Improved inversion of Bragg Coherent Diffraction Data using a Diffusion model

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For inversion of X-ray Free Electron Laser (XFEL) diffraction data, we previously developed a U-Net convolutional neural network (CNN) method that was optimized for arithmetic with complex numbers and called a Complex-CNN (C-CNN) [1]. This was found to perform better than a non-complex decoder where separate channels (amplitude and phase) of a complex image were generated. This made sense because the amplitude and phase of the domains within the thin-film $La_{1-x}Sr_xCuO_4$ sample, as used in the experiment, are intimately connected through the formalism of Bragg Coherent Diffractive Imaging [2,3].

The physics problem under investigation is the "phase domain problem" (PDP) illustrated in Fig 1. Within a single crystal, there exist side-by-side regions which are shifted relative to each other. When coherent X-rays diffract from this sample, their phases become shifted as shown and then interfere to form to form a speckled diffraction pattern in the far field. Inversion of this diffraction pattern is classically achieved by iterative minimization methods, for example Fienup's Hybrid Input-output method [4], or more recently by CNN approaches [5], but these are found to often fail in practice for the PDP which is particularly challenging. The uncertainty present in the PDP is one of uniqueness of the solution more than its sensitivity to missing data or noise. In our earlier publication [1], different levels of detail of the PDP were investigated. The first model was 15 elliptical domains of random phase in a regular array; this was found to be inverted reliably by the C-CNN even in the presence of noise added to the simulated diffraction pattern up to a certain level. The second model of 50 elliptical domains randomly distributed also performed well. The methods worked well for the experimental data, but the solution uniqueness was not fully explored [1].

Here we present early results from the application of the Diffusion Model (DM) to the same problem. We build on recent successes of DMs in generative modelling [6] and integrate them with physical constraints to solve inverse problems. We train the DM to denoise the complex amplitude and phase images corrupted by Gaussian noise, conditioning on the measured diffraction pattern via channel-wise concatenation. During inversion, reconstructions are obtained by initializing from random noise and then running the learned reverse diffusion process, in which each denoising step is supplemented by a physics-based update of the measured-simulated intensity mismatch, thereby combining the generative prior with data-fidelity constraints. The DM has already been applied to X-ray Ptychography, related to BCDI, with success [7].

So far, we have only looked at the 15-domain model, described above. We performed a side-by-side comparison with the C-CNN model in Fig 2. The same set of simulated training data (same model, different random phases) were used to train the C-CNN and the DM. The C-CNN result is the immediate supervised result without any learning iterations. High levels of agreement are seen in all cases with the biggest discrepancy in the phase channel of the C-CNN. All four random starts of the DM gave better levels of agreement.

In the near future, we will extend this work to the 50-domain model and XFEL experimental data.

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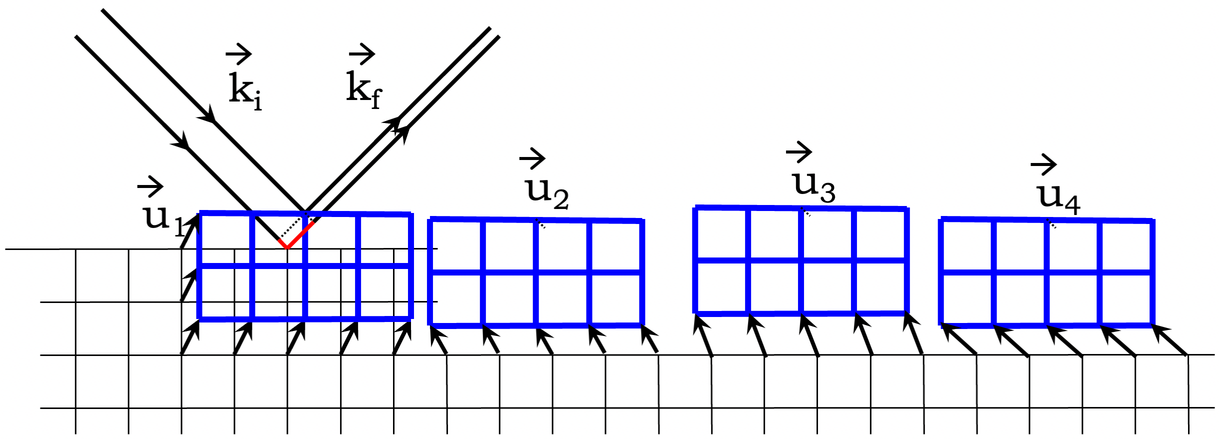

Figure 1. Schematic illustration of Bragg Coherent Diffraction Imaging (BCDI) applied to an array of crystal domains with different positions [2]. The vectors k_i and k_f represent the incident and exit wavevectors, while the u_i vectors represent the shifts of crystal pieces with respect to a reference lattice. The phase shift (red) can be seen to be $\phi_i = (k_f - k_i)$. u_i

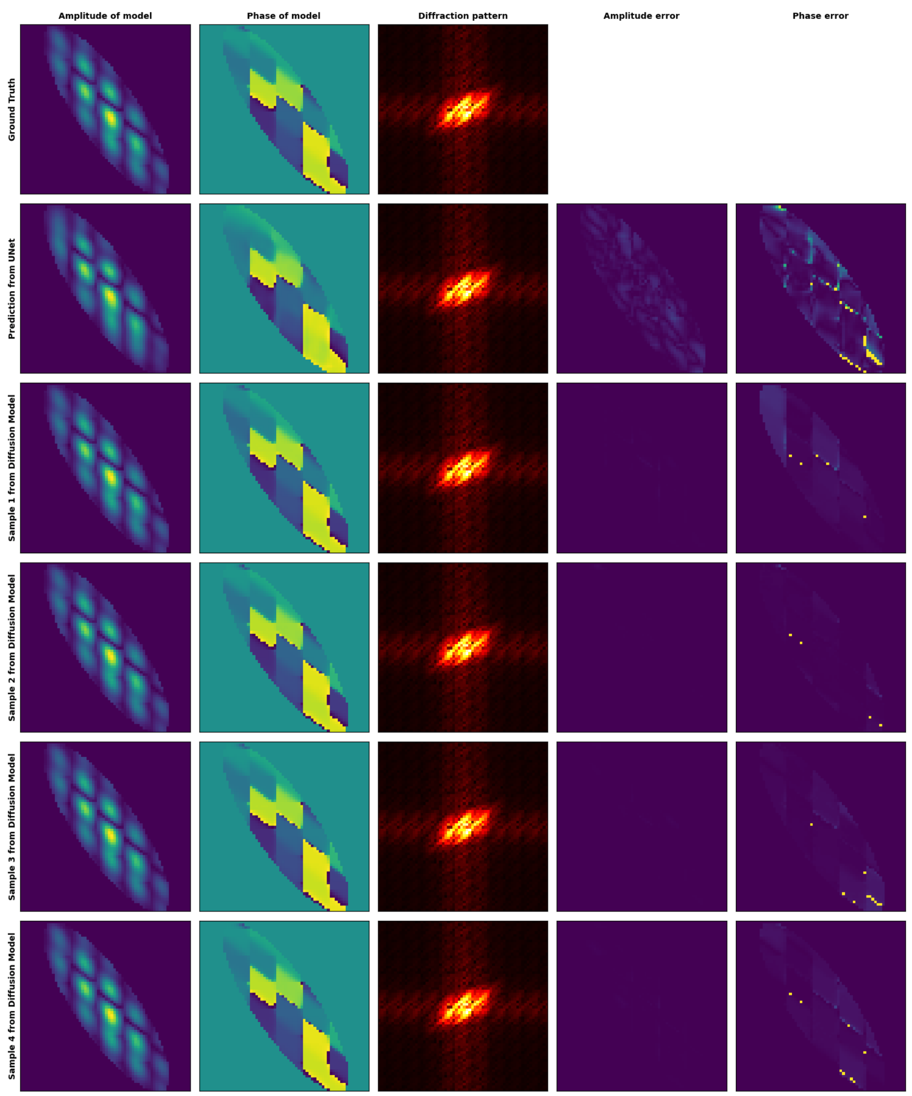

Figure 2. Results of applying the Diffusion Model (DM) to the 15-domain array simulation. The rows show the ground truth diffraction pattern and results from the DM and C-CNN. Columns represent the image amplitude, phase, the diffraction patterns and differences in amplitude and phase. Four random starts of the DM are shown.