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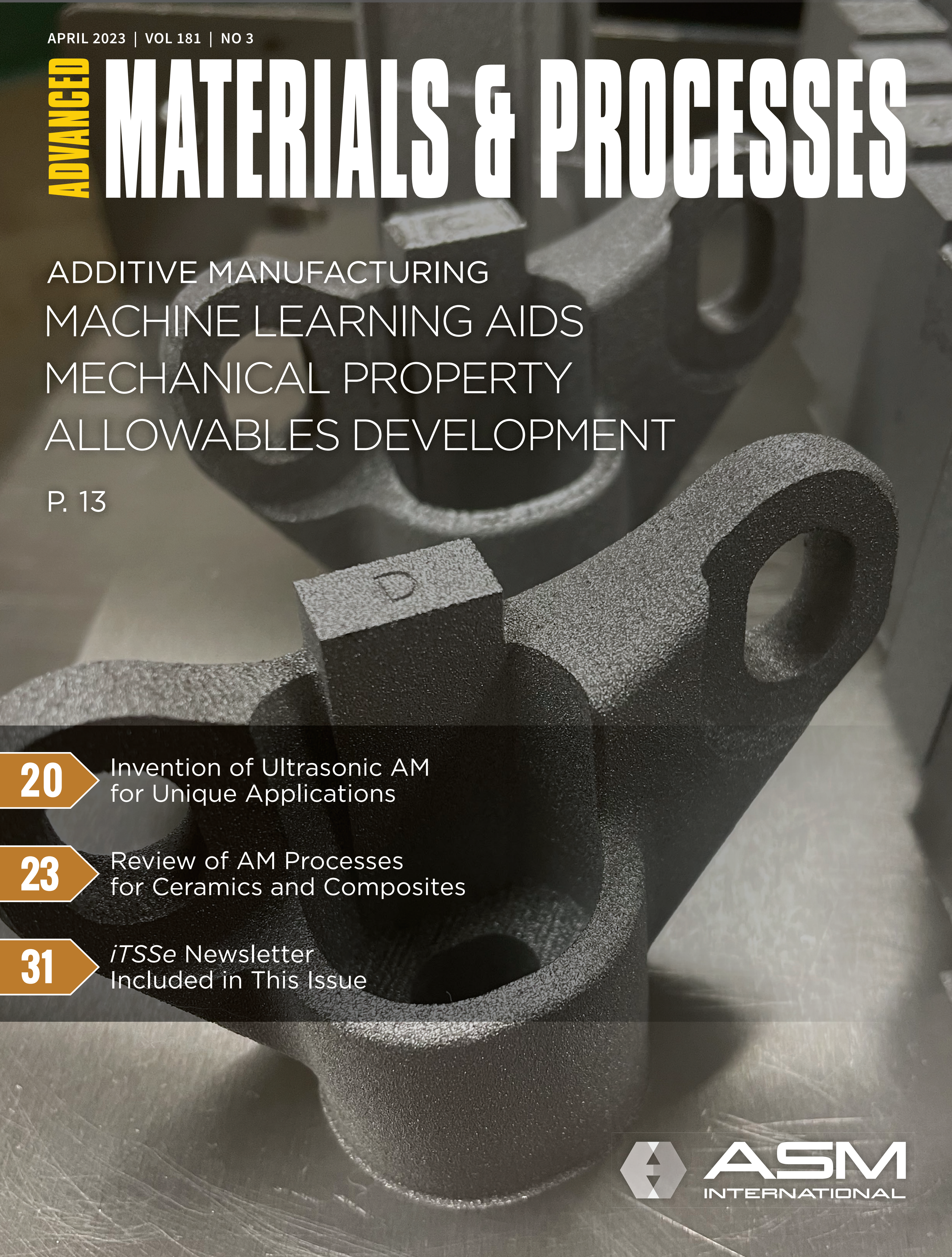
ADVANCED MATERIALS & PROCESSES



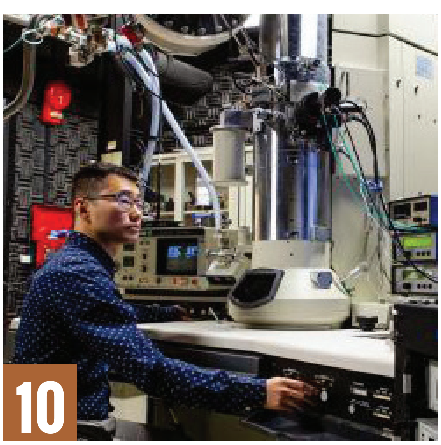
ADDITIVE MANUFACTURING
MACHINE LEARNING AIDS MECHANICAL PROPERTY ALLOWABLES DEVELOPMENT

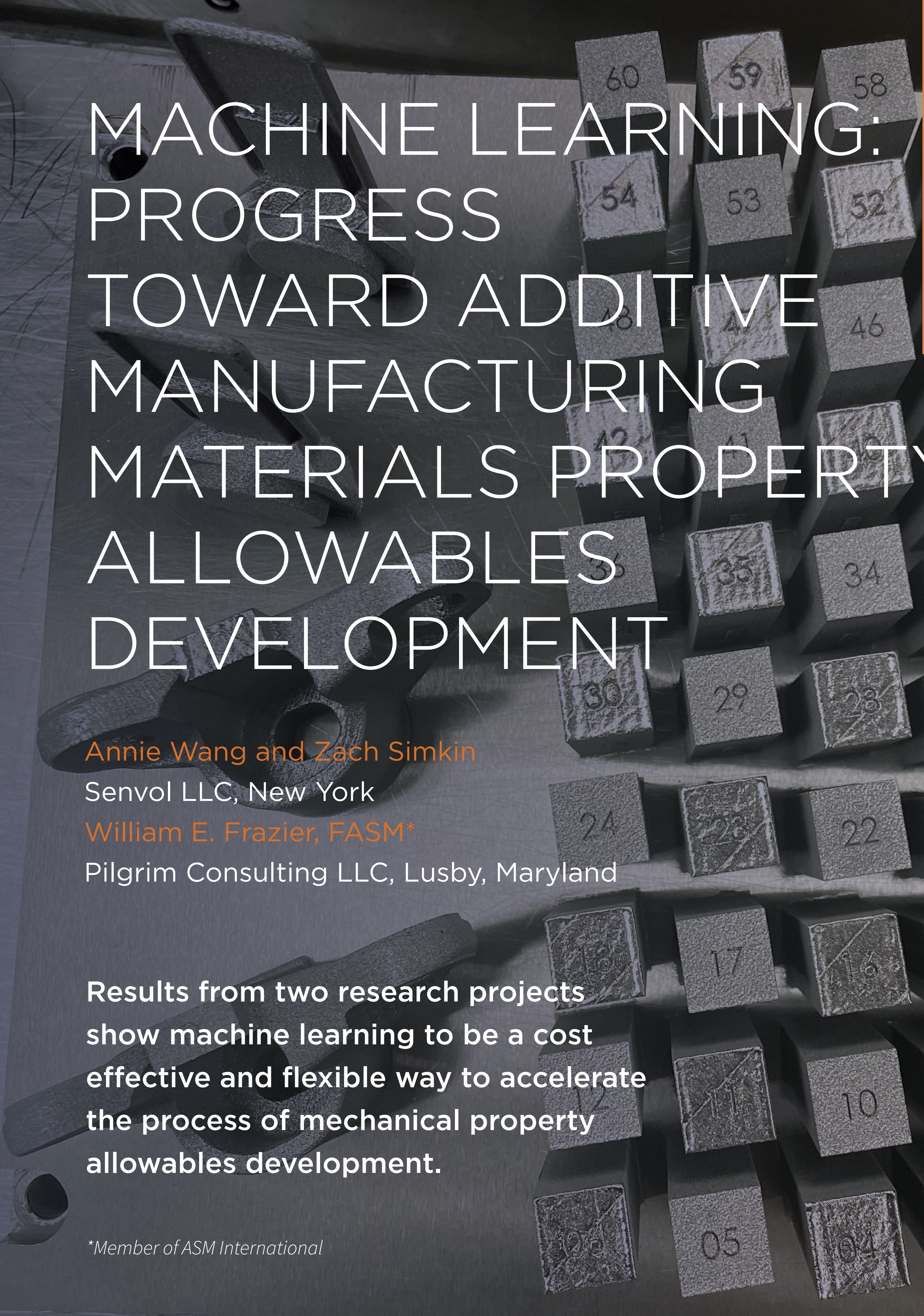
P. 13

ASM INTERNATIONAL

On the Cover:

Senvol recently led an additive manufacturing program for the U.S. Army. Image of one of the builds, done by EWI, using 17-4 PH stainless steel on an EOS M290 machine. Courtesy of Annie Wang, Olga Elsieeva, and William E. Frazier, FASM.





MACHINE LEARNING: PROGRESS TOWARD ADDITIVE MANUFACTURING MATERIALS PROPERTY ALLOWABLES DEVELOPMENT

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Results from two research projects show machine learning to be a cost effective and flexible way to accelerate the process of mechanical property allowables development.

**Member of ASM International*

The application of machine learning (ML) in the field of materials science and engineering has rapidly matured over the past decade. However, the full potential of this methodology has yet to be unleashed. This article starts with a succinct synopsis of ML and explores its many diverse characteristics. The results of two recently completed research projects investigating the potential use of ML to establish additive manufacturing (AM) materials property allowables are described. Although continued research and development (R&D) work is required, the results are very promising. The authors' thoughts on the maturation of ML for this application are then delineated.

BACKGROUND

The technologies involved in ML are illustrated in Fig. 1 and may be conveniently divided into seven broad areas: (i) data, (ii) ML categories, (iii) environment/infrastructure, (iv) data science and ML libraries, (v) algorithms, (vi) quality, and (vii) models. For the qualification of AM materials, the goal of ML is the development of accurate predictive models. Models may be thought of as human artifacts, i.e., representations of reality within prescribed limits.

The generation of ML models is based on the analysis of data. AM is a digitally intense process generating an abundance of data. Data quality, type, and quantity is important, and data must be scrubbed to ensure its pedigree and provenance. This is not trivial and can consume 85% of a data scientist's time[1,2]. The type of data (continuous or categorical/discrete) must be established. Further, prior to deciding upon an ML approach, the quantity of data needed to derive a meaningful model and the required data environment and infrastructure should be considered carefully.

Mathematical algorithms are then used to transform data into models. There are many algorithms used in ML, and each has their appropriate applications, strengths, and weaknesses. Table 1 provides a representative partial list of ML algorithms and their notional characteristics[3,4]. Common types of algorithms include regression, neural nets (NN), deep learning (DL), decision trees (DT), k nearest neighbors (KNN), and support vector machines (SVM)[5]. This article discusses regression, which has broad application, and polynomial regression algorithms, which were used in the research reported by the authors in this work.

Regression analysis encompasses a large variety of statistical methods to estimate the relationship between input variables and their associated features. Typical regression methods include a) linear regression, b) multilinear regression, c) polynomial regression, and d) logistic regression. Regression analysis is not a new technique but its application to big data sets with large numbers of independent variables to establish (with statistical confidence) a set of dependent materials properties allowables is novel.

ML can be applied to AM in a variety of ways in varying stages of maturation. Currently the lowest hanging fruit

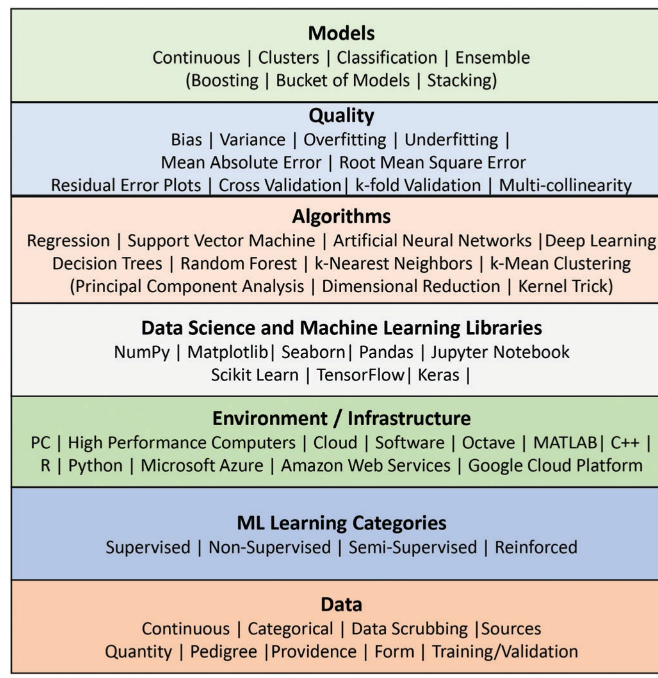


Fig. 1 — Machine learning technology stack.

TABLE 1 – GENERAL CHARACTERISTICS OF MACHINE LEARNING ALGORITHM[3,4]

Algorithm	Algorithm type*	Learning type**	Data required	Computational time to learn
Linear regression	R		Low	Low
Polynomial regression	R		Low	Low
Logistic regression	C		Low	Low
Naïve Bayes	C	S	Low	Low
Neural network	C	S, U, R	High	High
Deep learning	C	S, U, R	High	High
Decision tree	C & R	S	Low	Low
k-Nearest neighbor	I	I	Low	Low
Support vector machine	C	S	Low	High
k-Means	C	U		Low

*Type of algorithm: Regression (R), Classification (C), Instance (I)

**Learning types: Supervised (S), Unsupervised (U), Reinforced (R), Instance (I) (applications that are most mature today) are AM process optimization and certain aspects of process management and control. Once an ML model is trained, AM users can interrogate the model with various questions, such as "what process parameter set should be used if we require ultimate tensile strength of Y?" or "what is the trade-off between the different process parameter inputs?" or "which process parameter inputs have a large influence on part density?" This allows the AM user to rapidly develop optimized process parameters. Additionally, by monitoring the AM manufacturing process through testing coupon samples at regular intervals, the model can be further trained to detect process drift as a function of time or other factors (e.g., room temperature, humidity, personnel).

More sophisticated but far less mature applications for process management and control could come from applying ML to real-time sensory inputs or measurements, such as using computer vision to monitor in-situ sensors, feature engineering of time-series based measurements or training a model to identify features in visual input (e.g., CT scans, microstructure images).

In the medium to long term, ML could be used to develop methods for allowable calculations and assist in qualification, requalification, or delta qualification. While the concept of ML allowables is novel, it could be useful today as a "gate check" to help AM users decide whether or not a certain process is stable enough to warrant the time and resources needed to develop conventional allowables using the Metallic Materials Properties Development and Standardization (MMPDS) or Composite Materials Handbook-17 (CMH-17) methods. In other words, ML allowables today could be an estimate of conventional allowables yet to be developed.

The ML approach could also be used to demonstrate equivalency, which would greatly aid with requalification or delta qualification. The ML approach allows the issue of equivalency to be easily inverted. Instead of fixing the process parameters and expecting future AM machines to achieve the same requirements with a frozen set of process parameters, the AM user can fix the requirements and ask the ML model to determine what process parameter window on the new AM machine would allow the AM user to achieve the desired requirements.

ML MATERIALS PROPERTY ALLOWABLES DEVELOPMENT

Introduction. Senvol recently completed two programs that focused on demonstrating an ML-enabled approach to support materials allowables development. The first project was an Army program [funded via the Advanced Manufacturing, Materials, and Processes (AMMP) consortium] focused on stainless steel 17-4PH. Project members included Senvol, Lockheed Martin Missiles & Fire Control, EWI, Pilgrim Consulting, and Battelle. The second program was an America Makes program focused on a flame retardant polymer, where the project members were Senvol, WSU-NIAR, Northrop Grumman, Stratasys Direct Manufacturing, and Pilgrim Consulting.

Both projects completed a side-by-side comparison that evaluated an ML-enabled approach to allowables development. Results showed that an ML-based approach can be more flexible, cost-effective, time-effective, and equivalent to the conventional (e.g., MMPDS in the case of metals, and CMH-17 in the case of polymers) approach to materials allowables calculation.

Despite the potential that AM offers, the rate of AM adoption is very slow due in part to the high cost and time associated with material allowables development. Furthermore, AM is an advanced manufacturing technique that is process-intensive by definition; the creation of the materials and the part occurs in the same process. As such:

- Conventional materials allowables development binds the user to a limited set of machines and build parameters.
- The current allowables paradigm freezes the technology and user in time.
- Deviations or multiple allowables require generation of large amounts of additional data.

This results in an AM process that is not only costly and time-consuming to implement the first time, but equally costly and time-consuming to maintain in the long run when there are inevitably changes to the AM process.

There were two primary objectives of these two projects.

1. Develop and demonstrate a new approach to calculate materials allowables that is not a fixed-point solution.
   - The projects developed an approach to AM allowables that leverages the digital nature of AM and leverages machine learning (ML).
2. Demonstrate an ML-enabled approach to statistically substantiating materials property predictions across an entire parameter range.
   - An ML approach is extremely flexible and is able to handle any change to the AM process, thus providing materials property predictions even when deviating from the point at which an allowable was developed.

These two projects demonstrated that:

1. An ML approach enables a user to do parameter development and materials allowables development in parallel using the exact same empirical dataset.
2. An ML approach enables a user to make statistically substantiated predictions about performance and scatter everywhere in a given parameter range. This is particularly useful if a user needs to make parts using different parameters (e.g., one parameter set for performance reasons, and a different parameter set for efficiency/cost reasons).
3. ML allowables predicted materials behavior consistently with the

conventionally developed allowables (i.e., ML allowables were just as accurate as conventionally developed ones).

These projects also included a validation portion, which included a performance assessment of the ML allowables against the conventional allowables, as well as a cost-benefit assessment.

While the word "allowable" is used in this article, the authors wish to highlight an important caveat, which is that no true allowables were generated in either of the two projects discussed. First, the term "ML allowable" is used for convenience, however it should be noted that an ML-based approach is not an approved methodology for allowable development. Second, due to cost and programmatic constraints, several simplifying decisions needed to be made in generating the conventional allowables based on MMPDS or CMH-17 guidelines (e.g., only one lot of powder was used in each project).

Project Steps. The project steps for the two projects are summarized in Table 2.

Results and Discussion. The ML approach is vastly different from the conventional MMPDS or CMH-17 approaches to materials allowables. To illustrate, imagine a parameter space, such as the three-dimensional parameter space in Fig. 2, consisting of parameters A, B, and C. The ML approach can be applied to n-dimensions and is particularly suited for high-

TABLE 2 – ADDITIVE MANUFACTURING ML ALLOWABLES PROJECT SUMMARIES

	U.S. Army funded (AMMP Consortium) project developing ML-allowables on stainless steel 17-4 PH	America Makes project developing ML-allowables on fire retardant polymer
Machine and material	Machine: EOS M290 Material: Stainless steel 17-4 PH	Machine: 3D Systems sPro60 Material: Nylon 11 flame retardant (FR-106)
Step 1: Build and collect training data to develop ML model	ML software was used for the DOE (design of experiments). 293 vertical coupons over 3 builds. All coupons were built on a single AM machine. Each coupon was a different parameter set.	ML software was used for the DOE (design of experiments). 6 builds of 50 coupons each (i.e., 300 coupons total). Half of the builds were on machine 1, half were on machine 2. Each coupon was a different parameter set.
Step 2: Select two optimized parameters based on two different engineering requirements	ML model was the basis from which two optimized parameters were selected. Parameter set A is optimal to achieve requirement A. Parameter set B is optimal to achieve requirement B.	ML model was the basis from which two optimized parameters were selected. Parameter set A is optimal to achieve requirement A. Parameter set B is optimal to achieve requirement B.
Step 3: Calculate ML allowables	ML model was used to calculate ML allowable A at parameter set A and ML allowable B at parameter set B.	ML model was used to calculate ML allowable A at parameter set A and ML allowable B at parameter set B.
Step 4: Develop conventional allowables	Followed MMPDS S-basis guidelines: Parameter set A: Three builds with 10 coupons per build (30 coupons total) Parameter set B: Three builds with 10 coupons per build (30 coupons total).	Followed CMH-17 B-basis robust sampling guidelines: Parameter set A: 10 builds of five coupons each (50 coupons total) Parameter set B: 10 builds of three coupons each (30 coupons total).
Step 5: Calculate conventional allowables	Based on MMPDs guidelines, calculate S-basis allowable A and S-basis allowable B.	Based on CMH-17 guidelines, calculate B-basis allowable A and B-basis allowable B.
Step 6: Build validation build (i.e., previously unseen data)	Four representative parts total. 60 witness coupons: 30 built with ML-selected parameter set A, 30 built with ML-selected parameter set B.	Eight representative parts total. 38 witness coupons total: 15 built with ML-selected parameter set A, 15 built with ML-selected parameter set B.
Step 7: Analysis and comparison	Accuracy and usability of ML allowables A and B was compared against those of MMPDS S-basis allowables A and B using data from the validation build.	Accuracy and usability of ML allowables A and B was compared against those of CMH-17 B-basis allowables A and B using data from the validation build.

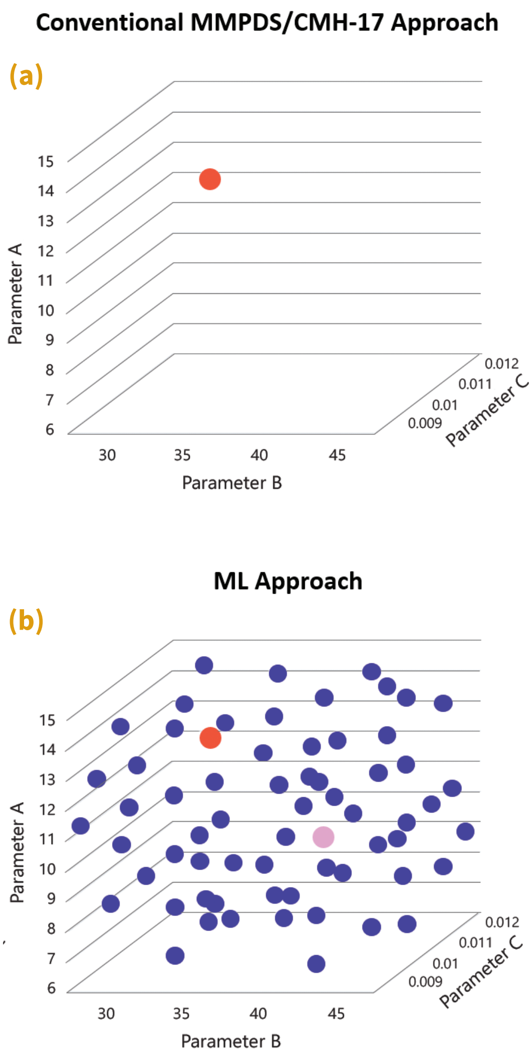


Fig. 2 — (a) Conventional allowable development; X (e.g., 30) samples at one parameter set (e.g., A1, B1, C1), so all 30 samples are repeats of the same parameter set; (b) ML approach; Y samples all over and evenly distributed over the parameter space; S-basis "ML-allowables" can be calculated at any parameter set even where there's no empirical data (e.g., red, pink dots).

dimensional problems (e.g., 4 dimensions and above), but for illustrative purposes only three-dimensional space is easiest to imagine.

In the conventional approach, many samples are collected at only one parameter point (illustrated by the red dot in Fig. 2a). In the ML approach (illustrated by the graph in Fig. 2b), the ML software was used to design the design of experiments (DOE) that consist of each of these blue dots. Each of these blue dots was built using a different parameter set. Each of the blue dots was used to develop a surrogate model (sometimes called a response surface) of the AM process. The ML model can point to parameter A and parameter B even though no empirical data has been collected at these dots.

Each of these blue dots is not just a point but is a processing window. The ML approach enables the user to conduct parameter development and allowables development simultaneously. In other words, the blue dots inform the parameter optimization and allow the AM user to select the optimal parameters to achieve the goals, but the blue dots also allow the AM user to make statistically substantiated predictions about the performance and the coefficient of variation of those predictions at any given point or process window. Hence, ML allowables could be calculated at the red dot for Goal A and done a second time at the pink dot for Goal B.

In comparing ML allowables against conventionally developed MMPDS or CMH-17 ones, the ML allowables predicted materials behavior consistently with the conventionally developed ones. In other words, ML allowables are just as accurate as those conventionally developed.

Table 3 presents an example comparing ML allowables against conventional MMPDS S-basis allowables for parameter A and B from the AMMP project on stainless steel 17-4 PH.

It is critical to recognize that the ML approach enables a user to do parameter development and materials allowables development in parallel using the exact same empirical dataset. Simultaneously, the single set of training data that is gathered in the ML approach can be used to generate an infinite number of allowables, thus the cost-benefit becomes even more favorable toward the ML approach if more than one allowable is generated.

Figure 3 provides a chart showing the total cost of allowable development (y-axis) for various quantities of allowables. For the purposes of this chart, the conventional MMPDS S-basis allowables were assumed to be developed using the minimum quantity of coupons required as per MMPDS (i.e., 30 coupons).

MATURATION OF ML FOR AM ALLOWABLES DEVELOPMENT

The future state of AM of mechanical property allowables development and AM process qualification is likely to involve the integrated use of the following technologies.

- Integrated computational materials engineering (ICME)
- Machine learning (ML) and artificial intelligence (AI)

TABLE 3 – CALCULATED MACHINE LEARNING ALLOWABLES RESULTS COMPARED TO CONVENTIONAL APPROACH

PARAMETER A – OPTIMIZED TO PRIORITIZE HIGH TENSILE STRENGTH OVER PRINT SPEED		
	ML allowable (MPa)	MMPDS allowables (MPa)
Ultimate tensile strength	154.9	159.4
Yield strength	153.0	153.2
PARAMETER B – OPTIMIZED TO BALANCE BETWEEN GOOD TENSILE STRENGTH AND FASTER PRINT SPEED		
Ultimate tensile strength	160.6	164.4
Yield strength	156.5	157.1

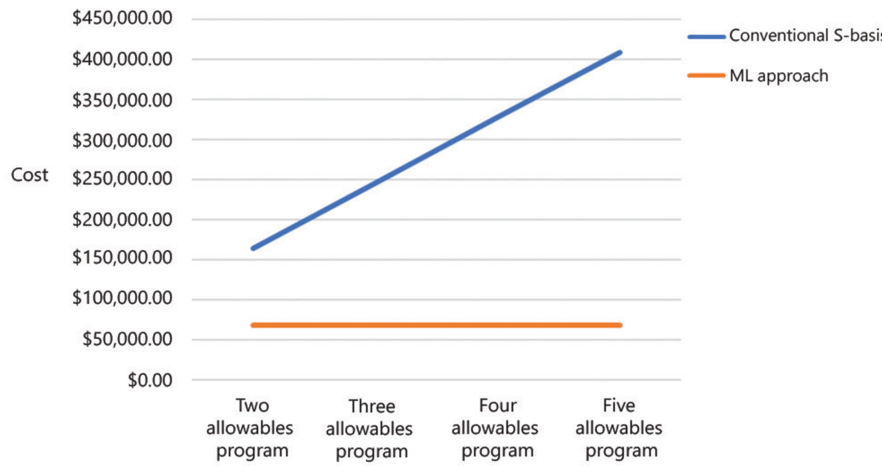
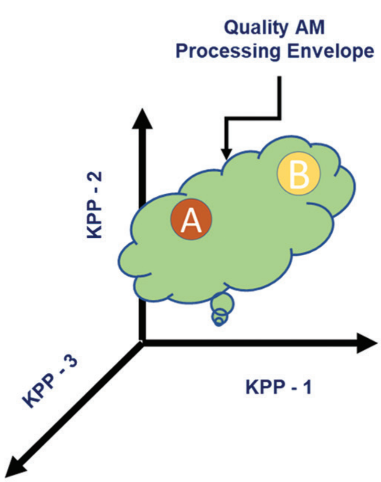


Fig. 3 — Cost comparison of machine learning and conventional allowables development.



Property	A	B
Yield Strength, MPa	≥ 400	≥ 450
Elongation, %	10 to 12	≥ 8%
Fracture Toughness, MPa$\sqrt{m}$	35 to 45	≥ 30
Fatigue Strength, MPa	120	150

Fig. 4 — Quality AM processing envelope in n-dimensional space for a hypothetical alloy.

- In situ process sensors and feed-forward, adaptive process controls
- Standards (process, control, sensor, data fusion, and informatics)
- Testing (statistically substantiated data)

While there appears to be community convergence on the tools to be used, there are countless approaches to their unified integration being explored.

The application of these tools to accelerate AM mechanical property allowables requires a paradigm shift in our thinking. The conventional approach to mechanical property allowables development is to a) freeze the materials process, b) produce multiple lots and heats, and c) conduct extensive mechanical property tests to generate statistically substantiated properties[6]. ML learning permits the concomitant assessment of AM key process parameters on a range of mechanical properties of interest. It thus provides both a means of converging on a set of optimal process parameters and establishing the robustness (sensitivity of properties to changes in process variables) of mechanical properties (Fig. 4). Within the "defect free" quality process envelope, process regions (A and B) can be identified to achieve a desired set of mechanical properties.

After ML has converged on a processing window to achieve the desired set of mechanical properties, ICME tools could be employed to further refine the processing window prior to investing in the development of statistically substantiated mechanical properties. The consistent and reproducible production of quality materials could then be ensured by employing adaptive, feedforward process controls. This would require real time data and analysis of information obtained from in situ sensors to be used in conjunction with predictive ICME tools.

For AM, this methodology has several advantages to "freezing" a process. Operating within the quality processing envelope helps ensure a defect-free material. Machine-to-machine or manufacturer-to-manufacturer qualification is made easier as one needs only to ensure that the process is operating in the predetermined quality envelope. The identification of optimal processing parameters required to achieve a new set of customer materials property requirements is made easier as the entire process space has been previously mapped to mechanical performance.

SUMMARY

Within this article, the authors provided a brief introduction to machine learning. ML allows engineers and scientists to tease out causal relationships from complex data sets. To develop a functional model, data scientists must first thoroughly scrub the data to ensure pedigree, provenance, quality, and form. Appropriate algorithms can then be applied to the data sets to develop a useful ML model, i.e., a representation of reality.

The potential of ML to accelerate the process of mechanical property allowables development was demonstrated in two recently completed, narrowly scoped projects. ML mechanical property allowables for laser powder bed fusion (LPBF) of a metal (17-4PH stainless steel) and a polymer (Nylon) were shown to be comparable to a conventional statistical based approach. The ML approach was shown to reduce the cost and time of an AM product deployment. The AMMP project demonstrated that development of two ML allowables was 58.7% less expensive than developing two conventional S-Basis MMPDS allowables. Using the exact same empirical dataset, ML allows the concomitant development of AM process parameters and materials allowables. The training data informs parameter optimization and allows for making statistically substantiated predictions about mechanical performance. Continued maturation of the technology is required, and a possible path forward posited.

The key takeaway is that the ML approach has the potential to be just as accurate as the conventional approach while also being much more cost-effective and flexible. **~AM&P**

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