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MACHINE LEARNING FOR MATERIAL CHARACTERIZATION WITH AN APPLICATION FOR PREDICTING MECHANICAL PROPERTIES

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ABSTRACT

Currently, the growth of material data from experiments and simulations is expanding beyond processable amounts. This makes the development of new data-driven methods for the discovery of patterns among multiple length scales and time-scales and structure-property relationships essential. These data-driven approaches show enormous promise within materials science. The following review covers machine learning (ML) applications for metallic material characterization. Many parameters associated with the processing and the structure of materials affect the properties and the performance of manufactured components. Thus, this study is an attempt to investigate the usefulness of ML methods for material property prediction. Material characteristics such as strength, toughness, hardness, brittleness, or ductility are relevant to categorize a material or component according to their quality. In industry, material tests like tensile tests, compression tests, or creep tests are often time consuming and expensive to perform. Therefore, the application ofML approaches is considered helpful for an easier generation of material property information. This study also gives an application of ML methods on small punch test (SPT) data for the determination of the property ultimate tensile strength for various materials. A strong correlation between SPT data and tensile test data was found which ultimately allows to replace more costly tests by simple and fast tests in combination with ML**.**

KEYWORDS

Machine Learning, Material Characterization, Small Punch Test, Tensile Properties, Ultimate Tensile Strength

INTRODUCTION

The field of materials science relies on experiments and simulation-based models as tools for material characterization [7]. Material properties, such as their structure and behavior, are critical to the potential application of the material of interest. More recently, the data generated by such experiments and simulations have created various opportunities for the application of data-driven methods. In addition to, for example, the experimental trial and error approach or a physical metallurgy approach, machine learning (ML) methods for property prediction and material design have attracted a lot of attention in recent years, see for example, [33, 109, 162]. While experimental investigations (the so-called first paradigm of materials science) have been carried out since the stone and copper age, scientists of the 16th century started to describe physical relations by equations (second paradigm). Thus,

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analytical equations became a central instrument of theoretical physics which were able to complement the empirical and experimental sciences. The 1950s marked the beginning of computational materials science and simulations, the third paradigm. Within this framework, computer experiments and simulations became possible, with the corresponding results being analyzed and interpreted like measured ones. It had to be recognized that many properties of materials cannot be described by a closed mathematical form as they are determined by several multilevel, intricate theoretical concepts. With the help of large amounts of data, hidden correlations, reflected in terms of structure and patterns in the data can be discovered that are not normally visible in small data sets. Thus, the fourth paradigm, data-driven science, of materials research was born [7, 34]. However, it is not only an advantage to have a large data volume but it can also be a challenge to cope with tremendous amounts of data. Today, data are indeed more andmore easily acquired and stored, due to huge progresses in sensors and ways to collect data on one side, and in storage devices on the other side.Nowadays, there is no hesitation inmany domains
in acquiring very large amounts of data without knowing in advance if they will be analyzed and how. The spectacular increase in the amount of data is not only found in the number of samples collected for example over time, but also in the number of attributes, or characteristics, that are simultaneously measured on a process. Data are gathered into vectors whose dimension corresponds to the number of simultaneous measurements on the process. Growing dimensions result in high dimensional data, as each sample can be represented as a point or vector in a high-dimensional space. Working with high-dimensional data means working with data that are embedded in high-dimensional spaces [159]. The curse of dimensionality is the expression of all phenomena that appear with high-dimensional data, and that have most often unfortunate consequences on the behavior and performances of learning algorithms. Contrary to the curse of dimensionality, databases in materials science are often limited in size due to expensive and
time consuming data acquisition via experiments or simulations [136]. Then the insufficient data size for the training of a ML model compromises the learning success and suitable new approaches for small datasets have to be found. Thiswork contains a literature survey which covers an overview ofML for materials science and specifically for metallic material characterization. As the measurement of such parameters is often expensive and time consuming obtained via experiments, alternative basic tests, such as the small punch test (SPT) can be an option if it can be shown that the same material property information can be extracted.
There is a wide range of ML approaches based on SPT data which will be presented.

STATE OF THE ART

Overview—ML for materials science

With ML, given enough data and a data-driven algorithm for rule discovery, a computer is able to determine physical laws which lead to the given data without human input [19, 68]. Traditional computational approaches use the computer for the employment of a hard-coded algorithm provided by a human expert. By contrast, ML approaches learn the rules that underlie a dataset by assessing a portion of that data and building a model to make predictions [19]. However, the human still needs to choose suitable ML models which supposedly represent the data well and do manual (sub-)tasks in preprocessing and feature generation. The existence of large amounts of data makes the use of ML models

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possible and enables data-driven knowledge to be obtained and patterns to be discovered. On the other hand, big data and their high dimensionality lead to difficult computational and statistical challenges, such as scalability and memory shortage, noise accumulation, interference correlation, incidental endogeneity, and measurement errors [40]. Materials science is an interesting field of application for big data methods and ML approaches which is beginning to show enormous promise. Four primary elements are critical in materials science and engineering: processing, structure, properties, and performance [110, 115]. There is no general agreement, however, on how these elements are interconnected. ML methods can be applied to the so-called process-structure-property-performance chain for learning more about the intrinsic interrelations of these components. One main goal is the enabling, acceleration, and simplification of the discovery and development of novel materials based on the convergence of high-performance computing, automation, and ML [27]. Another aim of using such approaches in the field of materials science is to achieve high-throughput identification and quantification of essential material properties [15]. Besides experimentally obtained datasets, numerous studies draw required information from simulation-based data mining. Altogether, it is shown that experiment- and simulation-based data mining in combination with ML tools provide exceptional opportunities to enable highly reliant identification of fundamental interrelations within materials for characterization and optimization in a scale-bridging manner [15]. For more detailed information on recent ML applications in materials science we refer to the general reviews of
Mueller et al Wagner et al , Dimiduk et al , or Wei et al . Examples for successful applications of ML techniques in materials science are, for example, to represent inorganic materials predict fundamental properties create atomic potentials , identify functional candidates analyze complex reaction networks or guide experimental design high-throughput phase diagrams and crystal structure determination

Open problem—interpretability

However, one of the major criticisms ofML algorithms in science is the lack of novel understanding and knowledge arising from their use. This ismostly becausemore complex ML algorithms are often treated as black boxes. Thosemachine-built models are hard to understand for humans. For a better acceptance ofMLmodels, data scientists aim to establish clear causal relations between materials structure defined broadly across length scales and properties. Especially scientific models have further constraints such as a minimal number of parameters and adherence to physical laws. It is the obligation of the data scientist to translate the results
of their work into knowledge other scientists can use in aiding for examplematerials discovery or deployment . Useful techniques for finding simple, reduced and interpretable models are for example principal component analysis (PCA) , cross-validation and regularization, and a thoughtful choice of model. PCA is a powerful technique for data dimensionality reduction. Large datasets are increasingly widespread. In order to interpret such datasets, PCA can be applied to drastically reduce their dimensionality in an interpretable way, such that most of the information in the data is preserved PCA extracts the orthogonal directions with the greatest variance from a dataset, the resulting principal components being linear combinations of the original variables. However, principal components are not necessarily simple to interpret physically but as the extracted features are linear combinations of the original variables they can still be intuitively explained.

Moreover, it allows a very straightforward data visualization
through data projection onto the main extracted components . However, PCA might be the wrong choice if features are not covariant. Another way to achieve interpretable ML models is intelligent feature selection for dimension reduction and thus easier interpretability. Regularization of a model entails adding a tunable penalty on model parameter size to the cost
function being minimized leading to a reduced feature space Furthermore, the choice of ML model has an immediate impact on its explainability. Regressions lead to coefficients whose size gives information about the relative size effect of modifying an input on the output. Decision trees are set up like flow charts and therefore easy to read. More complex models such as artificial neural networks (ANNs) are missing a clear explanation of the machine's "thinking" due to complex node interactions. But methods such as feature visualization or attribution exist, which allow a better understanding and interpretability of black box models. However, sometimes it might be reasonable to trade model accuracy for better explainability.

DISCUSSION AND CONCLUSIONS

This survey addresses applications of machine learning strategies inmaterials science for material characterization. There exists a wide range of promising applications for ML in materials science, for example, material discovery, molecular dynamics, and global structural prediction. The demand for new approaches dealing with limited data is huge. It was shown that data-driven approaches play a significant role in materials research in order to find relationships between the structure of amaterial and its properties. These relationships are often not linear. It is difficult to find generic patterns among multiple length scales and timescales. With experiments only, this cannot be achieved Therefore, data-mining techniques are indispensable for the recognition of correlations in the (experimental and simulated) data. As the amount of publicly available materials data grows, ML techniques in particular will be able to extract from these data sets scientific principles and design rules that could not be determined through conventional analysis. The majority of early ML applications to materials science employed straightforward and simple-to-use algorithms, like linear kernel models and decision trees. Now, these proofs-of-concept exist for a variety of applications even though there is a lack of benchmarking datasets and standards. To date,MLoften cannot realize the expected accuracy when applied to some tasks due to insufficient material data. Therefore, a more accurate model that was trained on a small but accurate data set is only meaningful within the input data space but does not generalize well while a less accurate model on a wide input data space is better at generalization but less exact. Therefore, accelerating the construction of publicly accessible material databases is highly important for the future development of ML in materials science. Another issue that holds back the development of precise ML models is the absence of failure data. In this case, a cultural shift toward the publication of all valid data, may it be positive or negative, is required. The majority of ML approaches in materials science is based on ANNs. However, conventional ANNs still suffer from several weaknesses such as the need for a large number of controlling parameters, the difficulty in obtaining stable solutions, the danger of overfitting and thus the lack of generalization capability [41]. However, ANNs have been enormously successful in understanding complex materials behavior, such as mechanical behavior (flow stress, hardness, tensile strength, fracture strength, and fatigue behavior) of metal alloys subjected to certain heat treatment and/or deformation procedures, as well as

in the prediction of micro-structures and phases resulting fromheat treatment and/or deformation processes. The most practical way to capture the complex dependence of a desired macroscopic property on the various process parameters is through such learning methods . ANNs have the potential to minimize the need for expensive experimental investigation and/or inspection of structural materials used in various applications, hence resulting in large economic benefits for organizations. In addition to ANN hybrid ML models or ensemble methods work well . For this, multiple independent models are built and the final regression or classification result is usually obtained as an average over the ensemble. In this way, additional noise is introduced into the fitting process and overfitting is avoided. However, there does not exist an overall solution that can be considered the best. The most appropriate model has always to be found specifically for the application and data situation. Furthermore, this paper focuses on ML based material property prediction from SPT data. Such simple material tests have gained popularity over the last couple of years because even though they are cheap and simple to perform, they make accurate material characterization possible, especially for failure analysis and remaining life assessment of in-service components or structural parts. Nevertheless, a few disadvantages have to be taken into consideration. The small sample size might not represent the bulkmaterial; the sample size effect influences thematerial properties; and the results of the SPT are sensitive to test parameters. However, also for SPT data, ML based models are popular for material parameter prediction.Most commonly found are ANNs, especially in combination with FEM for data generation. No application of traditional ML models to SPT data was found in the literature. The paper concludes with an application example which uses FDCs of structural materials as the basis for predicting he UTS. SimpleML approaches presented here, such as linear regression models or RFs provide good results for predicting the UTS based on SPT data, even for a very small database. As a consequence, it is possible to confirm the benefit of simple ML techniques in predicting mechanical properties such as the UTS based on as simple material tests as the SPT and the authors are sure that ML will positively shape materials science for the years to come.

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