International Journal of Advances in Scientific Research and Engineering (ijasre)

E-ISSN : 2454-8006

DOI: 10.31695/IJASRE.2025.11.3

Volume 11, Issue 11
November- 2025

Artificial Intelligence in Materials Characterization: Methods, Applications, and Future Perspectives

Meric Eren Cakar

Department of Materials Science and Engineering

Faculty of Engineering and Architecture

Izmir Katip Celebi University

Turkey

ABSTRACT

Materials characterization relies on techniques such as electron microscopy, diffraction, and spectroscopy to extract structural, chemical, and physical information from materials. While these traditional methods provide essential insights, their manual interpretation is time-consuming, operator-dependent, and difficult to scale for high-throughput analysis. In recent years, artificial intelligence (AI) has emerged as a transformative approach, enabling automation in image and pattern recognition, improving reproducibility, and accelerating property inference from experimental data. This paper reviews the current applications of AI in materials characterization, including microscopy, spectroscopy, and mechanical testing, and explains how algorithms assist in segmentation, phase identification, peak analysis, and predictive modelling. The review also discusses challenges such as data quality, model interpretability, and standardization, along with future opportunities like physics-informed learning, multimodal data fusion, and self-driving laboratories. Overall, AI is shown not only to enhance existing characterization workflows but also to redefine how materials data are generated, interpreted, and utilized in scientific decision-making.

Key Words: Artificial Intelligence, Data Analysis, Materials Characterization, Microscopy, Machine Learning, Spectroscopy.

1. INTRODUCTION

Materials characterization is a cornerstone of materials science and engineering, providing essential insights into physical, chemical, and mechanical properties of substances. Traditional characterization techniques, such as electron microscopy, X-ray diffraction (XRD), and spectroscopy, remain indispensable for analysing structure and composition. However, these approaches are often labour-intensive, require expert interpretation, and are limited in handling large datasets. With the rapid development of computational methods and data-driven science, artificial intelligence (AI) has emerged as a transformative tool to overcome these challenges [1, 3].

AI enables automatic recognition of patterns, prediction of material properties, and optimization of experimental processes. In the context of materials characterization, AI can analyse microscopy images, diffraction patterns, and spectral data with exceptional accuracy, thereby minimizing human bias and reducing analysis time [2, 4]. Furthermore, the integration of AI with high-throughput experimental systems accelerates the discovery of new materials, enhances data reproducibility, and supports decision-making in materials design [1, 5]. As industries increasingly adopt smart manufacturing and digital twins, AI-assisted characterization is expected to become a fundamental component of modern materials research.

This paper presents an overview of how artificial intelligence reshapes materials characterization techniques and methodologies. It reviews recent progress in machine learning and deep learning applications across microscopy, spectroscopy, and mechanical testing. The paper also discusses the challenges of model generalization, interpretability, and standardization while highlighting future opportunities for physics-informed and autonomous AI systems in materials research.

2. BACKGROUND AND RELATED WORKS

Materials characterization has undergone a major transformation in recent years due to the integration of data-driven approaches and artificial intelligence (AI). Traditional methods, such as scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray diffraction (XRD), have long been the foundation of materials analysis, enabling researchers to investigate microstructures, crystal phases, and elemental compositions. However, these methods often generate large volumes of complex data that are difficult to interpret manually. To address this challenge, AI and machine learning (ML) techniques have been increasingly applied to automate data analysis, reduce human error, and enhance reproducibility [1, 3].

One of the earliest comprehensive reviews of AI applications in materials science was presented by Butler et al. [1], highlighting the use of supervised and unsupervised learning for property prediction and materials discovery. Later, Ramprasad et al. [3] introduced the concept of "materials informatics," which utilizes machine learning algorithms to analyse experimental and computational data, improving the understanding of structure–property relationships. In microscopy, Kalinin and Ziatdinov [2] demonstrated that deep learning models, particularly convolutional neural networks (CNNs), can be trained to recognize defects, grains, and other microstructural features in real time, reducing the need for manual annotation.

In addition, Ziletti et al. [4] achieved accurate crystal structure classification using deep neural networks, outperforming traditional symmetry-based algorithms. Similar approaches have been implemented in spectroscopy and mechanical testing, where AI algorithms can identify spectral peaks, predict stress–strain behaviour, and detect anomalies in datasets. These studies collectively suggest that AI not only accelerates the interpretation of experimental data but also contributes to predictive modelling and autonomous experimentation.

The integration of AI into materials characterization has also promoted the emergence of "self-driving laboratories," where experimental design, data acquisition, and analysis are optimized through closed loop learning systems [5]. This paradigm represents a shift from manual experimentation to fully automated research cycles, improving both speed and consistency. While significant progress has been achieved, challenges remain, such as ensuring data quality, standardizing datasets, and enhancing model interpretability. Current efforts are therefore focused on combining AI models with physical principles (physics-informed learning) to produce scientifically reliable and explainable results.

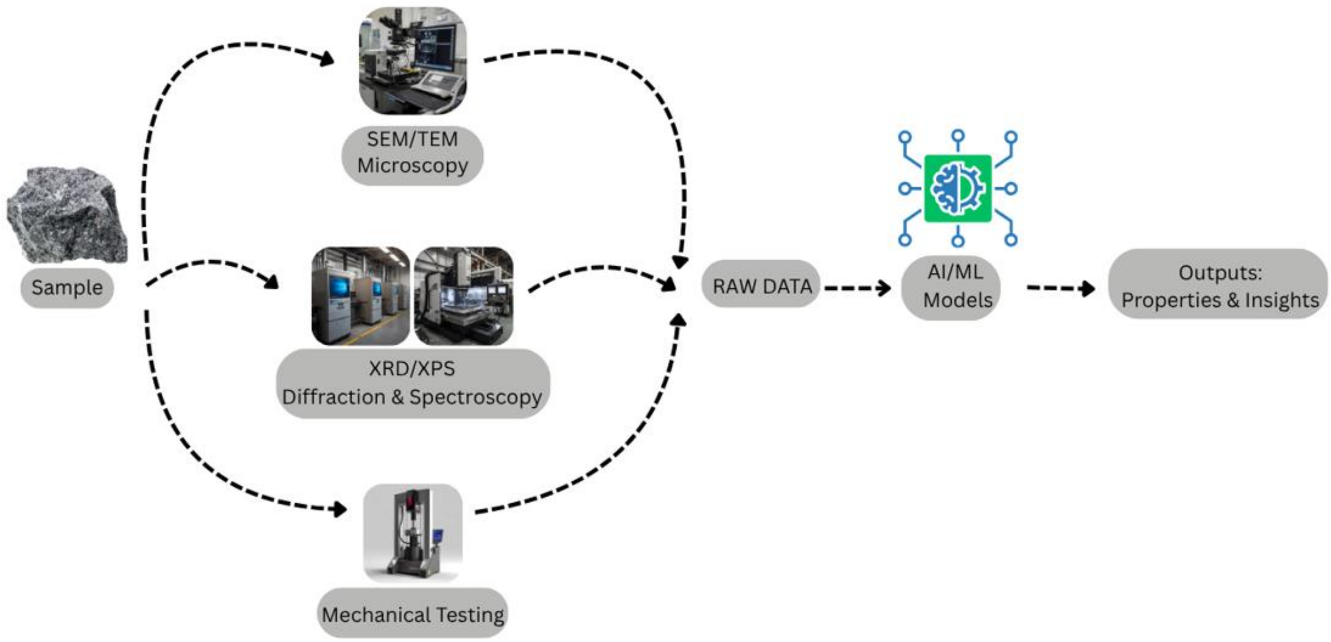

Figure 1. Schematic representation of the role of Artificial Intelligence in materials characterization (Created by the author)

DOI: 10.31695/IJASRE.2025.11.3

3. METHODS

Artificial intelligence (AI) applications in materials characterization primarily rely on supervised and unsupervised learning algorithms trained on high-resolution experimental data derived from techniques such as scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), and various spectroscopic analyses [6]. These techniques generate large volumes of complex data that require systematic preprocessing, feature extraction, and model training for meaningful interpretation. The overall workflow of AI-assisted materials characterization can therefore be divided into four key stages: data preprocessing, feature extraction, model training, and prediction or interpretation.

During the data preprocessing stage, raw data obtained from microscopy or spectroscopy are refined to eliminate experimental artifacts and background noise. This process involves filtering, normalization, and contrast enhancement. In image-based datasets, such as those obtained from SEM or TEM, preprocessing often includes edge detection, binarization, and segmentation of grains, phases, or defects [7]. For diffraction and spectroscopy data, baseline correction and peak deconvolution are essential to isolate relevant signal features and ensure quantitative accuracy. A properly pre-processed dataset establishes the foundation for all subsequent modelling efforts, as data integrity directly affects prediction reliability.

The feature extraction stage involves converting experimental data into numerical or image-based descriptors that represent the essential physical characteristics of materials. Traditional approaches employ manually designed statistical or morphological features, while deep learning methods, particularly convolutional neural networks (CNNs), automatically learn hierarchical representations from raw data. For example, CNN architectures can distinguish grain boundaries or dislocation structures in microscopy images, whereas algorithms such as Support Vector Machines (SVM), Random Forest (RF), and k-Nearest Neighbours (k-NN) are widely applied to spectral and mechanical data analysis. This combination of classical and deep learning approaches allows flexible adaptation to different characterization modalities.

In the model training phase, datasets are typically divided into training, validation, and test subsets to evaluate model generalization and robustness. Optimization algorithms such as stochastic gradient descent and Adam are used to minimize error functions while preventing overfitting. Performance metrics including accuracy, F1-score, and mean absolute error (MAE) are applied to assess predictive quality. Moreover, cross-validation techniques and uncertainty quantification frameworks ensure that model performance remains consistent across independent datasets [8].

Finally, in the prediction and interpretation stage, trained models are deployed to infer material properties or identify microstructural features from new experimental inputs [7, 9]. AI systems can automatically recognize unknown phases, predict mechanical behaviour, and identify morphological anomalies that may escape human observation. In recent years, physics-informed machine learning (PIML) has gained attention for integrating physical constraints into data-driven models, thereby improving interpretability and scientific reliability [9]. These hybrid approaches are particularly valuable in materials characterization, where physical consistency and experimental reproducibility are critical for advancing trustworthy AI-driven discoveries.

4. APPLICATIONS

Artificial intelligence (AI) has become an essential component of modern materials characterization, supporting a wide range of experimental techniques. From microstructural imaging to spectroscopy and mechanical property prediction, AI provides tools that enhance efficiency, accuracy, and scalability. This section outlines key applications of AI across different domains of characterization, emphasizing its role in image analysis, diffraction and spectroscopy, mechanical testing, and integrated laboratory automation.

4.1. AI in Microscopy and Image Analysis

Microscopy techniques such as scanning electron microscopy (SEM) and transmission electron microscopy (TEM) are fundamental in materials characterization because they allow scientists to observe microstructural details like grain boundaries, precipitates, and dislocation networks at very high resolutions. However, analysing these images manually is often slow and highly dependent on the operator’s experience, leading to inconsistencies between different researchers or laboratories.

DOI: 10.31695/IJASRE.2025.11.3

Artificial intelligence (AI), particularly deep learning-based image analysis, has significantly improved this process. Convolutional neural networks (CNNs) can automatically detect and classify microstructural features by learning directly from large sets of labelled images [10]. This removes the need for hand-crafted rules or subjective visual interpretation. For example, CNN-based segmentation models can identify inclusion phases or surface defects with a level of precision comparable to trained metallographers. Durmaz et al. [11] demonstrated that using such a deep learning model on titanium alloy datasets achieved more than 90% segmentation accuracy, while reducing manual labelling effort by over 80%. This means that tasks that used to take several hours can now be completed in minutes, with higher repeatability.

Beyond accuracy, AI also enhances reproducibility and standardization. Open-access datasets such as *Micro Net* [10] provide benchmark micrographs from various materials systems, enabling fair comparisons between algorithms and laboratories. Such shared data platforms make it easier to develop and validate models that generalize across different imaging conditions, magnifications, and materials.

AI is also beginning to support real-time and in-situ microscopy, where microstructural changes are captured as they happen during mechanical testing, heating, or corrosion. Real-time CNN analysis allows researchers to track grain growth, crack propagation, or void formation as the experiment progresses—something that was previously impossible to monitor at high frame rates. This advancement transforms the microscope from a simple observation tool into an intelligent system capable of automatic analysis and decision-making during experiments.

Overall, AI has revolutionized how microscopy data are handled. Instead of being limited by human interpretation speed and bias, scientists can now use machine learning to process massive image datasets, detect features with high precision, and even monitor microstructural evolution dynamically. These developments not only improve the efficiency of materials research but also establish a foundation for more autonomous, data-driven laboratories in the future.

4.2. AI in Diffraction and Spectroscopy Analysis

Diffraction and spectroscopy are among the most widely used analytical techniques in materials characterization, as they provide quantitative information about the structural, crystallographic, and chemical nature of materials. However, interpreting such data often requires complex peak fitting, background subtraction, and signal deconvolution — all of which are highly sensitive to noise and experimental variations. These challenges make manual analysis time-consuming and sometimes inconsistent, particularly when dealing with multi-phase or disordered systems.

Artificial intelligence (AI) has emerged as a powerful tool to overcome these limitations by automating data analysis, identifying hidden patterns, and improving peak resolution in diffraction and spectroscopy datasets. Machine learning (ML) models can rapidly classify unknown phases, predict crystal structures, and even detect subtle compositional changes that may not be visually distinguishable in the spectra. For instance, Lee et al. [12] applied deep convolutional neural networks to complex oxide systems, enabling accurate phase identification even in overlapping X-ray diffraction (XRD) peaks that traditional Rietveld refinement methods failed to resolve. This demonstrates AI's capability to handle nonlinear relationships and noise better than purely mathematical fitting models.

In Raman and infrared spectroscopy, AI-based algorithms have proven particularly valuable for analysing large sets of spectral data obtained from heterogeneous materials. Through unsupervised learning methods such as clustering or principal component analysis (PCA), researchers can automatically group spectra based on chemical similarity without prior labelling [13]. This allows rapid detection of impurity phases, local compositional gradients, or reaction intermediates in complex systems such as catalysts, ceramics, and polymers. Cordero et al. [13] demonstrated how machine learning could successfully distinguish multiple vibrational modes within a single spectrum, enabling fine chemical differentiation at sub-micrometre scales.

DOI: 10.31695/IJASRE.2025.11.3

Another key contribution of AI lies in quantitative prediction and simulation. Instead of merely classifying data, regression-based models can estimate physical parameters such as lattice strain, grain size, or defect concentration directly from spectral features. This approach reduces dependence on empirical calibration curves and allows for more flexible and adaptive analysis pipelines. Furthermore, by combining experimental and simulated data, *transfer learning* enables models trained on synthetic spectra to perform robustly on real-world measurements, effectively compensating for limited experimental datasets.

The integration of AI into diffraction and spectroscopy workflows has also accelerated high-throughput materials screening. Automated data pipelines can process hundreds of diffraction or Raman spectra per hour, making them ideal for combinatorial studies of alloy compositions or thin-film libraries. Such automation transforms characterization from a bottleneck into a continuous feedback loop for material discovery, where AI continuously refines data interpretation, feeds predictions to synthesis modules, and iteratively improves experimental design.

In summary, the application of AI in diffraction and spectroscopy bridges the gap between raw experimental data and physical understanding. By enabling rapid, reproducible, and high-resolution analysis, it supports the development of next-generation materials with greater efficiency and scientific insight.

4.3. AI for Mechanical Property Prediction

Mechanical characterization is one of the most essential yet time-consuming processes in materials engineering. Traditional mechanical testing methods, such as tensile, hardness, and fatigue tests, require precise specimen preparation, repeated measurements, and long testing durations. In recent years, artificial intelligence (AI) has been introduced to this field to accelerate the prediction and evaluation of mechanical properties using computational models trained on experimental or image-based datasets.

Machine learning (ML) algorithms such as Support Vector Machines (SVM), Random Forests (RF), and Neural Networks (NN) have been applied to correlate microstructural features with macroscopic mechanical properties. For instance, SEM or optical micrographs can be processed to extract parameters such as grain size, phase fraction, or defect density, which are then used as inputs for ML models predicting hardness or yield strength [14]. This approach eliminates the need for destructive testing in many early-stage studies, providing a faster and more cost-effective estimation of mechanical performance.

Deep learning architectures, including Convolutional Neural Networks (CNNs) and Graph Neural Networks (GNNs), have also expanded the predictive capabilities of AI in this area. CNNs are particularly effective for analysing two-dimensional micrographs, learning to recognize texture and pattern variations that correspond to material strength or ductility. In contrast, GNNs are designed to handle complex three-dimensional data, such as porosity networks or crack paths in additive manufactured materials, where spatial relationships between features significantly influence mechanical behaviour [15]. These models can simulate and predict fatigue life, crack propagation, or deformation behaviour under different loading conditions without the need for extensive experimental cycles.

Another application of AI in mechanical characterization is the integration of multi-source data, combining structural, compositional, and thermodynamic information to create unified predictive frameworks. For example, datasets containing both composition and microstructural features can be used to predict yield stress or elastic modulus with higher accuracy than single-input models. This data fusion approach allows researchers to design materials with targeted mechanical performance using computational screening before any physical testing.

Furthermore, AI techniques are being implemented in real-time testing and monitoring systems. During mechanical tests, machine learning models can analyse stress–strain curves as they are generated, detecting anomalies such as premature yielding, instability, or fatigue crack initiation. This capability not only improves data reliability but also enables adaptive testing—where experimental parameters are adjusted automatically based on AI feedback.

DOI: 10.31695/IJASRE.2025.11.3

Overall, AI-driven mechanical property prediction enhances efficiency, reduces experimental costs, and provides new insight into the relationships between microstructure and performance. These advancements are gradually shifting the field from purely empirical testing toward intelligent, data-driven materials design.

4.4. Autonomous and Self-Driving Laboratories

The concept of autonomous or *self-driving laboratories* represents one of the most advanced applications of artificial intelligence (AI) in materials research. These systems integrate robotics, high-throughput experimentation, machine learning algorithms, and automated data analysis to conduct research with minimal human intervention. The primary goal is to accelerate the cycle of materials discovery, from synthesis and characterization to optimization, by allowing AI to guide each experimental step.

In a self-driving laboratory, experimental instruments such as chemical reactors, coating systems, or analytical microscopes are digitally connected through an automation platform. Machine learning models analyse incoming data in real time, determine trends or deviations, and suggest the next optimal set of experimental parameters. For example, an algorithm may instruct a robotic arm to modify the precursor ratio or heating temperature to achieve a desired material property. This creates a *closed-loop workflow* in which the AI continuously refines its understanding of structure–property relationships through iterative experimentation [16].

High-throughput synthesis and characterization tools are essential to these systems. Automated X-ray diffraction (XRD) and spectroscopy modules can produce and analyse thousands of samples per week, generating massive datasets for model training. Reinforcement learning algorithms have been particularly successful in managing such workflows, enabling systems to “learn by doing” — adjusting their actions based on experimental outcomes rather than predefined rules. This approach allows the laboratory to evolve dynamically, improving accuracy and efficiency with each iteration.

Another critical application of AI in autonomous laboratories is multimodal data fusion. Data from different sources—microscopy, spectroscopy, mechanical testing, and even simulation outputs—can be integrated into a single decision framework. By merging these heterogeneous datasets, AI models can identify correlations between structure, chemistry, and performance that would be impossible to detect manually. This capability has led to faster optimization in catalysis, thin-film deposition, and battery materials development [17].

AI-enabled self-driving laboratories also promote reproducibility and standardization in materials research. Each experiment is logged with detailed metadata, ensuring that the same procedure can be repeated under identical conditions. This not only improves data reliability but also facilitates global collaboration, as experiment scripts and AI workflows can be shared across laboratories. Ultimately, these systems embody a transition toward intelligent research infrastructures where AI acts not as an assistant, but as an autonomous collaborator in the scientific process.

5. RESULTS AND DISCUSSION

The integration of artificial intelligence (AI) into materials characterization has led to a measurable transformation in how data are collected, processed, and interpreted. Across different experimental domains—microscopy, spectroscopy, mechanical testing, and autonomous laboratories—AI has improved both the speed and accuracy of analysis, while reducing human intervention and subjectivity.

In microscopy, for example, AI-driven image segmentation has replaced manual annotation, enabling quantitative microstructural analysis within minutes rather than hours. Deep learning models trained on large-scale datasets can distinguish grain boundaries, inclusion phases, and surface defects with accuracies exceeding 90% in many reported studies. These results demonstrate not only computational efficiency but also improved reproducibility, as AI eliminates the variation caused by human interpretation.

Spectroscopy and diffraction data have similarly benefited from machine learning algorithms capable of identifying subtle peak shifts and compositional variations that may go unnoticed in conventional analysis. Such improvements

DOI: 10.31695/IJASRE.2025.11.3

have been particularly evident in Raman and X-ray diffraction applications, where AI models have successfully differentiated overlapping peaks, leading to more accurate phase identification. The consistency of these findings across multiple studies indicates that AI can act as a reliable analytical assistant, significantly reducing error rates associated with manual fitting and interpretation.

In mechanical property prediction, AI methods such as support vector machines and neural networks have achieved high correlation with experimental data for hardness, tensile strength, and fatigue behaviour. These results underline the growing potential of AI to replace or supplement destructive testing, particularly in early-stage materials screening. While traditional methods remain the gold standard for final validation, AI-based predictions enable faster and more resource-efficient pre-selection of candidate materials.

The advent of autonomous or self-driving laboratories further expands these achievements by integrating AI-driven decision-making into the experimental loop. Early implementations have demonstrated that automated systems can independently design experiments, analyse outcomes, and propose new synthesis conditions, achieving optimization cycles several times faster than human researchers. This level of automation marks a critical shift toward continuous, self-improving research infrastructures.

However, despite these advances, challenges persist. Many of the published results rely on institution-specific datasets that limit the generalizability of AI models. Data standardization, model transparency, and interpretability remain active areas of concern. There is also a need for interdisciplinary collaboration to bridge the gap between materials science expertise and AI algorithm development. Encouragingly, recent studies highlight the growing trend toward open-access datasets and explainable AI frameworks, suggesting a collective movement toward more trustworthy and scalable AI systems in the near future.

The results reported across the literature consistently demonstrate that AI does not simply accelerate existing workflows—it redefines them. By coupling computation with experimentation, AI enables a more iterative and data-centric approach to materials research, paving the way for autonomous discovery and next-generation materials design.

6. CONCLUSION

Artificial intelligence (AI) has rapidly evolved from a computational tool to a transformative driver in materials characterization. Its integration across microscopy, diffraction, spectroscopy, mechanical analysis, and autonomous laboratory systems has enabled faster, more accurate, and more reproducible insights into complex materials behaviour. By automating data interpretation and linking structure to properties through predictive modelling, AI has significantly reduced human bias and experimental inefficiencies. Although challenges remain in data standardization, model transparency, and generalization across diverse materials systems, current progress clearly indicates that AI will continue to redefine how materials research is conducted. Future efforts focused on open data sharing, explainable models, and interdisciplinary collaboration will be essential to achieving fully autonomous, intelligent materials discovery pipelines.

REFERENCES

[1] Butler, K. T., Davies, D. W., Cartwright, H., Isayev, O., & Walsh, A. (2018). *Machine learning for molecular and materials science.* Nature, 559, 547–555.

[2] Ziletti, A., Kumar, D., Scheffler, M., & Ghiringhelli, L. M. (2018). *Insightful classification of crystal structures using deep learning.* Nature Communications, 9, 2775.

[3] Kalinin, S. V., & Ziatdinov, M. (2021). *Machine learning in microscopy: A user's guide.* Annual Review of Materials Research, 51, 149–173.

DOI: 10.31695/IJASRE.2025.11.3

[4] Ramprasad, R., Batra, R., Pilania, G., Mannodi-Kanakkithodi, A., & Kim, C. (2017). *Machine learning in materials informatics: Recent applications and prospects.* npj Computational Materials, 3, 54.

[5] Jha, D., Ward, L., Paul, A., Liao, W. K., Choudhary, A., Wolverton, C., & Agrawal, A. (2019). *ElemNet: Deep learning the chemistry of materials from only elemental composition.* Scientific Reports, 8, 17593.

[6] Kalinin, S. V., & Ziatdinov, M. (2021). *Machine learning in microscopy: A user's guide.* Annual Review of Materials Research, 51, 149–173.

[7] Ramprasad, R., et al. (2017). *Machine learning in materials informatics.* npj Computational Materials, 3, 54.

[8] Li, Z., et al. (2018). *Deep learning in spectroscopy data analysis.* Analytical Chemistry, 90(12), 7075–7082.

[9] Karniadakis, G. E., Kevrekidis, I. G., Lu, L., Perdikaris, P., Wang, S., & Yang, L. (2021). *Physics-informed machine learning.* Nature Reviews Physics, 3(6), 422–440.

[10] Stuckner, J., et al. (2022). *MicroNet: Materials microscopy dataset and benchmarking.* npj Computational Materials, 8, 45

[11]Durmaz, A. R., et al. (2021). *Deep-learning microstructure segmentation in titanium alloys.* Acta Materialia, 206, 116562.

[12] Lee, J.-W., et al. (2020). *Deep learning for phase identification in inorganic compounds from XRD.* Nature Communications, 11, 6163.

[13] Cordero, M. L., et al. (2025). *Machine learning of Raman data in multi-component systems.* Journal of Raman Spectroscopy, 56(3), 417–429.

[14] Mińkowski, M., et al. (2023). *Predicting elastic and plastic properties using ML.* Scientific Reports, 13, 2041.

[15] Shi, X., et al. (2024). *GNNs in materials science: Porosity networks and fatigue prediction.* Materials Graphene Engineering & Analysis, 6, 113–124.

[16] Häse, F., Roch, L. M., & Aspuru-Guzik, A. (2019). *Next-generation experimentation with self-driving laboratories.* Trends in Chemistry, 1(3), 282–291.

[17] Chowdhury, M. A., et al. (2021). *Machine-learning-guided materials research: A review.* Results in Materials, 13, 100230.

AUTHOR PROFILE

Meric Eren Cakar, a student of Materials Science and Engineering at Izmir Katip Celebi University, Turkey, is passionate about research and the continuous advancement of materials characterization. He aims to develop his academic and professional skills in parallel with the rapid growth of technology, focusing particularly on the integration of Artificial Intelligence (AI) into materials science. In the future, he looks forward to becoming a skilled materials engineer and researcher, dedicated to advancing data-driven and technology-oriented approaches in materials science. Email: mericerencakar@hotmail.com

DOI: 10.31695/IJASRE.2025.11.3