Novel applications of Generative Adversarial Networks (GANs) and Convolutional Neural Networks (CNNs) in the analysis of ultrafast electron diffraction (UED) images

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We employ generative adversarial networks (GANs) and convolutional neural networks (CNNs) in the study of ultrafast electron diffraction images. Polycrystalline bismuth, that is subjected to 800 nm pump laser pulses and undergoes thermalization, is probed by time-resolved electron diffraction. The diffraction images are collected and analyzed using deep learning techniques. Through the employment of a GAN, we are able to convert the experimental diffraction images into idealized diffraction patterns that are subsequently analyzed by a CNN. The network is trained on a limited dataset of only 408 diffraction images. Temperature changes are predicted with a deviation of less than 6% from theoretically estimated values, a remarkable result given the size of the dataset. Our novel method is promising for several reasons: (1) It provides a consistent method to train CNNs solely using synthetic data, which can be created without restriction as opposed to labelled experimental data, and to employ them in a neural network (NN) for the analysis of experimental diffraction patterns. (2) It shows that GANs trained on a small data set can still provide reliable results. (3) It provides a fast routine to analyze changes in diffraction data instead of undergoing a full analytical analysis of the images. (4) This method can be utilized for a wide range of data types with different image features.

I. INTRODUCTION

In recent years the study of neural networks (NNs)1 has opened the way for an ever-growing list of applications,2,3 owing to the exponential growth of computational power in modern processors compared to their predecessors. The digitization revolution has provided a constant stream of useful data to train NNs and enable advancements in algorithms that are more efficient computationally. These applications range from speech recognition4 to autonomous driving5 and medical diagnosis.6 At the heart of deep learning lies the idea that any complex task that requires an input and an output can be modelled with a sufficiently complex function. The parameters of this function can be ‘learned’ using labelled data to produce the desired output. The architecture of the function and its training methods are the subject of ongoing research.7 However, in all cases, the process of ‘training’ requires the minimization of some loss function. The loss function is designed to yield high loss if the predictions of the NN significantly deviate from the correct outputs of the labelled data. The loss is reduced as the NN predictions of the labelled data improve.

In chemistry and biology, scientists are often faced with molecules that have many degrees of freedom, yet there are only a few key modes that direct the chemical processes.8,9 This reduction in dimensionality is governed by a complex matrix of forces between the individual atoms inside the molecule and there is no theoretical derivation for it so far. This, in a way, resembles the minimization of a loss function in machine learning. Hence, one would naturally think that a machine learning algorithm that learns how this reduction in dimensionality takes place could provide significant insights into a theoretically intractable problem. One of the dream goals of time-resolved crystallography is to understand the dynamics along the key modes that govern chemical processes through time-resolved observation techniques.10 Typically, short electron pulses11, produced by DC and RF electric fields,12–16, or x-rays17,18 are used as probe pulses to study photochemical reaction pathways that are triggered through pump laser pulses. The obtained diffraction patterns are analyzed to extract information about the molecular dynamics.

However, one major obstacle is that it is impossible to directly invert reciprocal diffraction space into real space without more information, such as the signal field, due to the well-known phase problem.19 Therefore, to create a molecular movie, a minimization function is usually used that combines the diffraction data with known information about the chemical structures involved in the phase transition.20 This approach can be expanded upon to exploit deep learning algorithms to aid in a theoretically ambiguous task.
Previous studies demonstrated the usage of deep neural networks (DNNs), typically convolutional neural networks (CNNs), on x-ray diffraction images to classify space groups, extract features, and identify certain materials. However, one application that would be very useful in the field of ultrafast science is a full structural analysis of the molecular dynamics extracted from diffraction images in a time-resolved pump-probe experiment. In this paper, we take a step toward this goal. We present results of using DNNs, combining CNNs and generative adversarial networks (GANs), to analyze diffraction patterns obtained in an ultrafast electron diffraction (UED) experiment. Nanometer-thin layers of bismuth were deposited on 20 nm SiN windows to enable sufficient electron transmission to probe the structural transitions using 95 keV electron probes. The bismuth sample was excited with 800 nm laser pulses in the strongly driven limit for the solid-liquid phase transition. The effective time resolution for this instrument is on the 100 fs time scale. Diffraction images obtained at various time delays between pump and probe and different laser fluences were used to train and test our NN. Our analysis method is generalizable and, thus, should serve as a step in a more general scheme to predict molecular behaviour at the ultrafast timescale through deep learning.

II. STUDYING BISMUTH MELTING TEMPERATURES USING NEURAL NETWORKS

Bismuth samples consisting of layers of various thicknesses on silicon wafers, processed to give an array of 20 nm thin SiN windows to act effectively as electron transparent windows, were prepared via sputtering. The samples were then subjected to 800 nm 100 fs laser pulses and probed with 95 keV electron pulses. The purpose of the study was to test the ultrafast dynamics of bismuth melting and compare it to previous studies.

The ultrathin bismuth metal sheets were excited at sufficient excitation to exceed the solid-liquid phase transition. In comparison to the previous free standing bismuth studies, the effect of the SiN solid substrate support was to retard the onset of melting such that the dynamics were well understood as a thermally driven process, the dynamics of which could be well modelled by the traditional Debye-Waller relations for lattice heating. Hence, it is predicted that, at various time points in the initial picoseconds after laser excitation, the temperature of bismuth would vary by first rising and then stagnating at some point before cooling off. The temperature can be theoretically estimated from the diffraction patterns directly via analytical calculations. However, it would be useful to build a NN that can predict the temperature from the diffraction patterns directly for several reasons:

1. This is a less complex problem that involves only temperature changes in one type of atom involved in electron scattering. Hence it can serve as a simpler test case as a step toward more complex problems.

2. Successful analysis of diffraction patterns via a NN architecture can be applied to other problems if trained with different data on the same or very similar NN architectures.

3. In diffraction experiments a large volume of data is collected, therefore, having a NN that can automatically sort it out and provide an initial assessment can save a lot of time and effort.

4. Generally, one of the bottlenecks of machine learning is providing enough data for a NN to be trained to a satisfactory level. Hence, being able to, at least partially, train the network on synthetically created data would eliminate the need to collect lots of experimental data and label them adequately for network training. The process of creating, potentially unlimited, synthetic data for diffraction, if applied correctly, can be extended to many other problems.

III. METHOD

To illustrate the difference between typical NNs containing only CNNs and our novel NN containing a CNN and a GAN and show the improvement brought about by GANs, we present both NNs and discuss their respective performances.

A. Neural network with CNN

Synthetic diffraction patterns for bismuth at different temperatures were created using the programs CrystalMaker and CrystalDiffract. First, plots of radial powder diffraction patterns were created for different $u_{\text{iso}}$, where $u_{\text{iso}}$ is the root-mean-square (RMS) velocity of the atoms in the bismuth crystal. Then, using some simple code, these plots were converted into ideal diffraction patterns, i.e., perfectly circular patterns without noise. Fig. 1 shows a graph of the plot and the images created for various values of $u_{\text{iso}}$. The images created were then modified to better resemble the experimental diffraction patterns obtained in the lab. Thus, a central diffraction spot, a synthetic beam stop modelled after the experimental one were added as well as a Gaussian background. Fig. 2 shows such images before and after modification. The images obtained were used to train the NN.

1. Network architecture

We used a CNN consisting of three alternating convolutional and max-pooling layers followed by three dense layers and one dropout layer to prevent overfitting. Fig. 3 shows a schematic of the CNN. The images were reduced to 250 x 250 pixels and were fed into the network which contained the following layers: (a) Three convolutional layers that scan multiple filters through the image
producing smaller images and highlighting certain features. (b) Three max-pooling layers that halve the dimension of the image by taking the brightest spot in 2 × 2 pixel grids across the image. (c) Three dense layers that flatten the image into a vector and apply an affine transformation to reduce each vector into a single number. (d) One dropout layer with a rate of 0.2 after the first dense layer, which drops out randomly 20% of the vectors produced by the previous layer on each training step. This reduces overfitting.

All convolutional and dense layers have rectified linear unit (ReLU) activation, which means that the outputs of these layers were passed through the function \( \text{ReLU}(x) = \max(0, x) \), except for the last dense layer which had no activation function. The network was trained using a mean squared error loss, and the gradient descent algorithm used to minimize this loss was RMSprop. The learning rate of RMSprop was initialized to 0.001, but was set to exponentially decay throughout training with a decay rate of 0.96.

2. Main results and discussion

After 100 epochs of training, both the training and validation accuracy reached 90% as shown in Fig. 4. The metric for the correctness of a prediction was to be within 0.03 of the true \( u_{iso} \).

Having trained the network on synthetically produced diffraction rings, we subsequently tested the accuracy of this network on real diffraction images obtained from the experiment. Electron diffraction images over a period of 20 ps and at various laser fluence levels were inputted into the trained NN. Fig. 5a shows a plot of the NN’s predictions. As expected, the predicted temperatures before the laser pulse hit the sample (\( t = 0 \)) are steady, but rise rapidly when the laser excites the sample. After a transient period the temperature reaches a steady state. In addition, we observe that, as the fluence level rises, the peak temperature also rises. This is expected as more energetic laser pulses cause more thermal motion in the bismuth molecules. Hence, the NN predicts the general trend successfully.

To quantitatively assess the accuracy of the network predictions, analytic methods to compute the true temperatures of the lab images were created. This would have several benefits. On the one hand, having labelled data to train experimental images was created. This would have several benefits. On the one hand, having labelled data to train experimental images was created. This would have several benefits.

To solve this issue, a different method of generating synthetic images was implemented. Since manually attempting to adjust the images did not yield quantitatively accurate results, a NN that outputs synthetic images that resemble the ideal diffraction patterns of experimental images was created. This would have several benefits. On the other hand, having labelled data to train NNs is often difficult to obtain. The ability to create labelled synthetic data would thus be very beneficial. On
the other hand, creating synthetic data from limited experimental data in a systematic manner could benefit many other applications.

**B. GAN-CNN network**

For the task of taking experimental diffraction images as input, converting them to ideal images similar to synthetic images created via CrystalDiffract and outputting a temperature value, we created a specific type of NN consisting of a GAN and a CNN.

1. **GAN basic structure**

A GAN consists of two NNs, a generator G and a discriminator D, training in tandem. The discriminator takes in a reference image and outputs the probability of it being a real image as opposed to a generated image. The generator takes in random noise and outputs generated images. The random noise input allows the generator to produce slightly different images for different noise vector inputs, hence introducing some variability in the output. The generator and discriminator compete against each other to raise each other’s performance. As the discriminator gets better at recognizing ‘fakes’, the generator has to get better to continue ‘fooling’ it. The generator tries to create more accurate generated images that resemble the reference images to trick the discriminator, i.e., to maximize the probability of the discriminator incorrectly labelling generator images as real. The discriminator, on the other hand, tries to minimize the probability of it incorrectly detecting the generated images as reference images. Mathematically, the loss func-
and is not always accurate. Such a GAN means improving the performance of the generator to recognize them. Fig. 4 shows plots of an experimental image, the corresponding generated image and the corresponding synthetic image created via CrystalDiffract.

For our specific task we used a modified version of the Pix2Pix Generative Adversarial Network architecture. 35 Pix2Pix is built on the U-Net architecture, which has 3 components: a decoder, an encoder, and skip-connections. The decoder greatly down-samples the model’s input until it reaches a bottleneck layer. The bottleneck layer is the layer with the fewest nodes in the network; placing it between the decoder and encoder forces the decoder to only retain essential information. The encoder up-

2. Network architecture

For our specific task we implemented a modified version of a GAN. While a basic GAN takes noise as input and outputs images, we implemented a GAN that takes experimental diffraction images and outputs ideal diffraction images similar to the ones synthetically created via CrystalDiffract. This is advantageous as this technique can be extended to many instruments and different experiments. Experimental diffraction images typically include background noise due to scattering off the substrate holding the samples and dead or oversaturated pixels in the detector. This noise is removed with several analytical techniques, such as creating special masks to cover certain pixels or using specific equations to remove baseline noise, 34 and is not always accurate. Such a GAN then provides a mapping between experimental images and ideal synthetic images, of which an unlimited quantity can be created for training purposes.

Generating synthetic images given a lab image is an example of an image-to-image translation task, in which a mapping from an input image distribution to an output image distribution is to be learned. The data used for this task consists of image pairs. The model learns the mapping from the input image to the output image. If trained, the model can then be applied to new images to generate totally new outputs.

The dataset for image to image translation was created by pairing up lab images and synthetic images with the same temperature values. The model was trained to go from lab images to synthetic images. The synthetic images were cropped to 128 × 128 pixels and a Gaussian background was added in order to match the lab images as closely as possible, which led to better overall GAN performance. A circular mask was applied to the centre of both the lab and synthetic images. In total, 408 diffraction images were collected, of which 10% (41 images) were used as the validation set. Usually, image-to-image translation requires large datasets, often orders of magnitude larger than the size of the dataset available to us. Remarkably, despite the important differences between the images being minute our GAN is still able to identify them. Fig. 4 shows plots of an experimental image, the corresponding generated image and the corresponding synthetic image created via CrystalDiffract.

For this task, we used a modified version of the Pix2Pix Generative Adversarial Network architecture. 35 Pix2Pix is built on the U-Net architecture, which has 3 components: a decoder, an encoder, and skip-connections. The decoder greatly down-samples the model’s input until it reaches a bottleneck layer. The bottleneck layer is the layer with the fewest nodes in the network; placing it between the decoder and encoder forces the decoder to only retain essential information. The encoder up-
samples this to get the model’s output. However, there is often some low-level information that may be lost in the down-sampling process. To reliably translate the input image to the output, these features may be needed. The U-Net does this by incorporating skip-connections that connect the $i^{th}$ decoding layer from the input to the $i^{th}$ encoding layer from the output. For example, there would be a skip connection from the first decoder layer to the last encoder layer. Information can bypass the bottleneck layer by passing through these skip connections. The Pix2Pix loss function is similar to the GAN loss function described previously, with the addition of a loss term that measures the euclidean distance between the pixel values of the generated images and the pixel values of the corresponding synthetic images.

In order to further increase performance on this task, further modifications were made to this loss function. Peak-signal-to-noise ratio (PSNR) and structural similarity index measure (SSIM) values between the generated images and synthetic images were also calculated. These terms were included in the loss function to penalize generated images that are dissimilar to the corresponding synthetic images. These three terms, along with the GAN loss, are primarily effective at the start of training, when the GAN learns the general structure of the output images. On their own, however, they are not sufficient for the task: the network fails to consistently learn some small details of the synthetic images.

A new loss term is introduced to address this. This loss term is calculated by using a new CNN identical to the network in section III A. This Conversion CNN (CCNN) is trained to predict the $u_{\text{iso}}$ of synthetic images. It takes a generated image as input and outputs a corresponding $u_{\text{iso}}$ value. The difference between this predicted $u_{\text{iso}}$ and the analytically calculated $u_{\text{iso}}$ of the lab image is

FIG. 5. The neural network’s prediction of the $u_{\text{iso}}$ values and temperatures of the experimental bismuth diffraction images. The laser pulse excites the sample at $t = 0$ fs, where a rapid rise in temperature is observed. The temperatures predicted by the CNN are inaccurate albeit they follow the general trend of rising after excitation.

FIG. 6. Diffraction images: lab image, generated image, synthetic image. The generator takes a lab image as input and is trained to output the corresponding ideal diffraction pattern emulating the synthetic image.
added as the new loss described in Equ. 4.

\[ \mathcal{L}_{ImageTranslation}(x, y, u_{iso}) = \alpha_1 \mathcal{L}_{GAN}(G, D) + \beta_1 \text{PSNR}(G(x), y) + \beta_2 \text{SSIM}(G(x), y) + \gamma_1 |y - G(x)| + \gamma_2 |u_{iso} - \text{CCNN}(G(x))|. \]  

(4)

Here, \( \alpha_1, \beta_1, \beta_2, \gamma_1 \) and \( \gamma_2 \) are manually-tuned hyperparameters, \( x \) is the vector of lab images, \( y \) is the vector of corresponding synthetic images created via CrystalDiffact, and \( u_{iso} \) is the vector of corresponding \( u_{iso} \) values.

The GAN outputs a generated image that emulates an ideal diffraction pattern. This generated image is used as input for the CCNN, which outputs the corresponding \( u_{iso} \) value. This predicted \( u_{iso} \) value is the final output of the entire NN. It is compared to the analytically calculated \( u_{iso} \) value, for images in the validation set, to quantify the percentage error of the NN. Fig. 7 shows a schematic of how the network operates to predict temperatures.

Fig. 8 shows a schematic of the training process of the NN. The generator takes a lab image as input and generates an image emulating an ideal diffraction pattern. The discriminator takes a generated image and a synthetic image containing an ideal diffraction pattern, with minimal processing, created via CrystalDiffact and outputs a value between 0 and 1 from which the discriminator loss is calculated. The total loss function of the NN is the sum of the Euclidean distance between the generated image and the synthetic image, the difference between the analytical value of \( u_{iso} \) and the value of \( u_{iso} \) predicted by the CCNN, SSIM and PSNR of the generated image and the conventional generator loss which includes the discriminator predictions.

3. Main results and discussion

After 18 epochs of training, a prediction error of 4.3% was reached on the training set and 5.72% on the validation set. These results vary by a few percentage points for different training runs. This is due to some randomness in the initialization of the generator and discriminator networks at the start of the training process. Fig. 9 shows the training and validation errors.

This is a significant improvement over the performance in section III A, where the temperature predictions were significantly inaccurate as seen in Fig. 5a. Although the general trend of temperature rise after excitation was predicted correctly by the CNN, the level of inaccuracy deemed this approach inappropriate for providing a reliable automated model replacing analytical calculations. For the model to be useful, its temperature predictions need to reliably be within a few percentage points of the analytical temperatures. This level of accuracy was achieved by our GAN-CNN network. This performance is notable, given the small size of the dataset. Despite the variation between the images being very little, the GAN can accurately recreate the small details of importance in each image.

Moreover, the GAN-CNN network is generalizable as it provides an image-to-image mapping between the experimental data and ideal diffraction patterns. This approach can be applied to data taken by many other instruments and in different experiments, and hence, is not limited to UED.

IV. CONCLUSION

We demonstrated a novel application of GANs and CNNs in the study of UED images. Polycrystalline bismuth, that was subjected to 800 nm pump laser pulses and underwent thermalization, was probed via time-resolved electron diffraction. The diffraction images were collected and analyzed using deep learning techniques. Through the employment of a GAN, we were able to convert the experimental diffraction images into idealized diffraction patterns that were subsequently analyzed by a CNN. Temperature changes were predicted with a deviation of less than 6% from the theoretically estimated values.

Typically, electron diffraction images contain back-
FIG. 8. Neural network schematic. (Top) The generator takes a lab image as input and generates an image emulating an ideal diffraction pattern. (Middle) The discriminator takes a generated image and a synthetic image containing an ideal diffraction pattern, with minimal processing, created via CrystalDiffract and outputs a value between 0 and 1 from which the discriminator loss is calculated. (Bottom) The total loss function of the network architecture is the sum of the Euclidean distance between the generated image and the synthetic image, the difference between the analytical value of $u_{iso}$ of the lab image and the value of $u_{iso}$ predicted by the CCNN, SSIM and PSNR of the generated image and the conventional generator loss which includes the discriminator predictions.

Ground noise consisting of scattering off the sample holder, variations in the detector response, dead and oversaturated pixels, etc. These effects typically have to be removed manually through various analytical steps and the procedure is not always accurate. The GAN can learn the mapping between the experimental images and the corresponding ideal diffraction patterns. This is very useful and could be applied to data taken in different experiments with many potential applications. Moreover, training the CNN part of the GAN-CNN network was done only with synthetic images, of which a virtually unlimited number can be created.

Furthermore, the application presented in this paper was performed by training the network on a very small dataset of only 408 images. Further studies could exploit the power of this network by training it on larger datasets and by extending it to more advanced applications performed using different instruments.

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1. Laith Alzuabaidi, Jinglan Zhang, Amjad J. Humaidi, Ayad Al-Dujaili, Ye Duan, Omran Al-Shamma, J. Santamaría, Mohammed A. Fadhel, Muthana Al-Amidie, and Laith Farhan. Review of deep learning: concepts, cnn architectures, challenges, applications, future directions. Journal of Big Data, 8(1), Mar 2021.

2. Weibo Liu, Zidong Wang, Xiaohui Liu, Nianyin Zeng, Yurong Liu, and Fuad E. Alsaadi. A survey of deep neural network architectures and their applications. Neurocomputing, 234:11–26, Apr 2017.

3. Samira Pouyanfar, Saad Sadiq, Yilin Yan, Haiman Tian, Yudong Tao, Maria Presa Reyes, Mei-Ling Shyu, Shu-Ching Chen, and S. S. Iyengar. A survey on deep learning. ACM Computing Surveys, 51(5):1–36, Sep 2018.

4. Ali Bou Nassif, Ismail Shahin, Imtinan Attili, Mohammad Azzez, and Khaled Shaalan. Speech recognition using deep neural networks: A systematic review. IEEE Access, 7:19143–19165, 2019.

5. Ying Li, Lingfei Ma, Zilong Zhong, Fei Liu, Michael A. Chapman, Dongpu Cao, and Jonathan Li. Deep learning for lidar point clouds in autonomous driving: A review. IEEE Transactions on Neural Networks and Learning Systems, page 1–21, 2020.

6. Md. Milon Islam, Fakhri Karray, Reda Alhajj, and Jia Zeng. A review on deep learning techniques for the diagnosis of novel coronavirus (covid-19). IEEE Access, 9:30551–30572, 2021.

7. Md Zahangir Alom, Tarek M. Taha, Chris Yakopcic, Stefan Westberg, Paheding Sidike, Mst Shamima Nasrin, Mahmudul Hasan, Brian C. Van Essen, Abdul A. S. Awual, and Vijayan K. Asari. A state-of-the-art survey on deep learning theory and architectures. Electronics, 8(5):292, Mar 2019.

8. R. J. Dwayne Miller. Mapping atomic motions with ultrabright electrons: The chemists’ gedanken experiment enters the lab frame. Annual Review of Physical Chemistry, 65(1):583–604, Apr 2014.

9. Anatoly A. Ischenko, Peter M. Weber, and R. J. Dwayne Miller. Capturing chemistry in action with electrons: Realization of atomically resolved reaction dynamics. Chemical Reviews, 117(16):11066–11124, Jun 2017.

10. John C. Polanyi and Ahmed H. Zewail. Direct Observation of the Transition State. Accounts of Chemical Research, 26(3):119–132, 3 Apr 1993.

11. Zheng Li, Sandeep Gyawali, Anatoly A. Ischenko, Stuart Hayes, and R. J. Dwayne Miller. Mapping atomic motions with electrons: Toward the quantum limit to imaging chemistry. ACS Photonics, 7(2):296–320, Dec 2019.

12. R. J. Dwayne Miller. Femtosecond crystallography with ultrabright electrons and x-rays: Capturing chemistry in action. Science, 343(6175):1108–1116, 2014.

13. Germán Sciaini and R. J. Dwayne Miller. Femtosecond crystal electron diffraction: heralding the era of atomically resolved dynamics. Rep. Prog. Phys., 74(9):096101, 2011.

14. P. Baum and A. H. Zewail. Breaking resolution limits in ultrafast electron diffraction and microscopy. Proceedings of the National Academy of Sciences, 103(44):16105–16110, Oct 2006.

15. Hazem Daoud, Klaus Fleittmann, and R. J. Dwayne Miller. Compression of high-density 0.16 pc electron bunches through high field gradients for ultrafast single shot electron diffraction: The compact rf gun. Struct. Dyn., 4(4):044016, 2017.

16. Ernst Pflügl, L. Ascher, T. Perner, and J. K. Thomas. High performance of the Free Electron Laser: Improved electron bunching. New Journal of Physics, 8(11):272–272, Nov 2006.

17. T. R. M. Barends, L. Foucar, A. Ardevol, K. Nass, A. Aquila, S. Botha, R. B. Doak, K. Falahati, E. Hartmann, M. Hilpert, and et al. Direct observation of ultrafast collective motions in co myoglobin upon ligand dissociation. Science, 350(6259):445–450, Sep 2015.

18. Massimo Altarelli, editor. XFEL, the European X-ray free-electron laser: technical design report. DESY XFEL Project Group, Hamburg, 2006. OCLC: 254657183.

19. Garry Taylor. The phase problem. Acta Crystallographica Section D Biological Crystallography, 59(11):1881–1890, Oct 2003.

20. T. Ishikawa, S. A. Hayes, S. Keskin, G. Corthey, M. Hada, K. Pichugin, A. Marx, J. Hirsch, K. Shionuma, K. Onda, and et al. Direct observation of collective modes coupled to molecular orbital-driven charge transfer. Science, 350(6267):1501–1505, 2015.

21. Pascale Marc Vecsei, Kenny Choo, Johan Chang, and Titus Neupert. Neural network based classification of crystal symmetries from x-ray diffraction patterns. Physical Review B, 99(24), Jun 2019.

22. Yuta Suzuki, Hideitsu Hino, Takafumi Hawai, Kotaro Saito, Masato Kotsugi, and Kanta Ono. Symmetry prediction and knowledge discovery from x-ray diffraction patterns using an interpretable machine learning approach. Scientific Reports, 10(1):21790, Dec 2020.

23. Kevin Kaufmann, Chaoyi Zhu, Alexander S. Rosengarten, Daniel Maryanovsky, Tyler J. Harrington, Eduardo Marin, and Kenneth S. Vecchio. Crystal symmetry determination in electron diffraction using machine learning. Science, 367(6477):564–568, Jan 2020.

24. Angelo Ziletti, Devinder Kumar, Matthias Scheffler, and Luca M. Ghiringhelli. Insightful classification of crystal structures using deep learning. Nature Communications, 9(1), Jul 2018.

25. Woon Bae Park, Jiyong Chung, Jaeyong Jung, Keemin Sohn, Su-pra M. Pal Singh, Myungwook Pyo, Namsoo Shin, and Reesun Sohn. Classification of crystal structure using a convolutional neural network. UCRJ, 4(4):486–494, Jun 2017.

26. Julian Zimmermann, Bruno Langbehn, Riccardo Cucini, Michele Di Fraia, Paola Finetti, Aaron C. LaForge, Toshiyuki Nishiyama, Yevheniy Ovcharenko, Paolo Piseri, Oksana Pleskan, Kevin C. Prince, Frank Stenkemeyer, Kiyoshi Ueda, Carlo Callegari, Thomas Möller, and Daniela Rupp. Deep neural networks for classifying complex features in diffraction images. Physical Review E, 99(6), Jun 2019.

27. Leslie Ching Ow Tiong, Jeongrae Kim, Sang Soo Han, and Donghun Kim. Identification of crystal symmetry from noisy diffraction patterns by a shape analysis and deep learning. npj Computational Materials, 6(1), Dec 2020.

28. Hong Wang, Yunchao Xie, Dawei Li, Heng Deng, Yunxin Zhao, Ming Xin, and Jian Lin. Rapid identification of x-ray diffraction patterns based on very limited data by interpretable convolutional neural networks. Journal of Chemical Information and Modeling, 60(4):2004–2011, Mar 2020.

29. M. Gao, Y. Jiang, G. H. Kassier, and R. J. Dwayne Miller. Single shot time stamping of ultrabright radio frequency compressed electron pulses. Applied Physics Letters, 103(3):033503, Jul 2013.

30. Germán Sciaini, Maher Harb, Sergej G. Kruglik, Thomas Payer, Christoph T. Hebeisen, Frank-J. Meyer zu Heringdorf, Mariko Yamaguchi, Michael Horn-von Hoenegen, Ralph Ernsterfer, and R. J. Dwayne Miller. Electronic acceleration of atomic motions and disordering in bismuth. Nature, 545(7624):56–59, Mar 2009.

31. CrystalMaker Software Ltd. Crystalmaker, 2022.

32. H. X. Gao and L.-M. Peng. Parameterization of the temperature dependence of the debeye–waller factors. Acta Crystallographica Section A Foundations of Crystallography, 55(5):926–932, Sep 1999.

33. Jan Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, and Yoshua Bengio. Generative adversarial nets. In Z. Ghahramani, M. Welling, C. Cortes, N. Lawrence, and K.Q. Weinberger, editors, Advances in Neural Information Processing Systems, volume 27. Curran Associates, Inc., 2014.

34. Laurent P. René de Cotret and Bradley J. Siwick. A general method for baseline-removal in ultrafast electron powder diffraction data using the dual-tree complex wavelet transform. Structural Dynamics, 4(4):044004, Dec 2016.

35. Phillip Isola, Jun-Yan Zhu, Tinghui Zhou, and Alexei A. Efros. Image-to-image translation with conditional adversarial networks. In 2017 IEEE Conference on Computer Vision and Pattern Recognition (CVPR), pages 5967–5976, 2017.
Alain Horé and Djemel Ziou. Image quality metrics: Psnr vs. ssim. In 2010 20th International Conference on Pattern Recognition, pages 2366–2369, 2010.