A neural network based *hkl* indexation of multi-grain Laue Patterns

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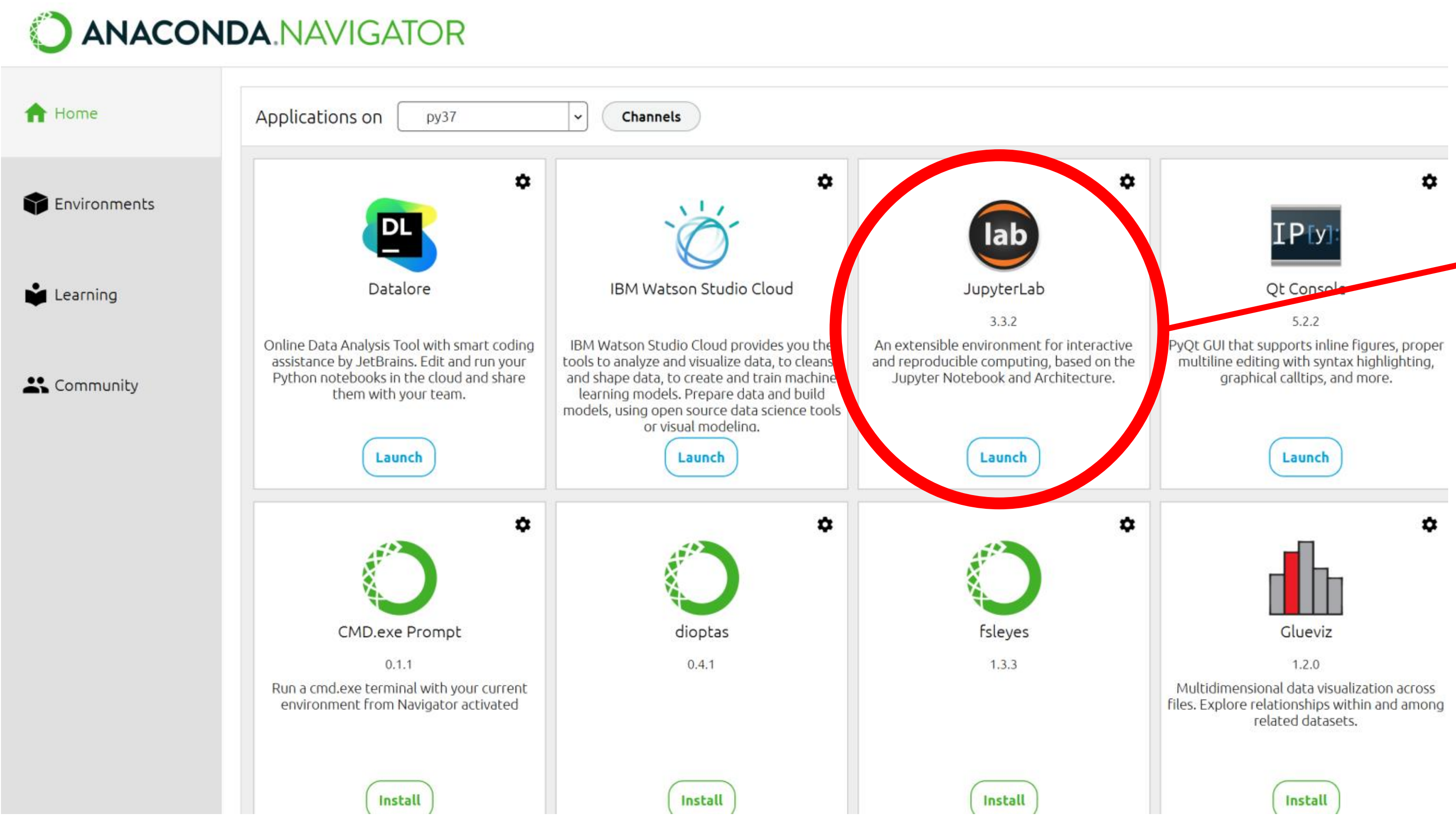
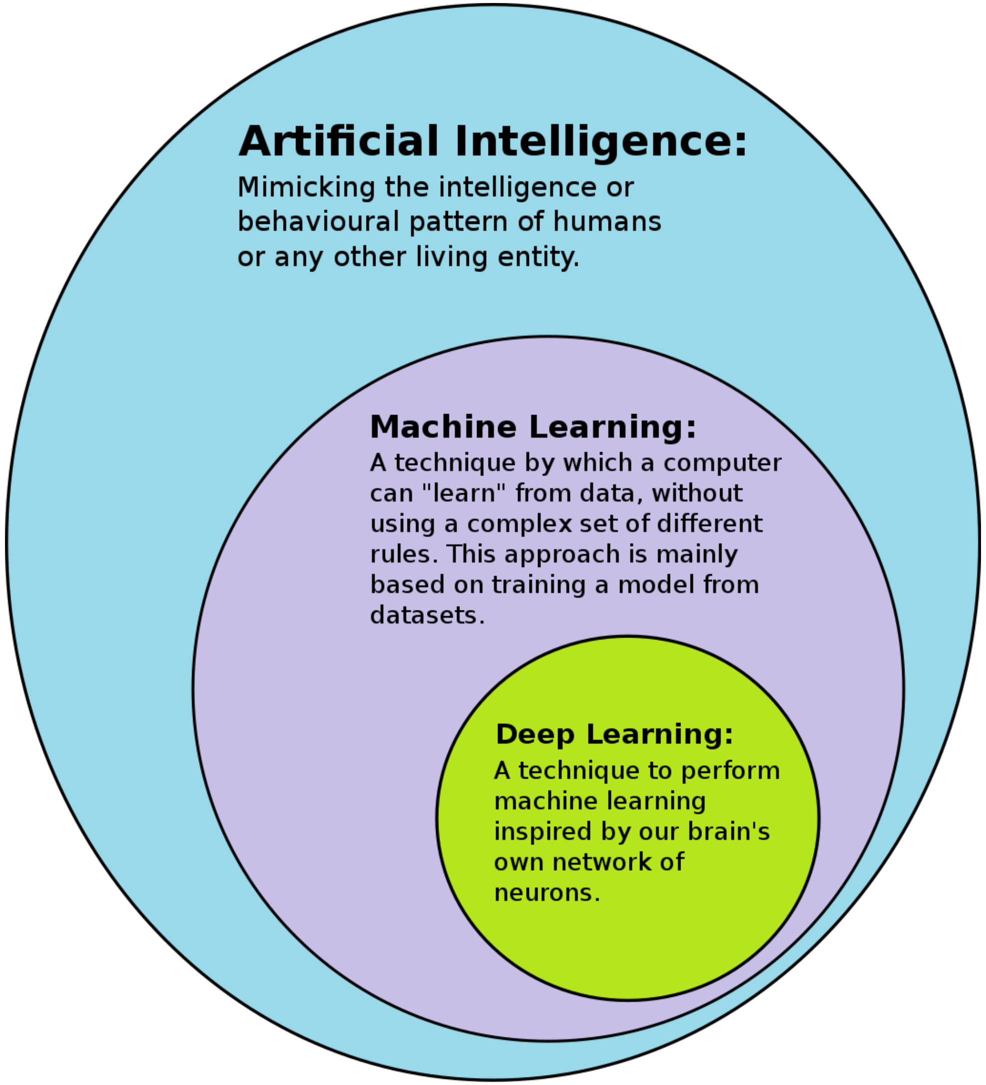
To work with the NEURAL NETWORK version of Laue indexation

- You can do **pip install lauetoolsnn** in your terminal where you have installed pip install lauetools → This is for the *Graphical User Interface* version of the code
- Additionally you will have to install tqdm (progressbar) library (**pip install tqdm**)



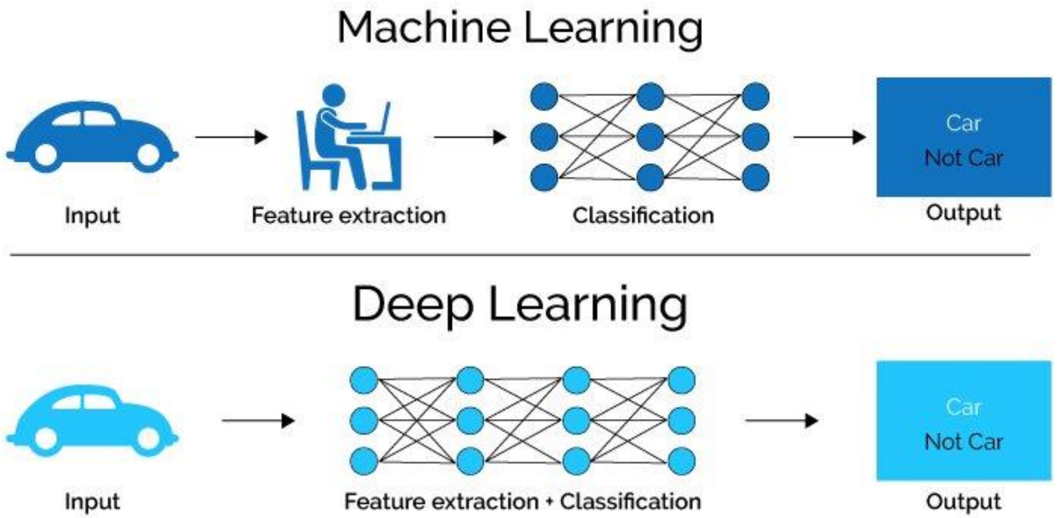
Additionally install JupyterLab / JupyterNotebook in anaconda navigator if you wish to run the notebook tutorial scripts

Gentle introduction to Machine learning



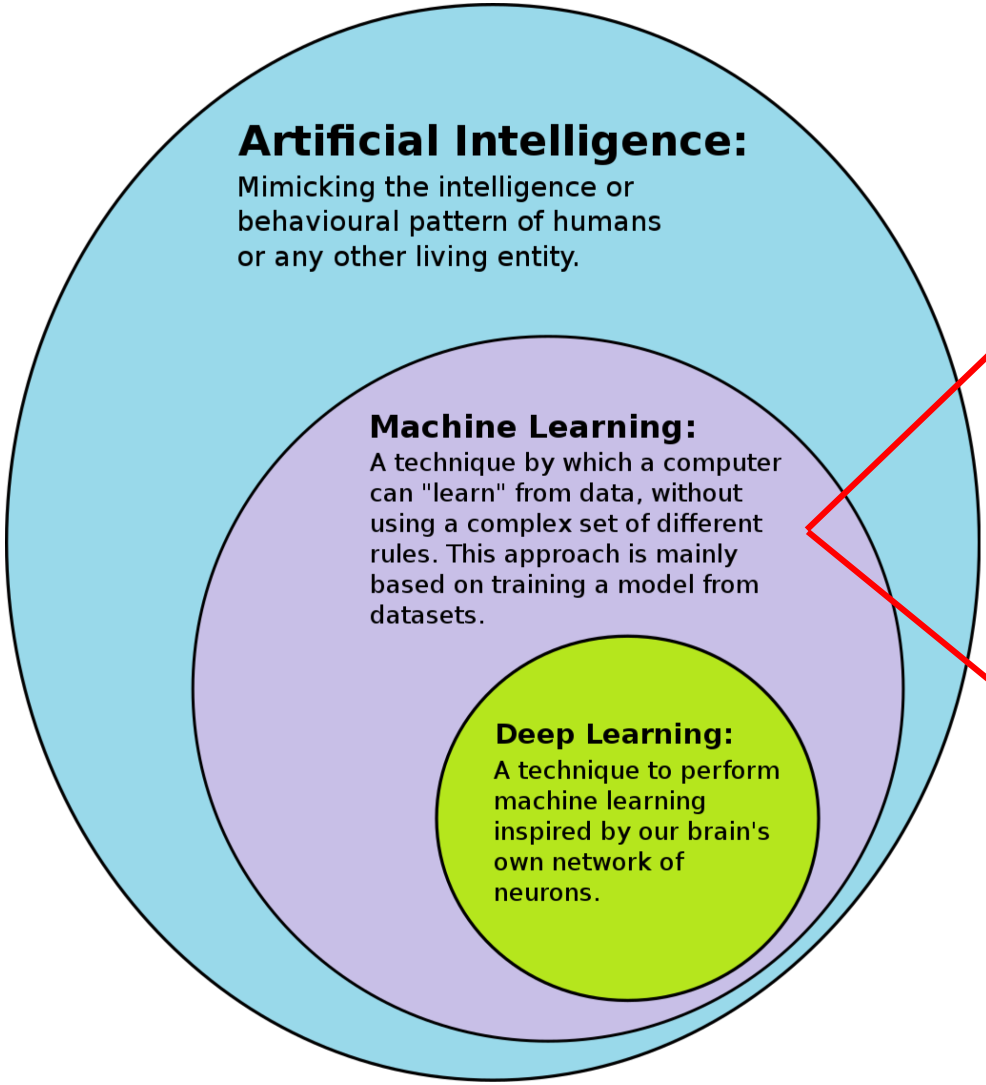
Machine Learning (ML): the **dataset** must be **preprocessed** to **extract** significant **features** that the model can be trained on.

Deep Learning (DL): refers to the training of artificial neural networks (**ANNs**) and the **feature extraction** is performed **automatically** during training.



https://datacatchup.com/artificial-intelligence-machine-learning-and-deep-learning/
https://towardsdatascience.com/deep-feed-forward-neural-networks-and-the-advantage-of-relu-activation-function-ff881e58a635

Gentle introduction to Machine learning



https://datacatchup.com/artificial-intelligence-machine-learning-and-deep-learning/
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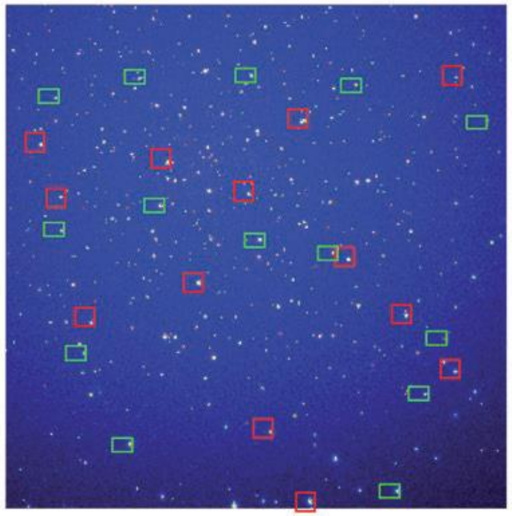
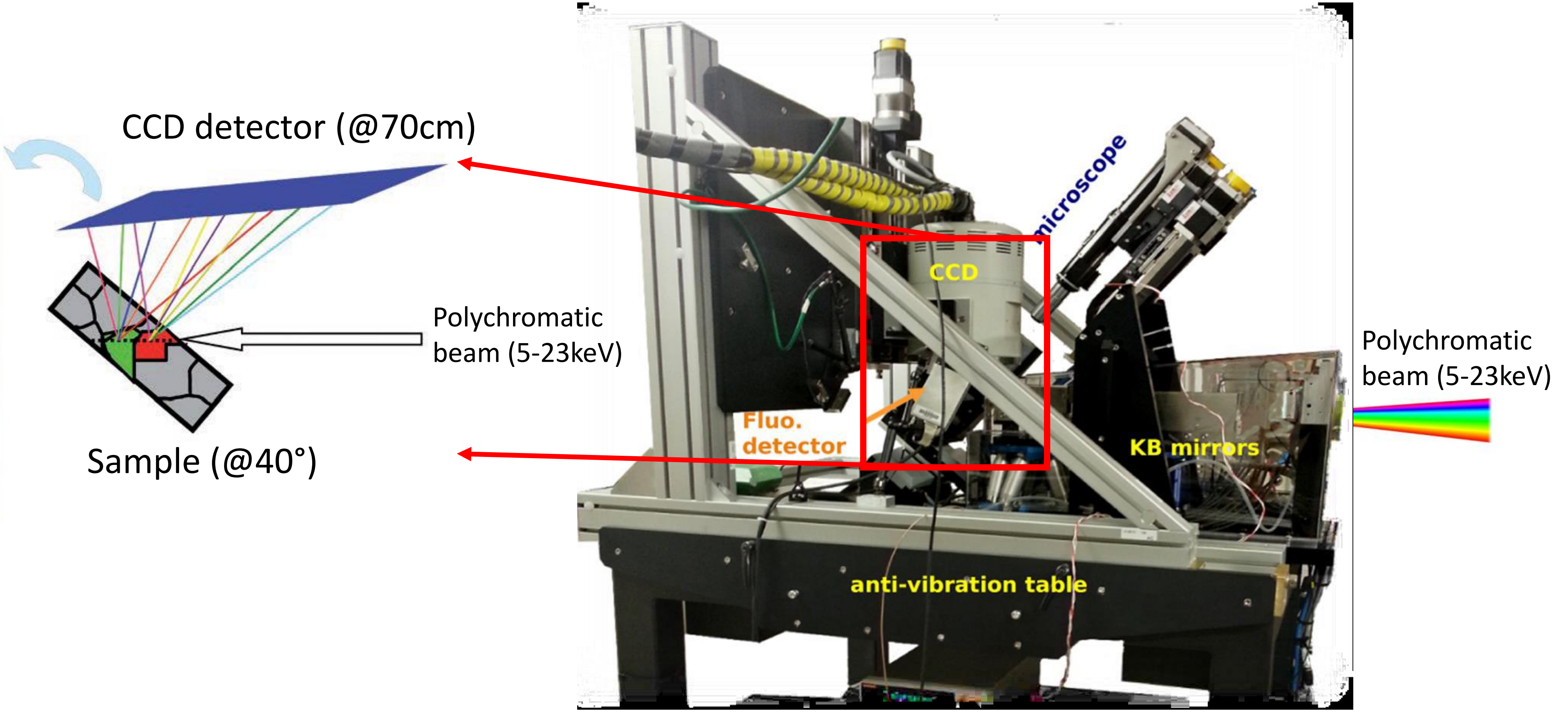
Feed forward Neural network: Application to Laue diffraction indexation





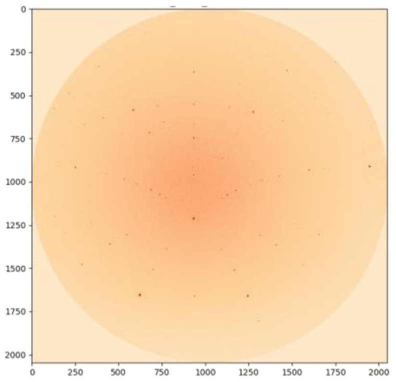
Laue Diffraction microscopy setup at BM32 beamline, ESRF

*Micha, J-S, and Odile R. "La microdiffraction Laue." *Reflets de la physique* 44-45 (2015): 68-71.

Introduction: Laue microdiffraction

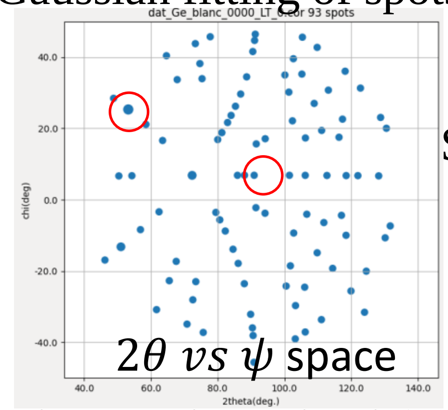
Classical indexation procedure for Ge

Raw detector image



Step 1

Thresholding and 2D Gaussian fitting of spots



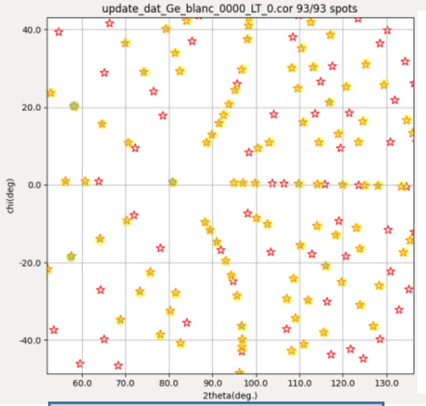
2θ vs ψ space

At this step we have no knowledge regarding the HKL indices of the detected spots

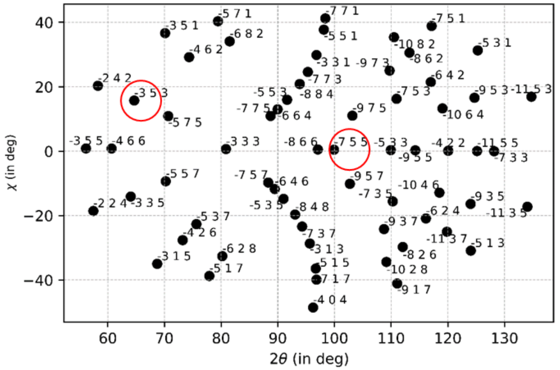
Step 2

Theoretical Look Up Table (LUT) of angular distances between two Miller indices

$\{h_2k_2l_2\}$	$\{h_1k_1l_1\}$ 100	110	111	210	211	221	310
100	0 90						
110	45 90	0 60 90					
111	54.7	35.3 90	0 70.5 109.5				
210	26.6 63.4 90	18.4 50.8 71.6	39.2 75.0	0 36.9 53.1			
211	35.3 65.9	30 54.7 73.2 90	19.5 61.9 90	24.1 43.1 56.8	0 33.6 48.2		
221	48.2 70.5	19.5 45 76.4 90	15.8 54.7 78.9	26.6 41.8 53.4	17.7 35.3 47.1	0 27.3 39.0	
310	18.4 71.6 90	26.6 47.9 63.4 77.1	43.1 68.6	8.1 58.1 45	25.4 49.8 58.9	32.5 42.5 58.2	0 25.9 36.9
311	25.2 72.5	31.5 64.8 90	29.5 58.5 80.0	19.3 47.6 66.1	10.0 42.4 60.5	25.2 45.3 59.8	17.6 40.3 55.1
320	33.7 56.3 90	11.3 54.0 66.9	61.3 71.3	7.1 29.8 41.9	25.2 37.6 55.6	22.4 42.3 49.7	15.3 37.9 52.1
321	36.7 57.7 74.5	19.1 40.9 55.5	22.2 51.9 72.0 90	17.0 33.2 53.3	10.9 29.2 40.2	11.5 27.0 36.7	21.6 32.3 40.5
331	46.5	13.1	22.0				



Experimental spots
Simulated spots
Exp & Sim spot overlap



Step 3

Refining structural parameters of crystal

Procedure for indexation:

1. Extracting peaks from the raw detector image → Quality of indexation depends on this step.

2. Indexation of spots (i.e. identifying the HKL miller indices) → angles matching with LUT

➢ Trial and error approach

➢ Time consuming process (depends on the maximum HKL index probed in the LUT & the two selected spots belong to same grain)

➢ Orientation matrix deduction : Comparing experimental and simulated Laue pattern to verify the validity (**matching rate similarity index**) of the proposed orientation matrix.

Crucial and most time consuming step

3. Model

Objective → **Employ neural network to automatize and speed up the HKL identification process with high reliability.**

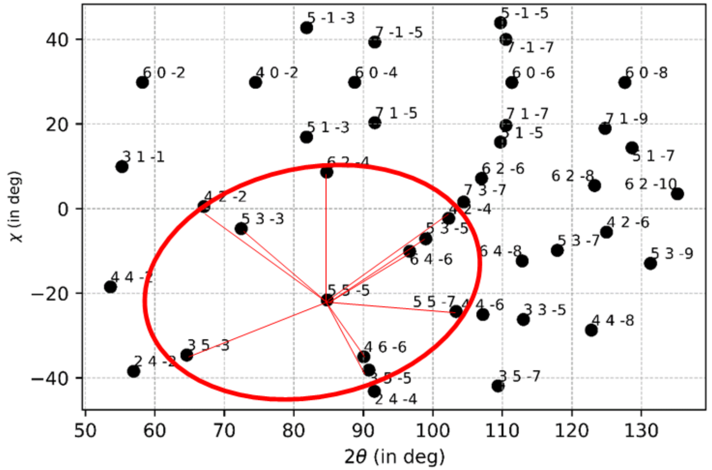
Neural network for indexation problem

Extracting Laue features for training

Ability of the neural network learning depends strongly on the applicability of the feature it is dealt with (garbage in garbage out)

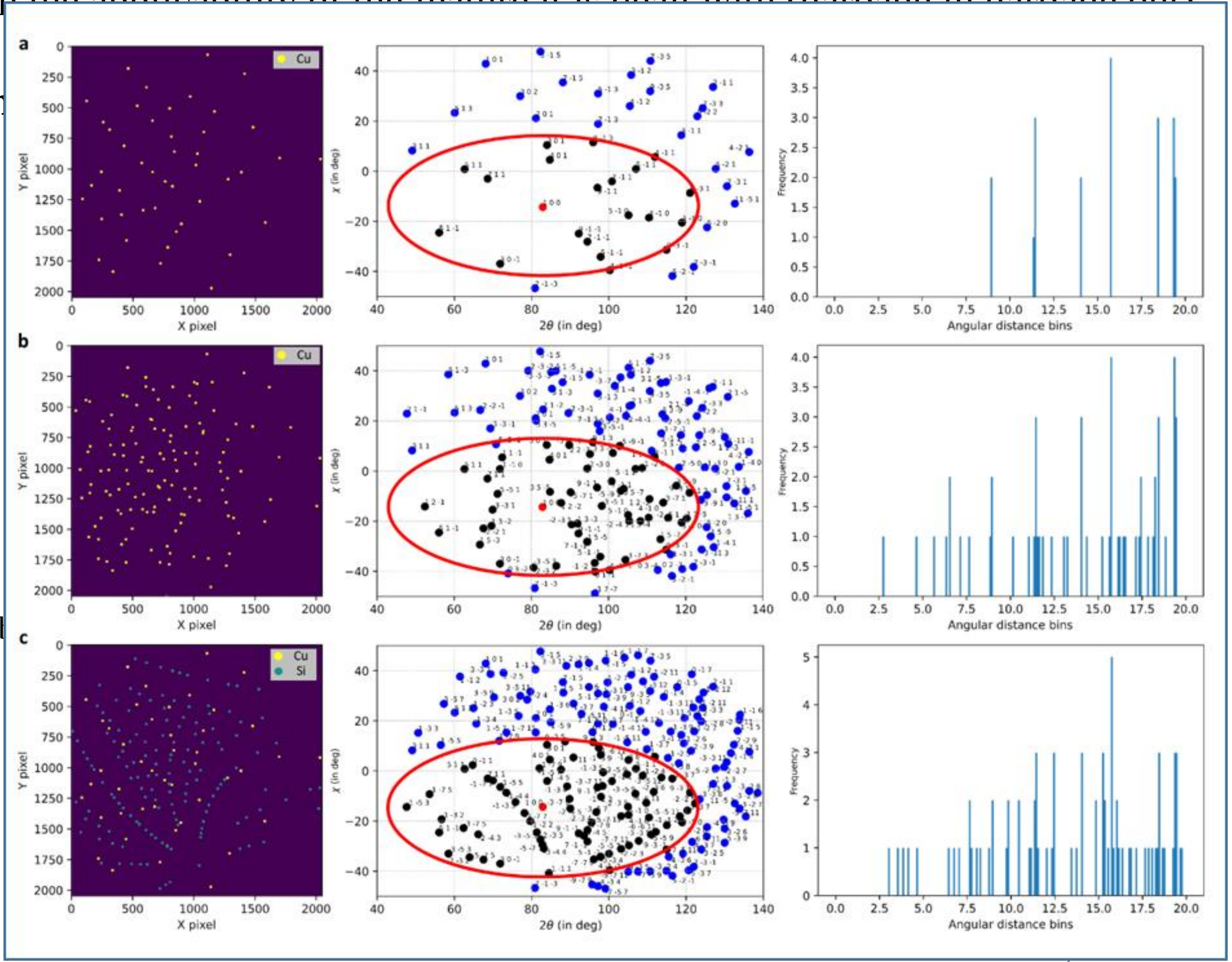
→ Often the **mutual angular distribution (or fingerprin**
on the *hkl* of the spot.

Simulated Laue Pattern for single crystal Cu



Binning of angular distance between neighbor spots

Neighbors defined b
limit search angle (here 20°)

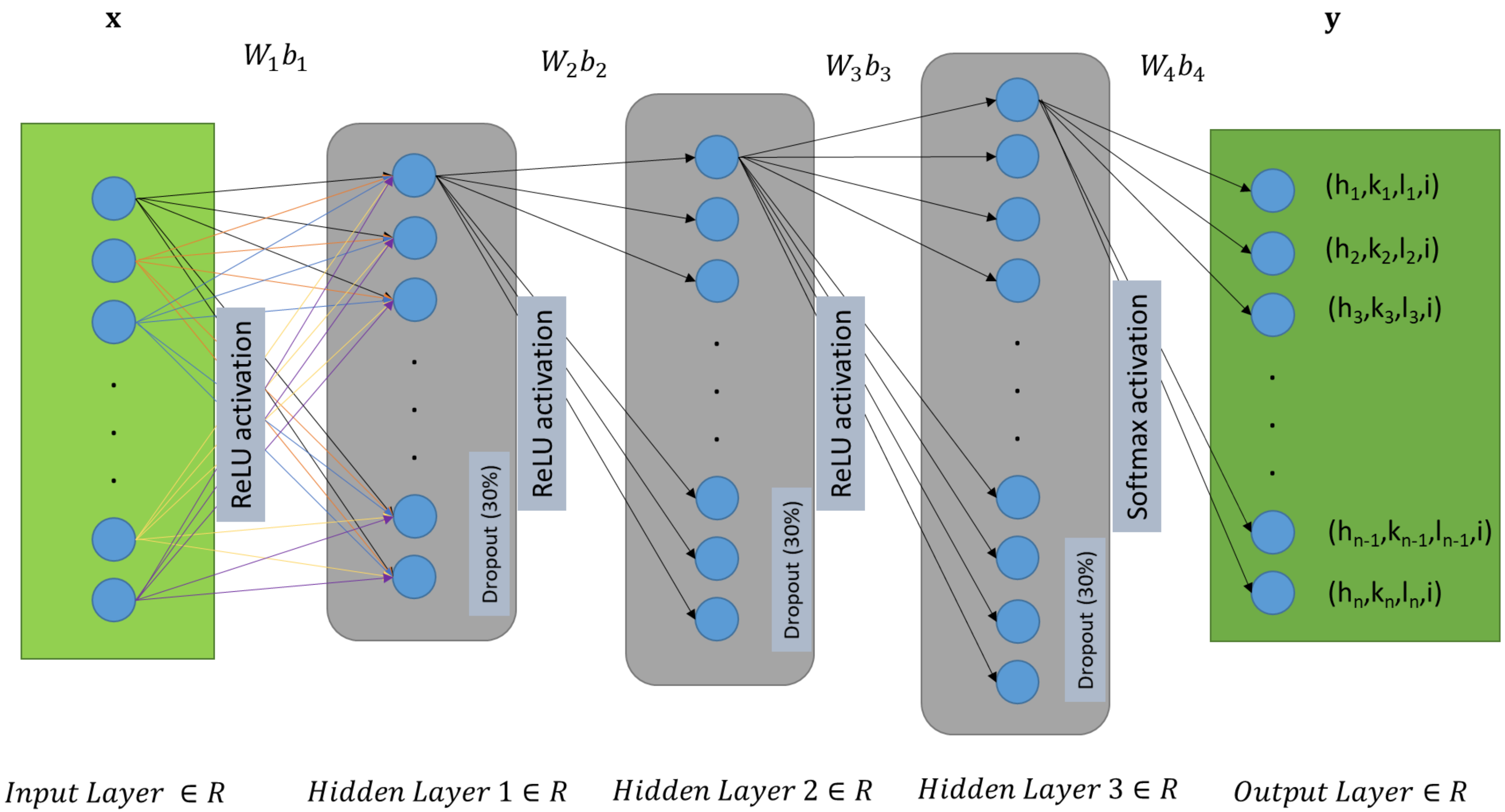


→ **Angular distance distribution is used as input for the Neural network.**

Neural network for indexation problem*

An optimized Deep Feed Forward model

A simple NN architecture → Faster prediction

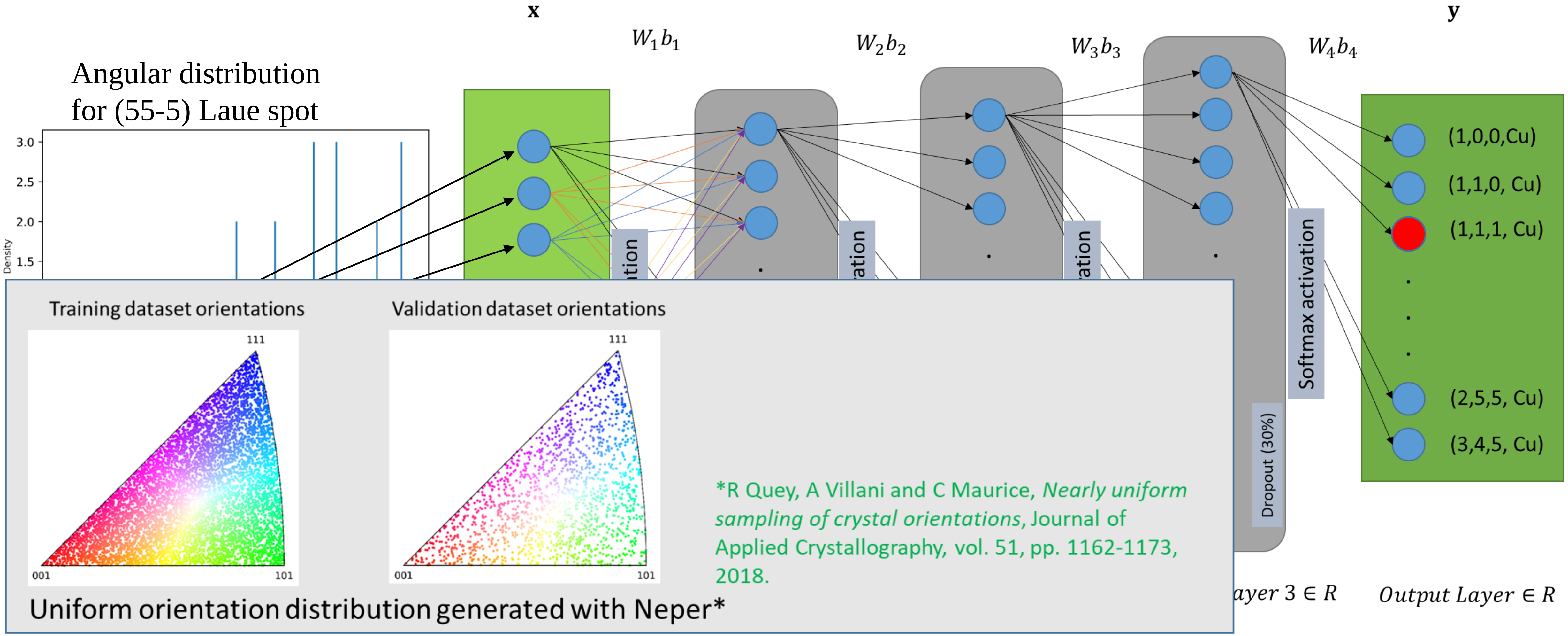


*Purushottam raj purohit R.R.P, et al. "Neural network based real-time *hkl* - indexation of Laue microdiffraction patterns recorded on polycrystalline samples". In preparation (2022).

Neural network for indexation problem*

An optimized Deep Feed Forward model

A simple NN architecture → Faster prediction



Uniform orientation distribution generated with Neper*

*R Quey, A Villani and C Maurice, *Nearly uniform sampling of crystal orientations*, Journal of Applied Crystallography, vol. 51, pp. 1162-1173, 2018.

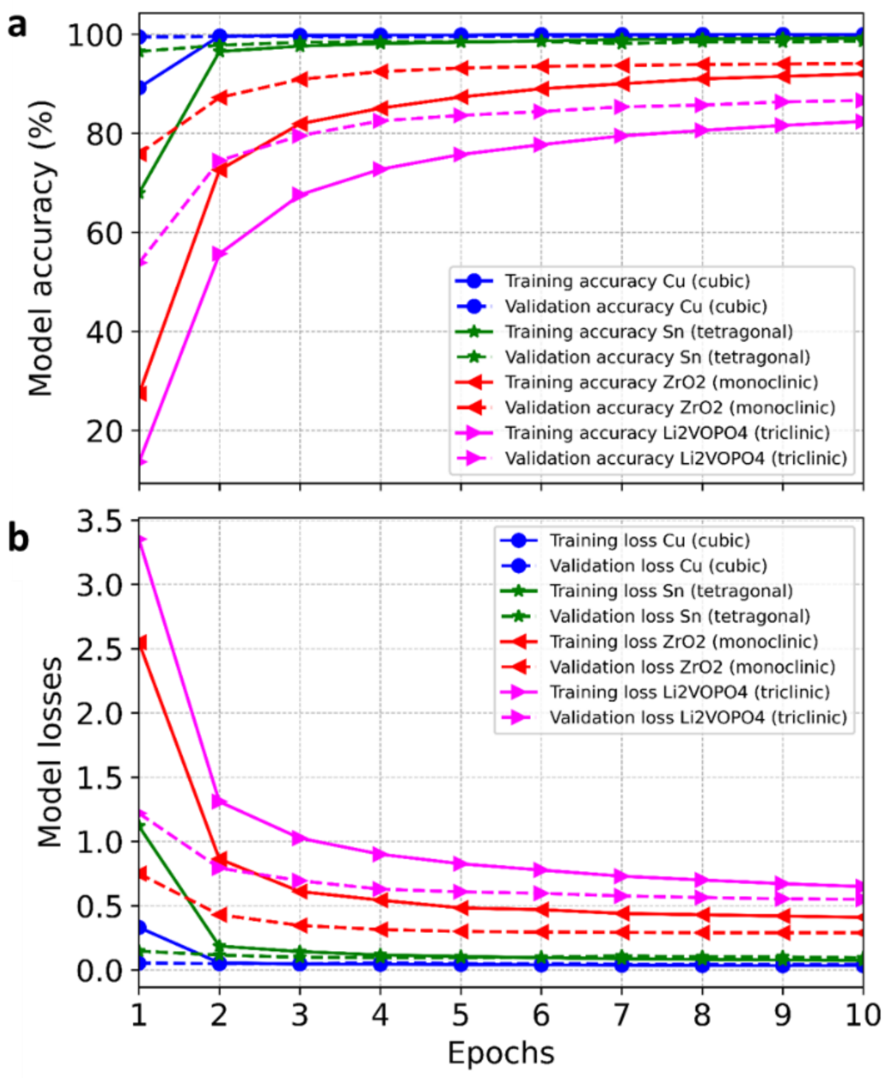
➢ Data augmentation: Gaussian noise and disappearance of spots (or **partial Laue patterns**) based on their energies

Neural network for indexation problem

An optimized Deep Feed Forward model

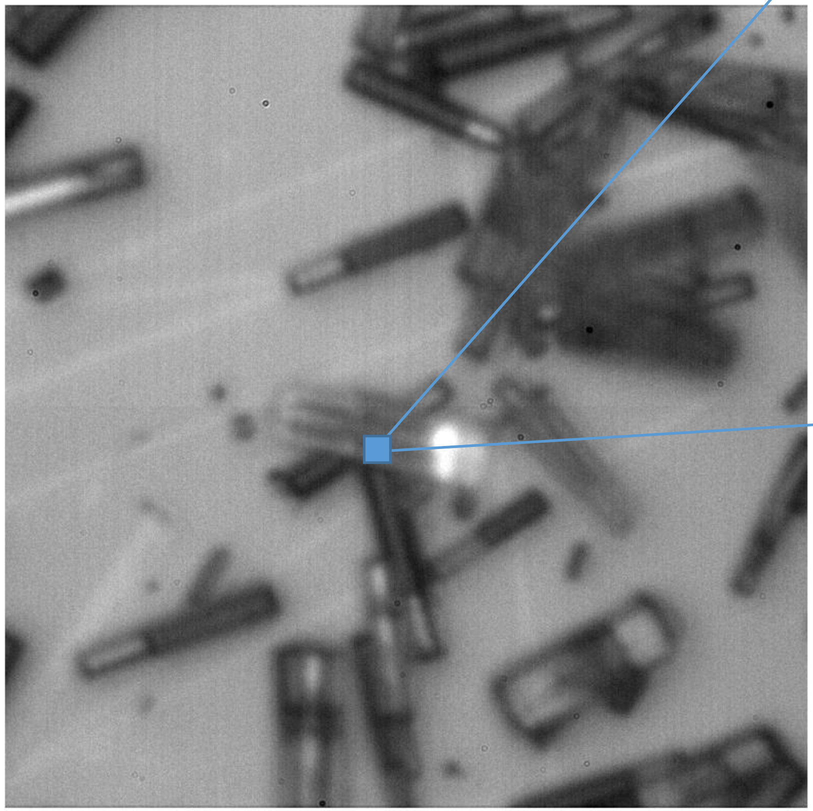
Crystal system	Crystal	Unit cell	Time to train the model (s)	Prediction time for single Laue image (s)
Cubic	Cu	a = 3.6 nm b = 3.6 nm c = 3.6 nm α = 90°; β = 90°; γ = 90°	25	0.06
Cubic (large unit cell)	UO_2	a = 5.47 nm b = 5.47 nm c = 5.47 nm α = 90°; β = 90°; γ = 90°	25	0.06
Hexagonal	Ti	a = 2.95 nm b = 2.95 nm c = 4.68 nm α = 90°; β = 90°; γ = 120°	180	0.15
Tetragonal	Sn	a = 5.83 nm b = 5.83nm c = 3.18 nm α = 90°; β = 90°; γ = 90°	180	0.1
Monoclinic	ZrO_2	a = 5.151 nm b = 5.212 nm c = 5.317 nm α = 90°; β = 99.23°; γ = 90°	750	0.2
Triclinic	Li_2VOPO_4	a = 7.096 nm b = 7.811 nm c = 7.101 nm α = 90.17°; β = 116.55°; γ = 90.72°	1200	0.2

- Single neural network architecture that works for all crystal symmetries

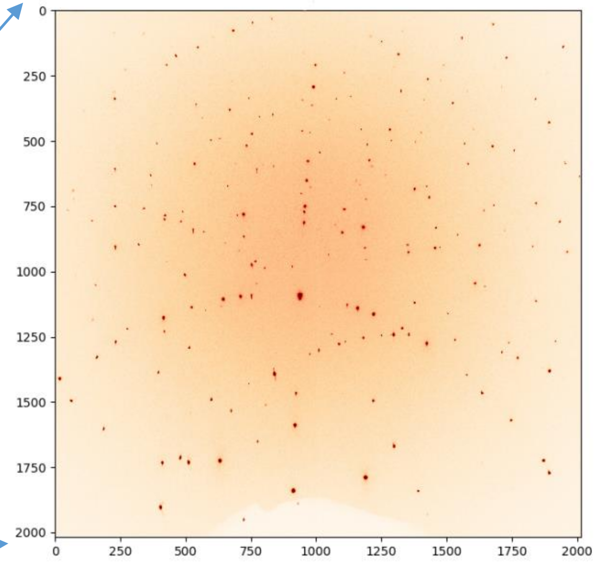


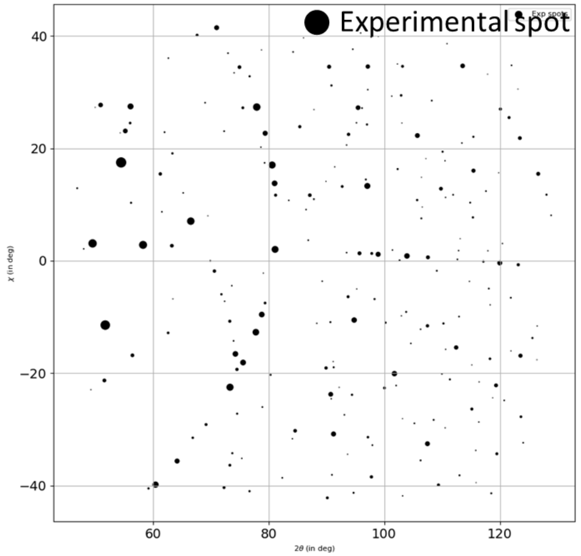
Characterization of GaN whiskers with micro-Laue

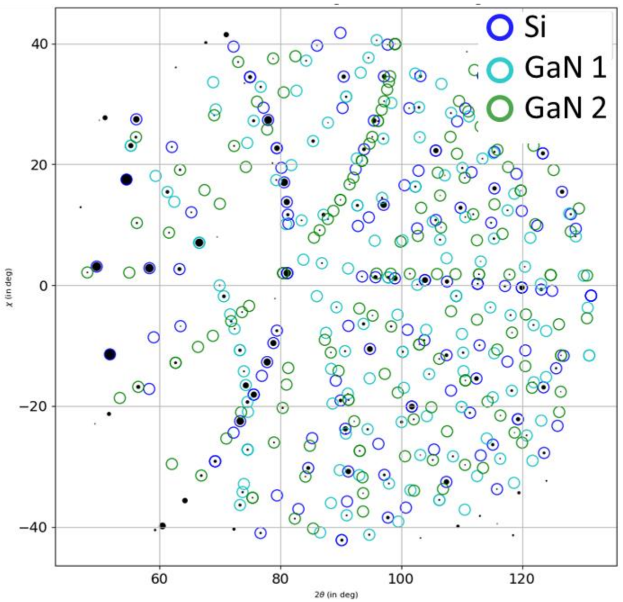
Optical microscopy image



Scan direction







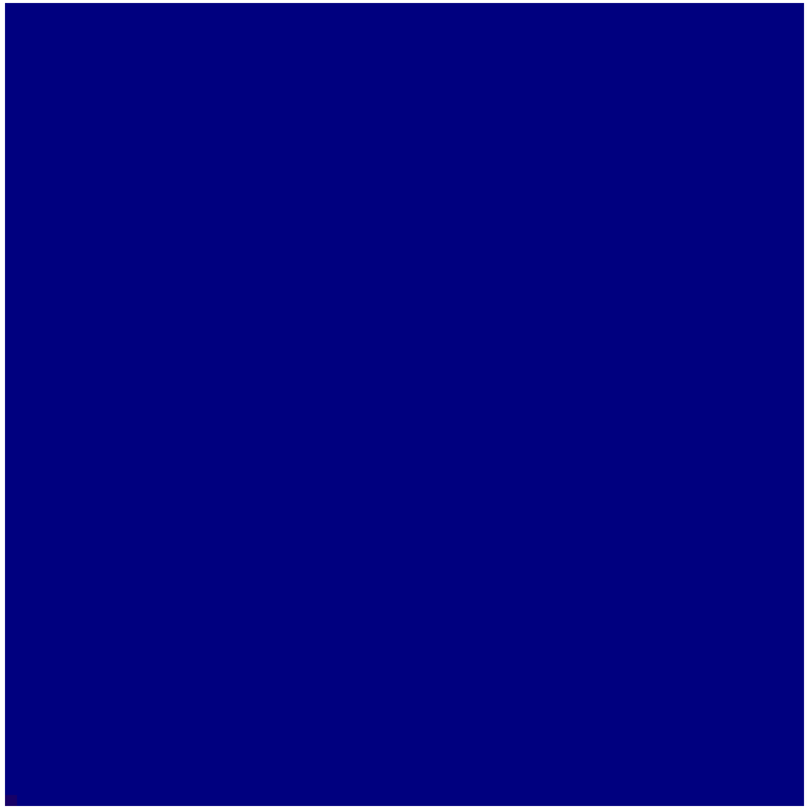
Neural network results

Micro-Laue campaign of Joël Eymery
Univ. Grenoble Alpes, CEA, IRIG-MEM, Nanostructures and Synchrotron Radiation Laboratory.

Characterization of GaN whiskers with micro-Laue

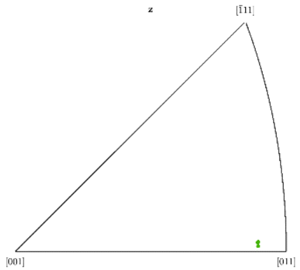
*IPF (Z) plotted with MTEX

Optical microscopy image

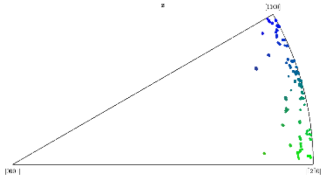


Scan direction

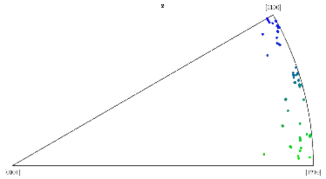
Si- phase



GaN- phase (grain 1)

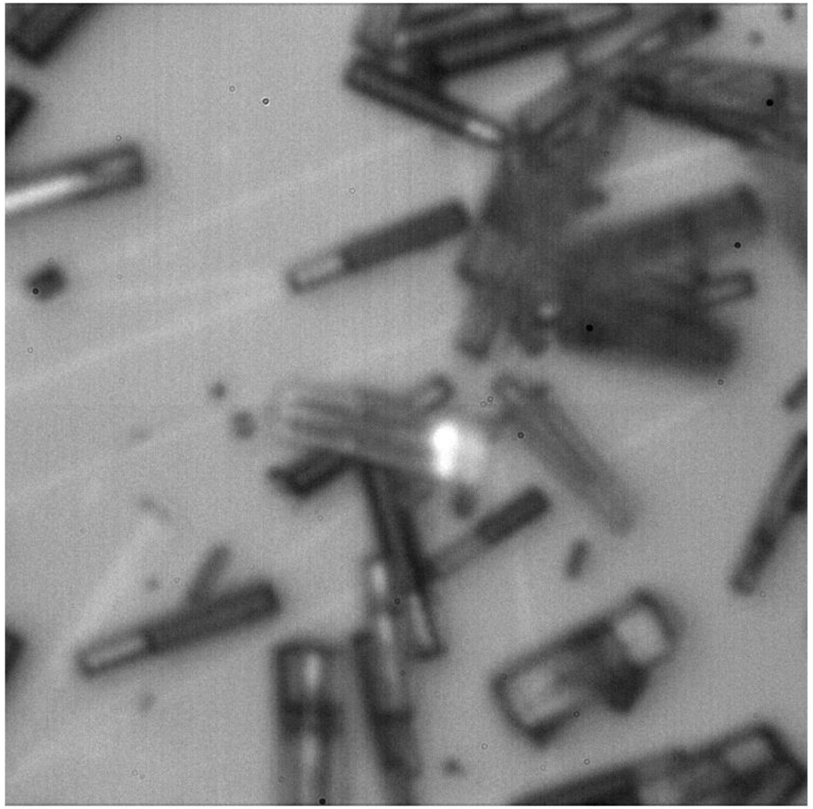


GaN- phase (grain 2)

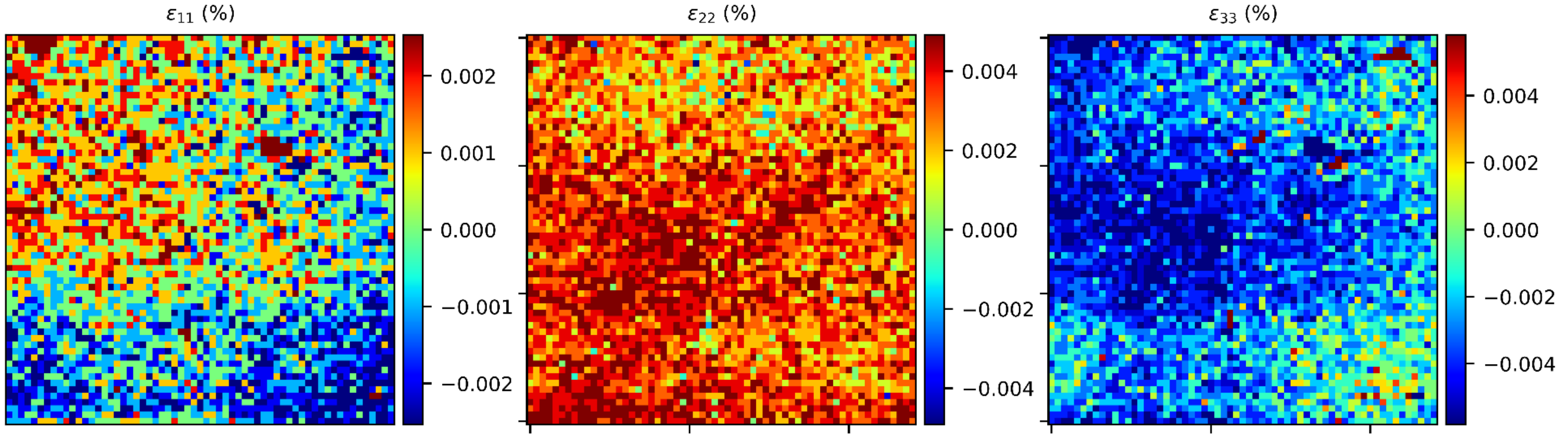


Characterization of GaN whiskers with micro-Laue

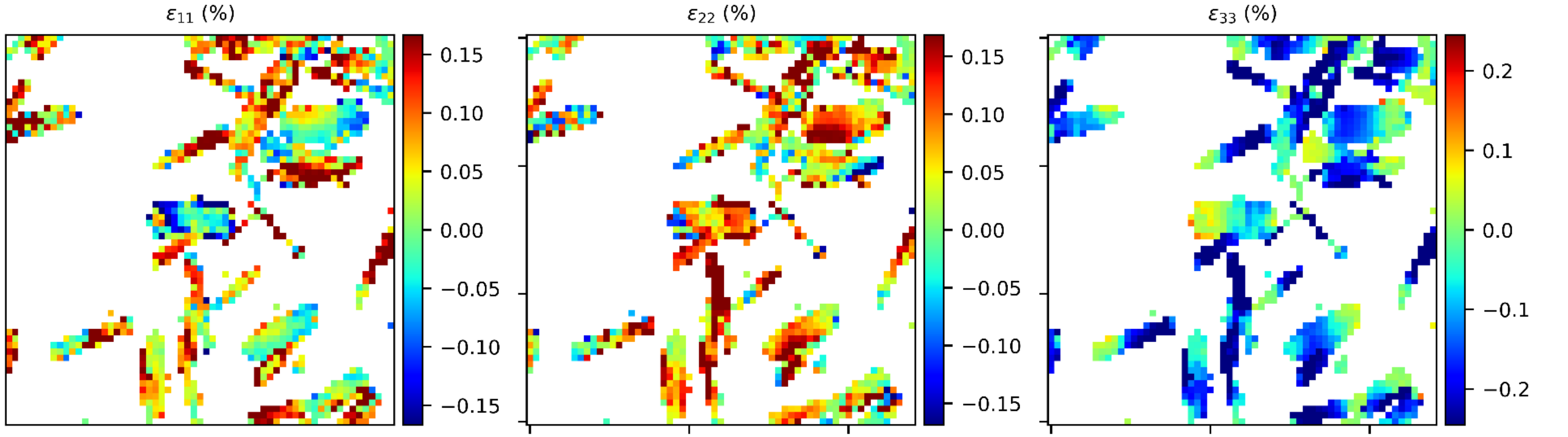
Optical microscopy image



Si- phase

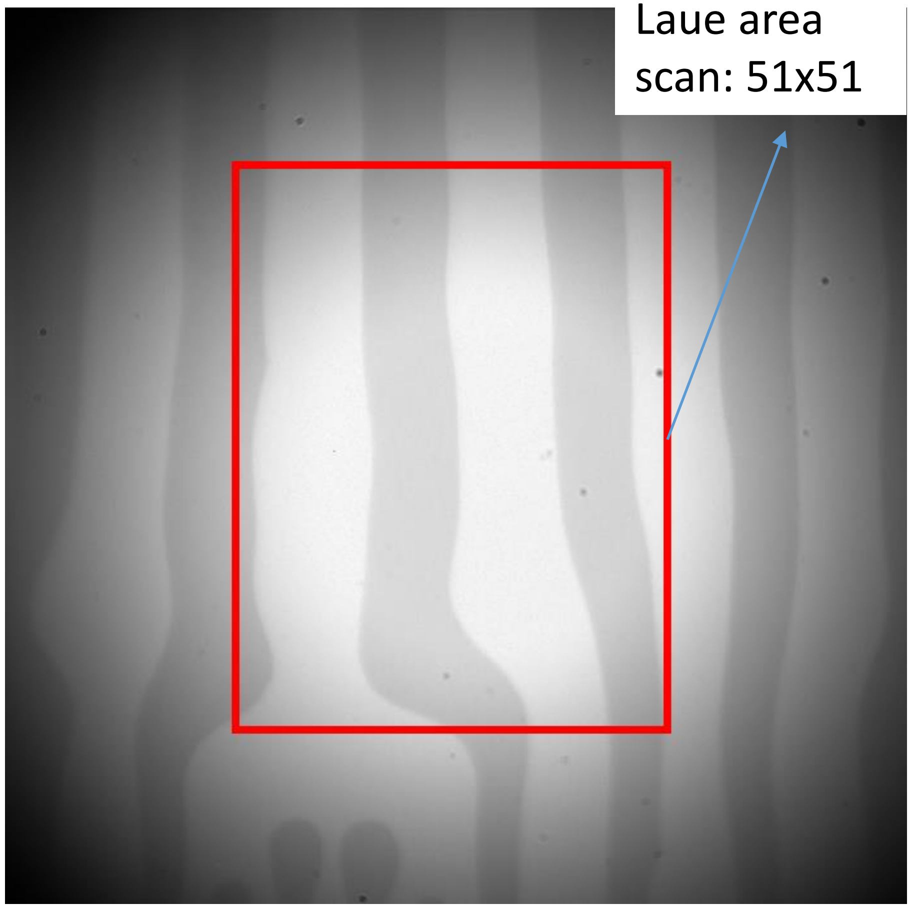


GaN- phase (grain 1)

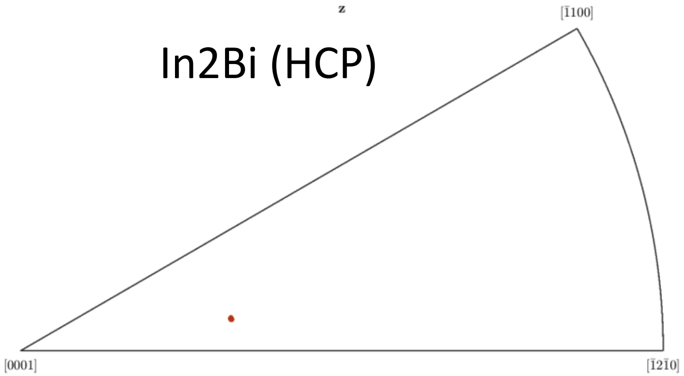


Characterization of In2Bi (HCP) and In (BCT)

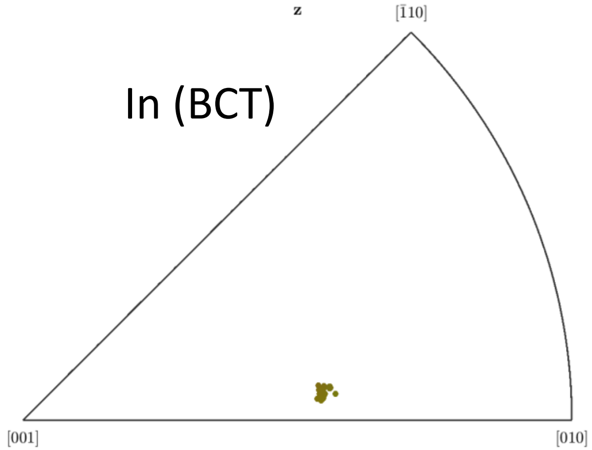
*IPF (Z) plotted with MTEX



In2Bi- phase

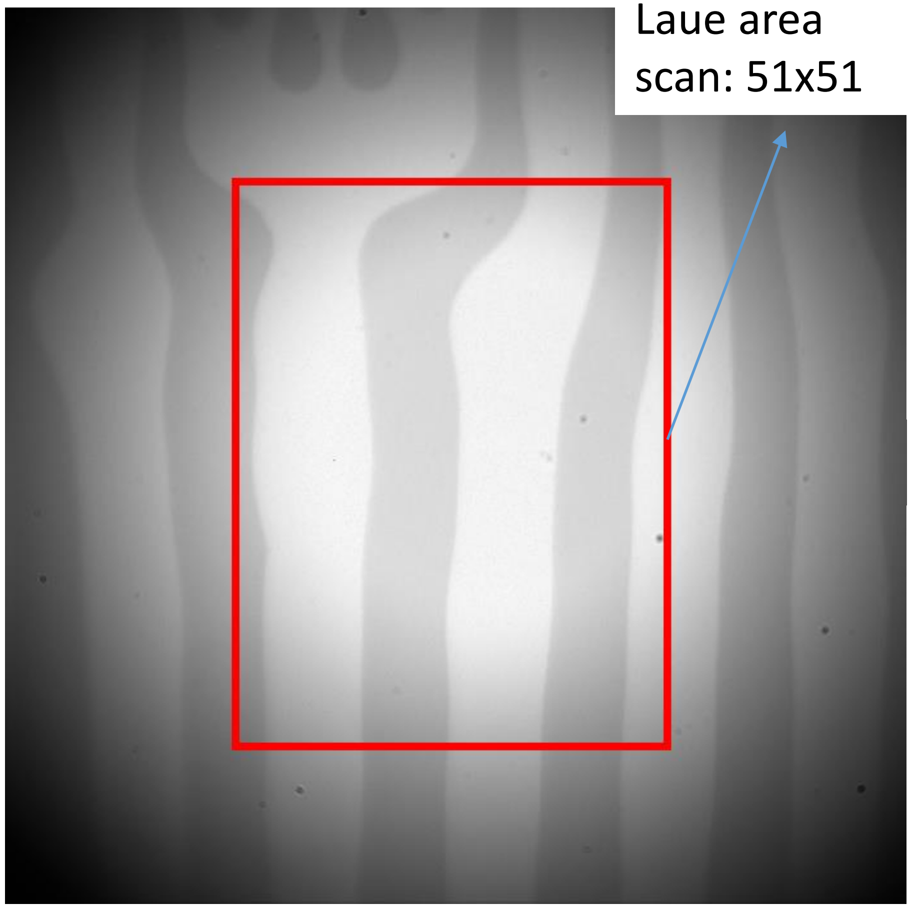


In- phase



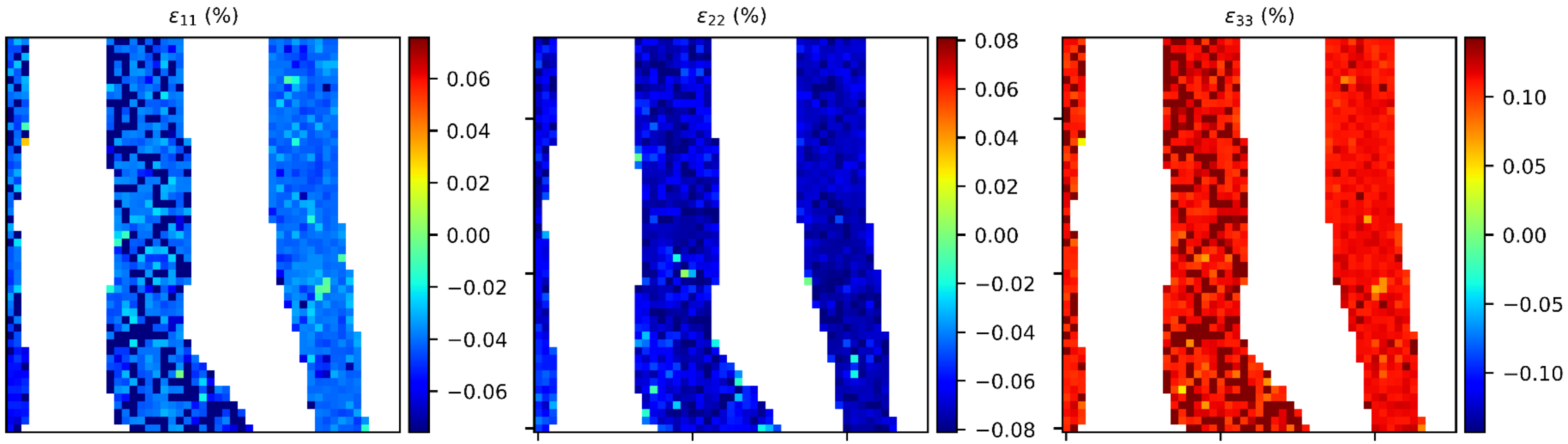
*Color does not represent texture here for Tetragonal phase but uniqueness in orientation

Characterization of In2Bi (HCP) and In (BCT)

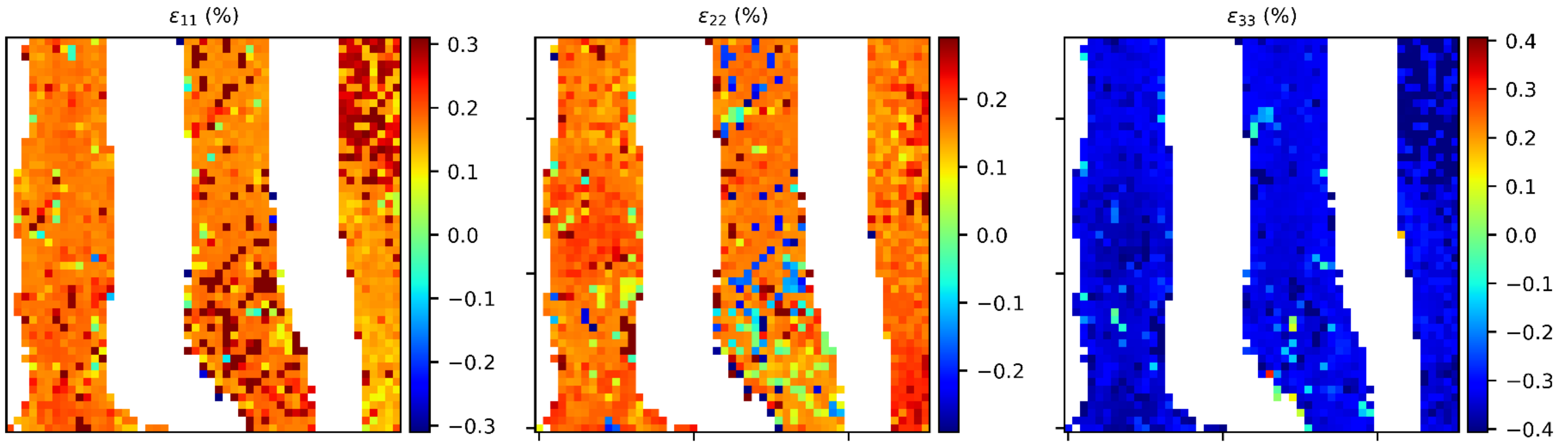


Laue area scan: 51x51

In2Bi- phase

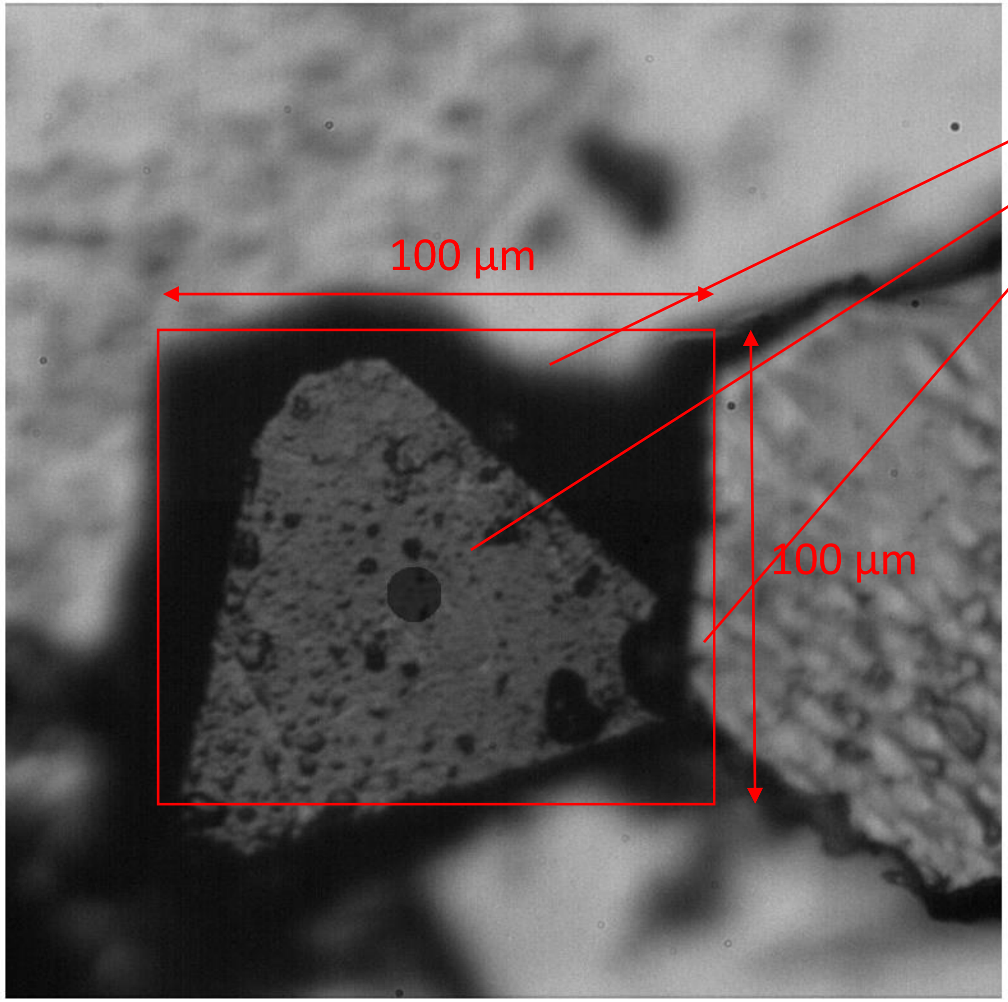


In- phase

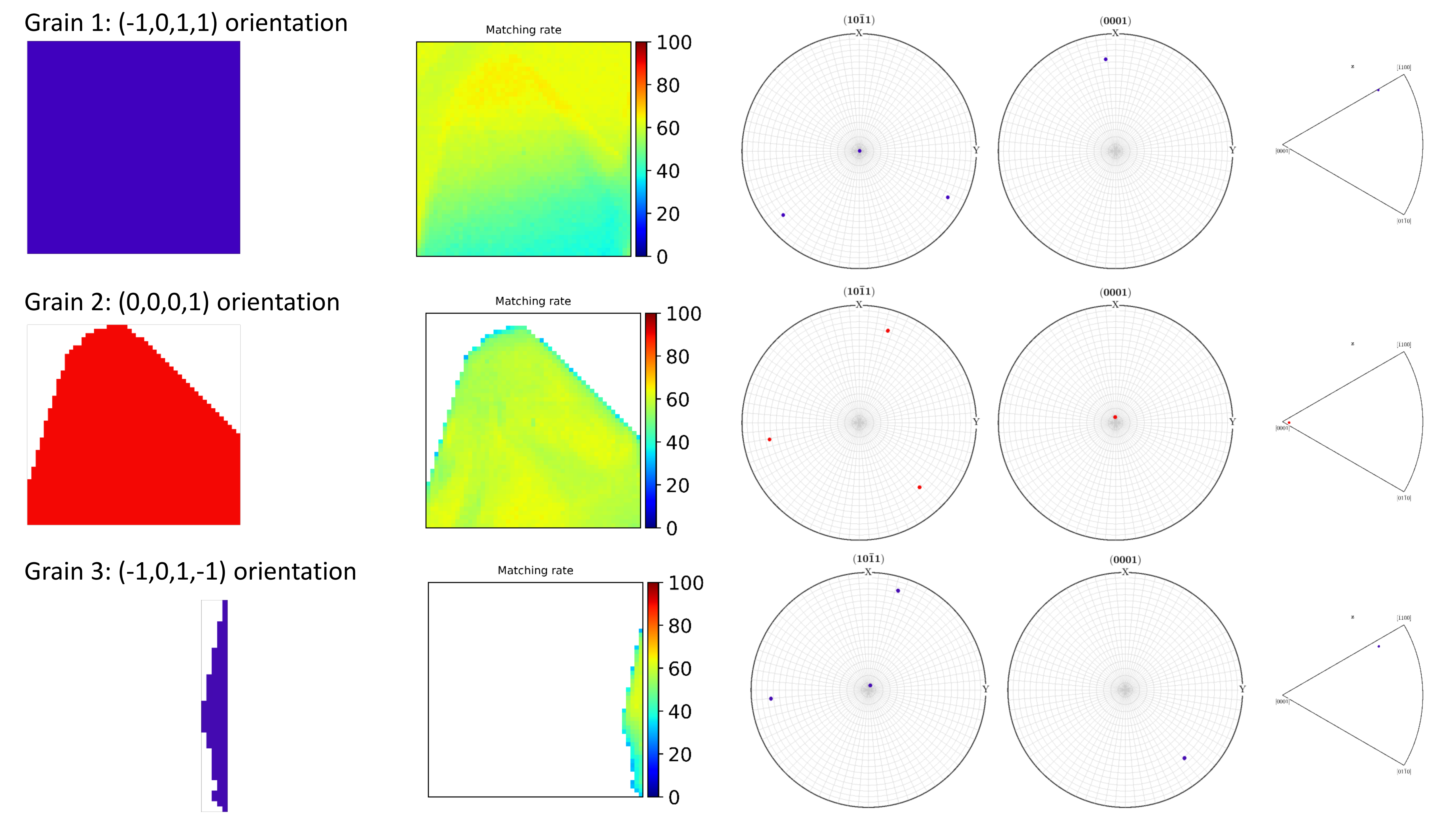


Herbertsmithite ZnCuOCl

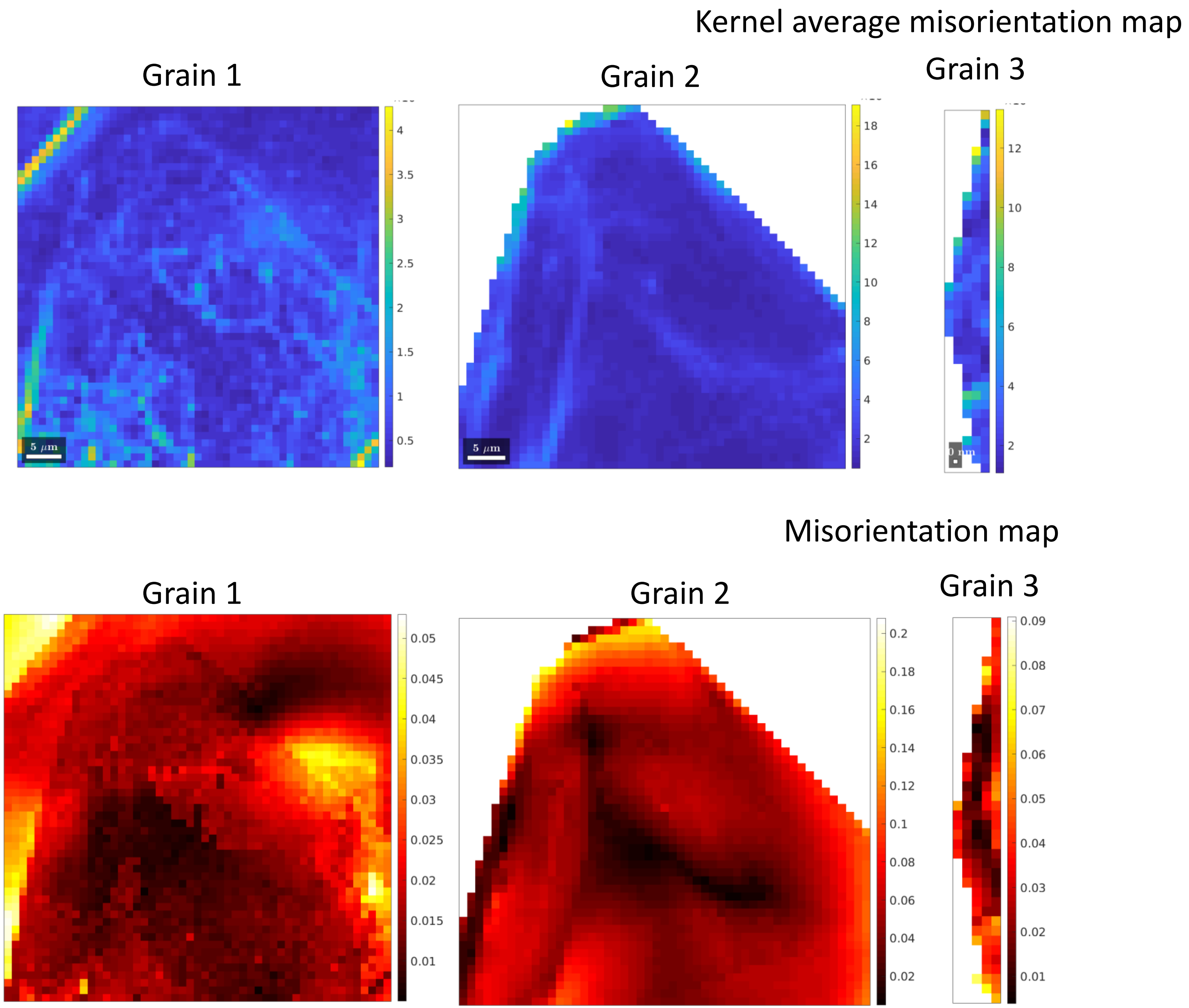
Optical microscope



Three grains are in the scanned ROI (**different DEPTH!**)

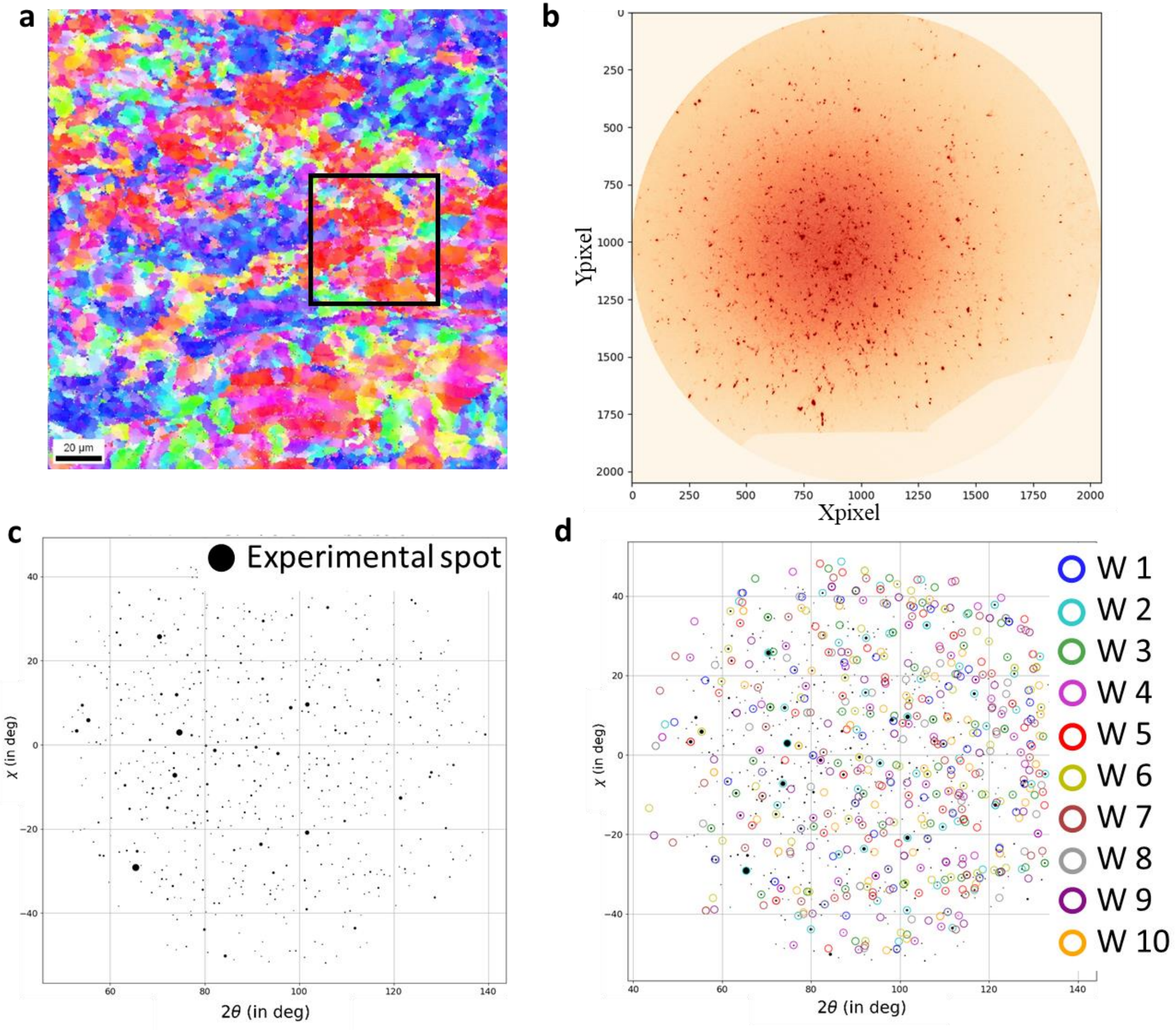


Grain 1: (-1,0,1,1) orientation
Matching rate
100
80
60
40
20
0
(101̄1)
X
Y
(0001)
X
Y
Grain 2: (0,0,0,1) orientation
Matching rate
100
80
60
40
20
0
(101̄1)
X
Y
(0001)
X
Y
Grain 3: (-1,0,1,-1) orientation
Matching rate
100
80
60
40
20
0
(101̄1)
X
Y
(0001)
X
Y



Kernel average misorientation map
Grain 1
Grain 2
Grain 3
5 μm
5 μm
Misorientation map
Grain 1
Grain 2
Grain 3

Polycrystalline Tungsten (W)

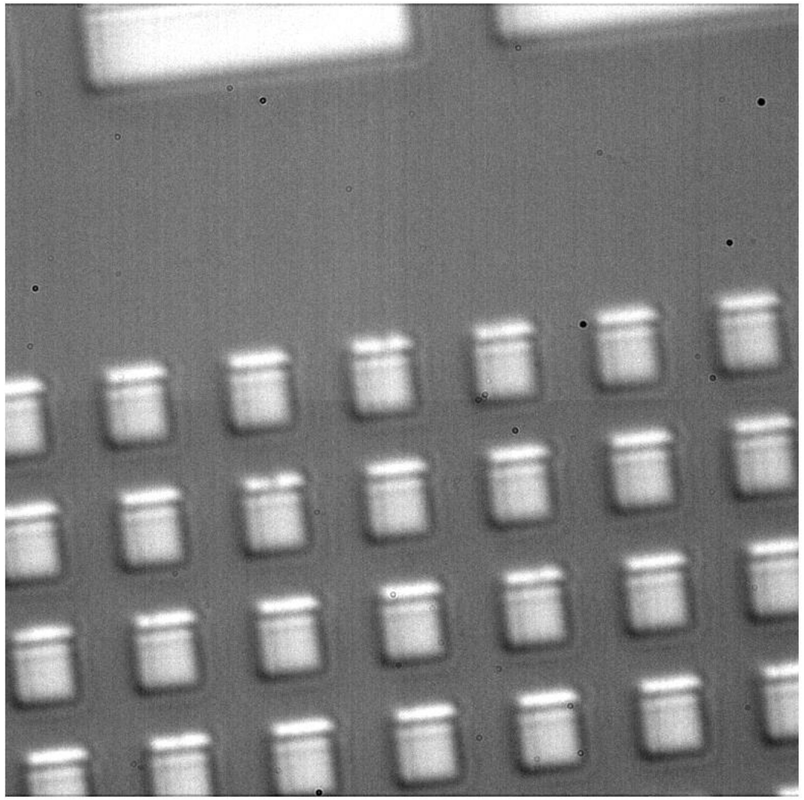


Appendix

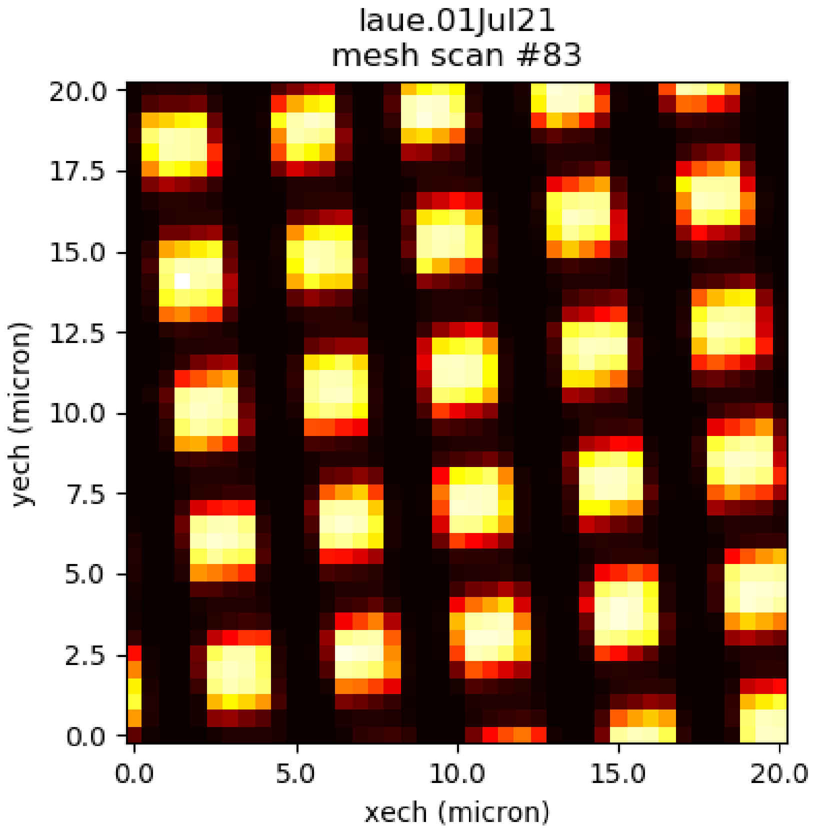
Multi-phase Detection

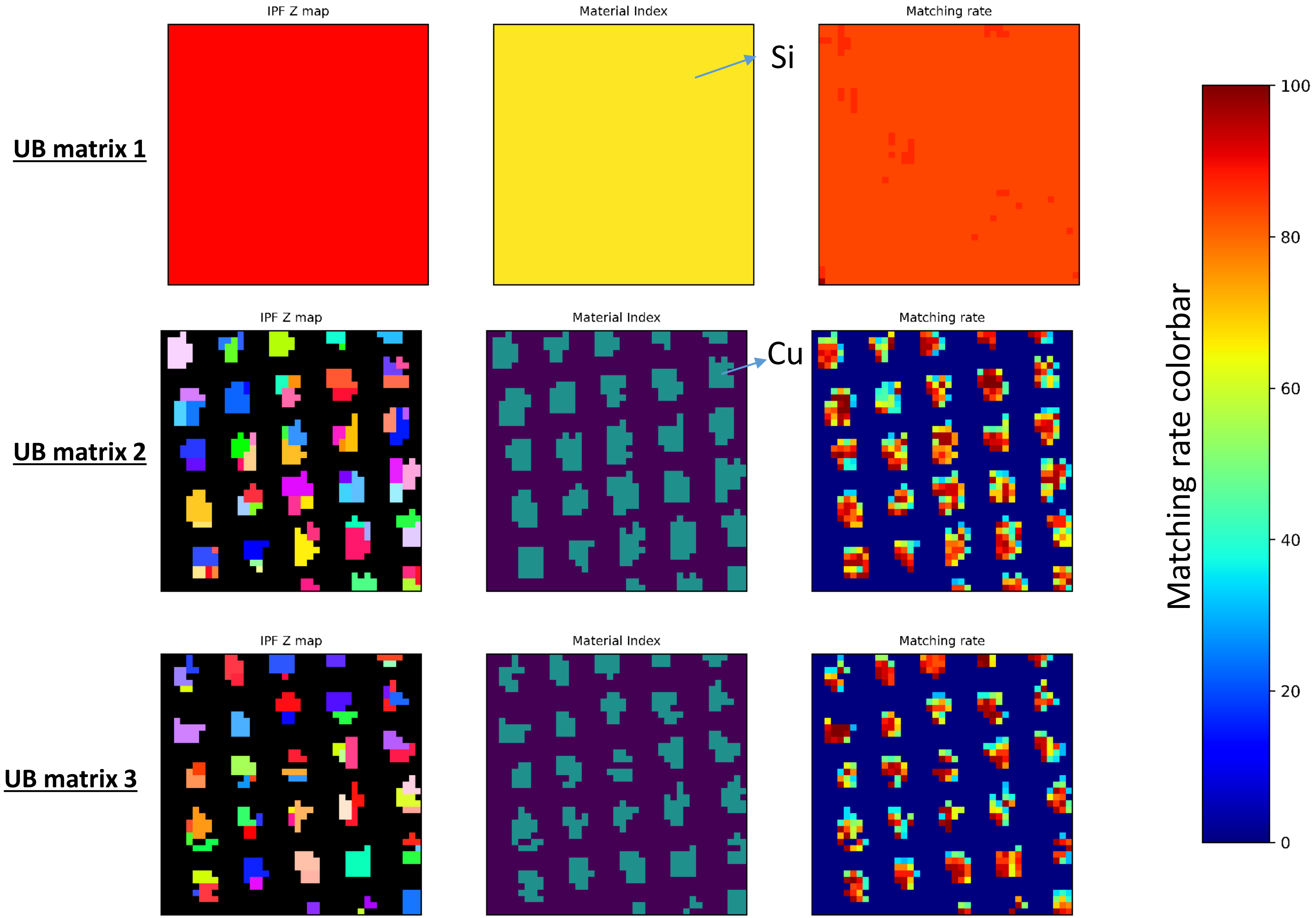
Cu-pads embedded in Si

Microscope image

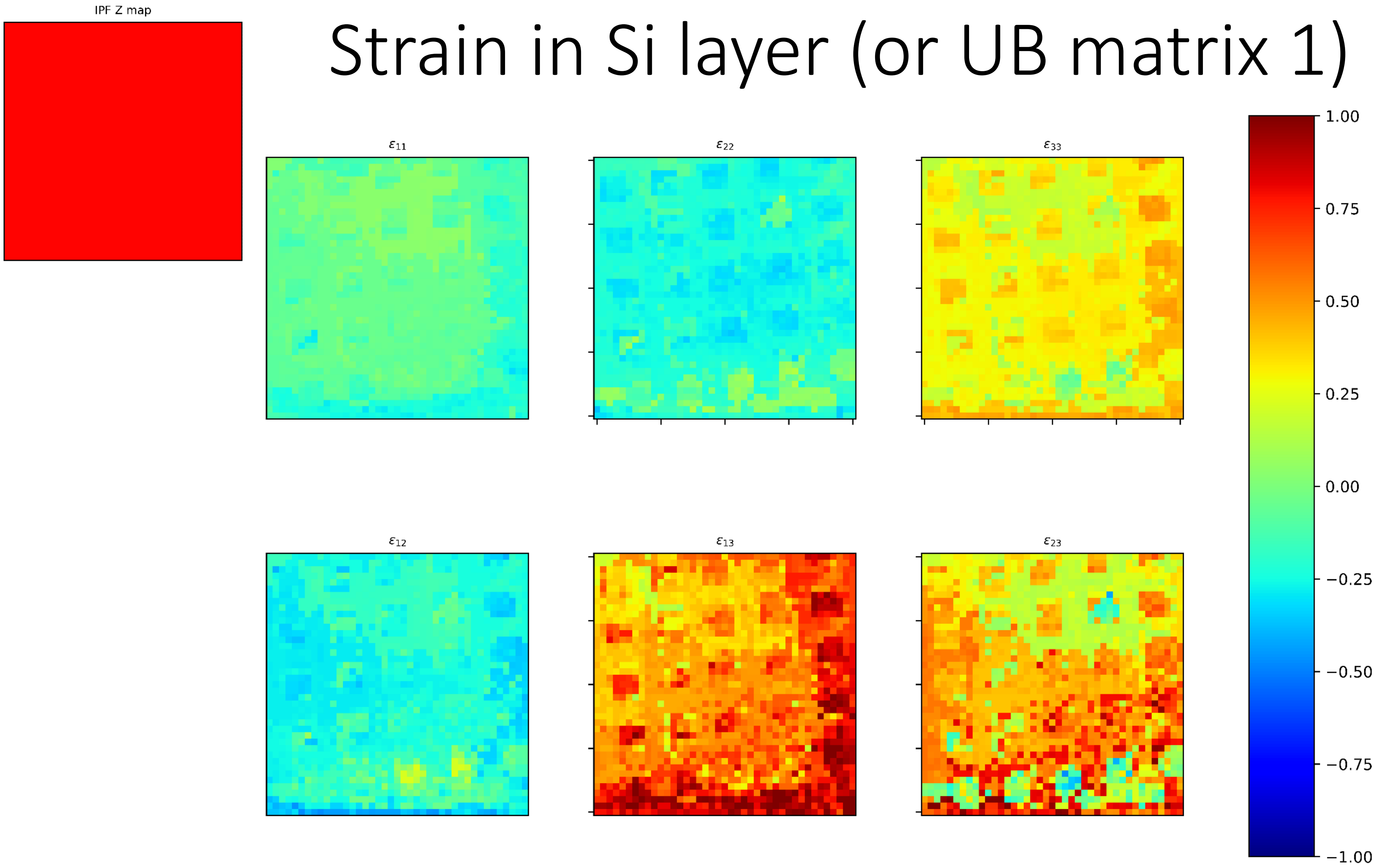


Fluorescence image




UB matrix 1
UB matrix 2
UB matrix 3
IPF Z map
Material Index
Matching rate
Si
Cu
Matching rate colorbar
100
80
60
40
20
0

Strain in Si layer (or UB matrix 1)



Strain in Cu layer (or UB matrix 2)