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Master thesis
in Materialsscience and Engineering

Four-Dimensional Scanning Transmission Electron Microscopy (4D-STEM) Analysis of NiCu alloy using py4DSTEM on High Performance Computing Cluster

submitted by

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September 14, 2024

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Zusammenfassung

Four-Dimensional Scanning Transmission Electron Microscopy (4D-STEM) Analysis of NiCu alloy using py4DSTEM on High Performance Computing Cluster

von Paul Jakob LOBPREIS

Hier Abstract!

UNIVERSITY OF SIEGEN

Abstract

Four-Dimensional Scanning Transmission Electron Microscopy (4D-STEM) Analysis of NiCu alloy using py4DSTEM on High Performance Computing Cluster

by Paul Jakob LOBPREIS

Here abstract!

Contents

Chapter 1

Introduction

1.1 Imaging with fast electrons

From TEM to 4DSTEM a brief description...

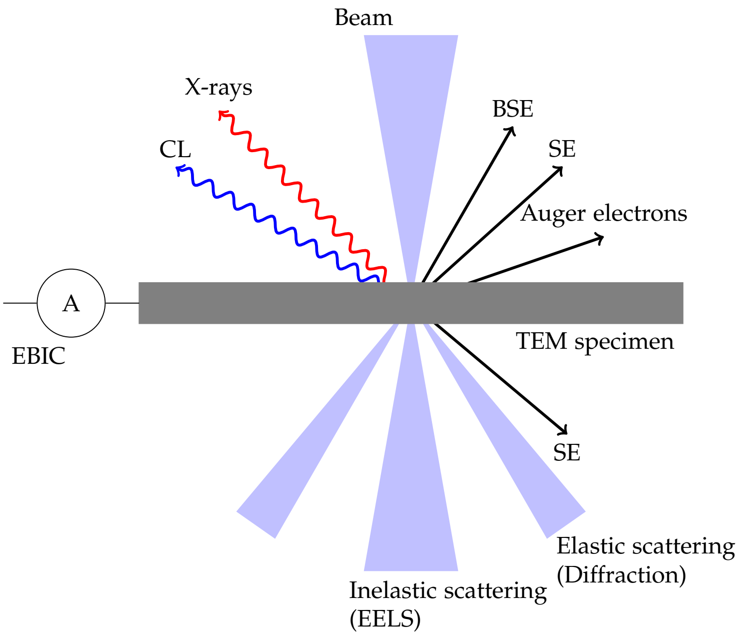


Figure 1.1: ww of elctrons with the sample, maybe exclude bc to trivial or another graph besides it

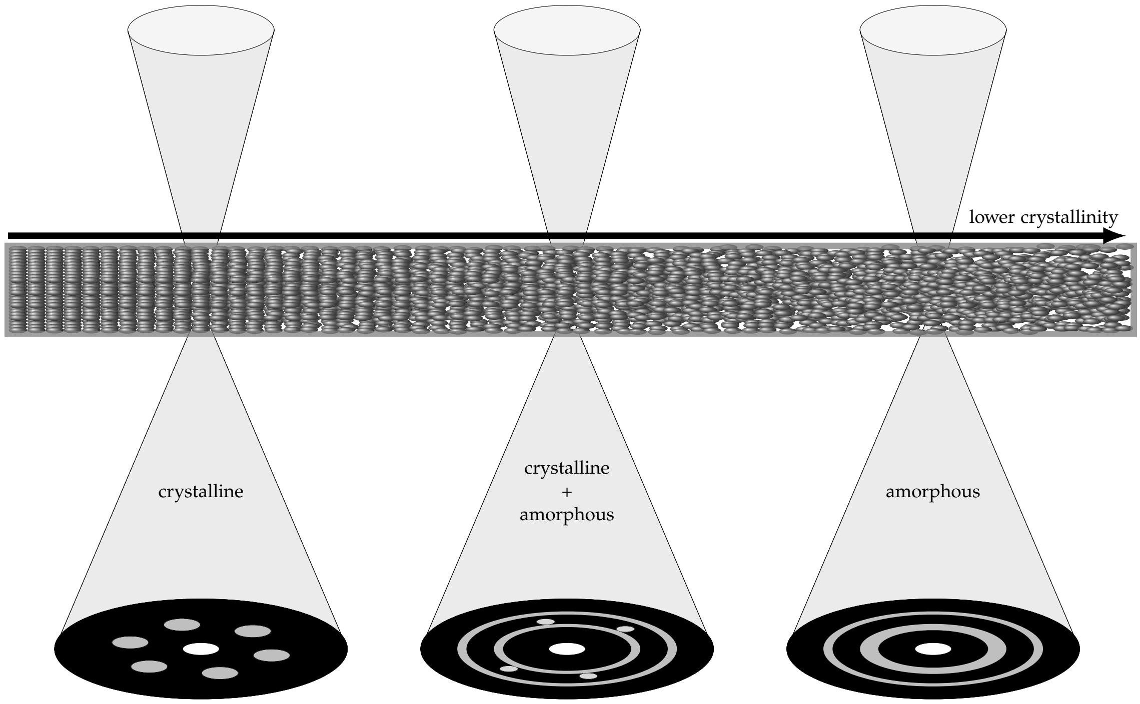


Figure 1.2: amorph to crystalline and changing patterns

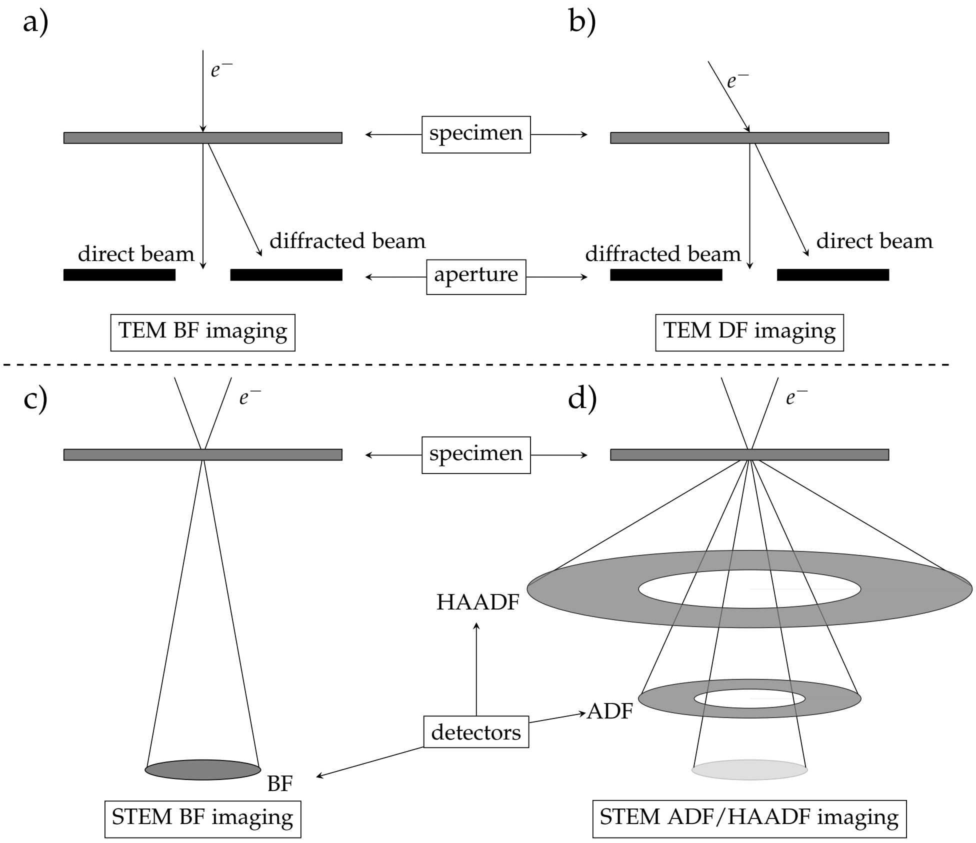


Figure 1.3: TEM modi

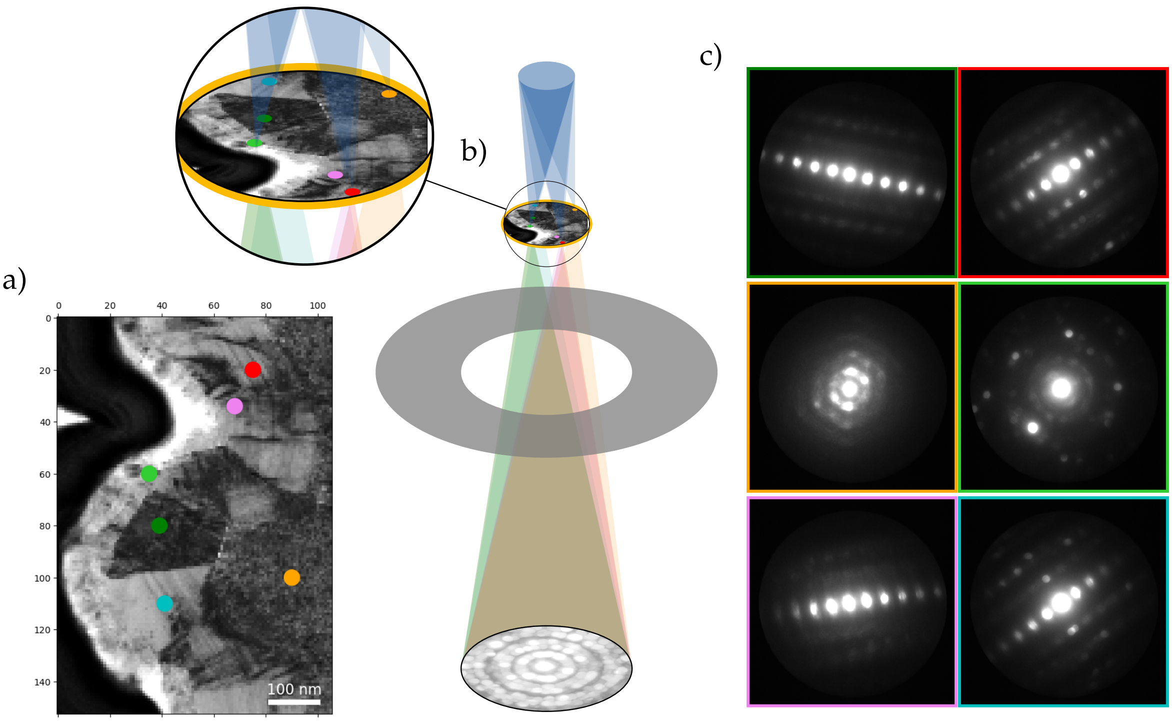


Figure 1.4: Overview 4DSTEM...

Figure 1.4 shows ...

1.2 Transmission electron microscopy

1.3 From STEM to 4D-STEM

1.4 Aim of this work

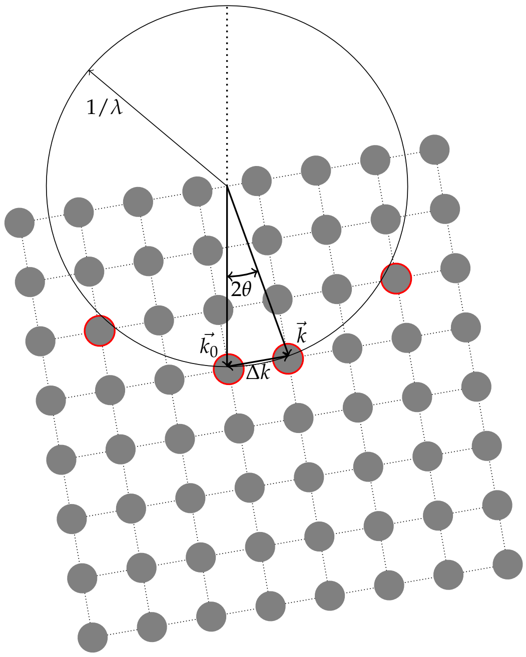
What did we do, what will be shown on the following pages, where to find the code etc.

Chapter 2

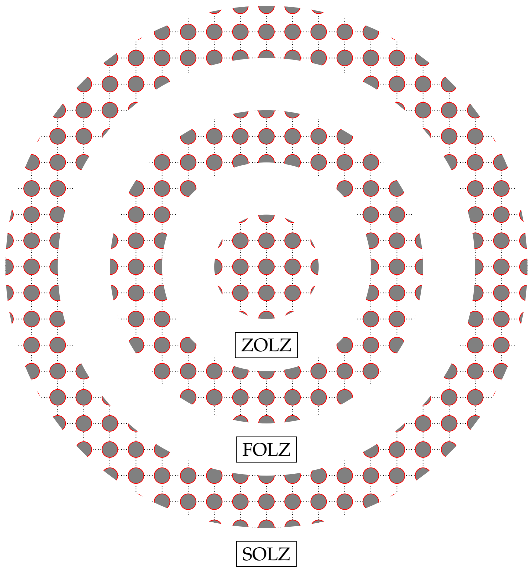
Theoretical introduction to 4D-STEM

2.1 Electron diffraction, Ewald sphere and Laue zones

Citing works per usual [1]



(a)



(b)

Figure 2.1: a) b)

2.2 Electron beam configuration and convergence angle

Convergence Angle and e dose/dwell time

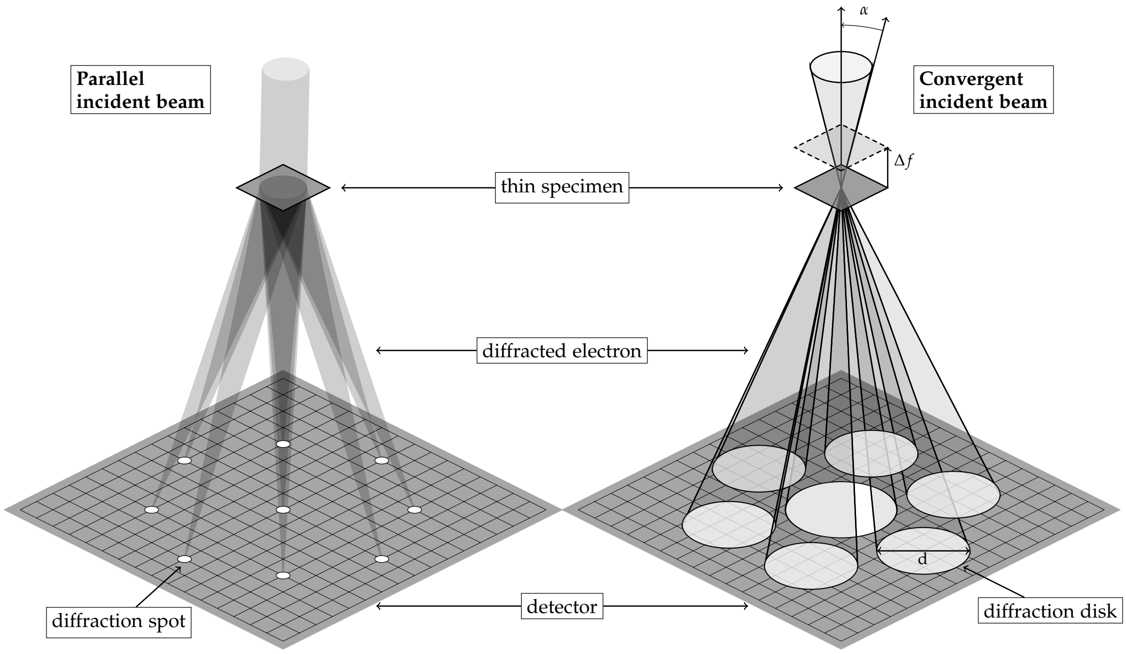


Figure 2.2: SAD vs. CBED

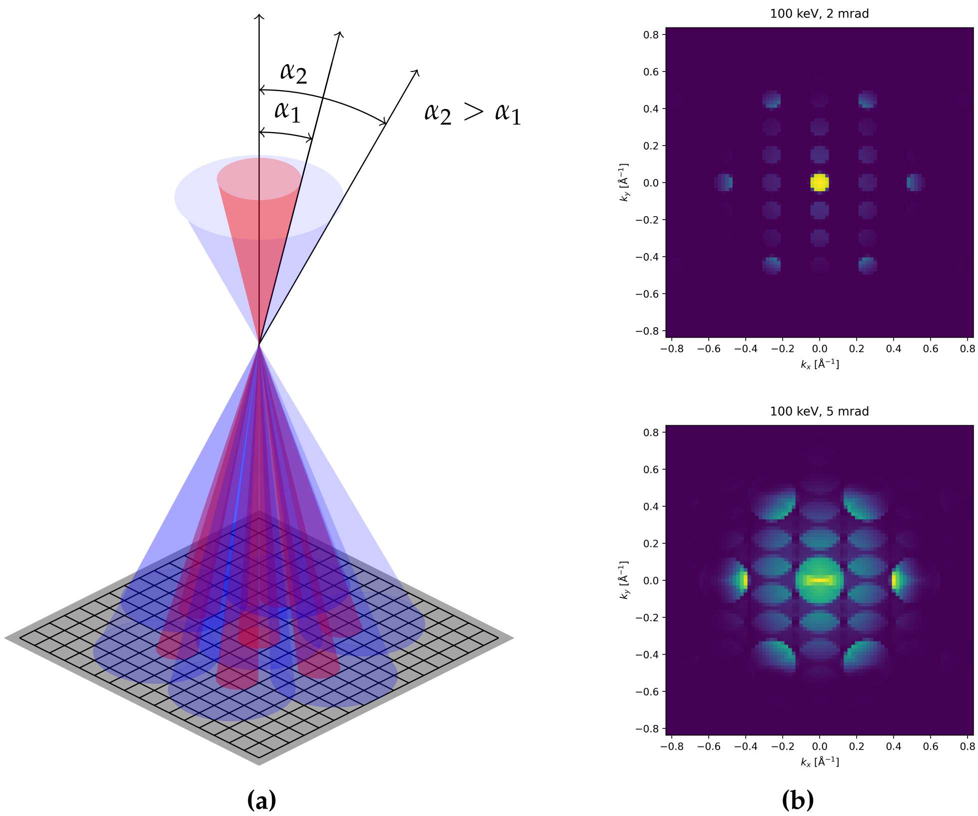


Figure 2.3: a) Two different convergence semiangles α resulting in different CBED patterns b) Simulated CBED patterns of silicium (111) choosing the zone axis as the propagation direction for two different convergence semiangles using abTEM, a python package for TEM simulation [2], see appendix A for corresponding notebooks/code

2.3 Possible detector configurations

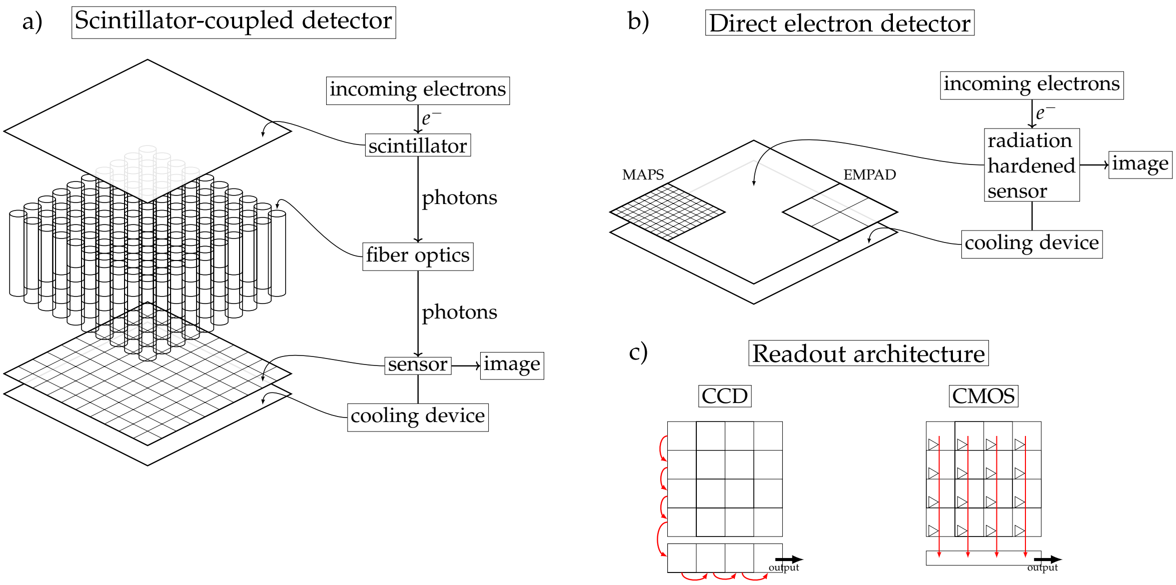


Figure 2.4: detectors, EMPAD,MAPS, CCD, CMOS

2.4 Scan strategy and measurement

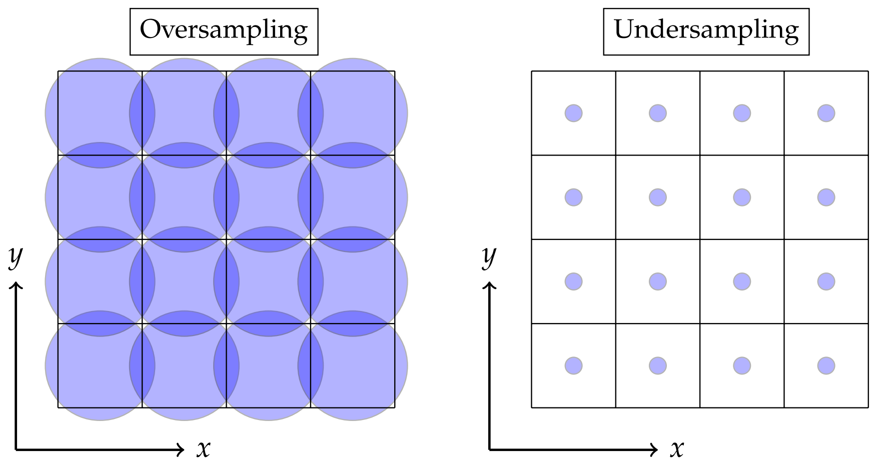


Figure 2.5: Over and undersampling...

Chapter 3

High performance computing for microscopy data analysis

3.1 Data management on HPC

High-pressure torsion HPT High performance computing (HPC) π

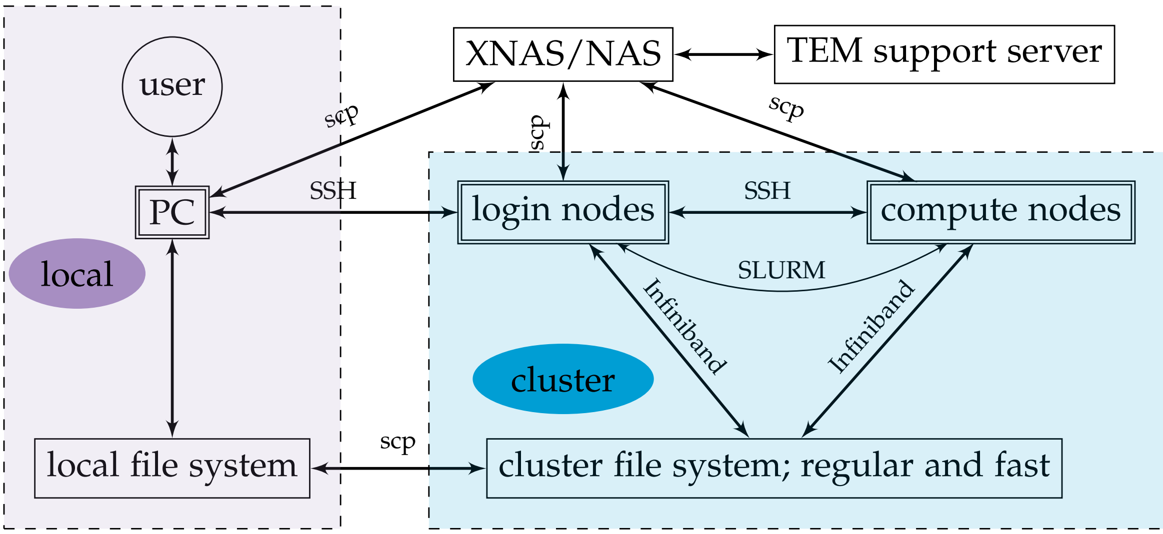


Figure 3.1: cluster

3.2 Data analysis using py4DSTEM

3.2.1 Load data and examine the datacube

```
# Import the needed packages
    import py4DSTEM

# This line displays the current version of py4DSTEM:
    py4DSTEM.__version__
```

The special method `__init__` ...

3.2.2 Basic visualization and virtual imaging

3.2.3 Reading, writing and file structure

```
4DSTEM_polyAu
├─ annular_dark_field
├─ bright_field
├─ dp_max
├─ dp_mean
├─ selected_area_diffraction_01
└─ virt_dark_field_01
```

Figure 3.2: Datensstrukturen in py4DSTEM darstellen mittels forest package

Chapter 4

4D-STEM utilizing a scintillator based CMOS detector

4.1 Experimental Setup and Instrumentation

4.2 High-pressure torsion (HPT) specimen

First sample provided by Description of HPT and FIB thinning of the sample?

4.3 Boron-doped diamond on graphene

Second sample by... as a proxy, ...

Chapter 5

Results and Discussion

5.1 Virtual imaging

5.2 Strain mapping

5.3 Automated crystal orientation mapping (ACOM)

Chapter 6

Conclusion and Outlook

6.1 Orientation and strain of HPT

6.2 Data analysis and challenges

6.3 4D-STEM at usi

Appendix A

Selected Jupyter notebooks with python code

A.1 Simulated CBED patterns of silicon in the (111) zone axis

- based on the abTEM tutorials; https://abtem.readthedocs.io/en/latest/user_guide/examples/notebooks/cbed_quickstart.html#cbed-quickstart

[1]:
```
import ase
import matplotlib.pyplot as plt
import numpy as np
from ase.build import bulk

import abtem
```

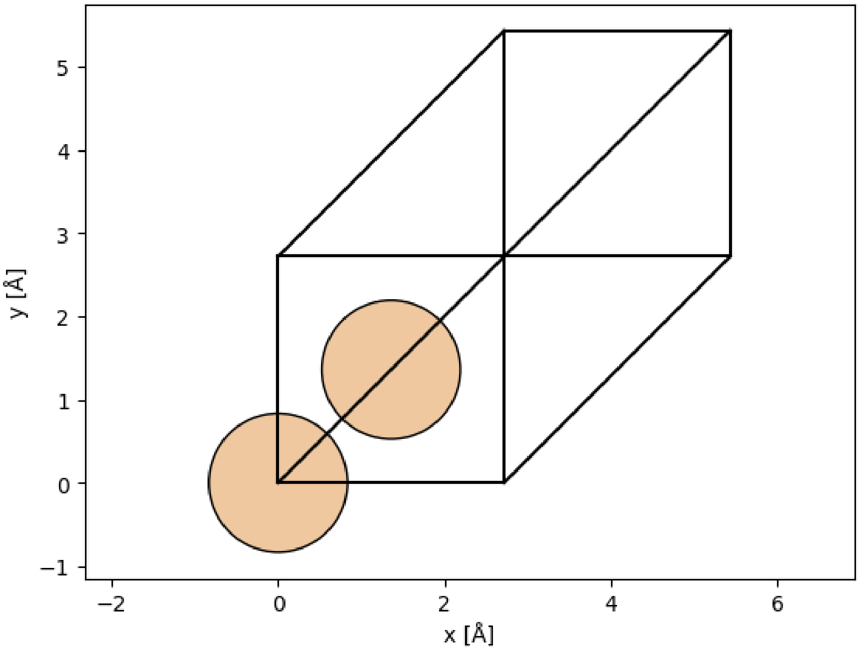
[2]:
```
# optional: set the configuration
abtem.config.set({"device": "cpu", "fft": "fftw"})
```

[2]:
```
<abtem.core.config.set at 0x146759790>
```

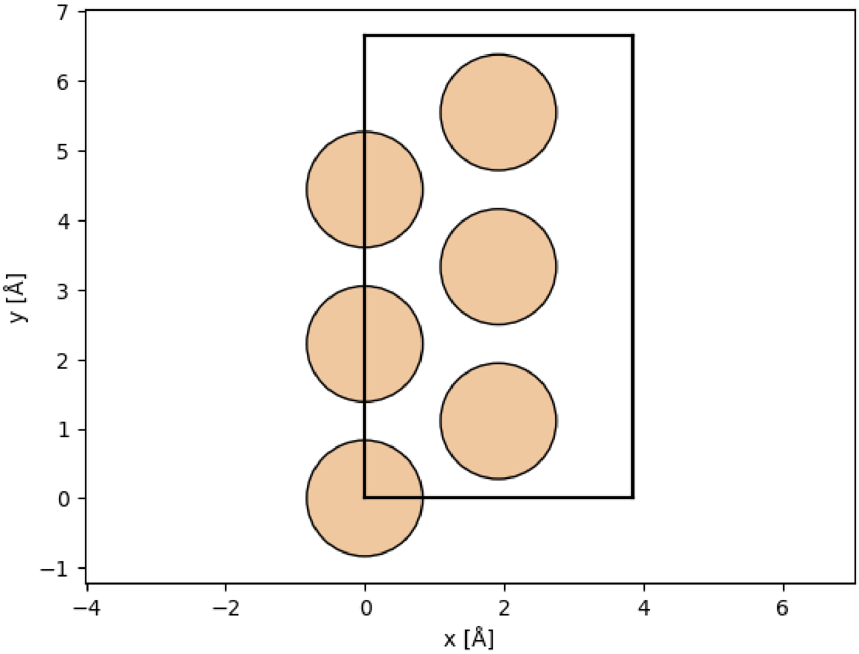
Atomic model

- create a atomic model of Si usinf the bulk function from ase
- Si atoms in a diamond lattice

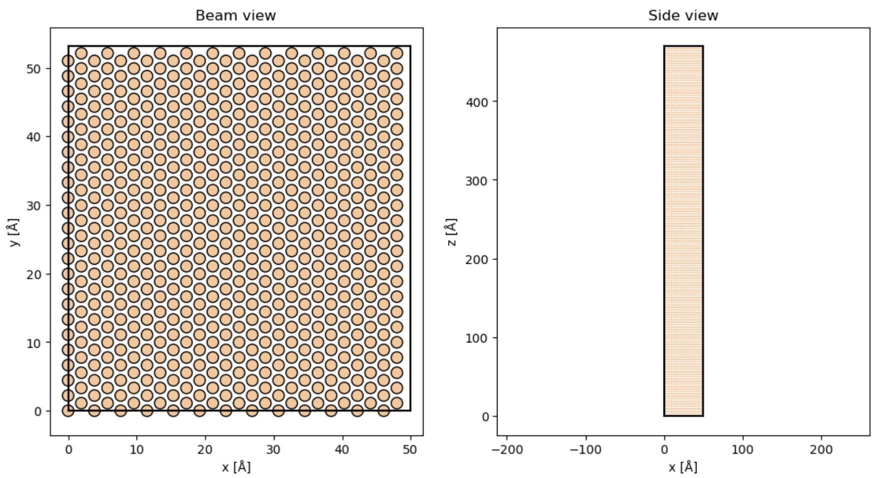
[3]:
```
silicon = bulk("Si", crystalstructure="diamond")

abtem.show_atoms(silicon, plane="xy");
```



[4]:
```
# choosing the zone axis as the propagation direction using the␣
↪surface function

silicon_111 = ase.build.surface(
    silicon, (1, 1, 1), layers=3, periodic=True
)  # create surface structure in the (111) direction

silicon_111_orthogonal = abtem.orthogonalize_cell(silicon_111)  #␣
↪make cell orthogonal

abtem.show_atoms(silicon_111_orthogonal);
```



[5]:
```
# repeat the structure in x, y and z, to improve the reciprocal␣
↪space resolution by simulating a thicker sample.

atoms = silicon_111_orthogonal * (13, 8, 50)

fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(12, 6))
abtem.show_atoms(atoms, ax=ax1, title="Beam view")
abtem.show_atoms(atoms, ax=ax2, plane="xz", title="Side view",␣
↪linewidth=0.0);
```



Potential

Frozen Phonons

- until now we assume that the atomic structures where the electrons scatter are static
- in reality they are not stationary but vibrate arround due to thermal and zero-point vibrations
- electron-phonon scattering is responsible for features sich as diffuse background and Kikuchi lines as well as high angle scattering in HAADF
- the frozen phonon model is a very simplified approach to phonons and electron scattering
- the exit-wave intensity is averaged over several frozen snapshots of the atomic model, emulating distinct vibrational configurations
- each frozen image is created by displacing its atoms by different random offsets from its equilibrium state

[6]:
```
frozen_phonons = abtem.FrozenPhonons(atoms, 8, {"Si": 0.078})
```

[7]:
```
potential = abtem.Potential(
    frozen_phonons,
    sampling=0.2,
    projection="infinite",
    slice_thickness=2,
    exit_planes=80,
)
```

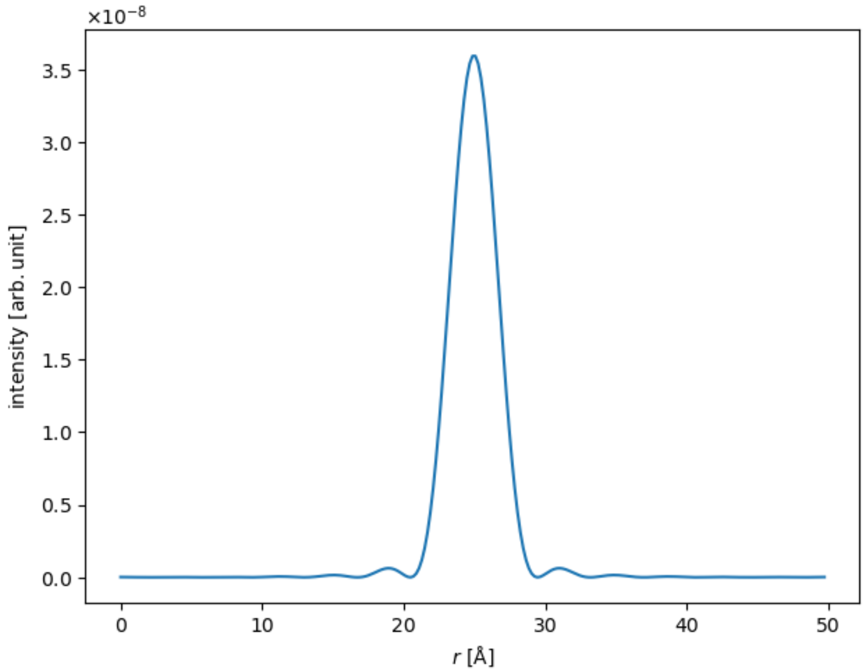
Wave function

- create a probe wave function at an energy of 200 keV
- two different convergence semiangles, to compare the resulting patterns

[8]:
```
# Version 1: 20 mrad
wave = abtem.Probe(energy=100e3, semiangle_cutoff=5)

# Version 2: 2mrad
# wave = abtem.Probe(energy=100e3, semiangle_cutoff=2)

wave.grid.match(potential)
```

[9]:
```
wave.profiles().show();
```

```
[########################################] | 100% Completed | 210.73 ms
```



Multislice

- run the multislice algorithm and calculate the diffraction pattern

[10]:
```
measurement = wave.multislice(potential).
↪diffraction_patterns(max_angle=30)
```

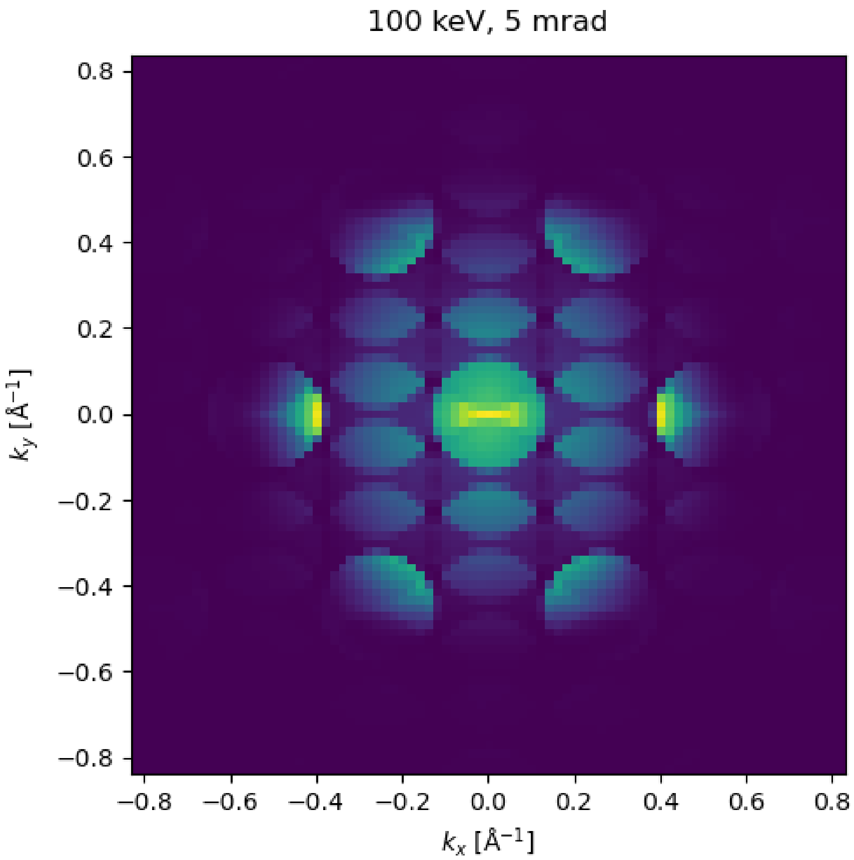
[11]:
```
measurement = measurement.mean(0)

measurement.compute()
```

```
[########################################] | 100% Completed | 3.28 sms
```

[11]:
```
<abtem.measurements.DiffractionPatterns at 0x14816e990>
```

Visualize

[12]:
```
visualization = measurement[-3].show(
    explode= True,
    title= '100 keV, 5 mrad'
)

# Save the visualization to a file
plt.savefig('CBED_100kV_5mrad.png', dpi=500, bbox_inches='tight',␣
 ↪pad_inches=0)
```



Appendix B

Setup for computing on HPC cluster

Bibliography

[1] K. C. Bustillo, S. E. Zeltmann, M. Chen, J. Donohue, J. Ciston, C. Ophus, A. M. Minor, *Accounts of Chemical Research* **2021**, *54*, Publisher: American Chemical Society, 2543–2551.

[2] J. Madsen, T. Susi, *Open Research Europe* **2021**, *1*, 13015.

List of Figures

List of Tables

Acronyms

HPC High performance computing. 7, 21
HPT High-pressure torsion. 7, 21

SEM Scanning Electron Microscopy. 21

TEM Transmission Electron Microscopy. 21

Symbolslist

π Geometrical value. 7, 21

Glossary

Python general-purpose programming language. 21

Acknowledgements

Prof. and CO

Others form group

My Family, Friends and Jessye

Declaration of Authorship

I hereby declare that the thesis submitted is my own unaided work. All direct or indirect sources used are acknowledged as references.

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