An Overview on Machine Learning for Characterizing Materials with A View of Predicting Their Mechanical Aspects

Amar C[1]
[1]*Lecturer, Department of Automobile Engineering, Government CPC Polytechnic Mysuru, Karnataka, India.*

***Abstract*—The current expansion of material data generated from experiments and simulations is surpassing manageable quantities. The advancement of innovative data-driven techniques for uncovering patterns across various length scales and time-scales, as well as structure-property relationships, is crucial. The application of these data-driven methodologies holds significant potential in the field of materials science. This review examines the applications of machine learning in the characterization of metallic materials. A multitude of parameters related to the processing and structure of materials significantly influence the properties and performance of manufactured components. This study aims to explore the effectiveness of machine learning techniques in predicting material properties. Characteristics of materials, including strength, toughness, hardness, brittleness, and ductility, play a crucial role in classifying a material or component based on its quality. In the industrial sector, conducting material tests such as tensile tests, compression tests, or creep tests frequently requires significant time and financial resources. Consequently, the utilization of machine learning approaches is regarded as beneficial for facilitating the generation of material property information. This investigation presents the application of machine learning techniques to small punch test data for the assessment of ultimate tensile strength across different materials. A significant relationship was identified between SPT data and tensile test data, which ultimately enables the substitution of more expensive tests with simpler and faster tests in conjunction with machine learning.**

***Index Terms*—Machine learning, Material characterization, Tensile properties, Ultimate tensile strength.**

1. INTRODUCTION

The field of materials science depends on experiments and simulation-based models as essential tools for material characterization. The characteristics of materials, including their structure and behavior, play a crucial role in determining the potential applications of the material in question. Recently, the data produced by these experiments and simulations has opened up numerous opportunities for applying data-driven methods. Alongside traditional methods such as experimental trial and error or physical metallurgy, machine learning techniques for property prediction and material design have garnered significant interest in recent years, as evidenced by various studies. Experimental investigations, known as the first paradigm of materials science, have been conducted since the stone and copper ages. It was during the 16th century that scholars began to articulate physical relationships through equations, marking the emergence of the second paradigm.

Consequently, analytical equations emerged as a pivotal tool in theoretical physics, effectively enhancing the empirical and experimental sciences. The 1950s heralded the advent of computational materials science and simulations, representing the third paradigm. Within this framework, computer experiments and simulations became feasible, with the resulting data being analyzed and interpreted in a manner akin to that of measured results. It is essential to acknowledge that numerous characteristics of materials cannot be encapsulated by a definitive mathematical expression, as they are influenced by various complex, multilevel theoretical frameworks. By utilizing extensive data, one can uncover concealed correlations that manifest as structures and

patterns, which typically remain obscured in smaller data sets. Consequently, the emergence of data-driven science in the field of materials research took place. However, it is not only an advantage to have a large data volume, but it can also be a challenge to cope with tremendous quantities of information. Today, data are increasingly accessible and can be stored with greater ease, thanks to significant advancements in sensors and methods for data collection on one hand, and storage devices on the other. Currently, there is a clear trend in various fields towards the acquisition of extensive data sets, often without prior knowledge of their potential analysis or application. The remarkable growth in data volume is evident not only in the quantity of samples gathered over time but also in the multitude of attributes or characteristics that are concurrently assessed in a process. Data are collected into vectors where the dimension aligns with the number of concurrent measurements taken on the process. Increasing dimensions lead to high-dimensional data, where each sample can be depicted as a point or vector within a high-dimensional space. Engaging with high-dimensional data involves navigating datasets that exist within high-dimensional spaces. The curse of dimensionality refers to the various phenomena that arise when dealing with high-dimensional data, often leading to adverse effects on the behavior and performance of learning algorithms.

In contrast to the challenges posed by high dimensionality, materials science databases frequently face constraints in size, primarily because data acquisition through experiments or simulations is both costly and time-intensive. Insufficient data size for training a machine learning model compromises the success of learning, necessitating the exploration of suitable new approaches for small datasets. This work presents a literature survey that provides an overview of machine learning applications in materials science, with a particular focus on the characterization of metallic materials. Given that measuring such parameters is frequently costly and labor-intensive through experiments, alternative fundamental tests, like the small punch test (SPT), may serve as a viable option if it can be demonstrated that equivalent material property information can be derived. A diverse array of machine learning methodologies derived from SPT data will be discussed. Additionally, Section 3 presents an example that utilizes machine learning to predict the tensile properties of a specific insert material type, drawing on SPT data. This study aims to explore the feasibility of identifying a machine learning model that can predict the tensile properties of a material based on SPT data [11]. Section sec4 wraps up this paper by providing insights into future research directions.

2. AN OVERVIEW

2.1 ML for materials science

Utilizing machine learning, when provided with sufficient data and an algorithm focused on rule discovery, a computer can identify physical laws that correspond to the given data autonomously. Conventional computational methods rely on the utilization of a fixed algorithm designed by a human specialist. In contrast, ML methods derive the principles that govern a dataset by evaluating a segment of that data and constructing a model to generate predictions [19]. However, the human still needs to select appropriate ML models that are expected to accurately represent the data and perform manual (sub-)tasks in preprocessing and feature generation.

The presence of substantial data facilitates the application of machine learning models, allowing for the extraction of data-driven insights and the identification of patterns. Conversely, the complexities associated with large datasets and their high dimensionality present significant computational and statistical challenges, including issues related to scalability and memory limitations, noise accumulation, interference correlation, incidental endogeneity, and measurement errors. Materials science represents a fascinating area where big data techniques and machine learning strategies are starting to reveal significant potential. Four essential elements play a crucial role in the field of materials science and engineering: processing, structure, properties, and performance. Nonetheless, there remains a lack of consensus regarding the interconnections among these elements. Machine learning techniques can be utilized within the process-structure-property-performance framework to gain deeper insights into the inherent relationships among these elements. A primary objective is to facilitate, expedite, and streamline the discovery and

development of innovative materials through the integration of advanced computing, automation, and machine learning. One of the goals of employing these methods in materials science is to attain efficient identification and measurement of critical material properties [15].

In addition to datasets obtained through experimentation, many studies extract necessary information from data mining based on simulations. In summary, the integration of experiment- and simulation-based data mining with machine learning tools reveals remarkable potential for the reliable identification of fundamental interrelations within materials, facilitating characterization and optimization across various scales [15]. For a comprehensive overview of recent machine learning applications in materials science, we direct you to the general reviews by Mueller et al, Wagner et al, Dimiduk et al, or Wei et al. Successful applications of ML techniques in materials science include representing inorganic materials, predicting fundamental properties, creating atomic potentials, identifying functional candidates, analyzing complex reaction networks, and guiding experimental design, as well as high-throughput phase diagrams and crystal structure determination.

2.2 Open problem—interpretability

One prominent critique of ML algorithms in research is the absence of innovative understanding and knowledge resulting from their application. This is mostly because more complex ML algorithms are often treated as black boxes. Humans struggle to comprehend machine-built models. To increase acceptability of ML models, data scientists try to demonstrate causal relationships between materials and structures across various length scales and attributes. Models in science face restrictions like limited parameters and conformity to physical rules. Data scientists must transfer their findings into useful information for other scientists, such as materials discovery or deployment. Effective methods for simplifying and interpreting models include principal component analysis (PCA), cross-validation, regularization, and careful model selection. Data dimensionality reduction is strong using PCA. Large databases are growing. PCA may be used to decrease the dimensionality of datasets, preserving most of the information. By extracting the orthogonal directions with the highest variance from a dataset, PCA creates linear combinations of the original variables. Although principal components may be difficult to physically grasp, the extracted features, which are linear combinations of the original variables, may be easily articulated. Additionally, data visualization is simplified by projecting data onto the primary extracted components. If features are not covariant, PCA may not be the best option. Intelligent feature selection may contribute to better interpretability of ML models by reducing dimension. Model regularization involves minimizing the cost function by placing an adjustable penalty on parameter size, resulting in a smaller feature space. Furthermore, ML model choice immediately affects explainability. Regressions provide coefficients that indicate the impact of input changes on output. Decision trees are simple to read and organized like flow charts. complicated models like artificial neural networks (ANNs) lack straightforward explanations of machine thinking owing to complicated node interactions. However, methods like feature visualization and attribution enhance the comprehension and interpretability of black box models. However, occasionally it may be acceptable to sacrifice model accuracy for improved explainability.

2.3 Open problem—small data

ML models often fit to tiny training sets, hindering their effectiveness and preventing replication of success. ML methods had in other fields. It is conceivable to apply ML algorithms for fitting tiny low-dimensional datasets. Few methods address this issue. For instance, ML models may be created by limiting material configurations, such as forecasting band gaps for certain semiconductor families with fixed composition or crystalline structure, rather than modeling compounds with a broad chemical space. Zhang et al suggest employing crude property estimate in feature space to create ML models with little materials data, improving prediction accuracy without increasing degree of freedom. Insufficient training data may be addressed by incorporating previous information into the training process, resulting in informed ML, or physics-informed ML. Domain knowledge frequently adds limits. By incorporating domain knowledge, a hybrid formulation of the ML problem may result in more accurate and relevant data interpretations. In addition to imposing limitations, expert knowledge may be incorporated in many ways. Until recently, it was

largely used for labeling data in supervised learning and establishing prior probabilities in Bayesian networks. Semi-supervised clustering programs may provide user advice via partial labeling information and hard limitations. Using data visualization to incorporate domain knowledge into ML model construction might enhance accuracy. Another method involves monotonizing ML functions using known physical relationships. Most ML systems are seldom considered with tiny data, since inadequate data size for training models might hinder learning performance. The database size barrier hinders applications, since building a database via experimentation is time-consuming and expensive. The recent development of materials databases may aid in addressing tiny data issues.

2.4 Existing data bases

The introduction of the Materials Genome Initiative in 2011 and the emergence of the Big Data era have led to huge databases of material characteristics, enabling engineers to easily access known material properties. The following databases exist: Materials Project, Inorganic Crystal Structure Database, Materials Genome Initiative, NOMAD archive, Topological Materials Database, Supercon, National Institute of Materials Science 2011, and National Institute of Standards and Technology with material class databases. A more complete list of material databases is in Correa-Baena et al. Negative outcomes are usually ignored. Negative data are frequently as critical for ML systems as positive outcomes to avoid bias. In areas with a history of data-driven study, such as chemistry, databases already exist. Additional data that are not necessary for a publication are typically not released, leading to publication bias. This wastes resources since other researchers must repeat the process to create a balanced dataset for ML applications. Due to the absence of consistent data formats or application programming interfaces, few databases are suitable for use with informatics approaches.

2.5 Materials informatics

Materials informatics relies on the databases above, which include data on many material characteristics. For a broad overview of materials informatics and big data in materials research, see. Materials informatics research includes standardization of representation and exchange of material data, organization, management, retrieval, filtration, and correlation of material data, material graphics, and data mining and knowledge discovery of material data. Another materials informatics review emphasizes atomic-scale modeling. However, it also encourages expanding materials databases to increase data accessibility for informatics. The increased use of materials data necessitates digitization and organization. Data must also be shareable and accessible. Evolving services like Materials Data Facility [14] and Citrination provide software interfaces for automated data searching, processing, and access. Wagner et al suggest a materials informatics approach that involves (a) initial feature assembly, (b) exploratory model development, (c) model refining for correctness, and (d) final training and deployment. Iteratively increasing complexity leads to a simpler ultimate model, boosting explainability and interpretability. Rajan et al provide a concise, philosophical study on materials informatics, which enables high-throughput, statistically robust, and physically meaningful surveying of complicated, multiscale information.

3. RESULTS AND DISCUSSION

ML for metallic material characterization

The characteristics of mechanical material properties must be accurately predicted and controlled, as they are closely related to and significantly influenced by process parameters and the resulting microstructures [15]. The fundamental concept behind employing machine learning techniques for predicting material properties involves examining and delineating the relationships—often nonlinear—between a material's properties and their associated characteristics, achieved by deriving insights from previously gathered experimental or simulated data. The mechanical behavior observed in simulations is frequently articulated through constitutive equations [15]. Investigation into the macroscopic performance of materials primarily emphasizes the relationship between their macroscopic (e.g., mechanical and physical) properties and their microstructure. Numerous material parameters can be approximated to within an order of magnitude by employing fundamental physical concepts. In instances where these parameters cannot be accurately estimated, machine learning methods can prove beneficial, necessitating the use of experimental or simulated

data. Experimental testing methods applicable to metals enhance our understanding of materials and their properties. Common destructive tests include the bend test, impact test, hardness test, tensile test, fatigue test, corrosion resistance test, and wear test, as illustrated in reference. The subsequent endeavors of the materials community to improve these tests and their outcomes through machine learning methods will be examined.

3.1 Corrosion

Detecting and monitoring corrosion is crucial for maintaining material health and decreasing life-cycle costs in various infrastructures, ships, planes, vehicles, and pipelines [6]. More recently, ML methods have showed promise in improving corrosion detection. They will aid a human inspector. This reduces inspection time and expense for civil infrastructure and eliminates the requirement for previous knowledge and human effort in feature design [12]. Popular methods include using ANNs for image processing-based corrosion detection. CNNs were used to detect corrosion by identifying rusty portions in pictures [12]. The CNN surpasses current corrosion detection methods based on texture and color analysis utilizing a multilayered perceptron network. The model uses a picture of the material and area of interest to classify it as corroded or not, using a sliding window. Pretrained networks help prevent overfitting from tiny datasets. Bastian et al. provide another CNN corrosion detection application [13]. As in Atha et al [12], pictures are divided into four classes: no corrosion, low-level corrosion, medium-level corrosion, and high-level corrosion. Additional CNN-based corrosion detection studies are available in [13]. Fang et al developed a hybrid technique using genetic algorithms and support vector regression to predict air corrosion depth in metals like zinc and steel. A hybrid technique may solve nonlinear regression estimation issues in materials science. Genetic algorithms are used to automatically identify suitable support vector regression hyper-parameters. The support vector regression inputs are temperature, wetness time, exposure time, sulfur dioxide concentration, and chloride concentration. The outputs are zinc or steel corrosion depth predictions.

An SVM technique was used by Hoang et al. to detect pipe corrosion using image processing. The pipe surface characteristics are extracted using picture texture, including statistical assessments of color, co-occurrence matrix, and run length. A decision boundary is created using SVM optimized by differential flower pollination to identify corroded and undamaged pipe surfaces by block-wise classification of the source picture. The corrosion rate of 3C steel in various environments was predicted using support vector regression and a smaller database of 46 samples. The model considered five seawater environment factors: temperature, dissolved oxygen, salinity, pH-value, and oxidation-reduction potential. The forecast error was low. Jimenez et al. evaluate ML methods (ANN, SVM, classification tree, and k-nearest neighbor) for 316L stainless steel pitting corrosion detection. Model inputs include environmental factors including chloride concentration, pH, and temperature, while outputs indicate material corrosion. Models based on ANNs and SVM with linear kernel were shown to be useful. For this application, ANN and SVM models outperform k-nearest neighbor and classification tree models in classification. The main benefit of this method over previous methods is that surface analysis is not required to examine corrosion behavior of a material.

3.2 Fatigue

ML techniques may also forecast fatigue, which is generated by cyclic loads and causes structural deterioration and fissures. Shiraiwa et al presented multi scale FEM and ML to forecast fatigue in welded constructions for various structural materials. Two algorithms are used: deterministic ML based on classical approaches and model-based ML. Deterministic ML, like multivariate linear regression and ANNs, forecast fatigue strength using chemical composition, processing parameters (e.g. reduction ratio, heat treatment), inclusion sizes, and fatigue strength. Microstructures and stress-strain curves from 40 low-carbon steels with varying chemical compositions and heat treatment conditions were utilized to train an ANN for model-based ML. This technique accounts for uncertainties like fatigue life scattering and incorporates previous structural and property information. Agrawal et al [8] used ML algorithms to predict fatigue strength of steel based on composition and processing parameters, including chemical composition, upstream processing details, heat treatment conditions, and mechanical properties. ML approaches included simple regression, decision

trees, SVM, and ANN. Successful strategies included ensemble and personalized approaches for various topics. The hold time in fatigue testing has been used to forecast material fatigue life for P91 steel base metal using machine learning methods. High accuracy is achieved by combining genetic algorithms and SVM to forecast fatigue life. Abdalla et al [2] provide a fatigue life model for steel reinforcing bars using an ANN radial basis function model, including maximum tensile strain and pressure ratio.

3.3 Creep

Metal creep occurs under strains below the yield strength, often at high temperatures. Creep rupture now poses a significant threat to power production systems in high-temperature and irradiated settings, such as nuclear reactors. Predicting creep rupture and usable life are necessary to prevent component failure and cost-ineffective operation. Analytical approaches struggle to represent the complex interdependencies between chemical composition, heat treatment parameters, product shape, tensile characteristics, and microstructure, which impact material behavior. Modeling using ML methods is a promising option. Additionally, ML eliminates costly and lengthy experimentation. For material design, creep is significant. Many designs just address one purpose, such as creep, without considering multi-property design. Another prominent model for creep rupture life and rupture strength of austenitic stainless steels is ANNs. The training database for predicting creep rupture life and stress for a given stress includes test conditions (stress and temperature), chemical composition, solution treatment temperature, time (limited availability), quench following, grain size, and ruptured life logarithm for various stainless steels. Chatzidakis et al. evaluate general regression neural networks, ANNs, and Gaussian processes to anticipate creep rupture tendencies. Results from experimental creep ruptures are input. The models' performance was inadequate. Shin et al used five ML models (RF, linear regression, k-nearest neighbor, kernelridge, Bayesian ridge) to predict creep behavior using Lambert-Miller parameters. Out of 466 available features, useful ones are identified via optimization and experimentation with various feature and model combinations. RF had highest accuracy with 5–21 top-ranking attributes. A multilayer perceptron neural network was used to forecast rupture and creep rupture stress of 9%Cr steels using chemical composition, heat treatment information, and geometrical shape.

3.4 Tensile properties

Material tensile properties reveal how it responds to tension. Understanding modulus of elasticity, elastic limit, elongation, proportional limit, area reduction, tensile strength, yield point, and other qualities requires tensile properties. Material condition, lifespan, and application performance depend on these qualities. Tensile properties must be accurately predicted to determine structural material service life. The ultimate tensile strength (UTS) of iron castings was predicted utilizing 25 factors, including composition, size, cooling speed, and thermal treatment, to forecast foundry defects and mechanical qualities. The many variables and conditions in casting make UTS estimate one of the hardest tasks in foundry manufacturing. UTS classification using Bayesian networks, k-nearest neighbor, and ANNs. All methods performed well, but ANNs outperformed others. Sterjovski et al. employed ANNs to forecast impact toughness of quenched and tempered pressure vessel steel, heat affected zone hardness in pipeline and tap fitting steels, and hot ductility and UTS of microalloyed steels over temperature. Inputs were composition, cooling rate, temperature, and thickness. All mechanical features were predicted using ANNs. ANNs may predict elongation, self-tempering temperature, and yield strength for reinforcing steel bars undergoing thermo-mechanical treatment using bar diameter and quenching duration, according to Sankaretal[130]. ANN numerical results match experimental data. Prune and predatorprey algorithms helped Datta et al. extract more data from input data than ANN analysis. Alloy composition, thermo-mechanical processing parameters, deformation in different temperature zones, final rolling temperature, and cooling rate were inputs for high-strength steels, while UTS, yield strength, and % elongation were anticipated. For this steel, solid solution hardening and microstructural components drive yield strength, whereas precipitation hardening drives UTS. Both strengthening procedures reduce ductility.

Tensile properties may be predicted using traditional machine learning. Shigemori et al. estimated hot-rolled steel tensile strength using locally weighted regression. The inputs were 18 chemical

composition, heating, rolling, and cooling temperature components. These variables clearly cause output. Least squares SVMs forecast material elastic modulus and yield stress. studies Al6061 and Al7075 FEM-simulated load-indentation curves to estimate material characteristics utilizing a training set of huge strain-large deformation FEM simulations. We employ load-indentation curve characteristics in ML. Using load-indentation data from dual conical indenters with different half-angles, the least squares SVM model predicts elastic modulus and yield stress. RAFM steel production material composition and treatment parameters were correlated with yield strength, impact toughness, and total elongation using an RF model and optimization algorithm. Tempering temperature, C concentration, time, and Cr content correlated well for yield strength and elongation. RF generalization and accuracy were high (R2 >85%). Fragassa et al. used pattern recognition analysis on experimental data and RF, ANN, and k-nearest neighbor to forecast cast alloys' yield strength, ultimate strength, ultimate strain, and Young's modulus. Every data originates from micrographs. UTS and yield strength prediction are better with ANNs. Acoustic emission data interpretation for failure prediction is another ANN usage. Christopher et al. predict Al/SiC composite strength using acoustic emission parameters and ANN analysis. Acoustic emission response and an ANN back propagation algorithm were used to evaluate unidirectional T-300/914 tensile specimen ultimate strength.

Hot ductility must be regulated to prevent cast steel surface cracks. Experimental work is challenging. Hot ductility prediction using ML models is advised. One research predicted hot ductility using a multivariate linear regression and grouped 12 chemical ingredients with similar experimental results. This model's cooling condition varies from continuous-casting conditions, making it difficult to utilize in industry. Hot ductility for microalloyed steels at continuous casting temperatures for strand or slab straightening is predicted using back-propagation ANN. Limited data preclude generalization. Since the ANN has one hidden layer, it cannot properly reflect the complex input-output relationship. Additionally, an ANN model predicted high-temperature ductility of steel grades based on composition and thermal history (five experimental parameters). The new model predicts ductility across a wider composition and heat history than previous studies. It works well in commercial manufacturing.

4. CONCLSIONS

In materials research, data-driven methodologies are crucial for identifying correlations between material structure and characteristics. Relationships are typically nonlinear. Finding common patterns across different length and durations is challenging. Experiments alone cannot do this. Thus, data-mining methods are essential for identifying correlations in experimental and simulated data. As publicly accessible materials data expands, ML approaches may extract scientific principles and design guidelines that traditional analysis cannot. Early ML applications in materials science mostly used basic methods like linear kernel models and decision trees. Despite the paucity of benchmarking datasets and standards, these proofs-of-concept exist for several applications. At present, ML may not achieve desired accuracy in certain jobs owing to inadequate data. A highly accurate model trained on a limited, accurate data set is only useful inside the input space, but lacks generalization, whereas a less accurate model trained on a larger data space is more generalizable but less precise. Accelerating the creation of public material databases is crucial for the advancement of machine learning in materials research. Lack of failure data hinders the construction of accurate ML models. A culture change towards publishing all legitimate facts, good or bad, is necessary.

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