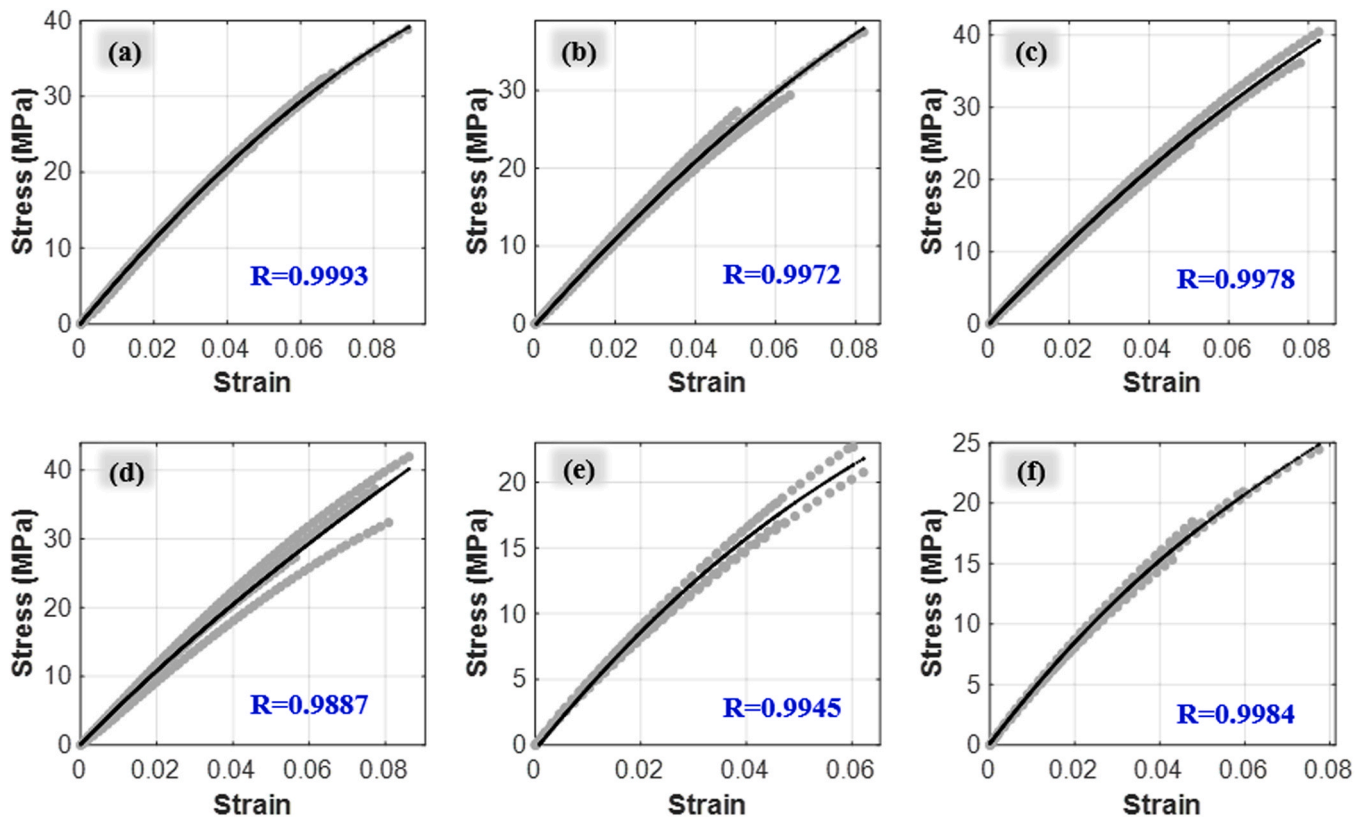


Fig. 4. Comparison between the experimental data (gray lines) and ANN predictions (black) of (a) neat photopolymer (PP), (b) PP/0.5 wt.% Fe_3O_4 , (c) PP/1 wt.% Fe_3O_4 , (d) PP/2 wt.% Fe_3O_4 , (e) PP/3 wt.% Fe_3O_4 , and (f) PP/4 wt.% Fe_3O_4 , showing overall excellent agreement between measured and predicted data.

for PP/3 wt.% Fe_3O_4 and PP/4 wt.% Fe_3O_4 samples. The elastic moduli for the latter two compositions were respectively 488 ± 25 MPa and 480 ± 38 MPa, reporting $\sim 22\%$ reduction compared to the modulus of the neat photopolymer samples. The further increase in brittleness and degradation of the mechanical properties due to the increase in the magnetic filler content are attributed to the non-uniform distribution of the magnetic particles within the polymer matrix due to agglomeration and settling.

The preceding discussion about the changes in the mechanical behavior and the inability of simplified micromechanics models (see for example Malley et al., 2021; Newacheck et al., 2021; Newacheck and Youssef, 2021, 2019) to reproduce such evolution highlights the superiority of the machine-learning approach. In other words, the incumbent micromechanics techniques frequently hinge on oversimplifying the analysis, leading to significant error. At the same time, the machine-learning approach takes into account the collective response of the samples, including the particle-matrix interactions, without imposing any simplifying assumptions. As a result, the classical theoretical approaches are capable of forecasting improvements to the properties but fail to account negative effects of the reinforcement phase on the overall mechanical behavior. On the contrary, the machine-learning algorithm was able to take into account the collective influence of the magnetic particles, including any potential strengthening or weakening processes (e.g., particle-matrix interface). Thus, the potential utility of machine-learning in mechanics, material analysis, and manufacturing is justified and substantiated.

Second is the statistical demeanor of the experimental data, showing low intra-composition variability (*i.e.*, low spread or low variance between the stress-strain curves within each composition) in the stress-strain data from one sample despite being printed into two batches, as discussed above. The low variability is observed in all

the stress-strain curves, except for the slight deviation shown in Fig. 4d and e (*i.e.*, 2 and 3 wt.%). This may be misleading from an additive manufacturing perspective since it implies that the LCD 3D printing process has high repeatability and consistent printing quality, which may be true for the neat photopolymer samples but not consistent with our experience manufacturing the composite samples. In a previous report, we noted significant inter and intra-batch variability when printing the composite structures due to the non-uniform distribution of the particles because of the pulsation action of the LCD printer. In the latter, the print bed continually moves towards and away from the printing screen to allow a fresh layer of the resin to cure upon exposure to the light source, displacing the magnetic particles away from the print region. The reader is referred to the work of Malley et al. (2021) for more discussion about this issue. Nonetheless, a significant difference was noted in the mechanical behavior of 3D printed neat polymer, and magnetic particles reinforced photopolymer samples, which is qualitatively evident in Fig. 4. Future research seeks to extend the machine-learning framework reported here to account for the effect of the printing conditions on the mechanical behavior of 3D printed materials. Even though the intra-composition variability can be considered negligible, the terminal stress and strain values were not consistent, exemplifying a larger variance in the properties and the size of the dataset from one sample to another. As discussed later, this poses a challenge for the traditional curve fitting of the stress-strain curves into conventional constitutive material equations and the data-driven approach, but it was not the case for the machine-learning model. Finally, and as reported above, the neural network model performed well in predicting the entire mechanical response irrespective of the composition with a near-unity correlation coefficient, as shown in Fig. 4. That is to say; the ANN prediction was insensitive to the significant difference in the ultimate strength and

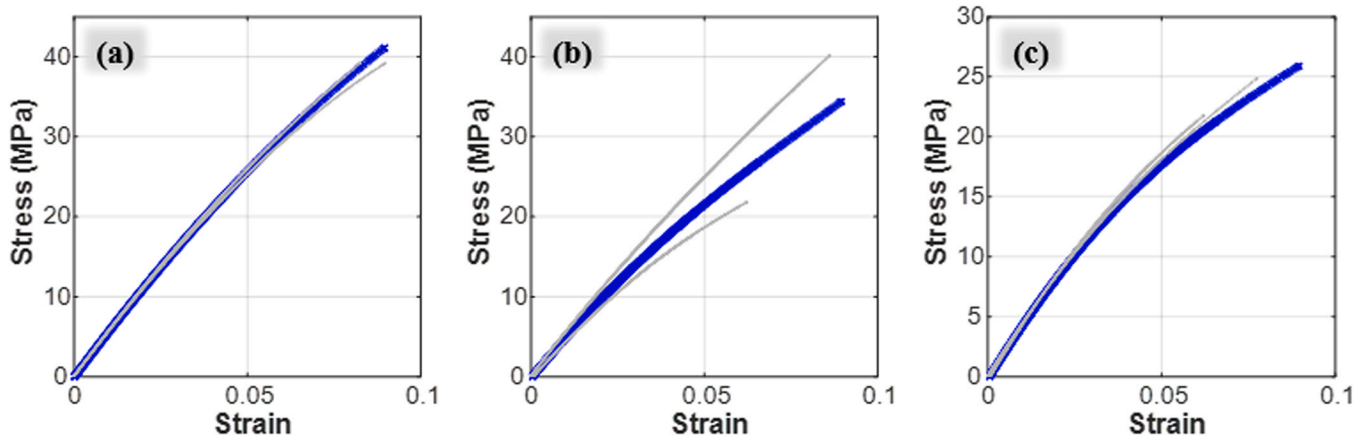


Fig. 5. The ANN model predictions (blue lines) of the stress-strain curves of (a) PP/0.75 wt.% Fe₃O₄, (b) PP/2.5 wt.% Fe₃O₄, and (c) PP/3.5 wt.% Fe₃O₄ compared to the composite compositions in the vicinity of the new compositions (gray lines).

strain-to-failure in the experimental datasets, *i.e.*, the variance of size in the datasets, where the ANN model was able to learn and correctly map the input-output relationships without tedious data preprocessing. This is consistent with the reported mean squared error of 4.3×10^{-4} during the training process.

It is reasonable to accept that the ANN model performs well in regurgitating the data it was trained, validated, and tested even though the testing data was internally hidden from the neural network during the training process. The remaining question is whether the ANN model can prognosticate the stress-strain behavior of new compositions. Therefore, the trained ANN model was used to forecast the mechanical behavior of three new compositions, namely PP/0.75 wt.% Fe₃O₄, PP/2.5 wt.% Fe₃O₄, and PP/3.5 wt.% Fe₃O₄. It is expected that the interpolation of the stress-strain curves of a new composition, *e.g.*, PP/2.5 wt.% Fe₃O₄, will lay in between the experimental data collected from and PP/2 wt.% Fe₃O₄ and PP/3 wt.% Fe₃O₄. Similar behavior is also forecasted for any new compositions bounded between those experimental data investigated herein and used to develop the ANN model. Such expectations are hinged on several mechanistic constitutive models for particulate composites, *e.g.*, see (Newacheck et al., 2021; Newacheck and Youssef, 2021). Fig. 5 is a comparison between the stress-strain curves of the newly predicted compositions and the data from experimental testing of compositions in the vicinity of the predictions. For example, Fig. 5a plots the neural network predictions of PP/0.75 wt.% Fe₃O₄ along with the experimental data collected from 3D printed composite sample of PP/0.5 wt.% Fe₃O₄ and PP/1 wt.% Fe₃O₄. In the absence of experimental data for the new compositions, *i.e.*, the overarching objective of this research, only intuitive qualitative analysis is introduced based on the foundations of mechanics of composite materials. Generally, the mechanical behavior of composite materials is strongly dependent (but admittedly nonlinear) on the ratio of the constituents, implying a change in the magnetic filler content results in a corresponding manipulation of the stress-strain response. At an intermediate weight fraction of Fe₃O₄ microparticles, the latter is bounded by the response with lower and higher weight fractions. The results in Fig. 5 are mostly consistent with this expected behavior, as for the cases shown in Figs. 5a and 5b for the 0.75 and 2.5 wt.% Fe₃O₄. On the other hand, the ANN predictions for 3.5 wt.% Fe₃O₄ are underperformed compared to the experimental data from 3 and 4 wt.%. It is worth noting that the physical testing data from the latter two compositions deviated significantly from their

preceding counterparts, as shown in Figs. 4e and 4f and discussed above. The change in the data demeanor affected the weights and biases impeded within the neural network model, resulting in the suboptimal predictions for higher magnetic filler compositions. Future research will focus on encoding physics objective functions to account for the change in the mechanics as a function of the constituents, *i.e.*, physics-informed machine-learning (Karniadakis et al., 2021).

Fig. 6 reports the predictions on the stress-strain curves of new compositions using the data-driven approach based on shape-preserving piecewise interpolations of the experimental stresses and strains as a function of filler content. Fig. 6a compares the predicted mechanical behavior of PP/0.75 wt.% Fe₃O₄ with the experimentally acquired stress-strain curves of the photopolymer with 0.5 and 1 wt.% Fe₃O₄ magnetic particles, while Fig. 6b-d are predictions for PP/1.5 wt.% Fe₃O₄, PP/2.5 wt.% Fe₃O₄, and PP/3.5 wt.% Fe₃O₄, respectively. First, it is important to note that the predictions were truncated to ~ 0.05 strains, constituting the minimal data length, as discussed above, which is the first drastic difference between the data-driven and ANN model approaches. The latter is agnostic to the premature failure of some of the samples, demonstrating the ability of machine-learning algorithms to capture the collective contributions (positive and negative) of the magnetic particles to the overall response. Second, the experimental data with lower and higher magnetic filler content bounded the predictions. For example, the stress-strain curve for PP/1.5 wt.% Fe₃O₄ is shown in Fig. 6b to be sandwiched between the experimental stress-strain curves of the 1 and 2 wt.%, respectively. The only deviation to this observation, *i.e.*, the boundness of the predictions with the experimental data, is the prognostication for the relatively high weight fraction, *e.g.*, 3.5 wt.%, which is attributed to the intermingling of the experimental stress-strain responses the 3 and 4 wt.% compositions. The latter was associated earlier with possible agglomeration and settling of the magnetic particles during printing, resulting in non-uniform distribution and heterogeneous curing. Finally, the predictions using the data-driven approach exhibit calculation artifacts (encircled regions in Fig. 6). While these artifacts might be filtered *a priori*, they are intentionally included since the ANN prediction did not undergo any postprocessing steps. The artifacts are a byproduct of the difference in data length from one composition to another. In general, the predictions using the data-driven were reasonable within the context of the measured stress-strain curves but underperformed the predictions of ANN approach.

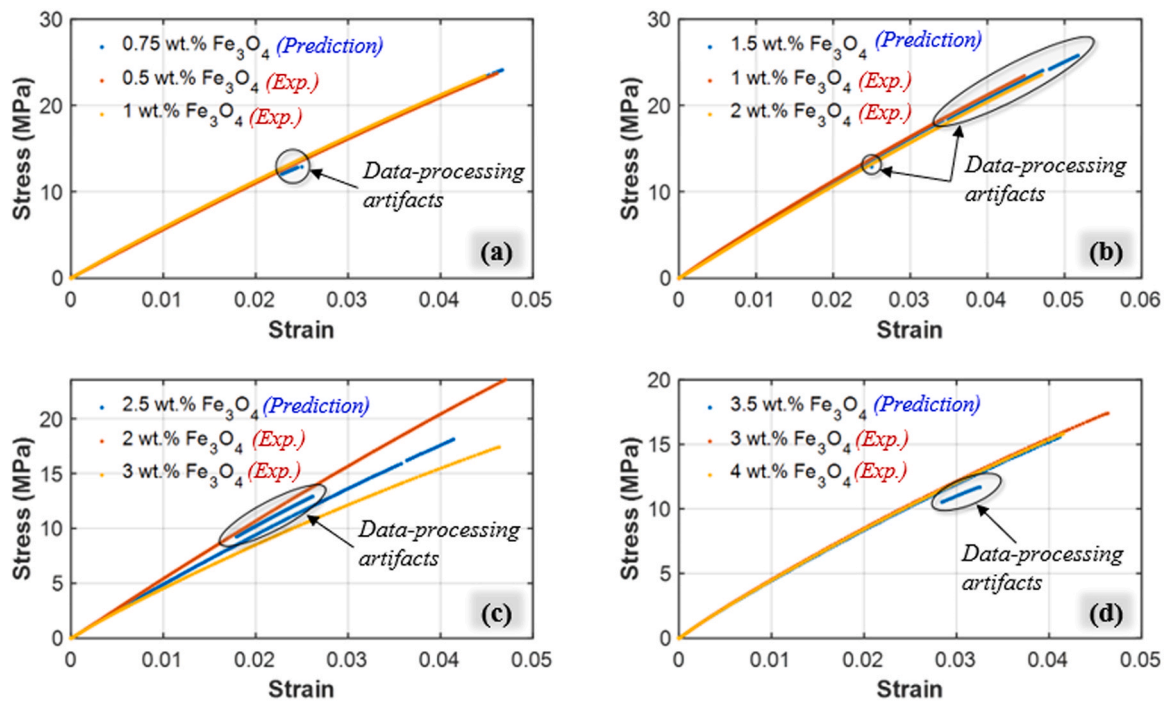


Fig. 6. The predicted stress-strain curves (blue lines) using the data-driven approach compared to the experimental mechanical behavior of the compositions (orange and yellow lines) in the vicinity of the predicted ratios with (a) PP/0.75 wt.% Fe_3O_4 , (b) PP/1.5 wt.% Fe_3O_4 , (c) PP/2.5 wt.% Fe_3O_4 , and (d) PP/3.5 wt.% Fe_3O_4 . The circled regions denote the artifacts from the interpolation process.

5. Conclusion

In this paper, we reported on the mechanical behavior of additively manufactured composite samples fabricated using the digital light projection process. The samples consisted of a composite of photopolymer and magnetic microparticles, where the latter included 0.5, 1, 2, 3, 4 wt.% weight ratios. The samples were mechanically tested using a load frame at a quasi-static loading rate under ambient environmental conditions. Subsequently, the data were synthesized using machine-learning and data-driven approaches to prognosticate the mechanical behavior of existing and new compositions. The machine-learning approach outperformed the data-driven method that suffered from unintended artifacts and truncated predictions due to limitations with interpolation and data, respectively. While the artifacts can be removed from the data-driven prediction by adding a postprocessing step, we refrained from doing so since the machine-learning forecasts did not undergo any additional processing; the truncated prediction challenge is irremediable, given the anisotropy of the mechanical response of the composite samples. On the other hand, the machine-learning stress-strain predictions were in excellent agreement with the experimental data and were consistent with mechanics-intuitions for the new compositions. Therefore, the machine-learning approach holds great potential for advancing additive manufacturing and the mechanics of materials.

Future research will emphasize two directions. First, improving the mechanical behavior of additively manufactured magneto-electric composite materials by enhancing the bonding interface through particle functionalization while introducing additional functionality. This new class of materials can potentially transform flexible and wearable electronics. To achieve the latter, a comprehensive multiscale physical characterization framework will be developed to elucidate the mechanical, electrical, and magnetic properties of the manufactured samples. Second is to amend the proposed machine-learning algorithm with physics and mechanics constitutive models, i.e., physics-informed machine-learning, to

improve the predictive-ability performance. The mechanical testing data used herein, and multi-physics experimental data will be used to train, validate, and test the new physics-informed models. Collectively, these research directions collate into the accelerated product development lifecycle, driving further progress in additive manufacturing processes and situating them as viable and intelligent replacements for conventional processed.

CRediT authorship contribution statement

Steven Malley: Data curation, Formal analysis, Investigation, Roles/Writing – original draft, Writing – review & editing, **Crystal Reina:** Data curation, Formal analysis, Investigation, Roles/Writing – original draft, Writing – review & editing, **Somer Nancy:** Data curation, Formal analysis, Investigation, Methodology, Software, Supervision, Roles/Writing – original draft, Writing – review & editing, **Jérôme Gilles:** Formal analysis, Methodology, Roles/Writing – original draft, Writing – review & editing, **Behrad Koohbor:** Formal analysis, Methodology, Project administration, Validation, Visualization; Roles/Writing – original draft, Writing – review & editing, **George Youssef:** Data curation, Formal analysis, Funding acquisition, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization; Roles/Writing – original draft; Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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