Accelerating Electron Diffraction Pattern Generation using Machine Learning

AI's Bridge between Structure and Pattern

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DisQS Disordered Quantum Systems

The Problem. When a beam of electrons is fired at a crystal they interact with atoms as they pass through it, deviating from their original path, leaving in an information rich pattern. These patterns can be analysed to learn about internal characteristics of the crystal.

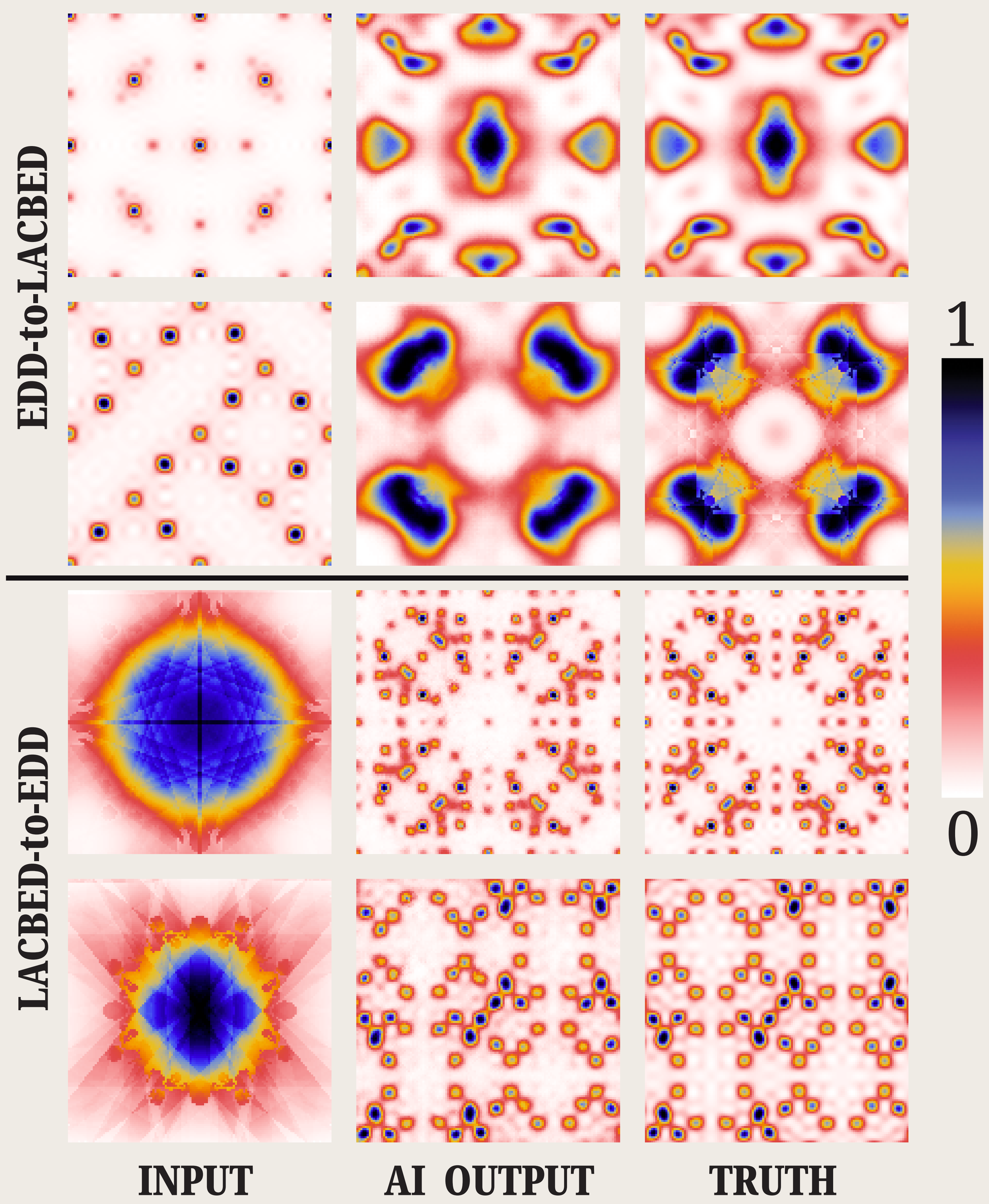
Electron diffraction experiments are expensive and existing simulations are time-consuming, and whilst the structure of the crystal is the determining factor of what the diffraction pattern looks like, finding the connection between the two is an extremely difficult problem.

The Preparation. The data acquisition required the collection of two images for each cubic crystal.

The first is the electron density distribution, obtained by an inverse Fourier transform of experimentally observed diffracted waves (from a large database):

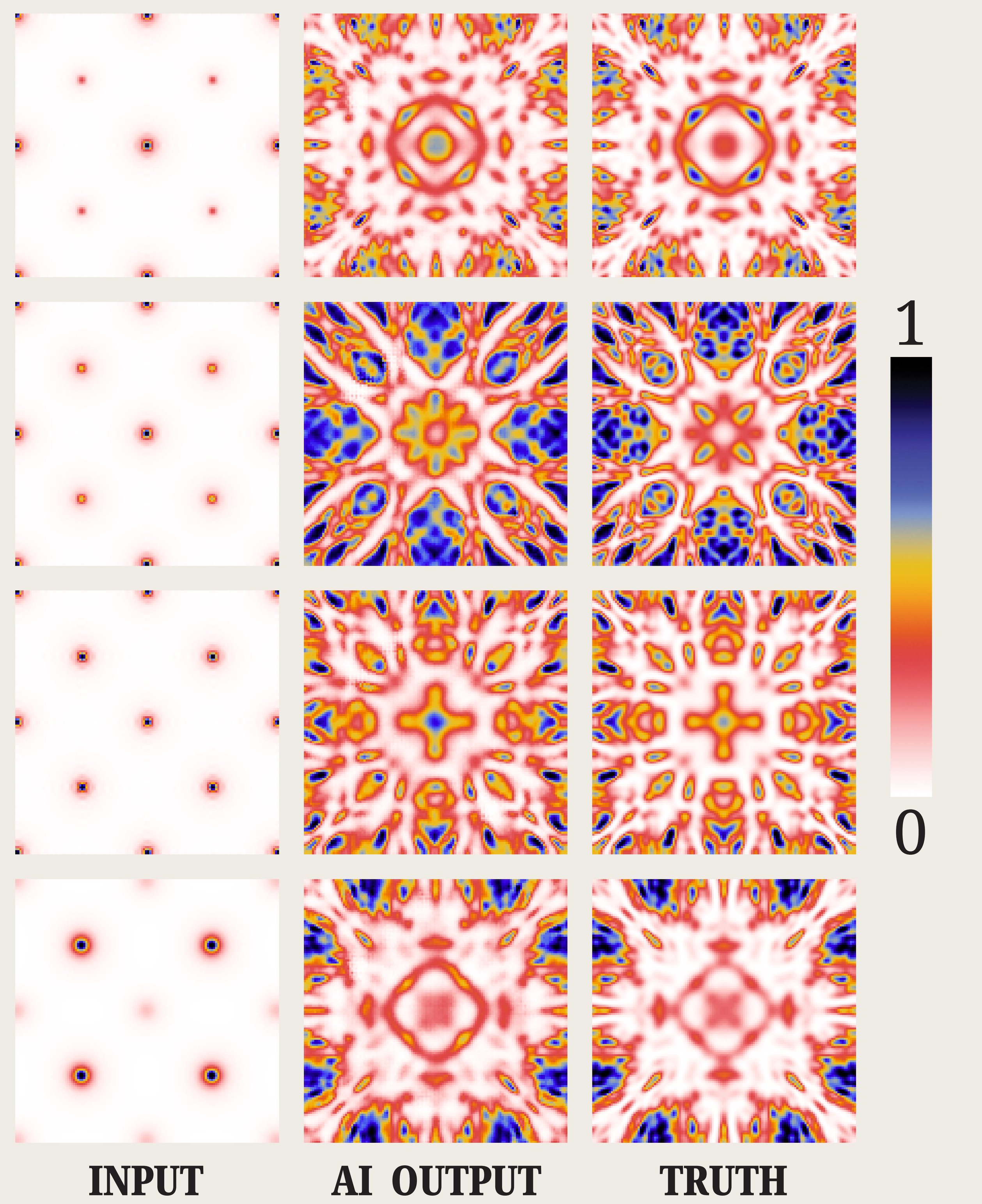
$$\boldsymbol{\rho}(\boldsymbol{x}) = \frac{1}{V}\sum_{\boldsymbol{h}} \boldsymbol{F}(\boldsymbol{h}) \quad \exp[-2\pi\imath\boldsymbol{h} \quad \boldsymbol{x}]$$

The second is the diffraction pattern—experimentally infeasible, so we opt to simulate using Felix [1, 2].



EXAMPLE RESULTS OF BOTH DIRECTIONS showing two models performing accurate image prediction. The two directions are going betwen the crystals' electron density disbtribution (EDD) and the LACBED pattern. The EDD images display normalised charge strength ranging from 0 to 1, and the LACBED pattern images show inverse intensity: white (0) is where the electrons are most likely to be found, and black (1) is where they are least likely to be found.

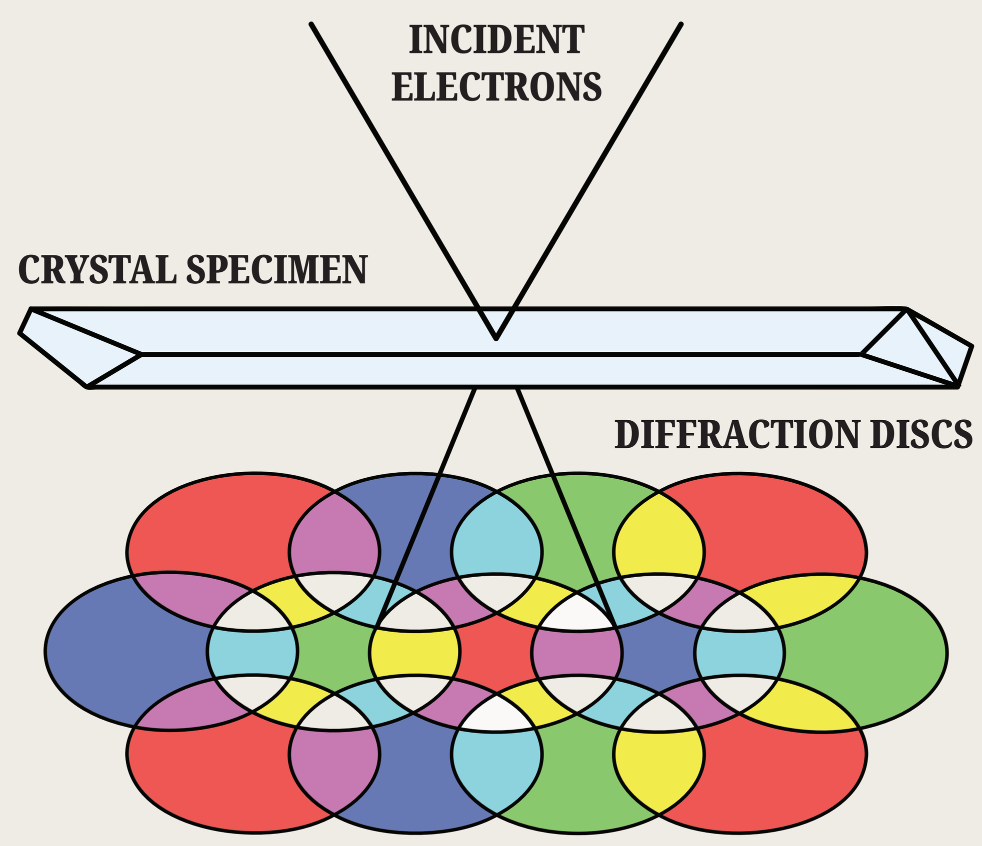
RESULTS ON A SPECIFIC SPACE GROUP displaying the model's ability to discern between very similar crystals with the same configuration but varying strengths of charges. All four crystals here lie in the F-43m space group. The discriminator in the model, when classifying images, uses a more sophisticated approach than just looking at each of the pixels individually, taking local convolutions to assess interdependencies between pixels that are spatially close, as this carries information about the nature of the image.



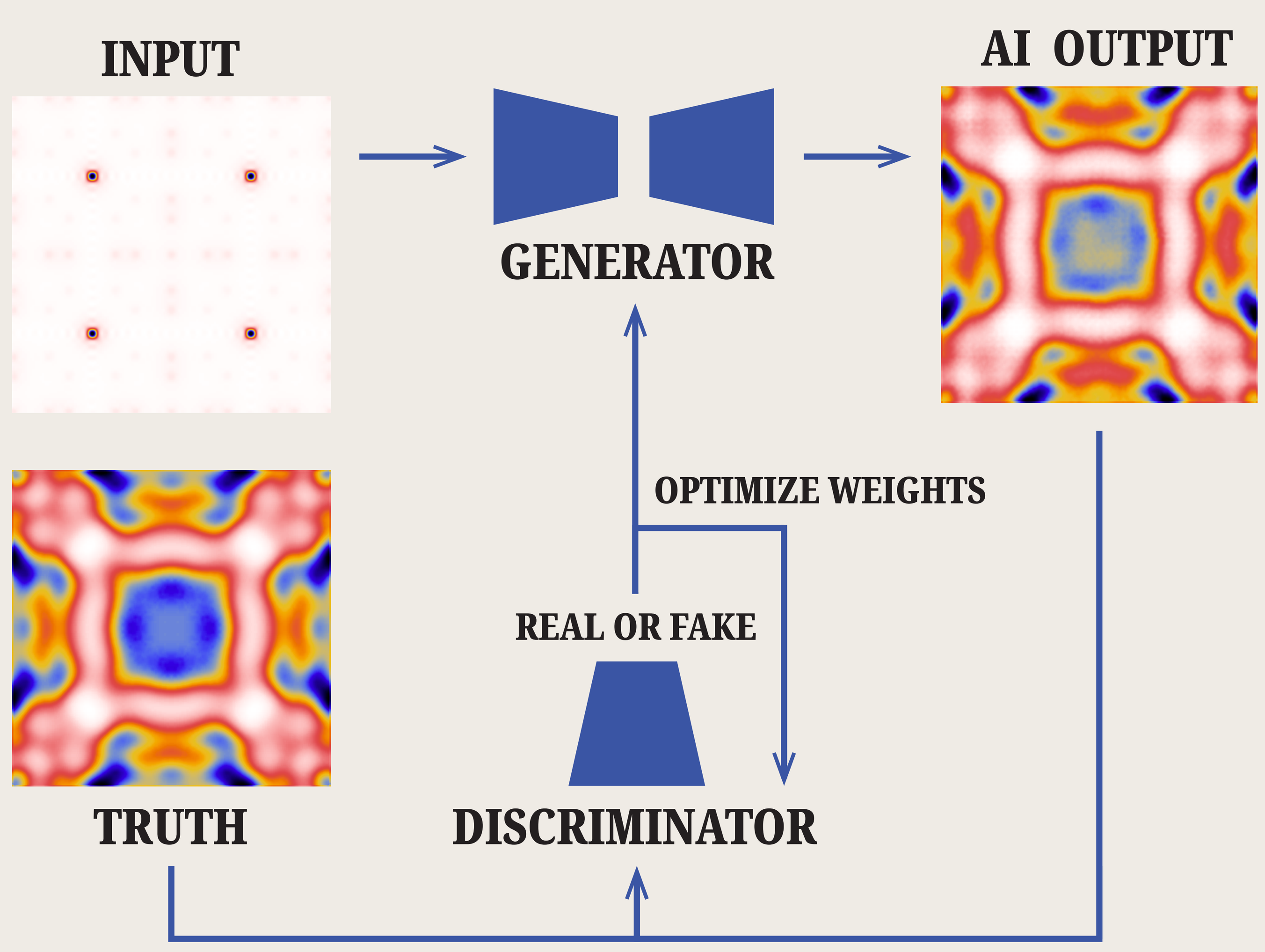
The Process. The project uses a conditional generative adversarial network (CGAN) architecture [3].

This image-to-image model features two main parts: a *generator*—analogously an artist whose main purpose is to fool the *discriminator*—a detective trying to discern between fake and real images.

Throughout training, the generator gets better at turning the input into the output, and the discriminator gets better at identifying real from fake, each constantly pushing the other to become more proficient in their task.



LARGE-ANGLE CONVERGENT BEAM ELECTRON DIFFRACTION (LACBED) wherein a beam is focussed to a small probe on the crystal. The discs in the resultant diffraction pattern overlap unlike regular CBED patterns. In experiments, the information in each disc can't be accessed separately; in using simulation software, we are able to extract individual discs. In this project we focus on the (0,0,0) disc, located in the centre, as it is the most information-rich part of the diffraction pattern.



Results. The machine learning model takes 20 milliseconds to predict an electron diffraction pattern, which is in constrast to 400 seconds for the simulation software, approximately four orders of magnitude faster.

Across multiple random seeds, the model achieves an average mean squared error loss below 0.02 when predicting diffraction patterns in the test set.

[1] Beanland, R. et al. (2012) 'Digital' electron diffraction - seeing the whole picture, https://arxiv.org/abs/1211.6571

[2] Felix: Bloch wave method diffraction pattern simulation software, https://github.com/WarwickMicroscopy/Felix

[3] Isola, P. et al. (2018) Image-to-image translation with conditional adversarial networks, https://arxiv.org/abs/1611.07004