Instamatic: a multi-purpose toolbox for collecting electron diffraction data

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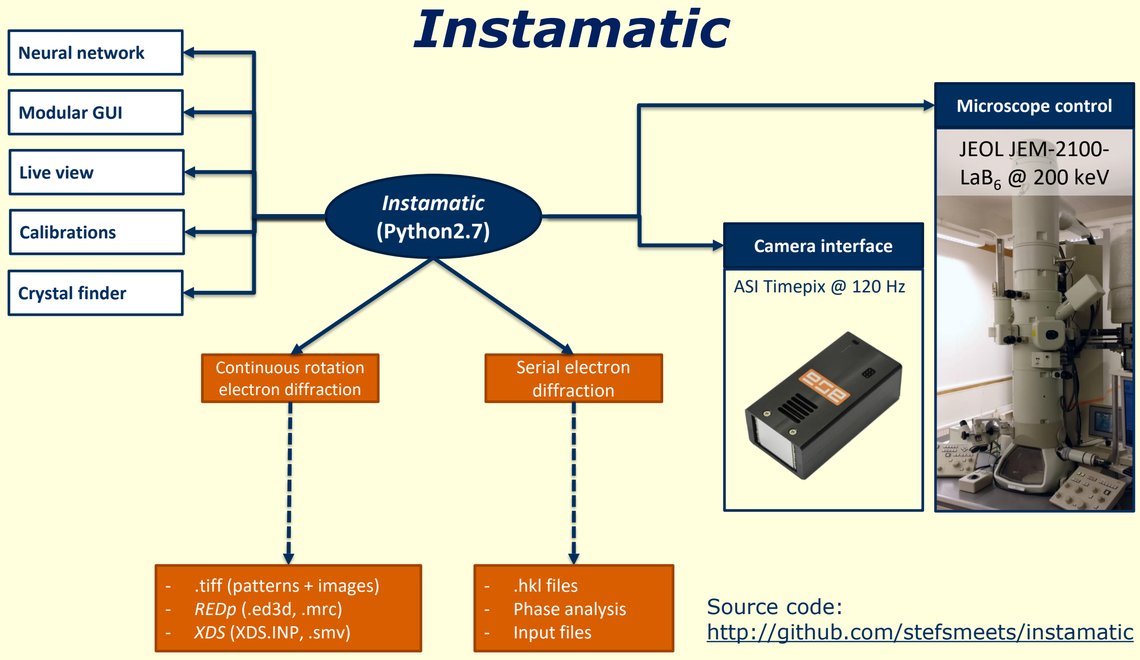
Introduction

We are developing software and methodology to automate the collection of electron diffraction data

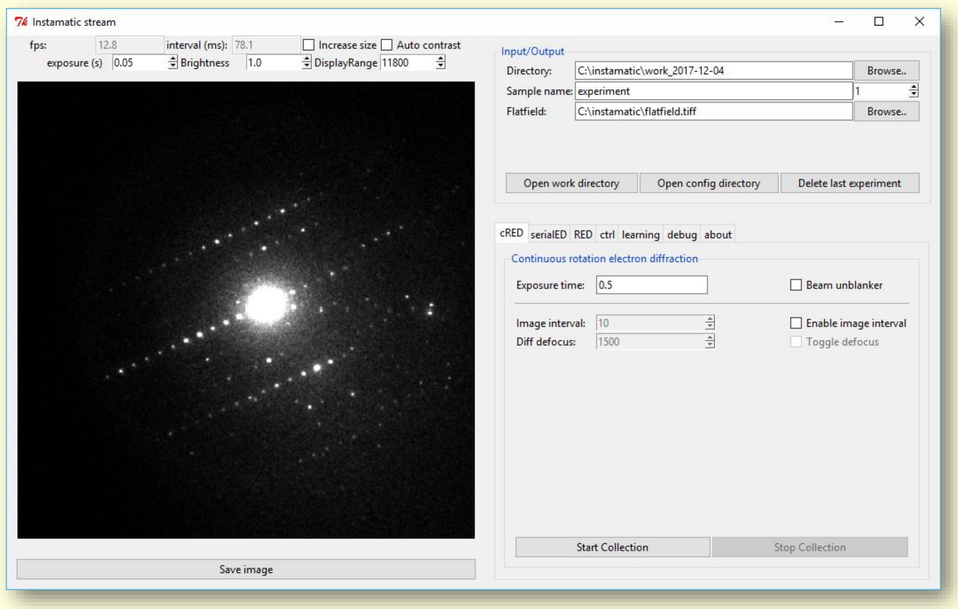
- **Single crystal electron diffraction**
  - Collect continuous rotation diffraction data on nano-sized crystals for structure determination
- **Serial electron diffraction**
  - Automatically collect diffraction data on ~3000 crystals per hour for screening and phase analysis
- **Machine learning**
  - Identify crystals suitable for further investigation

Instamatic



Source code: http://github.com/stefsmeets/instamatic

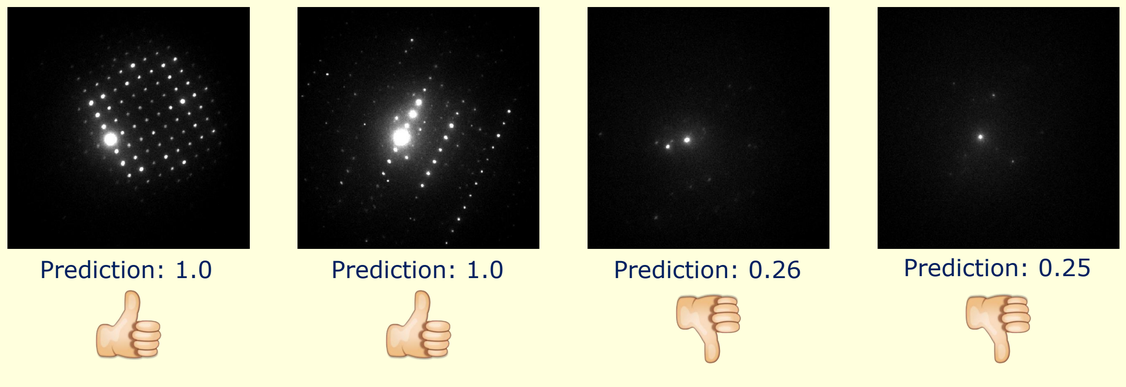
Instamatic is a python library for microscope and camera control with implementations for collecting serial and rotation electron diffraction data



GUI for collecting electron diffraction data

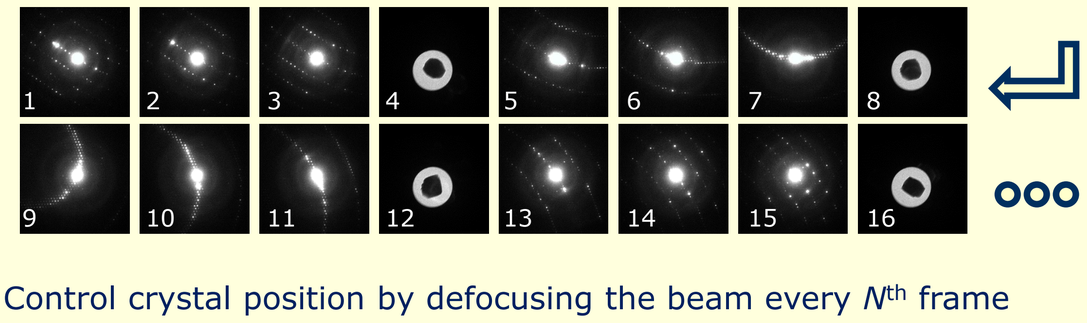
Machine learning

A deep convoluted neural network trained on >70.000 diffraction patterns predicts which crystals are suitable for collecting cRED data



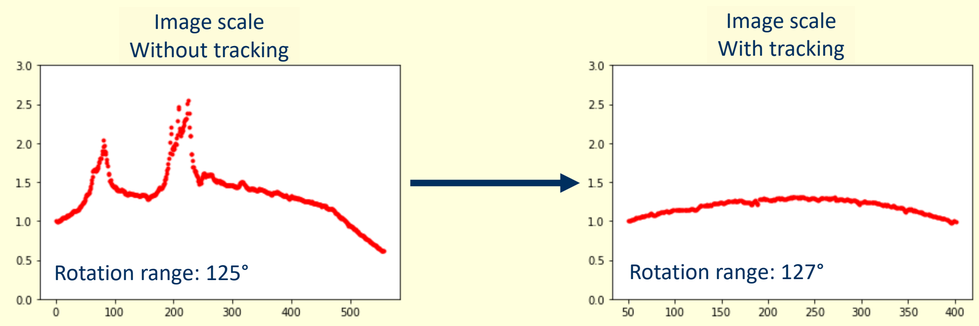
Continuous rotation electron diffraction

Collect data (SAED) while continuously rotating the crystal in the beam

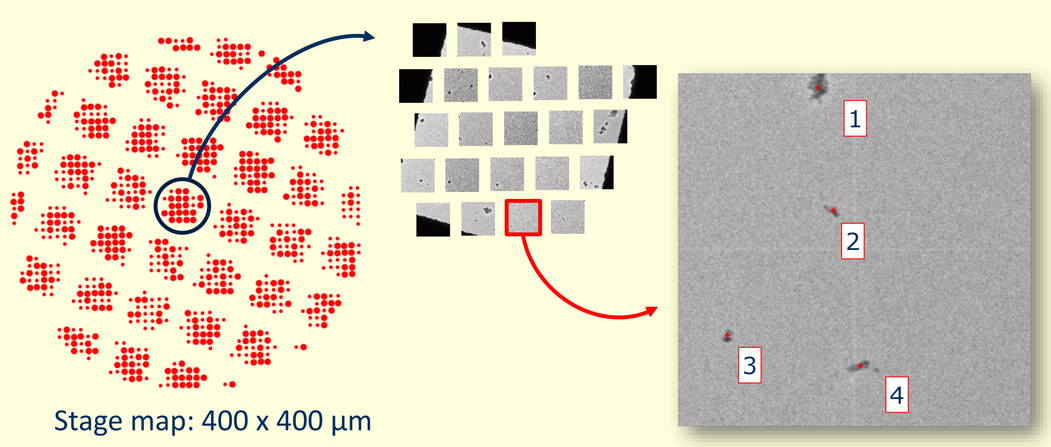


Control crystal position by defocusing the beam every N^{th} frame

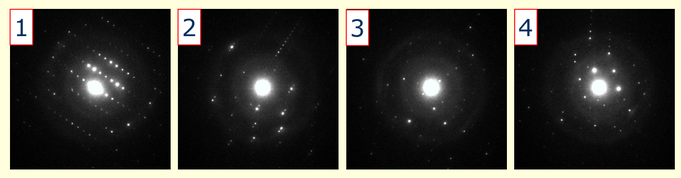
- Collect image and diffraction data on the same crystal
- More successful and reliable data collections
- Higher completeness because of larger rotation angles
- 10% of diffraction data are lost (N=10)



Serial electron diffraction



Stage map: 400 x 400 µm
836 images



Collect data on 1019 crystals in 80 minutes

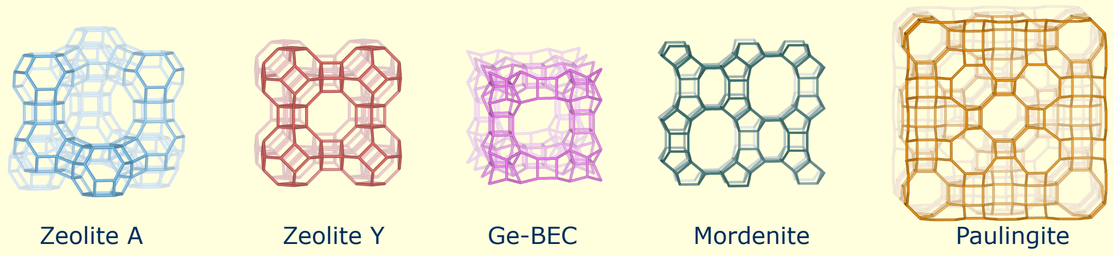
Applications

Screening
Identify crystals for cRED using machine learning

Crystal identification
Quantitative phase analysis on multiphasic materials

Structure determination
Combine ~200 diffraction patterns for structure determination

Structures solved



Acknowledgement

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