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Orientation, Pattern Center Refinement and Deformation State Extraction through Global Optimization Algorithms

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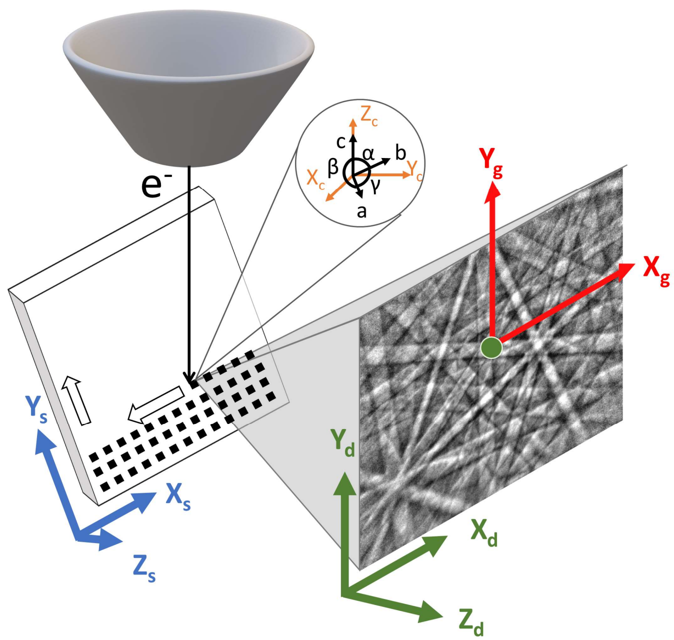
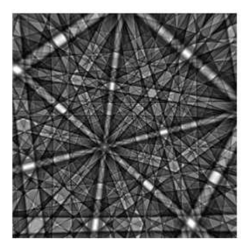
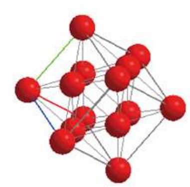
Electron Backscatter Diffraction

Electron backscatter diffraction is a fully automated SEM-based characterization technique to extract structural information from materials to study their microstructure, texture, defect density, residual strain, etc.







0.5% in pattern center
->
Strain uncertainty ~$3*10^{-3}$

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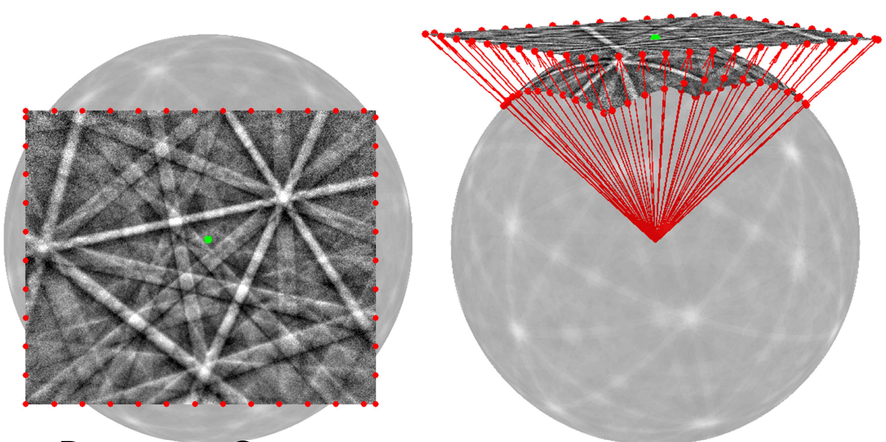
Zhu et al, Microscopy and Microanalysis, 2019

The Pattern Matching Problem

Forward model (f) describing the accurate diffraction physics:

$I_{simulated}$=f (keV, phase, geometry, orientation, pattern center, elastic deformation)

Known Partially known Unknown



Pattern Center

How do we improve the similarity between $I_{simulated}$ and $I_{experimental}$?

- Realistic forward model (f)
- Improve the accuracy of orientation and PC
- Determine the elastic deformation tensor

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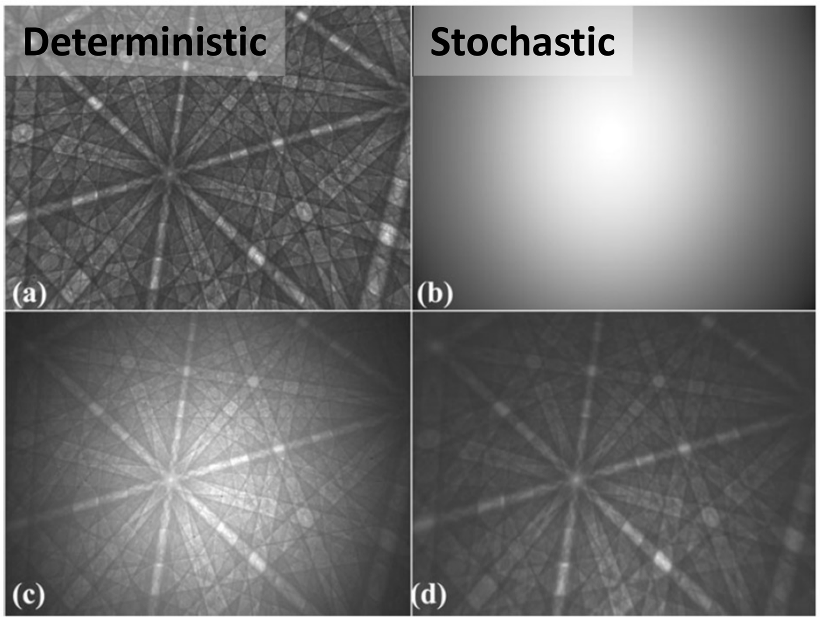
Dynamical Simulation of EBSD Pattern: Forward Model



Ground truth: Ni @ 30keV

Deterministic part: dynamical scattering model uses scattering matrix to predict probability of BSE distribution.

Stochastic part: Monte Carlo electron trajectory simulation to predict spatial and energy distributions for BSEs.

Geometric part: geometrical parameters-detector tilt, sample tile, crystal orientation, pattern center, deformation tensor.

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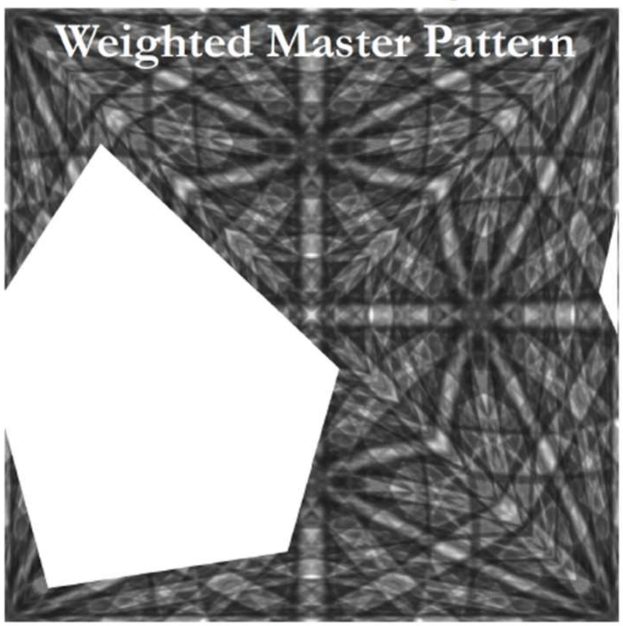
Callahan and De Graef, Microscopy and Microanalysis, 2013

Approximate Model for Deformation Tensor Inclusion

$$(X,Y)_L = \ell(F^{-1}(L_q[p]))$$



Approximate Deformation Model

Rotated and Undeformed Pattern Coordinates:

$$(X,Y)_L = \mathcal{L}(L_q[\widehat{\boldsymbol{p}}])$$

$\hat{p}$: detector pixel coordinates
L_q:quaternion rotation operator
q: (passive) rotation required to rotation
$\mathcal{L}$: square Lambert transformation.

Rotated and Deformed Pattern Coordinates:

$$(X,Y)_L{}' = \mathcal{L}(F^{-1}(L_q[\widehat{\boldsymbol{p}}]))$$

F^{-1}: interpolation on the undeformed master

Zhu et al, Ultramicroscopy, 2020

Formulation of the Optimization Problem

Definition of an optimization problem:

$$\max_{x \in S} \ \text{sim}\,(\text{f}(\mathbf{x}) \,,\, \text{I}_{\text{experimental}})$$

seek for a minimizer $\boldsymbol{x}^*$ that gives best match with the experimental pattern:

$$\text{sim}\,(\text{f}(\boldsymbol{x}^*) \,,\, \text{I}_{\text{experimental}}) \geq \text{sim}\,(\text{f}(\boldsymbol{x}) \,,\, \text{I}_{\text{experimental}})$$

Bounded optimization problem:

Initial estimate: orientation=$(\varphi_1, \Phi, \varphi_2)$, PC=(PCx, PCy, DD)

Optimized values: orientation$*$=$(\varphi_1, \Phi, \varphi_2) \cdot s$, PC $*$ =(PCx, PCy, DD) +pc

What about deformation?

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sim: similarity metric; x: n-dimensional parameter vector; S: subset of $\mathbb{R}^n$

Formulation of the Optimization Problem

Elastic deformation tensor contains the rotation and stretch:

Optimized values : PC* =(PCx, PCy, DD) +pc

Elastic deformation tensor **(8 degrees of freedom):**

$$F = I + \begin{pmatrix} \Delta\beta_{11} & \beta_{12} & \beta_{13} \\ \beta_{21} & \Delta\beta_{22} & \beta_{23} \\ \beta_{31} & \beta_{32} & 0 \end{pmatrix} + \beta_{33} I$$

EBSD insensitive to spherical strain!!!

For isotropic elastic material ($\sigma_{33} = 0$; orientation=[0,0,0]):

$$\boxed{\beta_{33} = \frac{-\lambda(\Delta\beta_{11} + \Delta\beta_{22})}{3\lambda + 2G}} \qquad \lambda = \frac{Ev}{(1+v)(1-2v)} \qquad G = \frac{E}{2(1+v)}$$

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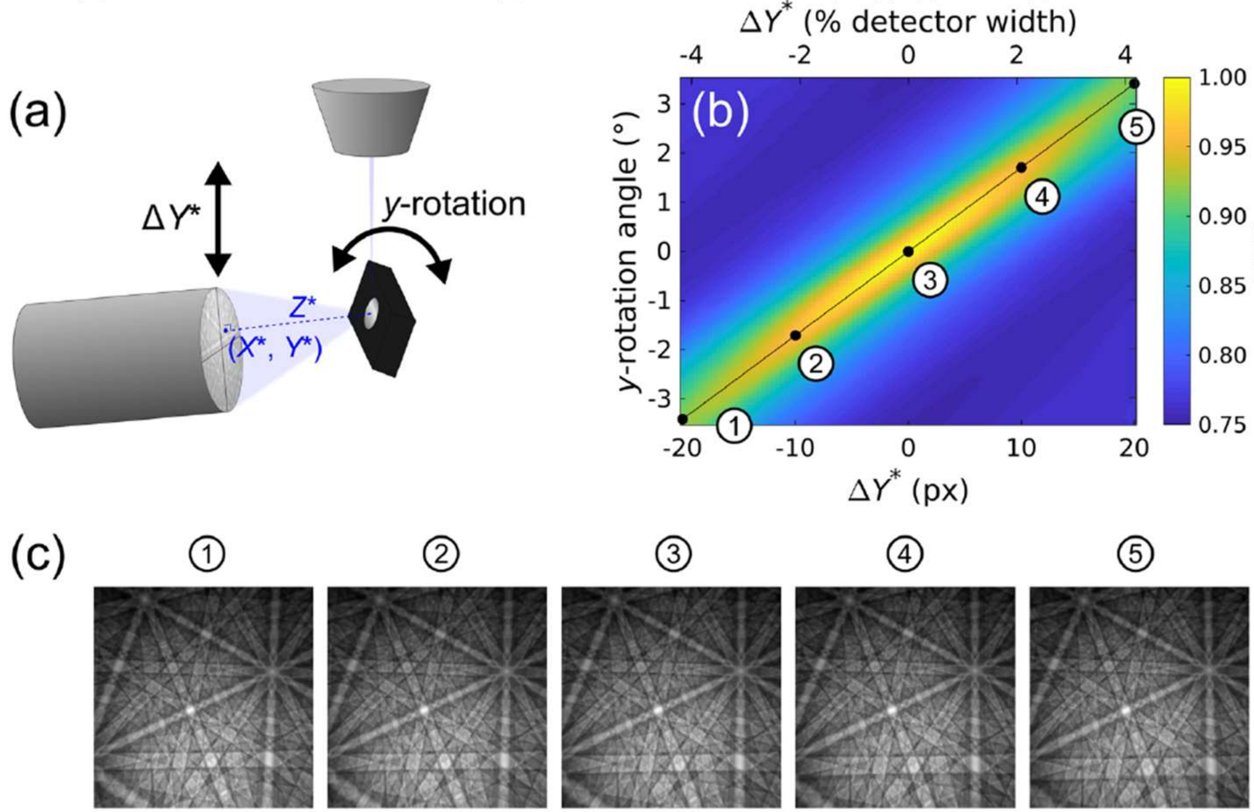
Hardin et al, Journal of Microscopy, 2015

Challenge in Convergence: Sloppy Optimization

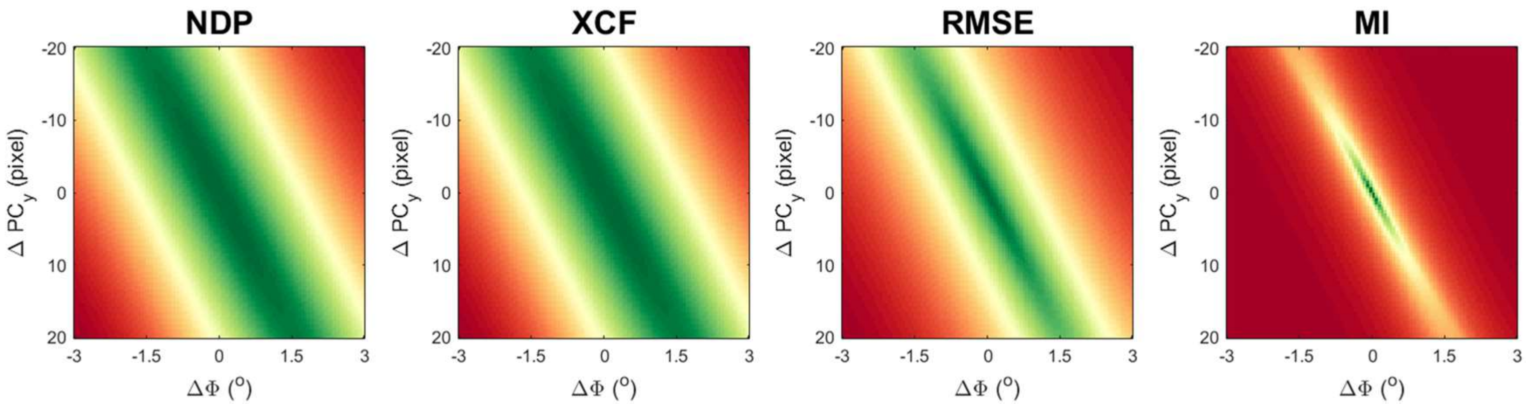


Pattern center shift can be compensated by small rotation.

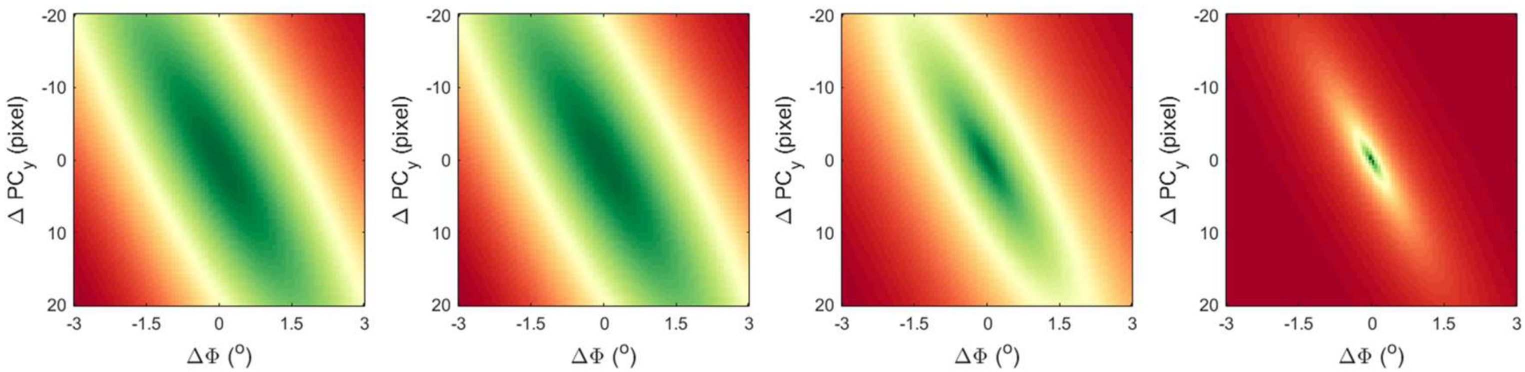
Nelder-Mead simplex can't converge efficiently

Pang et al, Ultramicroscopy, 2019

Sloppy Feature Scaling: Rotation Correction



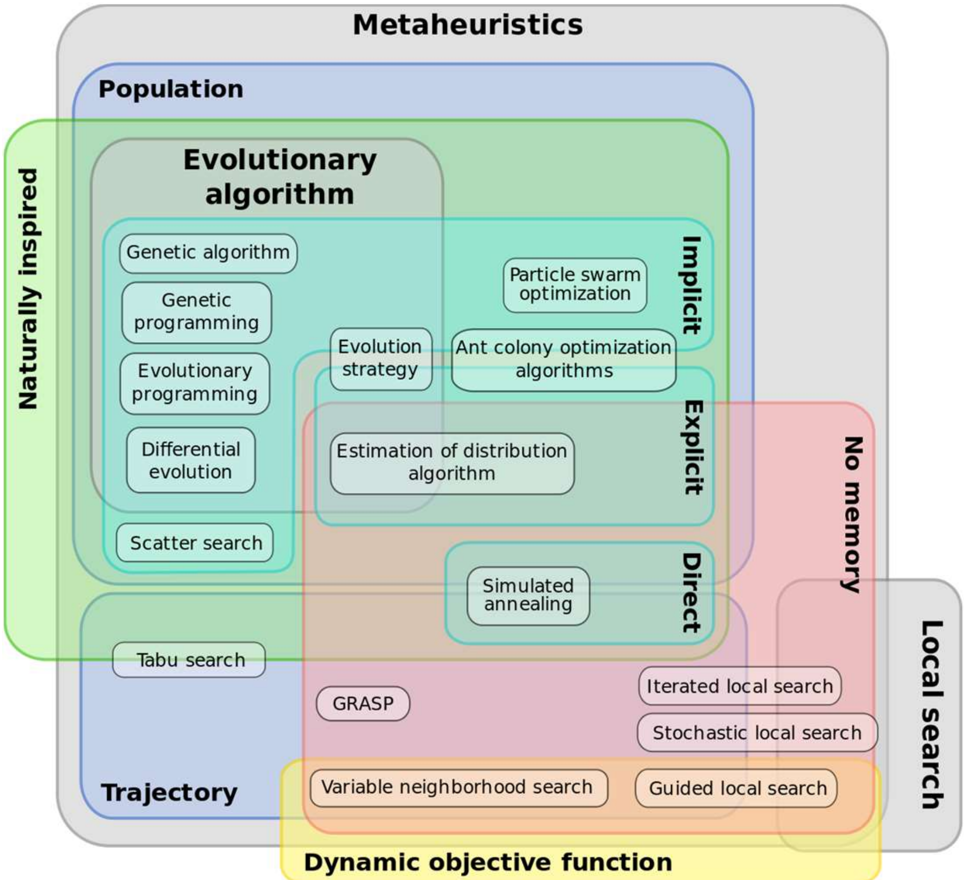
Rotation correction

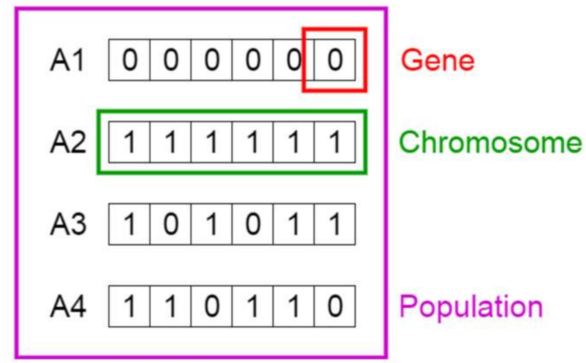


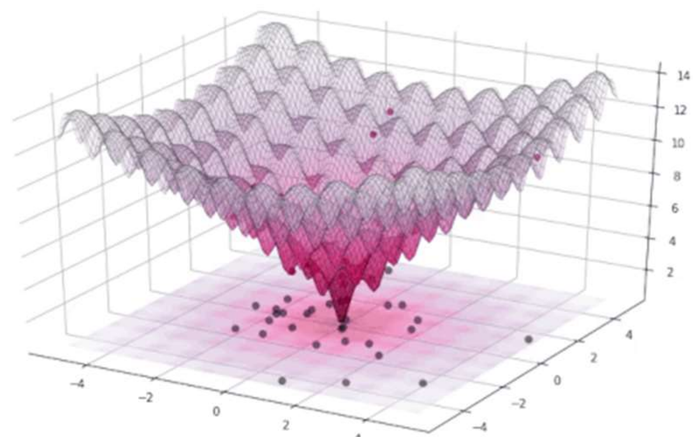
The sloppiness is universal to all the similarity metrics.

Singh et al, Journal of Applied Crystallography, 2017

Population Based Global Optimization







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Wikipedia.com/ Tanaka et al, Ultramicroscopy, 2019

Differential Evolution Algorithm

Initialization $\boldsymbol{x}_{i,g} = x_{j,i,g} \quad \mathrm{j} \in \{1, \dots, D\}, i \in \{1, \dots, N_p\}, g \in \{1, \dots, g_{max}\}$

Mutation

$$\boldsymbol{v}_{i,g+1} = \boldsymbol{x}_{r_1,g} + F(\boldsymbol{x}_{r_2,g} - \mathbf{x}_{r_3,g}) \qquad \text{DE/rand/1}$$

$$\boldsymbol{v}_{i,g+1} = \boldsymbol{x}_{r_1,g} + F(\boldsymbol{x}_{r_2,g} + \boldsymbol{x}_{r_3,g} - \boldsymbol{x}_{r_4,g} - \boldsymbol{x}_{r_5,g}) \qquad \text{DE/rand/2}$$

$$\boldsymbol{v}_{i,g+1} = \boldsymbol{x}_{i,g} + F(\boldsymbol{x}_{best,g} - \boldsymbol{x}_{i,g} + \boldsymbol{x}_{1,g} - \boldsymbol{x}_{r_2,g}) \qquad \text{DE/rand-to-best/1}$$

$$\boldsymbol{v}_{i,g+1} = \boldsymbol{x}_{best,g} + F(\boldsymbol{x}_{r_1,g} - \boldsymbol{x}_{r_2,g}) \qquad \text{DE/best/1}$$

$$\boldsymbol{v}_{i,g+1} = \boldsymbol{x}_{best,g} + F\left(\boldsymbol{x}_{r_1,g} + \boldsymbol{x}_{r_2,g} - \boldsymbol{x}_{r_3,g} - \boldsymbol{x}_{r_4,g}\right) \qquad \text{DE/ best /2}$$

Crossover

$$\boldsymbol{u}_{i,g+1} = u_{j,i,g+1} \begin{cases} v_{j,i,g+1} & if \;\; rand_j \le C_r \; or \; j = j_{rand} \\ x_{j,i,g} & otherwise \end{cases}$$

Selection

$$\boldsymbol{x}_{i,g+1} = \begin{cases} \boldsymbol{u}_{i,g+1} & if \;\; f(\boldsymbol{u}_{i,g+1}) \le f(\boldsymbol{x}_{i,g}) \\ \boldsymbol{x}_{i,g} & otherwise \end{cases}$$

R. Storn, K. Price, Journal of Global Optimization, 1997

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Hyperparameter Tuning

- Crossover probability (C_r): 0.7-0.9 (default:0.9)
- Mutation factor (F): 0.2-0.5 (default:0.5)
- Number of generations (g_{max}): 50-100 (default:100)
- Initial Population size (N_p): 10D

Zhu et al, Ultramicroscopy, 2021 (Under review)

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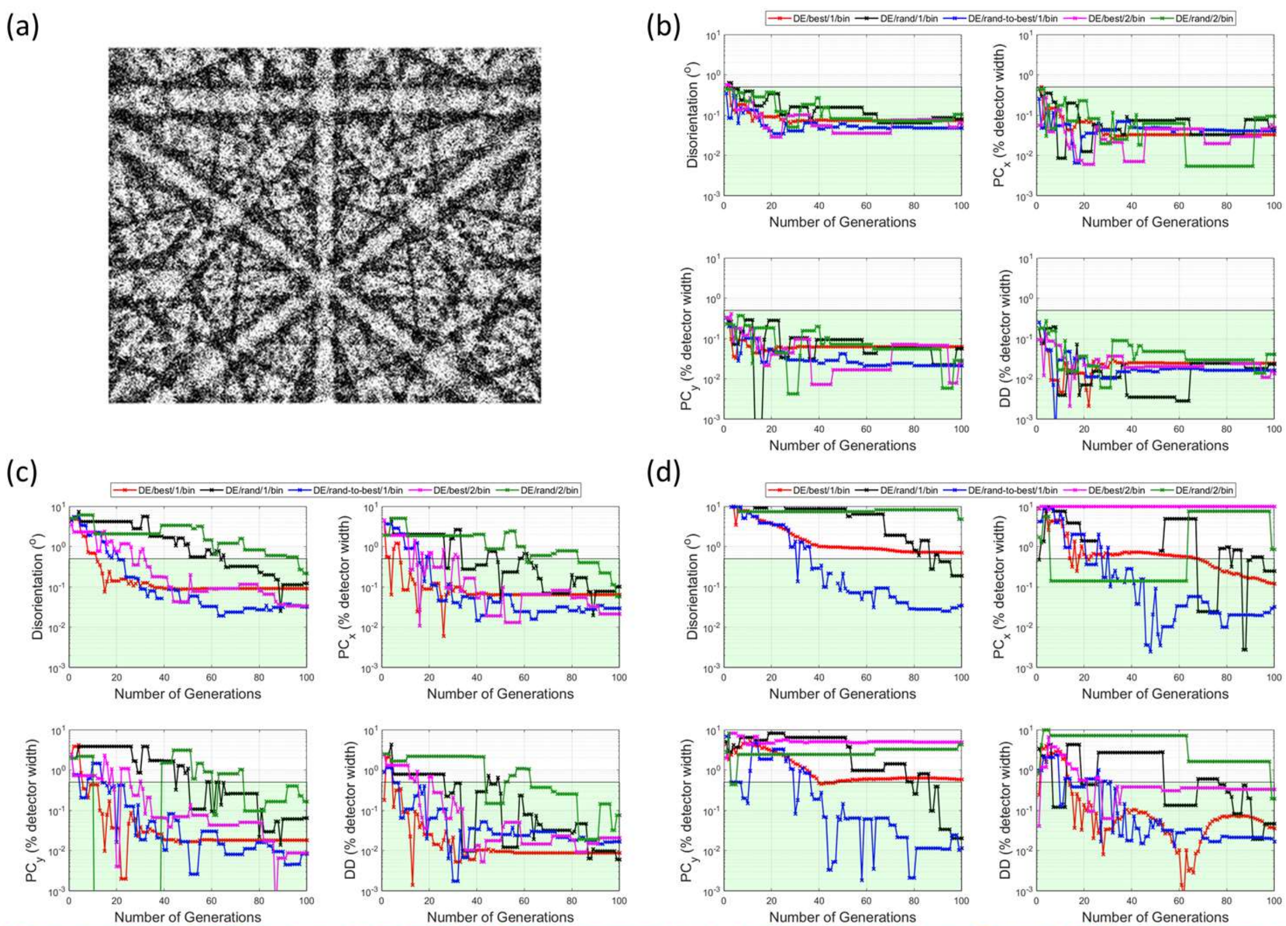
Mutation Schemes



Search spaces:

(a) 11.72 dB noise

(b) ±0.5° , ±0.5%

(c) ±10° , ±5%

(c) ±20° , ±10%

DE/rand-to-best/1

Zhu et al, Ultramicroscopy, 2021 (Under review)

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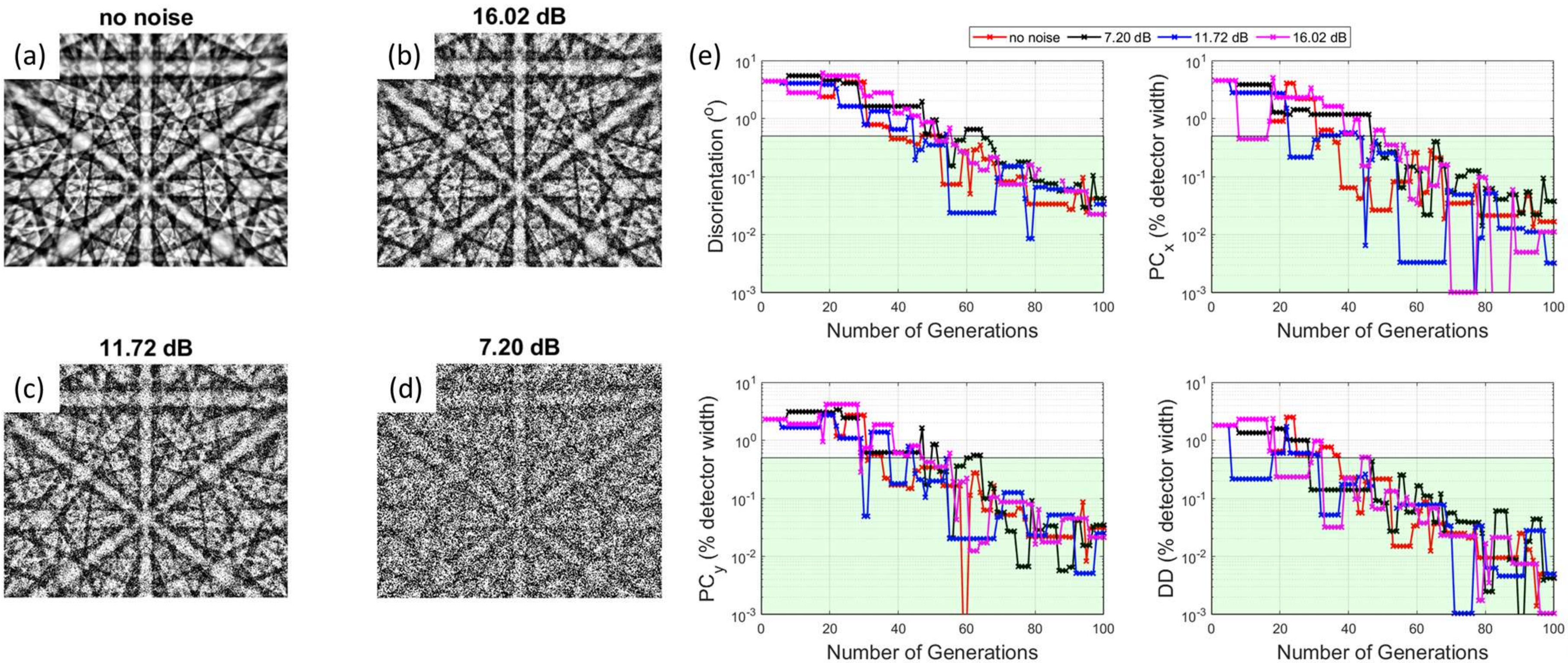
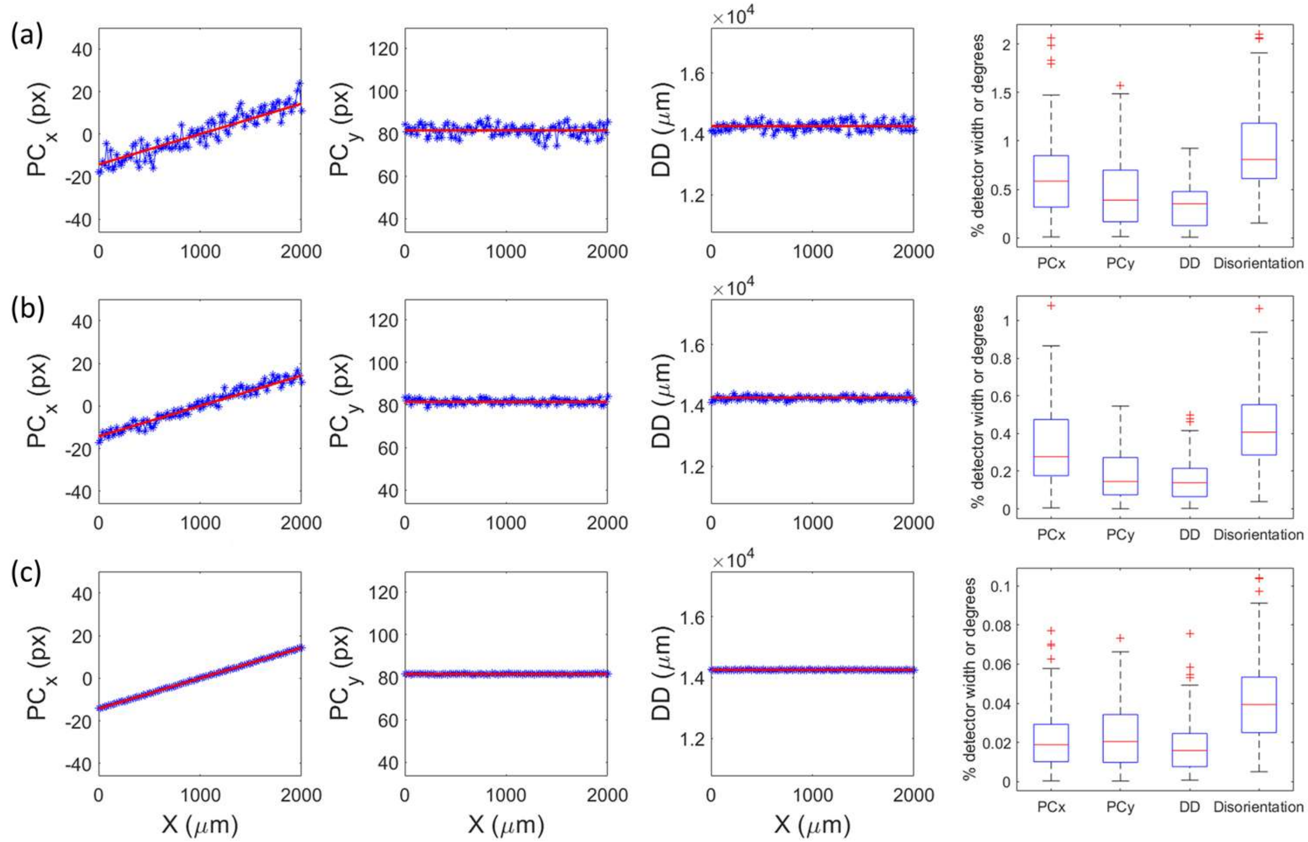
Noise sensitivity

g_{max}=100, Np=60, Cr=0.9 and F = 0.5 (DE/rand/1)



Zhu et al, Ultramicroscopy, 2021 (Under review)

Hybrid Optimization: DE+NMS



g_{max}=50

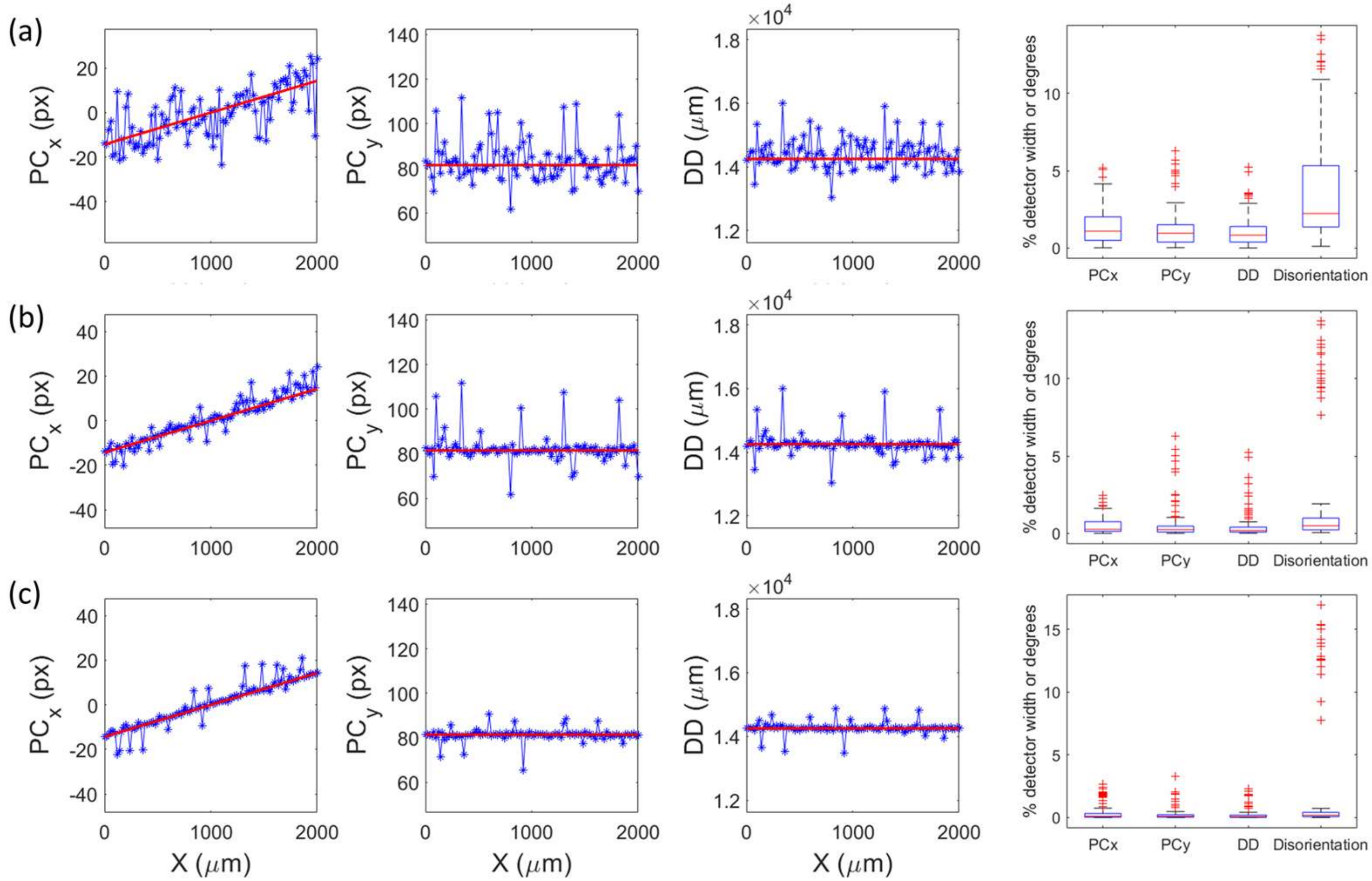
g_{max}=50 + NMS

g_{max}=100 + NMS

0.02% d.w. for pattern center and 0.04 degrees for the orientation

Zhu et al, Ultramicroscopy, 2021 (Under review)

Hybrid Optimization: PSO+NMS



g_{max}=50

g_{max}=50 + NMS

g_{max}=100 + NMS

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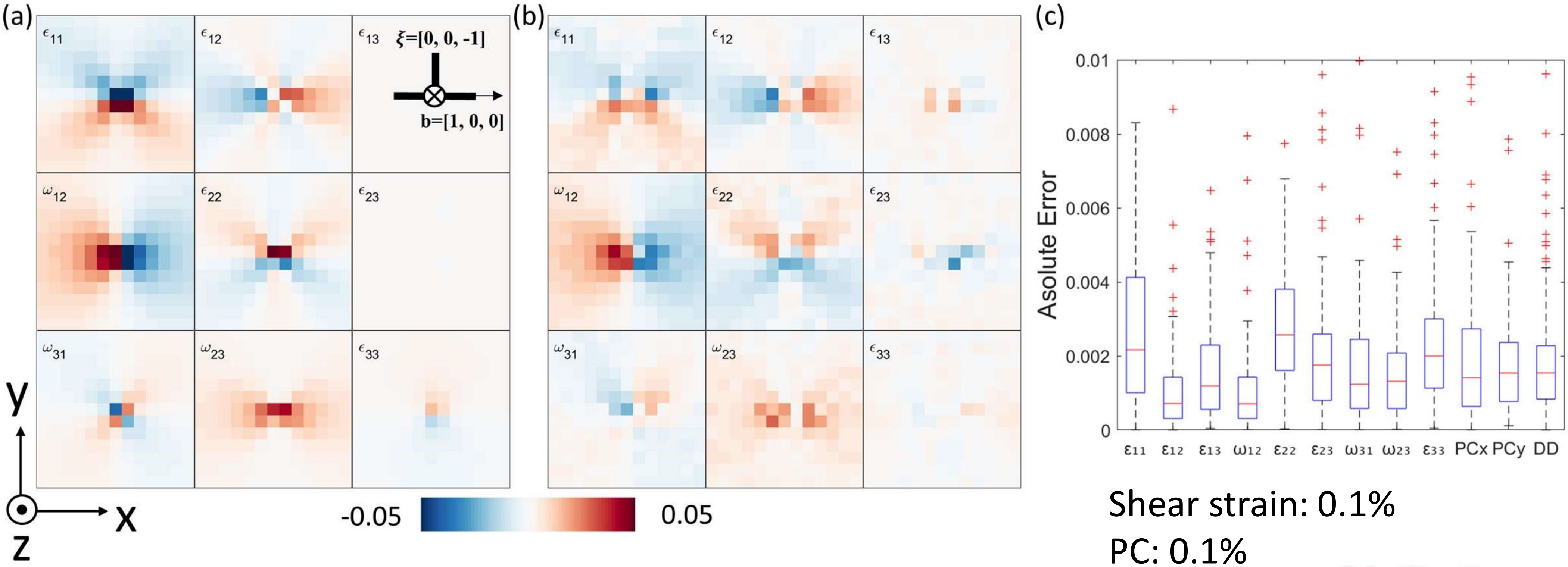
Deformation Tensor Inference: Simulated Patterns



Shear strain: 0.1%

PC: 0.1%

Zhu et al, Ultramicroscopy, 2021 (Under review)

Absolute Strain Mapping with Any Reference Pattern

1. Pattern pre-processing: adaptive histogram equalization, high-pass/low-pass filter
2. Determine the reference pattern to be used and optimize its PC and orientation
3. Use optimized PC and determine the strain tensor of reference pattern
4. Use cross-correlation based HR-EBSD to determine the strain map relative to reference
5. Strain state correction based on strain state of the reference pattern

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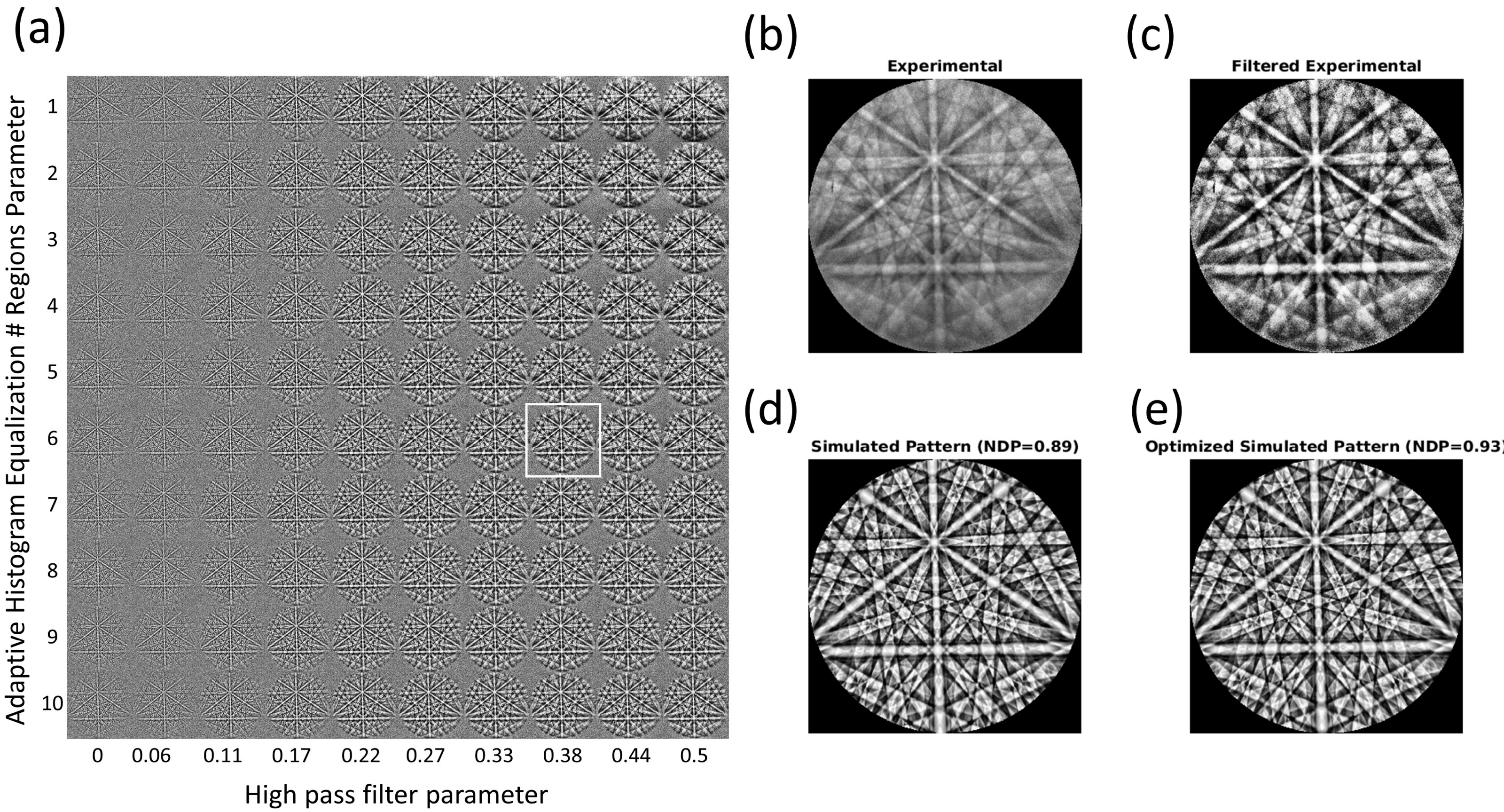
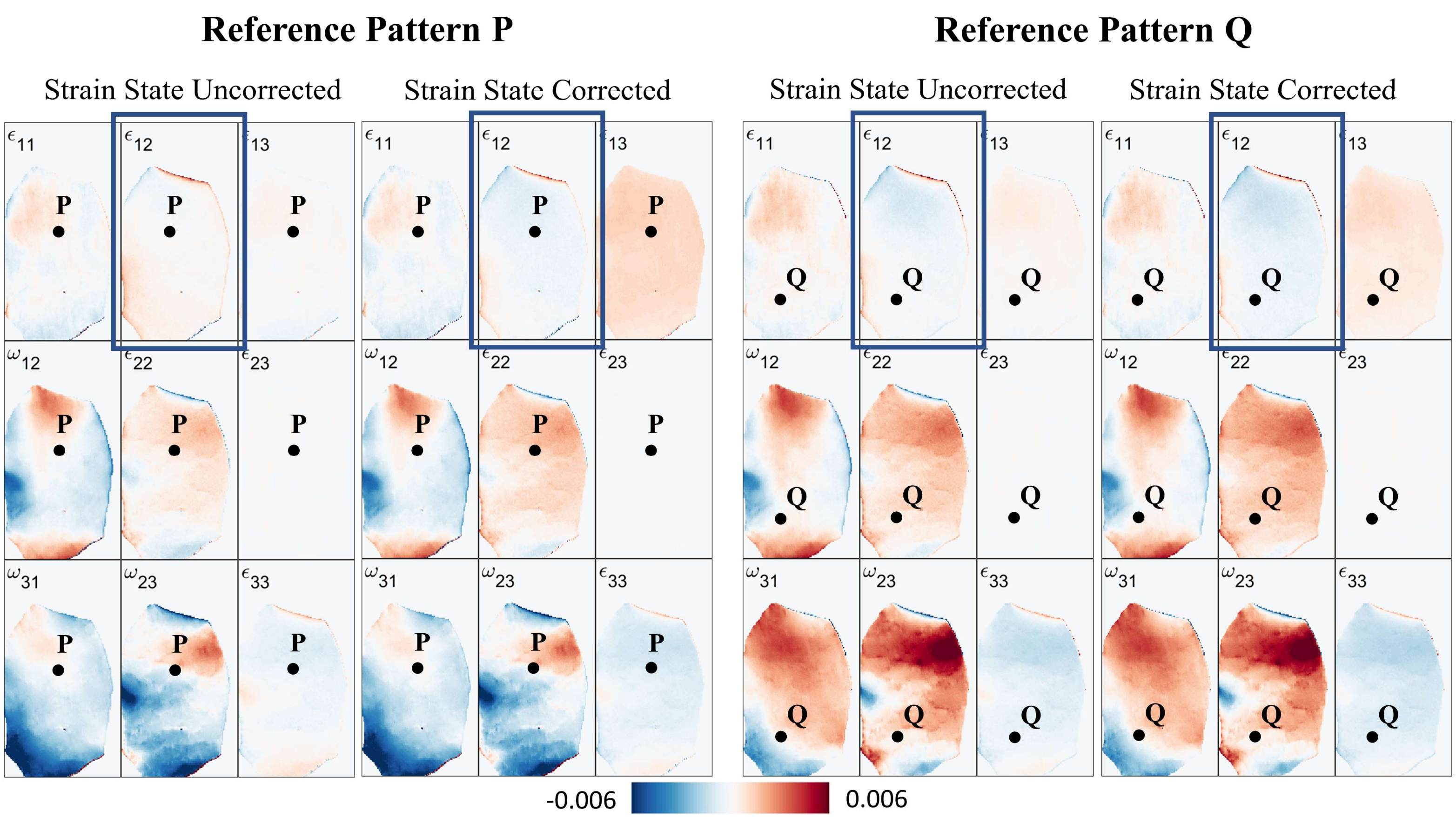
Zhu et al, Ultramicroscopy, 2021 (Under review)

Experimental Pattern Pre-Processing



Zhu et al, Ultramicroscopy, 2021 (Under review)

Experimental Validation: Low Cycle Fatigued TRIP Steel



Zhu et al, Ultramicroscopy, 2021 (Under review)

Summary

• The differential evolution algorithm outperforms particle swarm algorithm due to the nature of mutation.

• The search space for differential evolution is feasible up to ±20 disorientation and ±10 % detector width.

• Simulated undeformed patterns demonstrate an accuracy of ~0.04° for orientation and ~0.02% detector width for pattern center.

• Noisy simulated deformed patterns reveal an accuracy of shear strain and rotation components ~0.001 and ~0.002 for the normal strain.

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Other people in the group: Marcus Ochsendorf, Christian Kurniawan, Maxwell Lee, Ke-wei Jin, Michael Kitcher, Clement Lafond

Github Link: https://github.com/EMsoft-org/EMsoft

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