Intelligent Data Analysis for Materials Obtained Using Selective Laser Melting Technology

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Abstract. In this study, we present a software solution (toolkit) for intelligent data analysis obtained using the selective laser melting (SLM) technology. We have developed a program that uses Data Science approaches and machine learning (ML) algorithms for analyzing and predicting the mechanical properties of materials obtained using the SLM method. The program was trained on a large dataset of SLM materials and was able to achieve an accuracy of 98.9% in terms of the average particle size, using a combination of crystal plasticity and finite element methods (CPFEM) for the Ti-6Al-4V alloy. It allows predicting mechanical properties, such as yield strength, ductility, and toughness, for the structures of Ti-6Al-4V and AlSi10Mg alloys. The study proposes an approach to intelligent data analysis of properties and characteristics of various materials obtained using the SLM technology, based on a formed multidimensional digital model of processes using the developed software solution. The developed set of technologies for intelligent data analysis aimed at optimizing the SLM process demonstrates the potential of machine learning algorithms for improving understanding and optimization of materials obtained through additive manufacturing technologies. Overall, our research emphasizes the importance of developing intelligent solutions for data analysis in materials science and engineering, especially for additive manufacturing technologies such as SLM. By using the developed toolkit that applies machine learning algorithms, specialists can minimize technological production and implementation costs up to 1.2 times, by optimizing the processes of designing and developing materials for various applications, from aerospace industry to biomedical engineering.

Keywords: Selective Laser Melting · Intelligent Data Analysis · Machine Learning · Data Science · Additive Manufacturing Technologies · SLM DS Framework

1 Introduction

The additive manufacturing technology, also known as 3D printing, has revolutionized the way products are produced. Among various additive manufacturing techniques, selective laser melting (SLM) is one of the most promising technologies for producing

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complex geometries with high part accuracy from metal powders. However, the quality and properties of the final product strongly depend on the process parameters and the properties of the raw materials used [1].

To address this issue, a suite of data analytics technologies has been developed to optimize the SLM process and predict the properties of the final product. In this article, we present an intelligent solution for analyzing material data obtained during the SLM process.

The developed solution allows for the collection, storage, and processing of data, including external and/or unstructured data, using artificial intelligence algorithms. This enables a better understanding of the processes involved in SLM and increases the accuracy of predicting the properties and quality of the final product.

The solution employs various artificial intelligence methods and algorithms, such as machine learning, statistical analysis, and clustering algorithms, to discover hidden patterns and predict material properties based on the raw material composition and process parameters. Furthermore, the developed solution also allows for the optimization of the SLM process by modeling conditions and predicting optimal process parameters [2] to achieve desired quality and performance criteria. This reduces the time spent on technological stages by automating the process and optimizing quality management, significantly increasing the efficiency of the SLM process.

The aim of this work is to investigate the potential of intelligent data analysis for materials obtained by SLM technology using the developed software solution and to evaluate its effectiveness. The research hypothesis is that the developed software solution will significantly improve the quality and conformity of the sample to the specified characteristics and reduce the stages of the technological process by implementing the prediction of the properties of the obtained material, which, in turn, can lead to improvements in the design and production process of products manufactured by SLM technology.

To achieve the set goal, the following tasks were addressed in this work:

- development of a software solution for collecting, storing, and processing data on materials obtained using SLM technology, using artificial intelligence algorithms;
- analysis of the effectiveness of the developed software solution based on data obtained in experiments with materials obtained using SLM technology.

2 Materials and Methods

To implement intelligent data analysis of the physical, mechanical, chemical, and technological properties of samples grown in different spatial arrangements within a selective laser melting chamber, with the aim of creating an intelligent database of material properties obtained through the selective laser melting process, a software solution was developed for data collection, storage, and processing, including external and/or unstructured data, using artificial intelligence algorithms [3]. For this purpose, a materials property database was created to support and collect information on metallic, polymeric, and ceramic materials at all stages of production, as well as to compare the characteristics obtained during material and/or structure use [4].

Metallic, polymeric, and ceramic materials produced using the SLM process were selected for the study. The description of the studied objects includes characteristics such as size, shape, structure, composition, and other properties.

The quality of the initial components is critical for predicting the mechanical, physical, chemical, and technical characteristics of the obtained samples. In this study, only high-quality components that meet all SLM technology requirements were used.

All data were collected at all stages, starting from the manufacturing stage, with the fixation of input parameters based on the applied source material and manufacturing parameters, and ending with the testing stage, including the methods and techniques of testing and the physical, chemical, mechanical, and other characteristics obtained, with the accumulation of this information in the materials property database.

The materials property database enables data collection from various sources using appropriate connectors, including open, closed, and external sources, and includes the following sections: sample acquisition modes, composition of source components, sample microstructure, stress-strain diagram, ultimate strength, elasticity, Young's modulus, endurance limit, physical characteristics (thermal conductivity, density), technological characteristics (bendability, cutting), impact toughness, hygroscopicity, gas permeability, gas evolution, and others.

The tools and techniques used for data collection and analysis include various data analysis methods, statistical analysis, and analysis of the obtained results.

The main method of data analysis in this study is machine learning and artificial neural networks, which allow for the creation and use of pre-trained machine learning models for predictive analysis of technological parameters to obtain a sample with specified characteristics.

Consider various ML approaches including neural networks, ensemble approaches, Image Processing Methods, clustering algorithms, classification and regression analysis which have proved to be a very useful tool in the study for material analysis.

Multilayer neural networks (MNN) trained on extensive datasets including experimental results and SLM process parameters have proved to be a highly effective tool. They facilitate the identification of complex and hidden relationships between various input variables and material structure. When investigating the accuracy of the model, we included ensemble methods in terms of combining several ML models: Random Forest, Gradient Boosting and numerical method Concurrent Processing Finite Element Model. This allowed us to gain a deeper insight into the processes underlying the creation of materials using SLM technology.

In addition, genetic algorithms and evolution-based optimization have been investigated - these methods can be used to find the best SLM process parameters based on given target material characteristics.

In addition to neural networks, image processing methods have also been actively introduced, which are designed to analyze microscopy of materials obtained during experiments. They help to identify and characterize structural features of the material, such as pores, microstructures and defects. The information obtained has proven to be very valuable in assessing the influence of material structure on its properties.

In addition, various clustering, regression and classification algorithms have been investigated in order to categorize different types of materials and to identify patterns depending on the process parameters, depending on the problems under consideration:

- to study the properties of materials obtained using SLM technology over time and predict their future values, time series analysis may be used;

- to determine the degree of correlation between various characteristics of composite materials and identify the factors that have the greatest influence on their properties to uncover hidden or explicit dependencies, correlation analysis is used;
- to study individual groups of materials based on their characteristics and determine which properties are characteristic of each group, classification algorithms are used.

When performing intelligent analysis of heterogeneous data sets of physical, mechanical, chemical, and technological properties of samples grown [5] at different spatial locations in the growth chamber, the following steps must be taken:

- data storage – this is the first step in intelligent data analysis, which includes developing a method of storing data that will be used in the study;
- data validation – this step involves checking the data for reliability and correctness. It allows you to exclude possible errors and ensure that the data is ready for use;
- data pre-processing and analysis – this step includes data processing to prepare them for use in the analysis, including cleaning the data from outliers, converting the data into a convenient format, and/or selecting a subset of features for further analysis;
- training – at this stage, machine learning models are trained on the processed data.

After training the machine learning models, they can be tested on data sets that were not used in the training process. Various approaches, such as cross-validation, data sampling, and others, can be used to improve the quality of the machine learning models. In cross-validation, the model is tested on multiple data sets, which allows for a more accurate assessment of its quality. Stratified data sampling may be used to consider the distribution of classes in the sample. If the model shows high accuracy and meets the criteria set for testing, this confirms its suitability for use in predicting material properties, classifying materials based on their properties, and identifying dependencies between different properties.

To conduct the study, a sample of 100 specimens was selected for static testing, which were produced using the SLM technology from the following materials: polyamide P2200, steel 316L, titanium alloy Ti6Al4V, and aluminum alloy AlSi10Mg. The test objects were characterized by material properties such as strength, elongation, elasticity, min-max bending, thermal properties, and others. Qualitative input components, as well as data on manufacturing process parameters, were used to predict [6] these characteristics. The specimens were made from different materials and with different manufacturing parameters, including melting temperature, printing speed, size, and shape of the specimen [7].

Various testing instruments and techniques were used to collect data on the materials being developed, such as strength, stability, and wear analyses under different operating conditions. Standard testing methods, such as tensile and bending tests, were used to measure mechanical characteristics. Differential scanning calorimetry (DSC) [8] and thermogravimetry (TGA) [9] methods were used to measure thermal properties. X-ray diffraction (XRD) [10] and scanning electron microscopy (SEM) [11] methods were used to study physical characteristics of the materials. Data was recorded at all stages, from manufacturing with input parameter fixation to testing stages, including testing methods and obtained physical, chemical, mechanical, and other characteristics [12].

To compare the obtained results with the data obtained during the operation of the material and/or constructions, standard testing and result comparison methods [13] were used. One of them is comparison with reference values, which serve as a reference point for comparing the obtained results [14]. These can be formed from standard regulatory technical requirements for materials/constructions, such as GOST, as well as from previous research. Comparison with reference values allows determining whether the obtained results meet the requirements and whether the research goals have been achieved. Another method is comparison with previous data on similar materials. This approach allows comparing obtained results with those obtained in previous studies, which helps to test hypotheses about the results of the research, as well as to identify any differences or unexpected results [15]. Comparison with data obtained from other testing methods is also used to compare results obtained using different methods to confirm the adequacy of testing methods and the possibility of replicating results in other conditions. These methods can be used together or separately to compare results and verify the accuracy of obtained data. They can also be used to assess the quality and accuracy of machine learning models trained on data obtained from experimental tests.

3 Results and Discussion

A solution for investigating materials manufactured using the SLM technology utilizes several ML approaches (Neural Networks, Image Processing Methods, Clustering and Classification Algorithms, and Regression Analysis), including two stages: defining the structure of input experimental and/or modeling data and predicting properties and process parameters that are necessary for understanding the fundamental material properties and fine-tuning the equipment. Exploring the correlation between the structure and properties of materials requires data collection that contains a feature space covering atomic and/or local structural descriptors. These descriptors are assumed to reflect characteristic physical mechanisms and microstructural details for the existing set of materials. They can include atomic properties of elements and atomic fractions in multi-component materials, as well as various indicators such as lattice distortion and local crystallography in metallic systems. This requires constant access to sufficient volumes of data, which include data obtained from high-performance modeling, extensive experiments, mechanical testing and microscopy, as well as from existing material databases and other heterogeneous sources.

The structure of the SLM material investigation process using the developed intelligent analysis solution (see Fig. 1).

Thus, the developed solution allows obtaining new knowledge and information from material properties databases, which can be used to improve the production process, develop new materials, and create innovative technologies.

Studying the relationship between material structure and properties requires collecting data that contains a feature space covering atomic and/or local structural descriptors. These descriptors presumably reflect characteristic physical mechanisms and microstructural details for the existing set of materials. This may include atomic properties of elements and atomic fractions in multicomponent materials, as well as various indicators such as lattice distortion and local crystallography in metallic systems. The "Experiment Settings" window (see Fig. 2).

Fig. 1. The SLM material analysis process using machine learning.

To record the results of sample analysis, the "PropertiesOfSamples" table is used, which stores the properties obtained from the analysis of each specific sample. After fixing the property values, they can be changed for a particular sample during subsequent analyses. Additionally, in the "Sample Production" section, there is the "Condition" table that contains information about the state of a specific manufactured sample at a given time. For instance, it can indicate that the sample is in the process of testing or has already passed a check for certain properties.

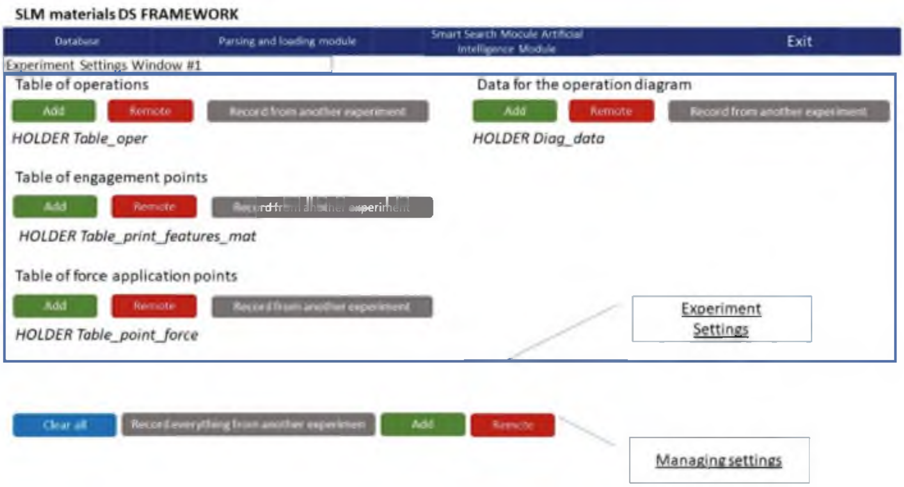

Fig. 2. The experiment settings window.

The “ProductionBatches” table is used to control the production of samples, storing information about the production batches of samples. It includes data such as the production date, the number of manufactured samples, and other necessary data for production control. Moreover, the “SampleRest” table stores information about the remaining samples, such as the date of manufacture, the number of manufactured samples, and the stock balance.

As evident from the description of these tables, the functionality of the solution allows for the use of a combination of local and global attributes to form a dataset of objects that can be analyzed to optimize the volumetric physical properties of materials [1]. For example, with a dataset of metal alloys, we can use information about internal interatomic interactions, hardness, elasticity, ductility, and impact toughness to determine the quantitative relationship between the alloy’s structure and its physical properties. The predictive aspect of machine learning enables this to be done without prior assumptions, solely based on existing data.

Such an approach plays a crucial role in studying new engineering materials, allowing for a quick and accurate assessment of how changes in structure can affect the physical properties of the material. Furthermore, based on the obtained data, the material’s structure can be optimized to achieve specific physical characteristics. Overall, the well-designed structure of tables and entities allows for efficient management of the sample production and analysis process, quality control, and research to improve material properties and production processes. Therefore, intelligent data analysis enables the acquisition of new knowledge and information from the material properties database that can be used to improve production processes, develop new materials, and create innovative technologies.

The solution uses several ML approaches, including supervised, unsupervised, and reinforcement learning methods, to analyze data. These methods allow for the determination of material properties, the prediction of their properties, and their management using appropriate models. The output data of the solution is presented in various formats, including electronic and print formats. The structure of the Data Science process for investigating the features of SLM materials using ML methods (see Fig. 3).

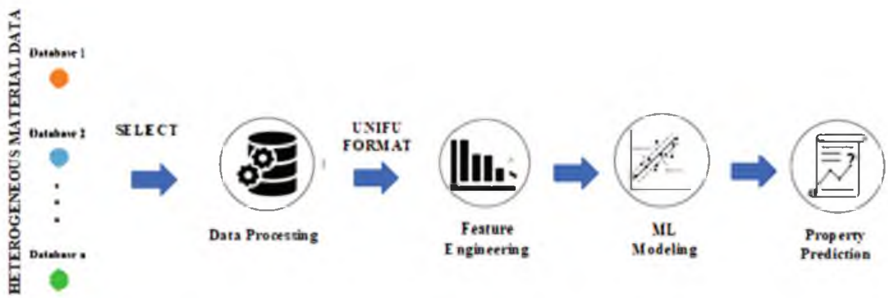

Fig. 3. Data Science approaches used in the study of SLM material traits by ML methods.

In addition, the system allows retraining existing machine learning models on added or existing datasets, providing the ability for more accurate predictions and optimization of material properties based on new data. The user interface provides a wide range of tools for flexible customization of the machine learning pipeline in modeling and research. It includes various tools such as connectors, visualization, preprocessing, models, saving reports to an external file, and evaluators. The number of pipeline steps is unlimited, and multiple visualizations or preprocessings [5] can be used in succession. When selecting a tool in the panel, the available parameters specific to that tool change. The list of tools is stored in a database (DB), where the module name, user name, and brief description of the method are stored. Python script files are stored under the same name.

Tools of the same type have the same input and output format, which allows for easy scaling of the number of tools as needed and according to the scale of the problem being solved. All steps are saved in the pipeline table and will be available for further editing. It is also possible to fix the final model by assigning it a necessary name and using it for quick predictions at any time. The workspace of the intelligent analysis pipeline of LSM materials (see Fig. 4).

The final generated model represents a single Python script that combines all data operations for a specific pipeline. The data should be passed to this model [1] in the format it was received from the connector/source. All data preprocessing will be performed by the script, which will output the results. This approach is a universal one, combining data analysis and DS methods, ensuring easy scalability and flexibility for solutions.

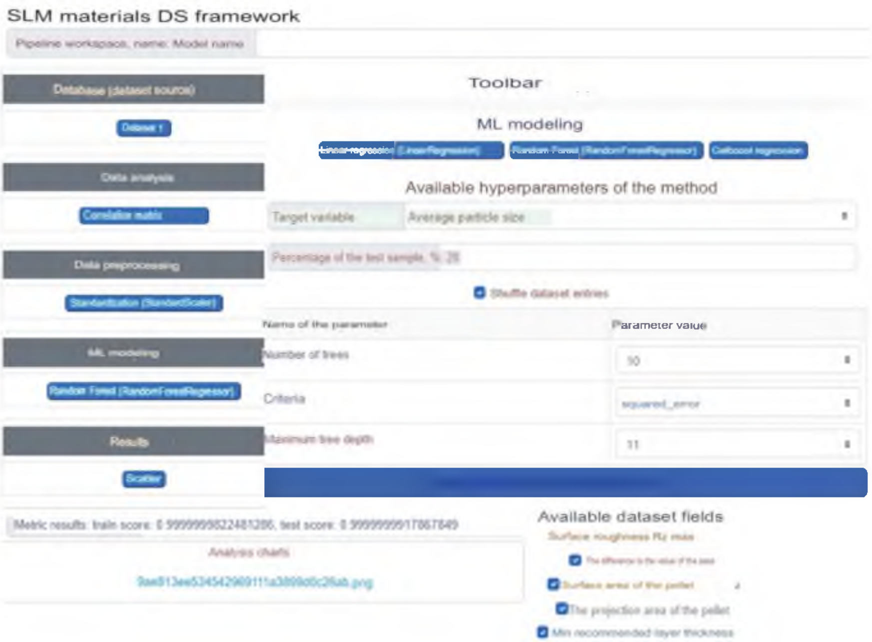

Fig. 4. The working area of the pipeline of intelligent analysis of LSM materials.

To evaluate the quality of prediction models, data on the operation of obtained materials and/or constructions was used. The research results showed that the use of intelligent data analysis can improve the quality of obtained materials and accelerate the process of their creation.

When it comes to SLM metals, volumetric elasticity is one of the functional properties that largely depends on electronic structures, chemical bonds, atomic-molecular arrangement, production history, and thermal treatment. This makes material design a complex task for materials scientists.

In our experiment, data analysis was performed to predict stresses during the tension of metallic materials, such as aluminum alloys, steel, and Ti-6Al-4V alloy at different temperatures, deformation rates, and applied deformations. To achieve accurate assessments of yield strength, hardness, ductility, elasticity, fatigue properties, and fracture toughness, a neural network [1] was used, which was trained to find the optimal alloy composition in combination with thermal treatment parameters.

In addition, intensive research work has been carried out in the field of amorphous metals. The modeling graph and yield strength evaluation of the composition were conducted with the use of solid solution strengthening structure in accordance with the specified strength properties that depend on the composition. Empirical measurements combined with a relevant set of parameters [16] were used to tune the parameters of the gradient boosting trees algorithm (see Fig. 5).

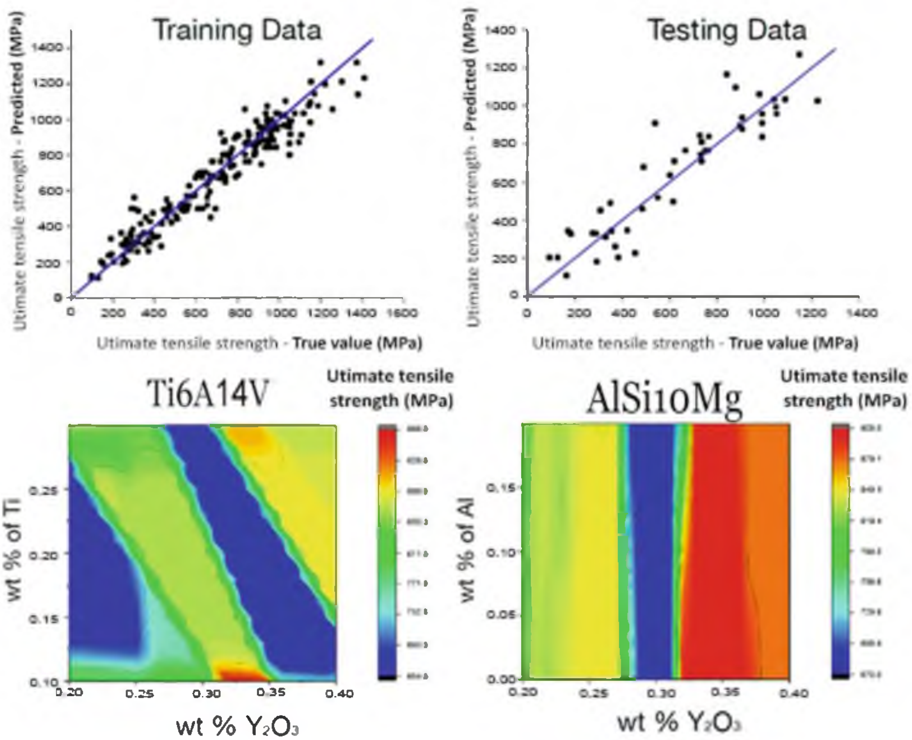

Fig. 5. Simulation and yield strength estimation graph of Ti-6Al-4V and AlSi10Mg composition.

In this research, we conducted experiments aimed at investigating crystal deformation in polycrystalline metals and alloys, with a focus on Ti-6Al-4V material. Our solution also allows the investigation of Digital Image Correlation (DIC) and Multiscale Material Modeling (MI) techniques combined with machine learning.

Initially, samples of Ti-6Al-4V material were prepared for subsequent analysis. These samples were subjected to experiments using a variety of previously reported techniques, including ultra-high resolution electron backscatter diffraction (EBSD) and surface profilometry. EBSD provides information about the microstructure of the crystals in the sample, while profilometry allows the measurement of surface strain.

The next step was to create models to analyze the deformation in the Ti-6Al-4V material. For this purpose, crystal plasticity and finite element modeling (CPFEM) techniques were used to create mathematical models to predict the deformation behavior of the material.

The next aspect of the study was the correlation between the data obtained from experiments (EBSD and profilometry) and the results predicted by CPFEM methods. In this step, a comparison between the deformation fields obtained from CPFEM models and real deformation measurements on the specimens was performed [17].

In addition, neural networks were employed to analyze and interpret the data obtained by DIC and MI in order to trace complex patterns and dependencies in the data, which in the final solution improved the accuracy of the analysis and provided a better understanding of the crystal deformation processes in Ti-6Al-4V material. The neural network was organized as a Convolutional Neural Network (CNN), which is a typical choice for image analysis.

The input layer accepts images obtained from DIC and MI methods. The convolutional layers were used to extract features from images (detect patterns and structures in deformed materials). Full-link layers accept the extracted features and performed analysis to further interpret the data. The output layer generates the analysis results including information about deformation and material behavior.

To optimize the neural network structure and its hyperparameters, we used a genetic algorithm. This method allowed us to systematically modify the network architecture, select optimal activation functions, the number of layers and their sizes, and tune other parameters to achieve the best results in analyzing deformation data.

Thus, very good agreements were obtained, and the solution demonstrates the application of CPFEM methods for studying plasticity and deformation in Ti-6Al-4V alloy with the use of ML (see Fig. 6).

Overall, the use of various data collection and analysis methods with the developed software solution toolkit has allowed for a more complete and accurate understanding of the properties of materials produced by SLM technology and to determine optimal manufacturing [18] parameters to achieve the required characteristics with sufficiently high levels of accuracy and efficiency in designing new SLM materials and products made from them.

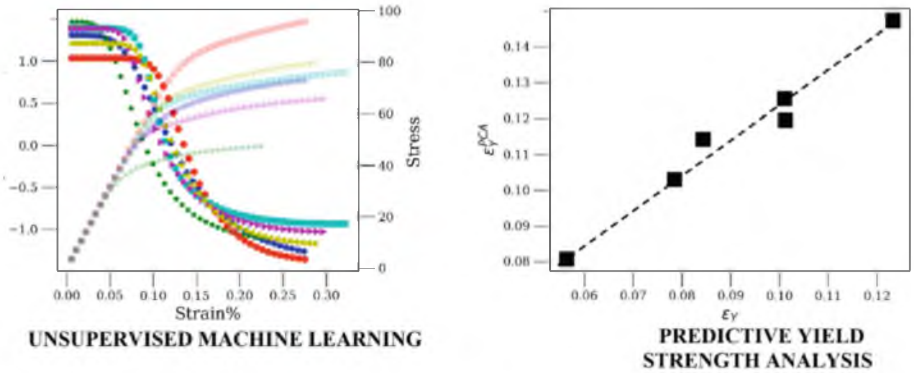

Fig. 6. A software environment for investigating and predicting the yield strength of Ti-6Al-4V, using ML methods.

4 Conclusions

This article is an intermediate step towards achieving the ultimate goal. As a result of the study, a software solution for intelligent data analysis of materials produced using SLM technology has been developed. This solution has significantly increased the efficiency and accuracy of the analysis, as well as revealed new patterns in the data. Within the study, experiments were conducted on a dataset obtained from studies of the structure of Ti-6Al-4V and AlSi10Mg alloys, (see Fig. 4, 5 and 6), and machine learning and data analysis methods were applied to determine the optimal parameters for the yield strength of the SLM process.

The results showed that our software solution enabled achieving a prediction accuracy of 98.9% for mechanical properties of materials obtained through SLM technology, in terms of the average particle size, by combining crystal plasticity and finite element methods (CPFEM) for the Ti-6Al-4V alloy, which surpasses the accuracy of previous studies in this field. Additionally, our solution allows reducing data analysis time by several times, significantly simplifying the analysis process and increasing the efficiency of using SLM materials in various application areas [19], through more efficient SLM process design using machine learning methods. Thus, our software solution can be further used for analyzing data for other materials obtained through SLM technology and for improving the design and production process of materials with desired properties.

Despite significant achievements, there are some limitations to our study. Firstly, we used data only from one source - the "https://viam.ru/review/5942" database. This may limit the generalization of results to other SLM materials that may have different compositions and properties. Additionally, our model does not consider the influence of other factors on material properties, such as ambient temperature, humidity, etc. Further research is necessary for a more complete understanding of the interaction between SLM process parameters and material properties. It should also be noted that the obtained results may be dependent on specific SLM process conditions and the data used, which will allow us to expand our model in the future to include additional factors, such as temperature and humidity, as well as use data from other sources [1].

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