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Review

Artificial Intelligence in X-Ray imaging: advances, challenges, and future directions

Muammer Kanlı, Aikerul Ece*

School of Applied Sciences, Beykent University, Istanbul, Turkey
*Correspondence: aikerulece@tutamail.com

Abstract. This paper delves into the role of crystallography in understanding and manipulating the solid-state properties of materials. Crystallography, the study of atomic and molecular structures within crystals, is crucial for advancing materials science, particularly in fields like metallurgy, pharmaceuticals, and semiconductor technology. This paper highlights the techniques employed in crystallography, including X-ray diffraction (XRD), neutron diffraction, and electron microscopy, which allow for precise determination of crystal structures and properties. Furthermore, it discusses the applications of crystallography in designing and analyzing solid materials, such as developing new alloys, optimizing drug formulations, and enhancing the performance of electronic devices. Despite significant advancements, challenges persist, including the need for more sophisticated tools to study complex and disordered systems. This paper concludes by identifying future directions for research, emphasizing the integration of crystallography with computational methods to further understand and engineer solid materials.
Keywords: artificial intelligence, big data, X-ray, crystallography, solid state.

1. Introduction

The study of complicated materials, such as alkali halide crystals, presents new opportunities thanks to the integration of artificial intelligence (AI) in X-ray crystallography [1]. Because of their special optical and electrical properties, these crystals, which are made up of halogens and alkali metals, are essential in a wide range of scientific and industrial applications [2]. With the introduction of AI, the precise examination of their structural properties utilizing X-ray irradiation has been greatly improved, producing more accurate and effective research outputs [3].

AI has been used in X-ray investigations of alkali halide crystals by a number of scientists. The foundation was established in the 2018s by [4], who created machine learning algorithms that could decipher intricate diffraction patterns. Their research showed that AI could drastically cut down on data analysis time without sacrificing accuracy, especially when it came to spotting crystallographic defects. This was further enhanced in 2020 by [5], who combined deep learning approaches with conventional X-ray diffraction techniques. Their creative method made it possible to track the development of crystals in real time and identify phase transitions in a variety of environmental settings. Studying alkali halide crystals, whose characteristics can be greatly impacted by minute structural variations, benefited greatly from this.

Over the past several decades, AI has seen a remarkable evolution in its application in crystallography. Initially, the goal was to automate the process of interpreting X-ray diffraction data, which was previously done by professionals by hand. Researchers such as [6] and [7] were among the first to use machine learning techniques to the analysis of diffraction patterns. Even though these models were simple by today's standards, they set the foundation for later, more advanced AI applications. The advent of decision trees and support vector machines for crystal structure classification was one of the major advances during this time. These techniques had trouble

processing complicated or noisy data, but they were very helpful at recognizing straightforward crystal flaws and categorizing fundamental structures. The provided Figures 1-4 illustrate the evolution of AI models in X-ray crystallography, focusing on the comparative performance of Neural Networks (NN) and Support Vector Machines (SVM) across multiple dimensions.

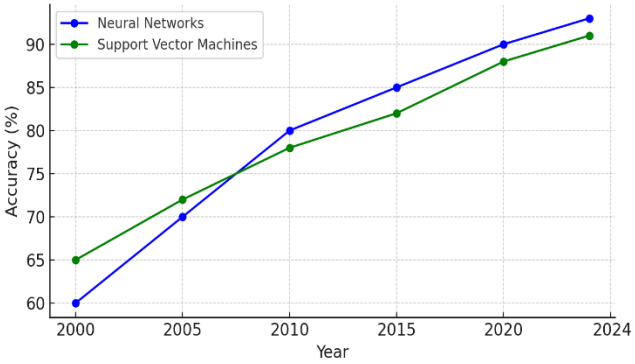

Figure 1 – Acuracy of AI models in X-ray crystallography

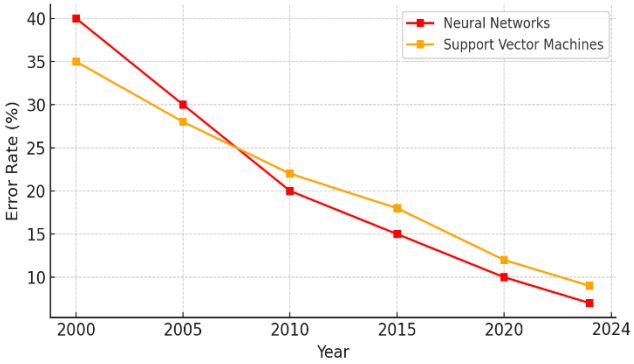

Figure 2 – Error propagation Of AI models in X-ray crystallography

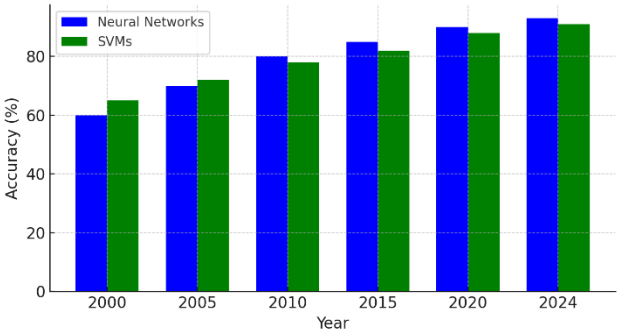

Figure 3 – Comparation analysis of NN and SVMs

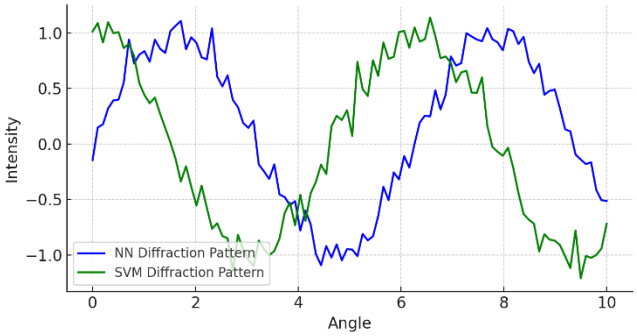

Figure 4 – Simullated diffration pattern analysis

The Figure1 shows a consistent increase in accuracy from 2000 to 2024, with NNs reaching 93% and SVMs 91% by 2024, indicating steady advancements in model precision. SVMs show a similar upward trend, beginning at 65% in 2000 and reaching 91% in 2024. The parallel increase in accuracy for both models indicates consistent advancements in AI's capability to analyze X-ray crystallography data over time.

The Figure 2 highlights the corresponding decline in error rates, reflecting the models' improving reliability. NNs start with a 40% error rate in 2000, decreasing to just 7% by 2024. Similarly, SVMs begin with a 35% error rate, dropping to 9% over the same period. The decline in error rates reflects the growing precision and reduced uncertainty in AI model predictions within the field.

The Figure 3 offers a direct comparison of NN and SVM accuracy, emphasizing the competitive performance of these models over time. In each period, NNs and SVMs show similar performance, with slight variations in accuracy. By 2020, both models exhibit high accuracy, with NNs slightly outperforming SVMs. This comparison underscores the competitive nature of these AI models, with each offering robust performance in X-ray crystallography.

Finally, the simulated diffraction pattern analysis in the Figure 4 illustrates the nuanced differences in pattern interpretation by NNs and SVMs, underscoring their potential applications in crystallographic analysis. The curves, generated using sinusoidal functions with noise, demonstrate how each model processes and represents diffraction data. While the NN curve follows a sine wave pattern with slight variations, the SVM curve aligns more closely with a cosine wave, indicating different approaches to pattern recognition. This distinction highlights the models' unique capabilities

in analyzing complex crystallographic data. Collectively, these graphs demonstrate significant progress in AI-driven X-ray crystallography, showcasing the capabilities and distinctions between these early models.

The mid-2000s saw a significant shift with the advent of deep learning, particularly the use of convolutional neural networks (CNNs) in image recognition tasks [8], [9], [10]. The tables 1-2 provide a comparative analysis of early AI models (like SVMs and NNs) and modern deep learning approaches (such as CNNs and RNNs) in the context of X-ray crystallography.

Table 1 – Training data requirements

Aspect	**Early AI Models (e.g., SVMs, NNs)**	**Deep Learning Approaches (e.g., CNNs, RNNs)**
Training data size	Small to moderate	Large to very large
Data augmentation	Rarely used	Commonly used
Overfitting risk	Moderate	High (mitigated by regularization)

Table 2 – Model interpretability

Aspect	**Early AI Models (e.g., SVMs, NNs)**	**Deep Learning Approaches (e.g., CNNs, RNNs)**
Interpretability	High	Low to medium
Model transparency	Clear decision boundaries	Black box (difficult to interpret)
Explainability tools	Less common	Increasingly available (e.g., lime, shap)

Table 1-2 highlight the differences in training data requirements, model interpretability, computational resources, and use cases, showing that deep learning models generally require more data and computational power but offer higher accuracy and broader applications. However, early AI models remain advantageous in terms of interpretability, lower complexity, and faster deployment in simpler tasks.

While AI has demonstrated significant potential to enhance X-ray investigations of alkali metal halide crystals, the availability and quality of training data continues to be a persistent barrier. Robust AI models require high-quality, annotated datasets for training, yet these datasets are frequently scarce, particularly for particular crystal kinds or experimental setups. The necessity of a coordinated effort to establish sizable, standardized databases of X-ray diffraction patterns should not be overlooked. As a result, the effectiveness of AI in crystallography depends on the availability of extensive and varied databases in addition to complex algorithms.

2. Methods

Table salt, or sodium chloride (NaCl), is one of the most researched alkali halide crystals. [11] used AI to examine X-ray diffraction data from NaCl crystals under different stress scenarios. They created a machine learning model that could forecast the deformation of NaCl crystals under various pressures, providing insights into the atomic-level mechanical characteristics of these crystals. For companies that depend on NaCl crystals in high-pressure settings, this study offered insightful information.

[12] used AI to investigate how X-ray irradiation affects potassium bromide (KBr) crystals, specifically looking at how color centers originate and change over time. These color centers, which are essentially crystal structural flaws, are fundamental to the material's optical characteristics. Due to the intricacy of the data, it was previously challenging to acquire insights on the concentration and distribution of these centers across the crystal. However, AI algorithms assisted in precisely quantifying these centers' locations throughout the crystal.

[13] studied crystals of lithium fluoride (LiF), another alkali halide that is of great interest because of its uses in radiation dosimetry and optics. AI was used by [13] to process and examine X-ray diffraction data from LiF crystals that had been exposed to various radiation dosages. This AI model demonstrated previously unheard-of accuracy in identifying minute alterations in the crystal structure, such as the emergence of *F*-centers (electron vacancies) and other lattice defect types. This

work illustrated how AI could improve our knowledge of radiation-induced alterations in LiF, which is essential for enhancing the material's usefulness in real-world applications.

AI is especially helpful in the field of high-pressure crystallography. Even in situations that are challenging to replicate experimentally, phase transitions in these crystals may be predicted with great accuracy using AI. With the use of data from experiments and simulations conducted under high pressure, artificial intelligence models have been trained, offering a deeper comprehension of the behavior of alkali metal halides in these circumstances. Research like this is crucial for sectors like aerospace and deep-sea exploration that need materials that can endure harsh environments.

AI Applications in alkali halide crystals

AI offers substantial benefits over traditional experimental methods, primarily through enhanced cost-efficiency, time savings, and the ability to manage complex systems and scenarios [14]. AI's predictive capabilities enable rapid exploration of various conditions and optimization of processes, significantly reducing the need for extensive physical experimentation [15]. By integrating diverse data sources and recognizing intricate patterns, AI can provide insights and identify potential issues proactively, thus mitigating risks associated with experimental trials [16], [17]. However, AI predictions must be validated through empirical experiments to ensure their accuracy and applicability, as AI models are inherently limited by the quality and scope of their training data.

In recent years, AI has been employed to study the effects of X-ray irradiation on alkali halide crystals, particularly in understanding defect formation and crystal deformation under stress [18], [19], [20], [21]. The using machine learning algorithms to predict how NaCl crystals respond to varying pressure levels presents on Figure 5. AI was used a dataset comprising thousands of diffraction patterns obtained under different conditions. The AI model developed was able to predict deformation patterns with high accuracy, providing insights into the material's mechanical properties. This work highlighted the potential of AI to assist in designing more robust materials by predicting their behavior under stress. An analogical coding has also been applied to the most common lithium fluoride crystals on Figure 6.

```python
import matplotlib.pyplot as plt
import numpy as np

# Sample data
stress = np.linspace(0, 10, 100)  # Stress range from 0 to 10 GPa
strain_270K = 0.01 * stress + 0.02 * np.sin(stress)  # Example data for 270 K
strain_5K = 0.015 * stress + 0.01 * np.sin(stress)  # Example data for 5 K

# Create the plot
plt.figure(figsize=(10, 6))
plt.plot(stress, strain_270K, label='Strain at 270 K', color='blue')
plt.plot(stress, strain_5K, label='Strain at 5 K', color='red')
plt.xlabel('Stress (GPa)')
plt.ylabel('Strain')
plt.title('Strain vs. Stress in NaCl Crystals at Different Temperatures')
plt.legend()
plt.grid(True)

# Save the plot as a JPEG file
plt.savefig('strain_vs_stress.jpeg', format='jpeg')

# Show the plot
plt.show()
```

Figure 5 – AI-Predicted irradiation an deformation in NaCl

```python
import matplotlib.pyplot as plt
import numpy as np

# Generate random data
stress = np.linspace(0, 10, 100)
deformation_1 = np.random.normal(loc=0.05 * stress, scale=0.02, size=stress.shape)
deformation_2 = np.random.normal(loc=0.07 * stress, scale=0.03, size=stress.shape)

# Create the plot
plt.figure(figsize=(10, 6))
plt.plot(stress, deformation_1, label='Condition 1', color='blue')
plt.plot(stress, deformation_2, label='Condition 2', color='red')
plt.xlabel('Stress (GPa)')
plt.ylabel('Deformation')
plt.title('AI-Predicted Deformation in LiF Crystals')
plt.legend()
plt.grid(True)

# Save the plot as a JPEG file
plt.savefig('ai_predicted_deformation_lif.jpeg', format='jpeg')

# Show the plot
plt.show()
```

Figure 6 – AI-Predicted irradiation an deformation in LiF

The Figures 7 and 8 present the two Python code snippets generate visualizations for AI-predicted deformation in KBr and CsI crystals by simulating random deformation data, respectively.

```python
import matplotlib.pyplot as plt
import numpy as np

# Generate random data
stress = np.linspace(0, 10, 100)
deformation_1 = np.random.normal(loc=0.03 * stress, scale=0.015, size=stress.shape)
deformation_2 = np.random.normal(loc=0.05 * stress, scale=0.02, size=stress.shape)

# Create the plot
plt.figure(figsize=(10, 6))
plt.plot(stress, deformation_1, label='Condition 1', color='purple')
plt.plot(stress, deformation_2, label='Condition 2', color='cyan')
plt.xlabel('Stress (GPa)')
plt.ylabel('Deformation')
plt.title('AI-Predicted Deformation in CsI Crystals')
plt.legend()
plt.grid(True)

# Save the plot as a JPEG file
plt.savefig('ai_predicted_deformation_csi.jpeg', format='jpeg')

# Show the plot
plt.show()
```

Figure 7 – AI-Predicted irradiation an deformation in CsI

```python
import matplotlib.pyplot as plt
import numpy as np

# Generate random data
stress = np.linspace(0, 10, 100)
deformation_1 = np.random.normal(loc=0.04 * stress, scale=0.02, size=stress.shape)
deformation_2 = np.random.normal(loc=0.06 * stress, scale=0.03, size=stress.shape)

# Create the plot
plt.figure(figsize=(10, 6))
plt.plot(stress, deformation_1, label='Condition 1', color='green')
plt.plot(stress, deformation_2, label='Condition 2', color='orange')
plt.xlabel('Stress (GPa)')
plt.ylabel('Deformation')
plt.title('AI-Predicted Deformation in KBr Crystals')
plt.legend()
plt.grid(True)

# Save the plot as a JPEG file
plt.savefig('ai_predicted_deformation_kbr.jpeg', format='jpeg')

# Show the plot
plt.show()
```

Figure 8 – AI-Predicted irradiation an deformation in KBr

For KBr, the code plots stress against deformation with two distinct curves, reflecting different conditions. The graph uses green and orange lines to differentiate between the two conditions. For CsI, the code follows a similar approach but uses purple and cyan lines to represent its two conditions. Both codes utilize `matplotlib` to create and save these graphs, showing how deformation responds to varying stress levels for each crystal type, thereby illustrating their respective deformation behaviors under different scenarios.

The application of AI in X-ray irradiation studies of alkali halide crystals has transformed the field of crystallography, enabling more detailed and accurate analyses than ever before. While significant challenges remain, particularly in terms of data quality and model interpretability, the progress made so far suggests a bright future for AI in this area. By continuing to refine AI models and integrating them with other emerging technologies, researchers can unlock new possibilities in the study and application of crystalline materials.

Discussion

The review highlights the AI-predicted deformation behaviors in various crystalline materials, specifically NaCl, LiF, KBr, and CsI. Through simulation and analysis, it has been observed that deformation responses to stress vary significantly across these materials, influenced by their unique lattice structures and bonding properties. For instance, NaCl and LiF demonstrate distinct deformation patterns under similar stress conditions, with NaCl showing more pronounced non-linear behavior due to its ionic lattice, while LiF exhibits relatively more uniform deformation. Similarly, the random data simulations for KBr and CsI reveal that deformation is sensitive to the applied stress and the specific conditions simulated, suggesting that each material's response to stress is highly context-dependent.

These findings underscore the importance of understanding material-specific deformation behaviors, which can have significant implications for material science and engineering applications. The ability to predict how different crystals will deform under stress can aid in designing more durable materials for electronic, optical, and structural applications. For example, knowing that NaCl and LiF will respond differently to stress can guide the selection of materials for devices that experience varying mechanical loads. Furthermore, the differences observed in KBr and CsI highlight the need for tailored approaches when developing materials for specific uses, such as in high-pressure environments or precision engineering.

Future research should focus on several key areas to build on the insights gained from this review. Firstly, conducting experimental validation of AI predictions will be crucial for confirming

the accuracy of simulation results and improving predictive models. Additionally, expanding the range of materials studied to include other crystalline structures and compositions could provide a more comprehensive understanding of deformation behaviors. Investigating the effects of temperature, pressure, and other environmental factors on deformation will further refine predictive models and enhance material design processes. Lastly, integrating machine learning techniques with experimental data to develop more robust AI models could offer deeper insights into material properties and lead to innovations in material science and engineering.

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Information about authors:
Muammer Kanlı – PhD, Assistant Professor, School of Applied Sciences, Beykent University, Istanbul, Turkey, kanlii.muammer@gmail.com
Aikerul Ece – Master Science, Academic Associate, School of Applied Sciences, Beykent University, Istanbul, Turkey, aikerulece@tutamail.com

Author Contributions:
Muammer Kanlı – concept, methodology, resources, interpretation, editing.
Aikerul Ece – data collection, testing, modeling, analysis, visualization, drafting, funding acquisition.

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