Deep Learning for Bragg Coherent Diffraction Imaging: Detector Gap Inpainting and Phase Retrieval

Thesis

présentée et soutenue publiquement le

Pour l'obtention du titre de

Docteur de l'Université Grenoble Alpes
(mention Physique du rayonnement et de la matière condensée)

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The present document is a draft of my PhD manuscript.

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Deep learning for Detector Gaps Inpainting

In this chapter the "detectors' gaps problem" in Bragg Coherent Diffraction Imaging and our approach to solve it using Deep Learning are discussed. The main state-of-the-art measures are presented briefly and the topic of image inpainting with Deep Learning is introduced. The focus will then shift to our works that led eventually to the optimal "Patching-based" approach that can also be found in the published paper entitled *"Patching-based deep learning model for the Inpainting of Bragg Coherent Diffraction patterns affected by detectors' gaps"* (https://doi.org/10.1107/S1600576724004163). The chapter is closed with some analyses of the performances of the DL models in a variety of simulated and experimental cases.

0.7 The "Gap Problem"

At time of writing, standard BCDI experiments employ pixelated photon counting detectors to acquire the diffraction patterns. These detectors can guarantee high spatial resolution, noise-free counting and fast read-out times. Two examples of these devices, currently used at the ID01 beamline are the MAXIPIX and EIGER detectors [1, 2]. These detectors are often built by tiling together several sensing chips in order to cover a larger area, and are typically bonded to an Application-Specific Integrated Circuit (ASIC) using bump bonding. This implies the presence, in the overall sensing region, of vertical and/or horizontal stripes that are not sensitive to the impinging radiation. The width of these lines varies depending on the device but normally does not exceed the equivalent of some tens of pixels. Specifically, for the MAXIPIX detector the gap size is of 6 pixels while the EIGER has larger gaps of both 12 pixels and 38 pixels. The detector gaps problem does not affect BCDI only, but it is shared among other x-ray techniques that deal with single photon-counting pixelated detectors and/or beamstops. We have seen in chapter 0.1 that during a BCDI scan the 2D images acquired by the detector are stacked to form a 3D array. This leads these lines to become planes of missing signal in the dataset. The problems arise when reconstructing the data affected by these gaps. In fact, these regions of non-physical zero intensity deceive the Phase Retrieval algorithms inducing the presence of artifacts in the reconstructions[3]

It follows that the reliability of the reconstructions in this case is compromised as the strain distribution can be deeply affected by the artifacts. A good practice during standard BCDI experiments is to avoid the gaps by moving the detector if possible. However, this tends to be problematic for the case of high-resolution BCDI, i.e. when the diffraction pattern measurement extends to higher q-values, thus covering more than one sensing chip and necessarily crossing a gap region. Under these circumstances it becomes important to reduce the amount of artifacts deriving from the gaps.

0.8 State of the art

Here we will discuss the current strategies employed to treat the detector gaps. As someone could argue, the simplest yet not practical, solution would be to slightly move the detector sideways and acquire a second full scan with the gap hiding a different region of the same Bragg peak, and then merge the two measurements into a single gap-less one. This would in turn increase the acquisition time of more than 2X making it de facto never an option during standard experiments. Iterative phasing algorithms like PyNX allow the user to define a mask of the gap regions and will.

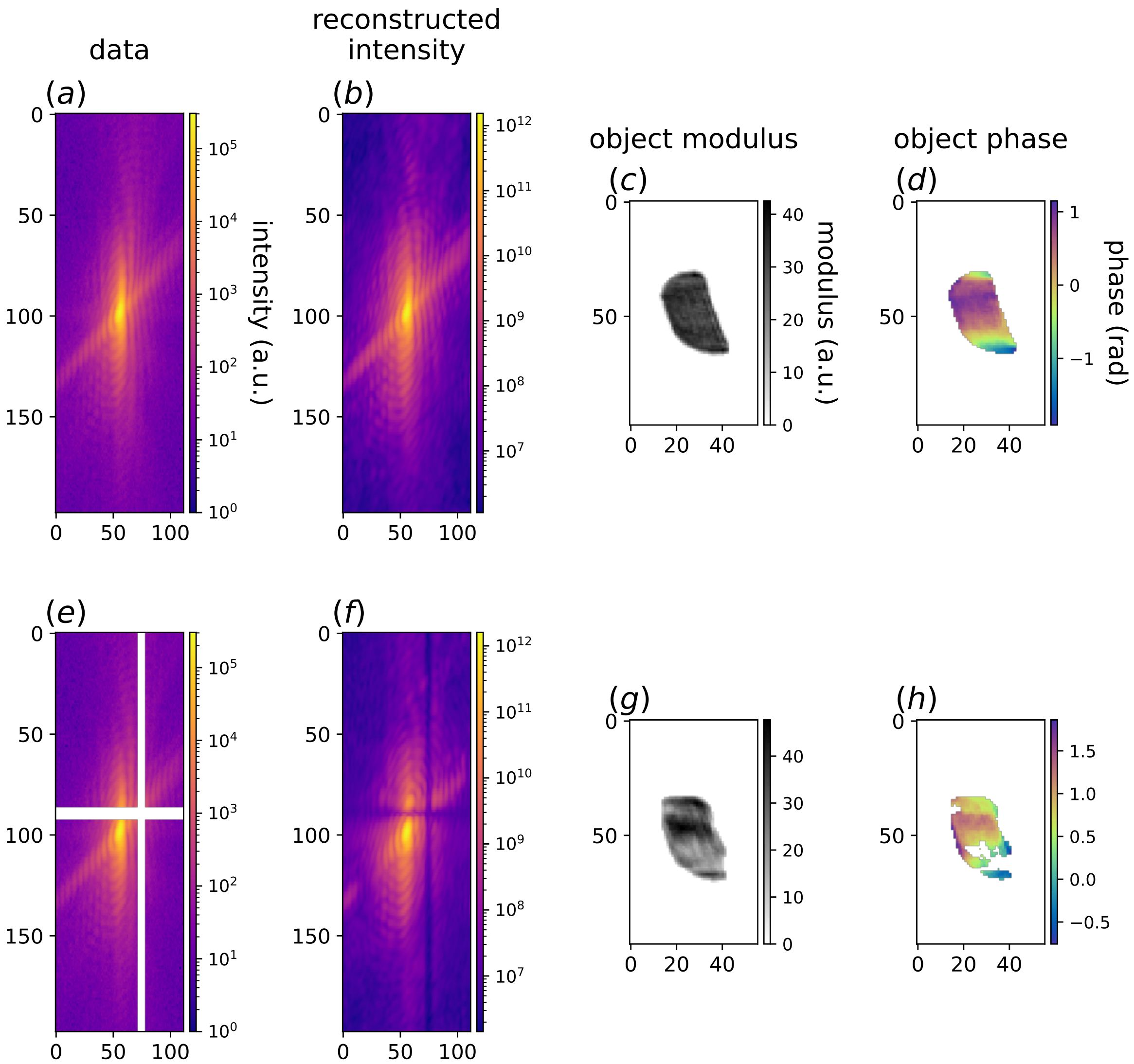

Figure 1: Effect of detector gaps in BCDI reconstructions (a) The central xz slice of an experimental diffraction pattern. **(b)** The same slice of the diffracted intensity calculated from the retrieved object. **(c - d)** xz slice of the modulus and phase respectively of the particle obtained from the phasing of the gap-less dataset. **(e)** Same slice as in **(a)** with an artificially added 6 pixel-wide, cross-shaped gaps to mimic the detector's ones. **(f)** The same slice of the diffracted intensity calculated from the retrieved object when not masking the gap regions. **(h - g)** xz slice of the modulus and phase respectively of the particle obtained from the phasing of the gap-affected dataset. The distortions caused by the gaps are evident.

0.9 Model design

0.10 Patching approach

0.11 Results in detector space

0.12 Results in real space

0.13 Fine-tuning

0.14 Performances assessment

Part IV

Deep learning for Phase Retrieval

We enter now the core topic of the thesis. Most of the efforts during this PhD have been dedicated to the Phase Problem.

0.15 State of the art

0.16 Highly strained crystals

0.17 Reciprocal space phasing

0.18 Phase symmetries breaking

0.19 Model design

0.20 Results on 2D case

0.21 Results on 3D case

0.22 Refinement with iterative algorithms

0.23 Experimental results

Part V

Conclusions

Bibliography

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3. Carnis, J. *et al.* Towards a quantitative determination of strain in Bragg Coherent X-ray Diffraction Imaging: artefacts and sign convention in reconstructions. *Scientific Reports* **9.** Publisher: Nature Research. ISSN: 20452322 (Dec. 1, 2019).

Annexes

Appendix A

Appendix