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

## Thesis

présentée et soutenue publiquement le

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## **0.1 Introduction**

The present document is a draft of my PhD manuscript.

# **Part I**

## **Bragg Coherent Diffraction Imaging**



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## **0.2 Single crystal diffraction**

## **0.3 Phase Problem**





## **Part II**

# **Convolutional Neural Networks**



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**0.4 Introduction on neural networks**

**0.5 Convolutional**

**0.6 U-Net and MSD-Net**



## **Part III**

# **Deep learning for Detector Gaps Inpainting**



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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 a dozen of pixels. 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] The typical artifacts caused by detector gaps are noticeable because of the presence of high-frequency oscillations in the amplitude and phase of the reconstructed object.

Moreover, these gaps tend 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.

**0.8 State of the art**

**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**



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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**



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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