Novel Remapping Method for HR-EBSD based on Computer Vision Algorithm

Chaoyi Zhu[1], *Kevin Kaufmann*[2], *Kenneth Vecchio*[1,2*]

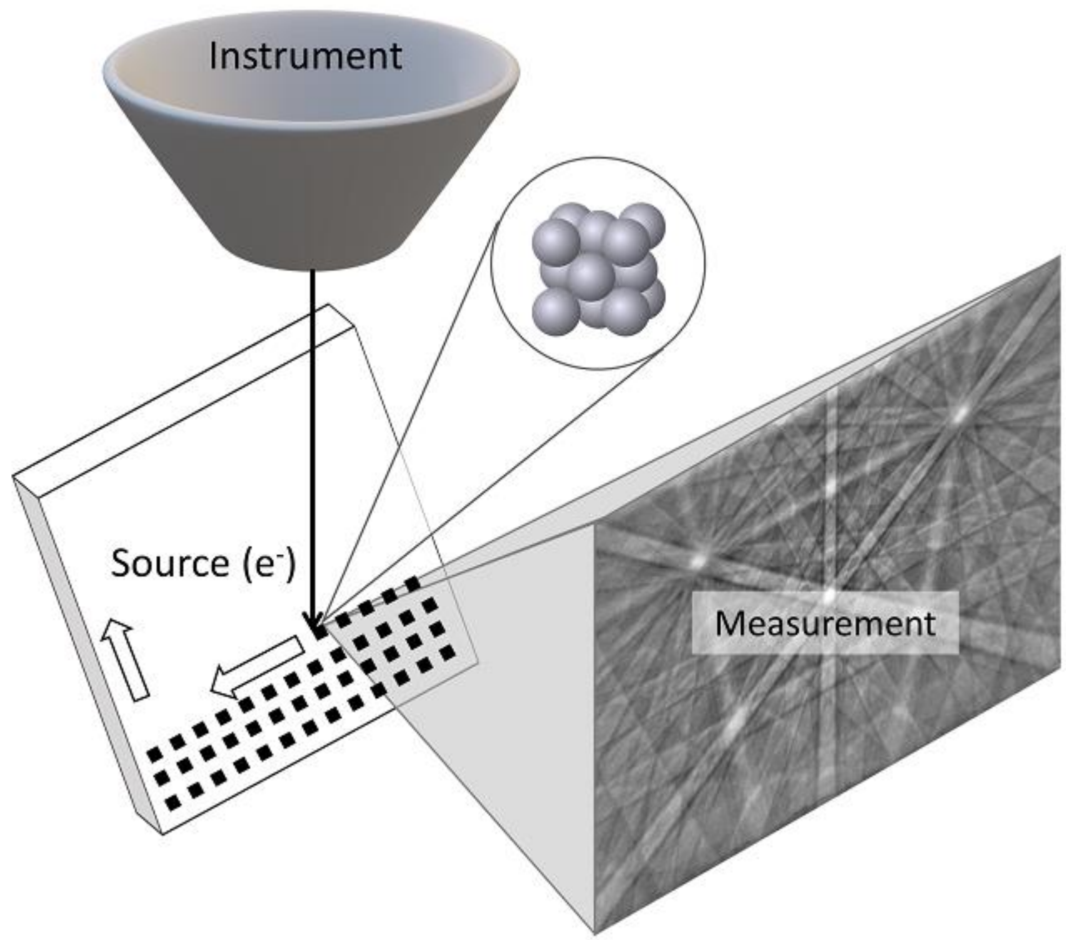
[1]Materials Science and Engineering Program, UC San Diego, La Jolla, CA 92093, USA

[2]Department of NanoEngineering, UC San Diego, La Jolla, CA 92093, USA

Technical Meeting and Exhibtion
MS&T20
MATERIALS SCIENCE & TECHNOLOGY

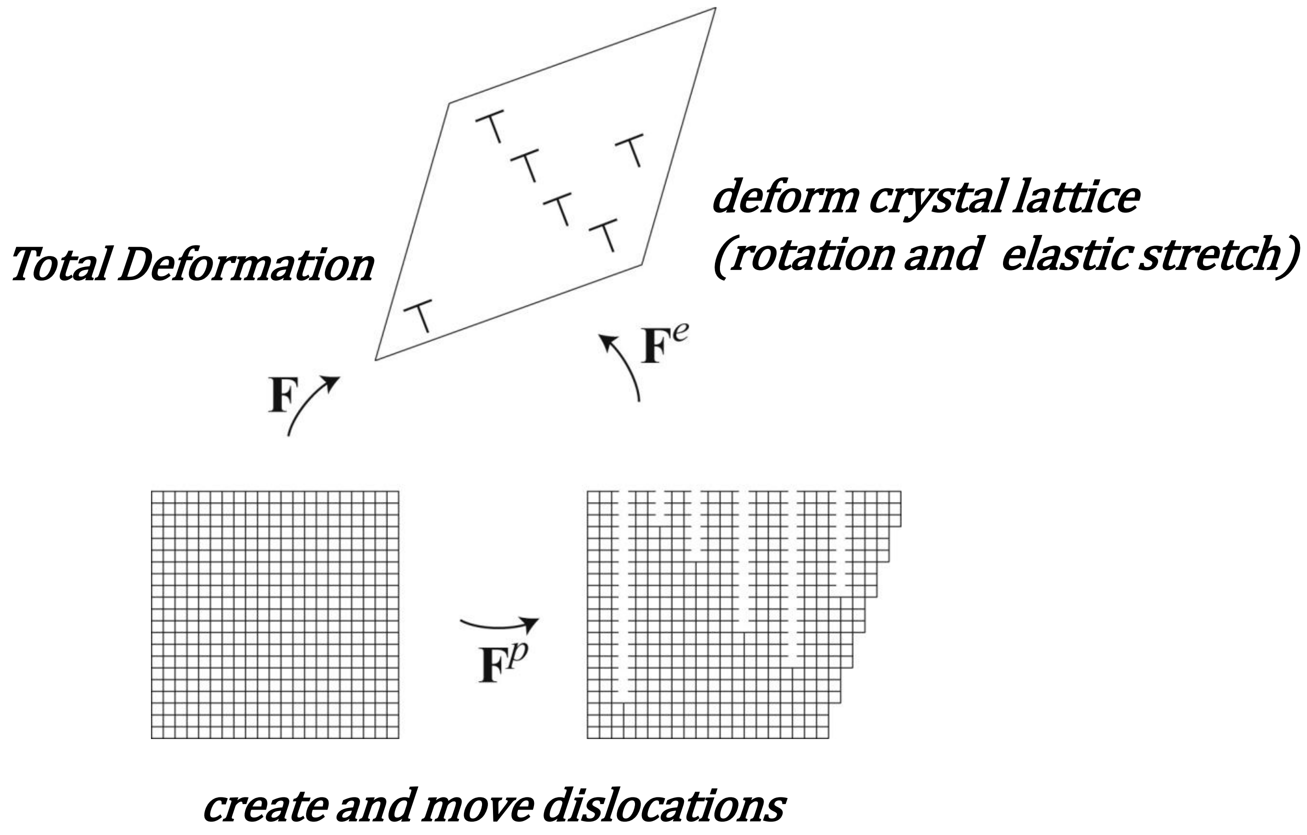
Materials Characterization

Electron Backscatter Diffraction



- Texture
- Microstructure
- **Deformation**

Crystal Deformation



Deformation gradient tensor:

$$\boldsymbol{F} = \boldsymbol{F}^{e}\boldsymbol{F}^{p}$$

Elastic stretch: shift of the zone axis and changes in the interplanar angles

$$\boldsymbol{\varepsilon} = \frac{1}{2}\left(\boldsymbol{F}^{e} + \boldsymbol{F}^{e^{T}}\right) - \boldsymbol{I}$$

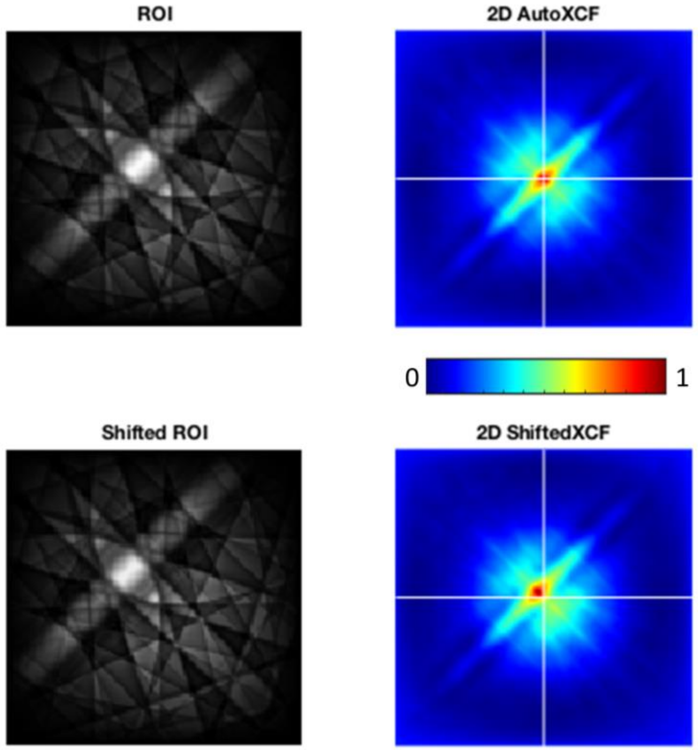
Lattice rotation: whole pattern rotation

$$\boldsymbol{\omega} = \frac{1}{2}\left(\boldsymbol{F}^{e} - \boldsymbol{F}^{e^{T}}\right)$$

K.C. Le *et al*., 2015;
Kröner, 1958;
B.C. Larson *et al*, 2007

HR-EBSD (Cross-Correlation)

Cross-Correlation



$$f_{test} * f_{ref} = \Im^{-1}[\Im(f_{test}) \cdot conj(\Im(f_{ref}))]$$

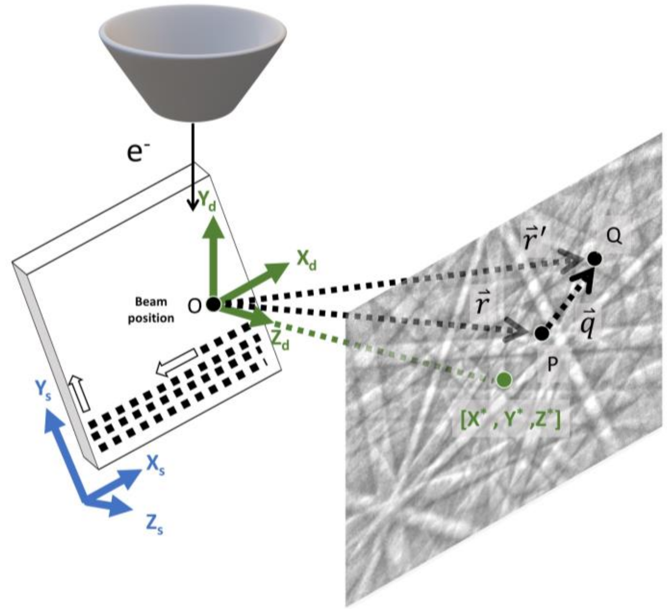
Wilkinson et al, 2006

Higher level of sensitivity:

- Rotation: 1×10^{-4} rad or 0.006 °
- Elastic strain: 1×10^{-4}
- GND lower noise floor:
  - Hough: $\Delta\rho \approx 10^{14}$ lines/m^2
  - HR-EBSD: $\Delta\rho \approx 10^{12}$ lines/m^2

Shift of the XCF peak from the origin represents the shift of the test ROI from reference ROI.

HR-EBSD (Cross-Correlation)

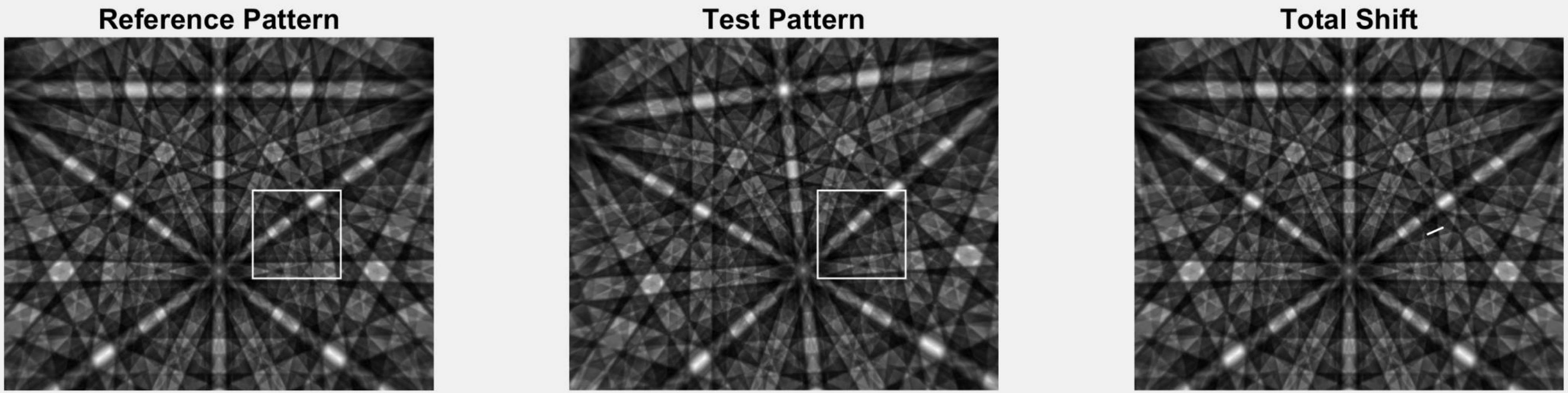


Non-linear minimization method to obtain deformation gradient tensor (F^e):

$$minf(F^e) = \sum_{\{ROI\}} \frac{1}{2} \left| \frac{Z^*}{(F^e \cdot \vec{r}) \cdot \vec{k}} F^e \cdot \vec{r} - (\vec{r} + \vec{q}) \right|^2$$

$\vec{r}$: center of ROI
Z^*: detector distance
$\vec{q}$: measured shift

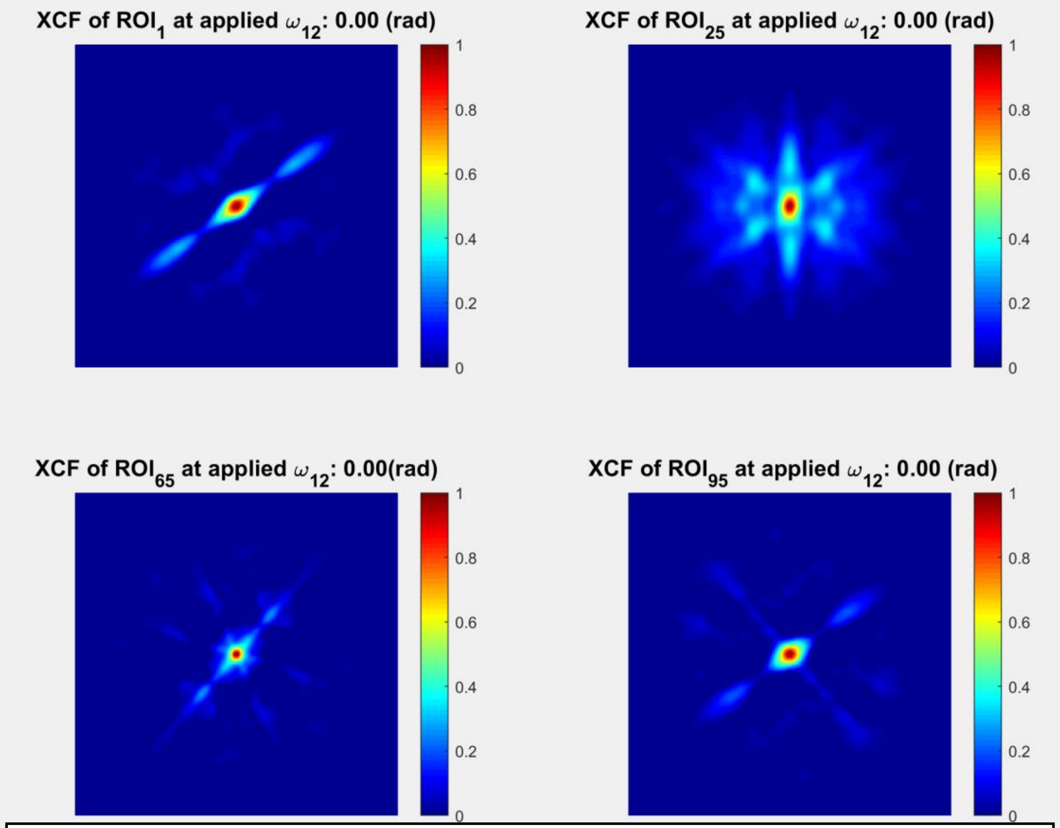
F^e between two images can be calculated from shifts measured between many regions of interest (ROIs).



Maurice *et al.*, 2012

Cross-Correlation: Limitation

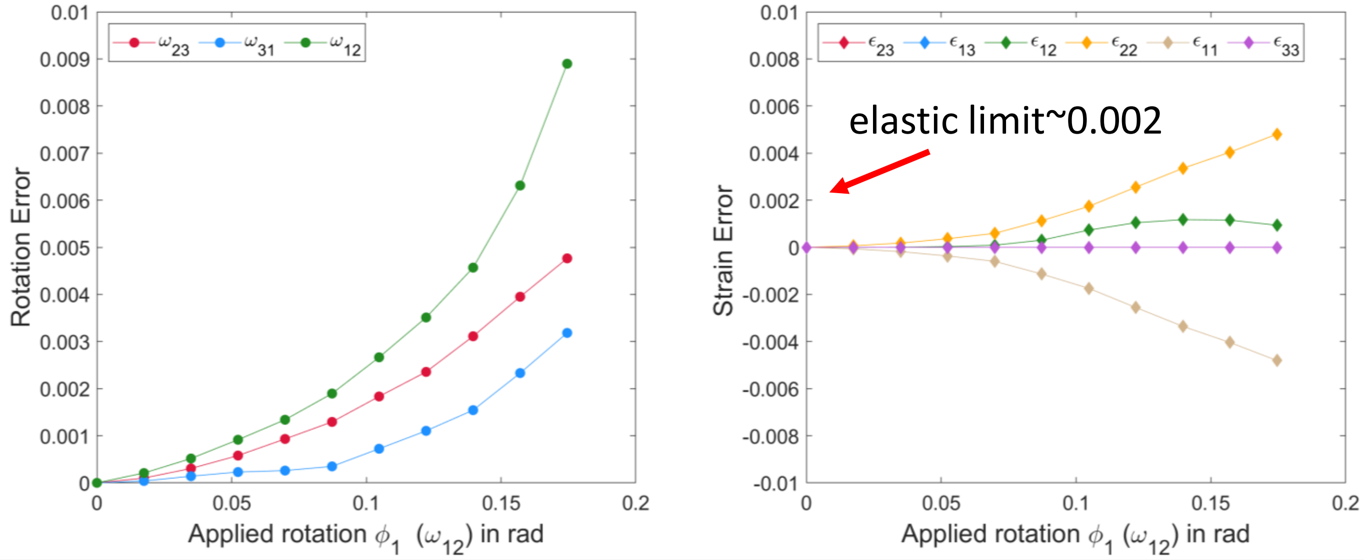
Cross-Correlation Between Patterns of Large Relative Rotations

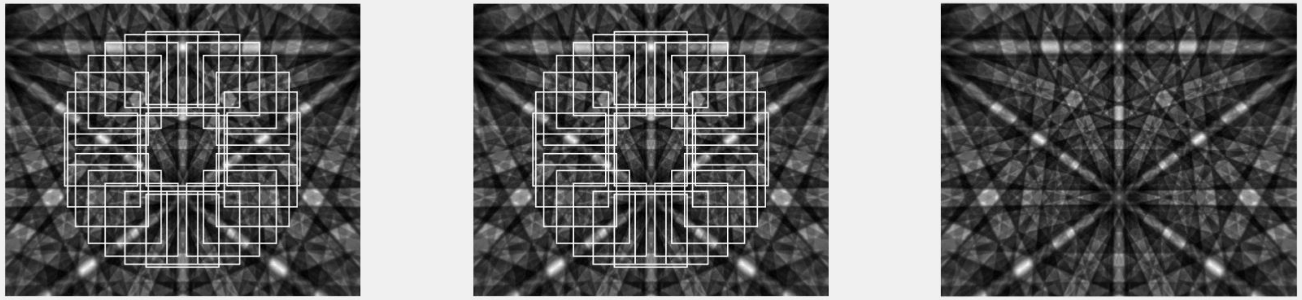


XCF peak changes at higher rotations

- Multiple peaks
- Peak shape distortion

Rotation and Strain Error

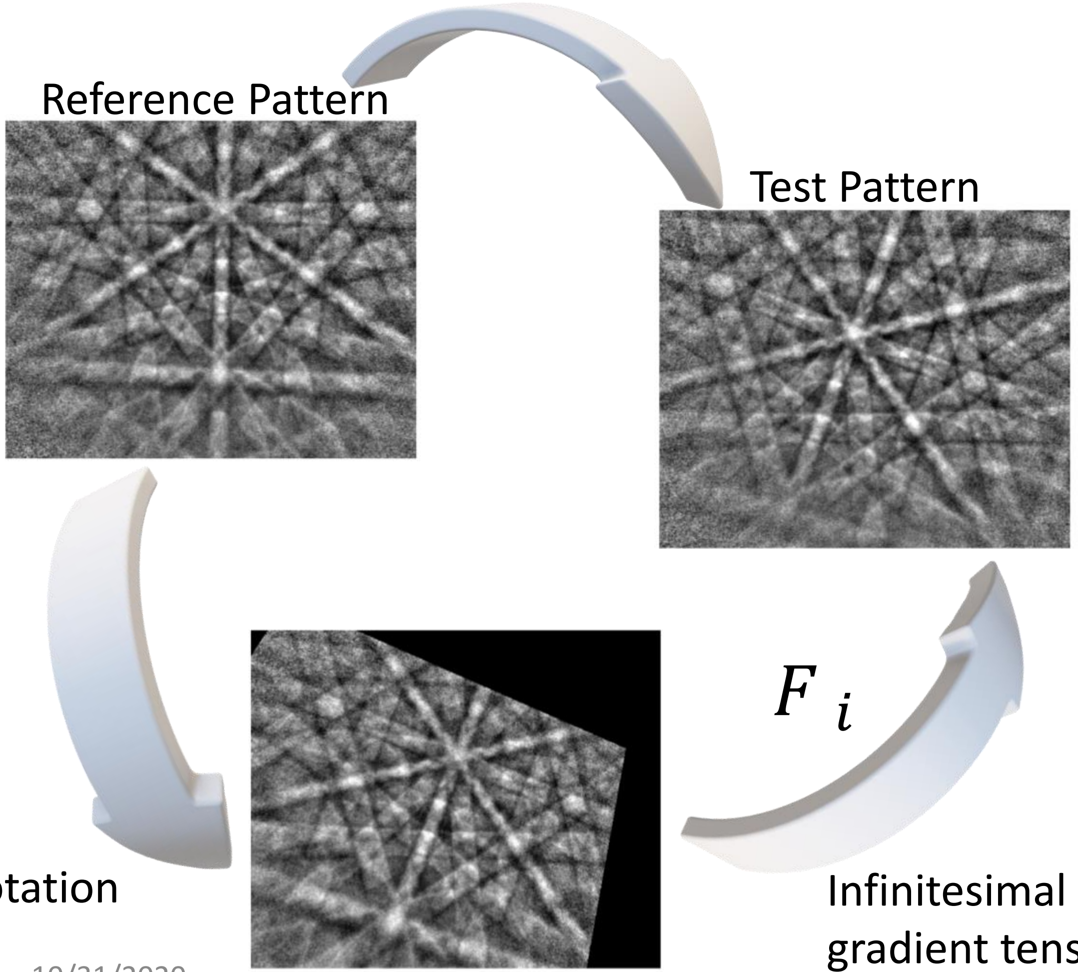




Pattern Remapping Technique

Total deformation gradient tensor

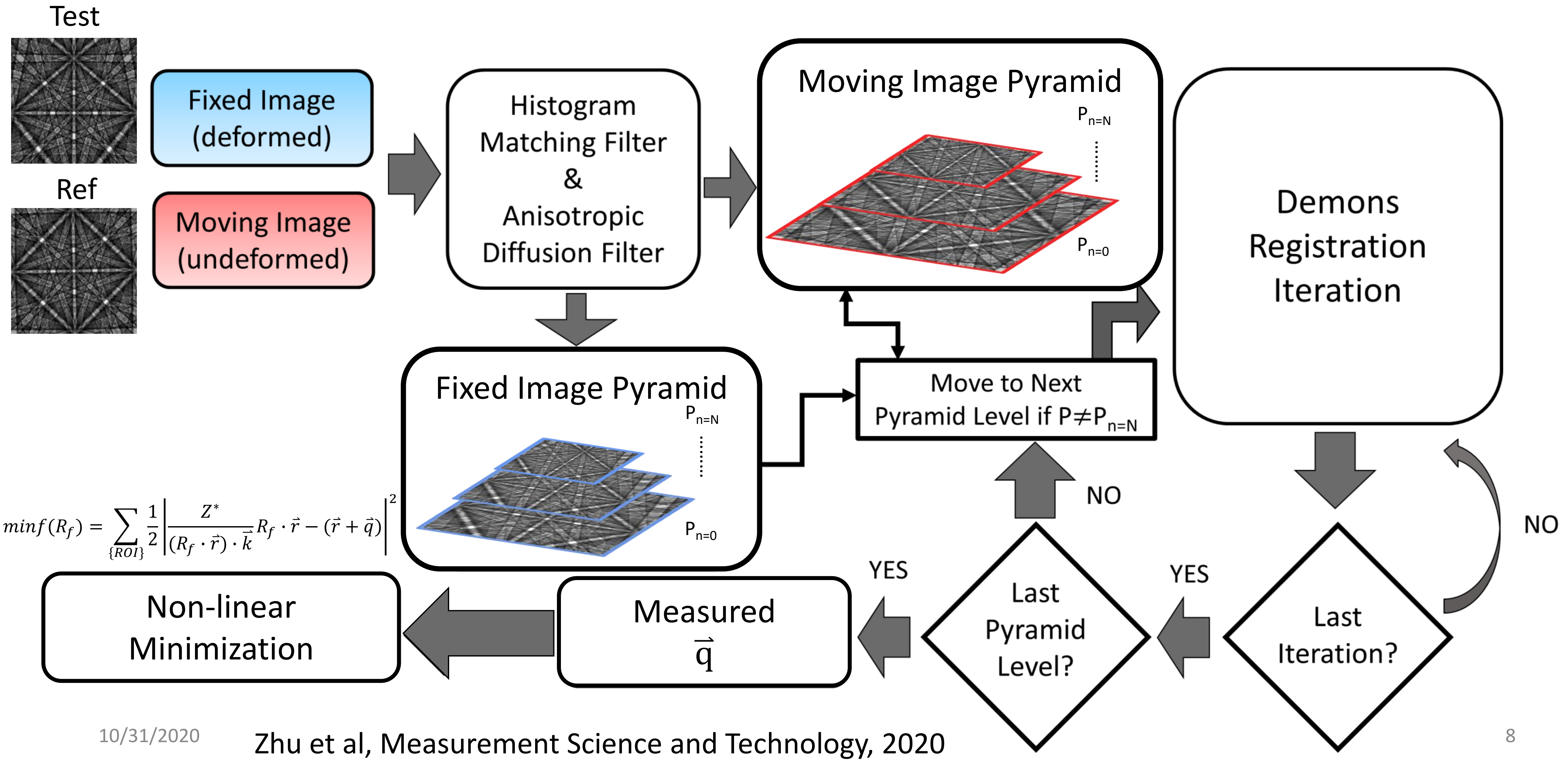
$$F_f = F_i \cdot R_{\mathrm{f}}$$



1. Remapping using orientation matrix (Maurice *et al*, 2012)
2. Remapping using cross-correlation (Britton *et al*, 2012)
3. Global matching using computer vision for remapping (Zhu et al, 2019)

Britton *et al*, Ultramicroscopy 2012
Maurice *et al.*, Ultramicroscopy 2012
Zhu et al, Ultramicroscopy 2020

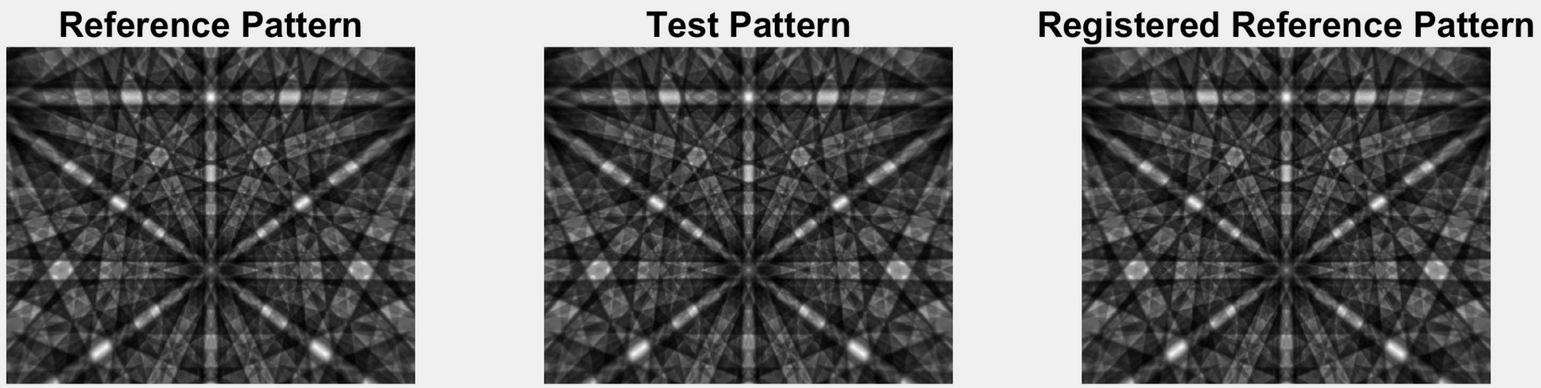
Image Registration Workflow to Extract Deformation Gradient Tensor



$$minf(R_f) = \sum_{\{ROI\}} \frac{1}{2} \left| \frac{Z^*}{(R_f \cdot \vec{r}) \cdot \vec{k}} R_f \cdot \vec{r} - (\vec{r} + \vec{q}) \right|^2$$

Zhu et al, Measurement Science and Technology, 2020

Determine the Remapping Rotation Matrix



$$minf(R_f) = \sum_{\{ROI\}} \frac{1}{2} \left| \frac{Z^*}{(R_f \cdot \vec{r}) \cdot \vec{k}} R_f \cdot \vec{r} - (\vec{r} + \vec{q}) \right|^2$$

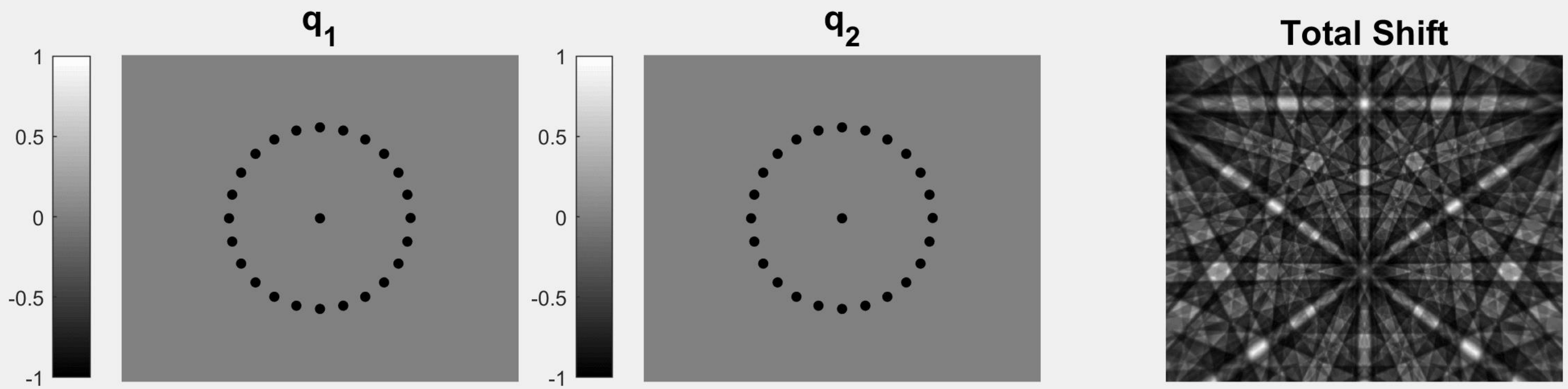


Image Registration Shift Field: $\vec{q} = [q_1, q_2]$

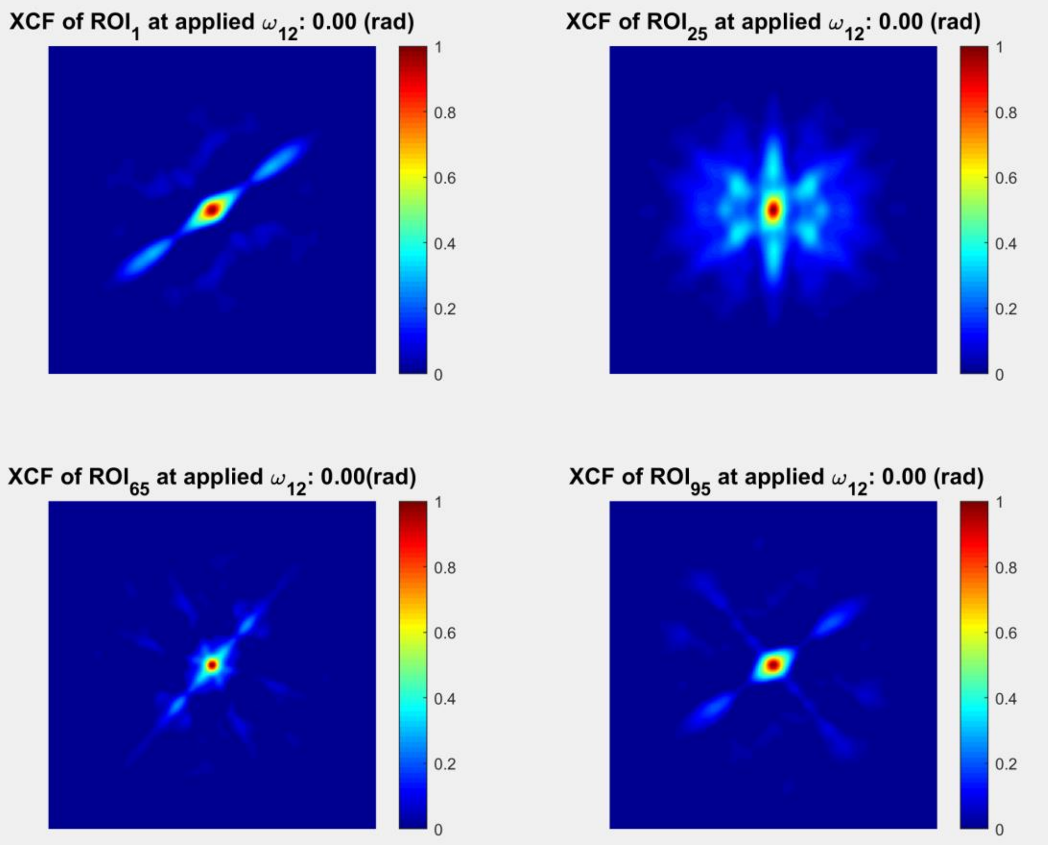
Zhu et al, Ultramicroscopy 2020

UC San Diego
JACOBS SCHOOL OF ENGINEERING
NanoEngineering

Cross-Correlation (after Remapping)

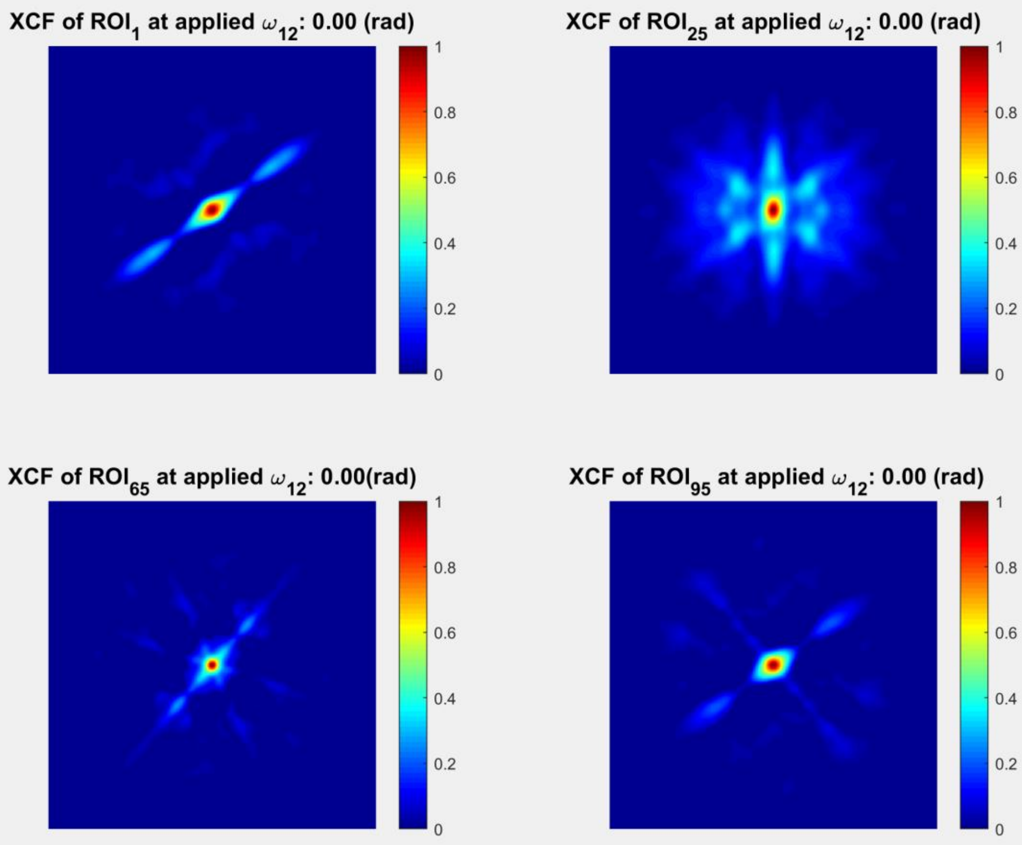
NanoEngineering
Materials Research Center

Cross-Correlation (No remapping)



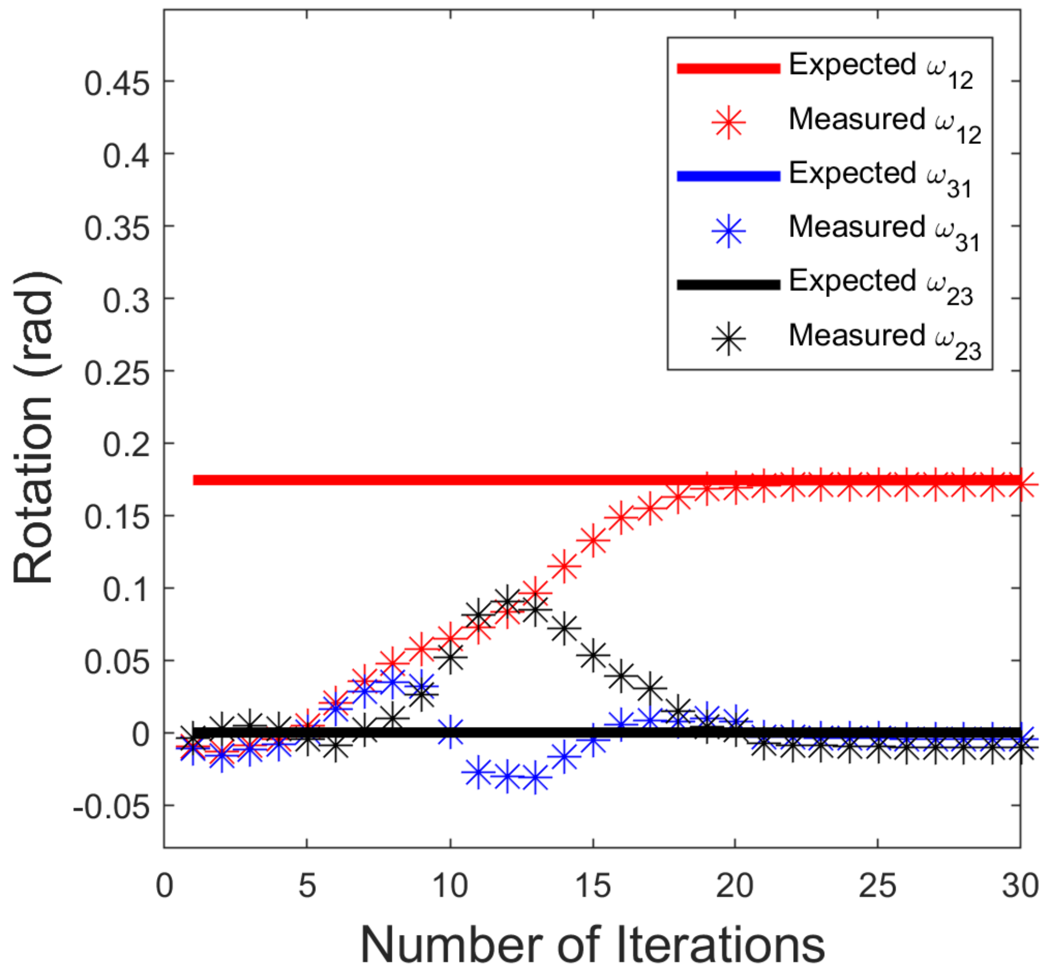
$$F_f = F_i \cdot R_f$$

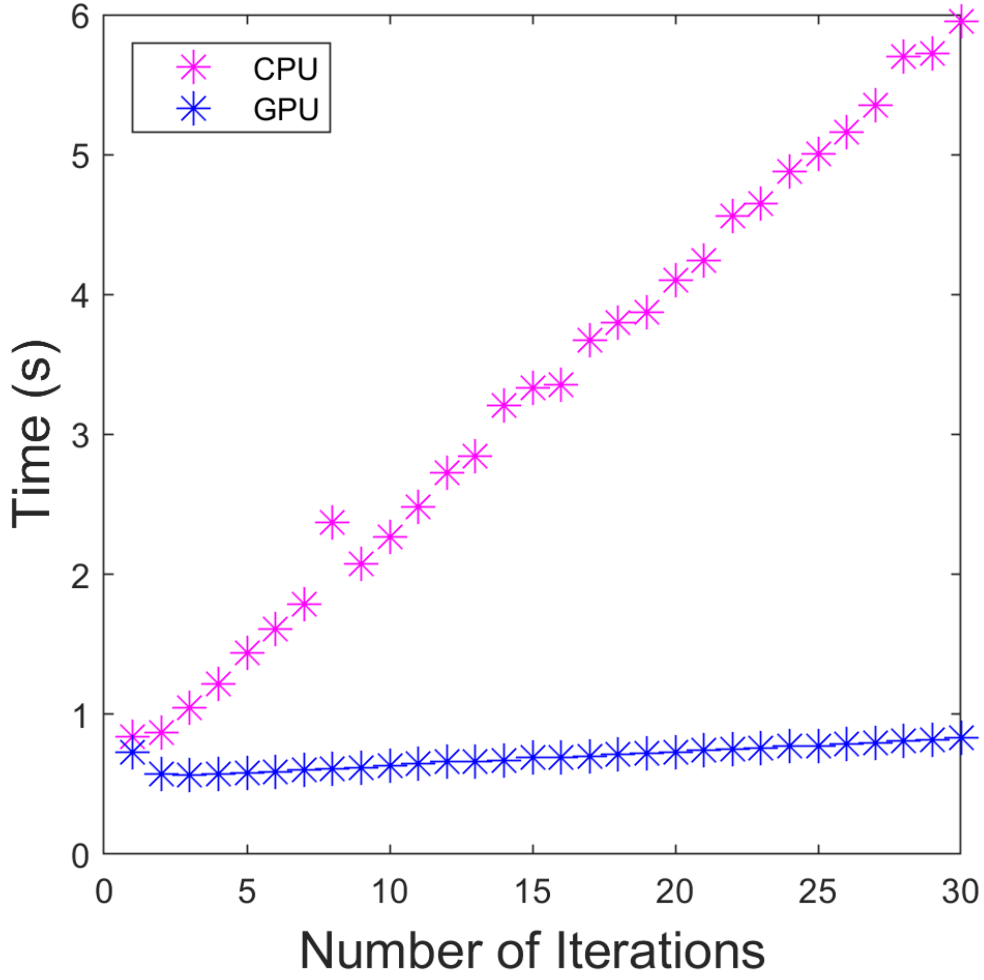
Cross-Correlation (After remapping)



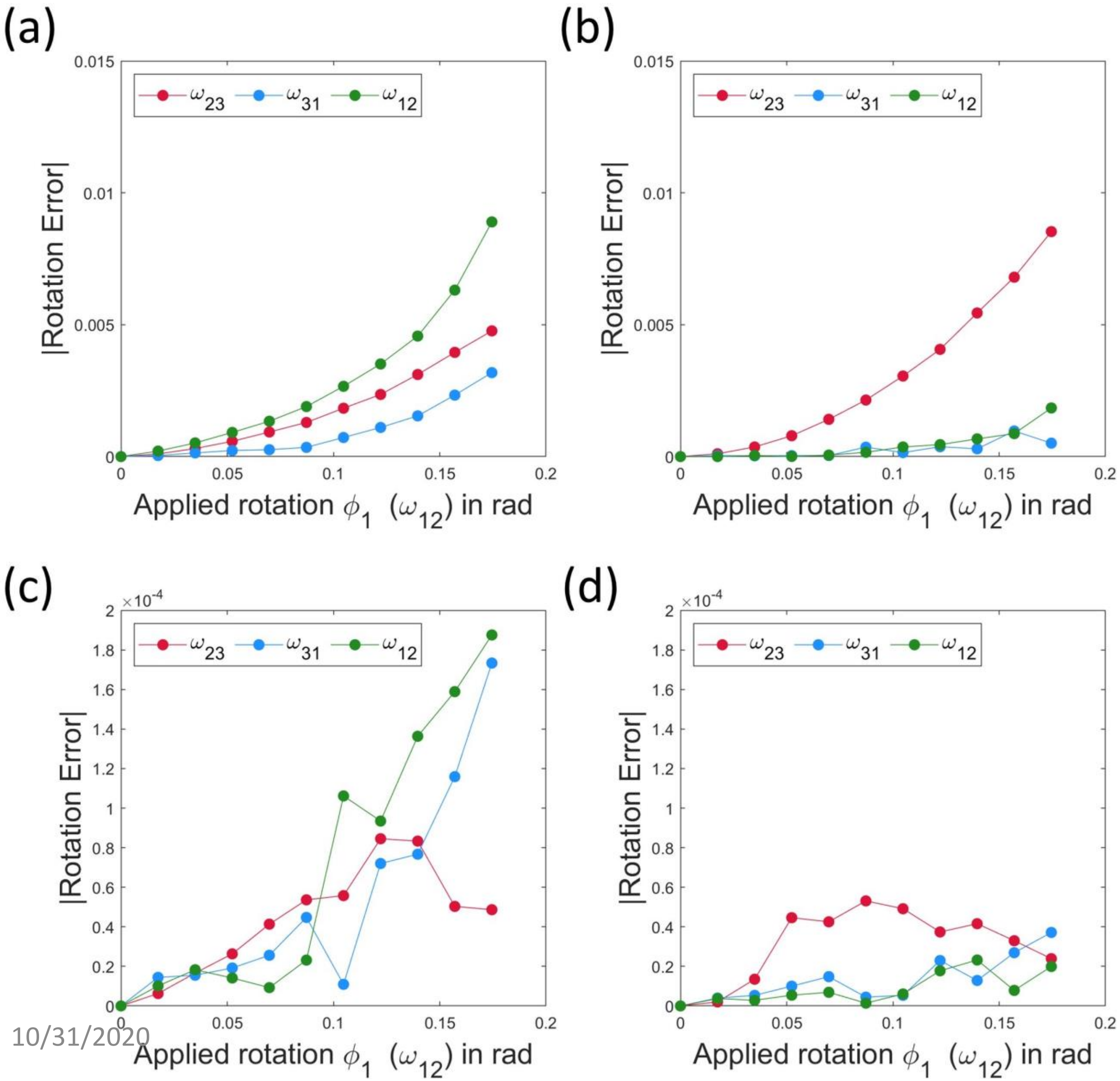
- No peak distortion for the cross-correlation after remapping
- Single high intensity peak only

GPU Acceleration for Image Registration

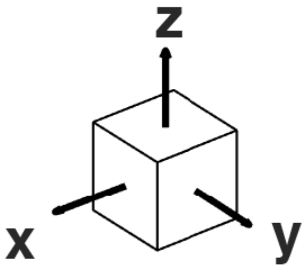




Angular Resolution of Different Methods



Reference pattern: [0,0,0,]
Test pattern: [i,0,0] i=0˚~10˚



(a) cross-correlation

(b) image registration

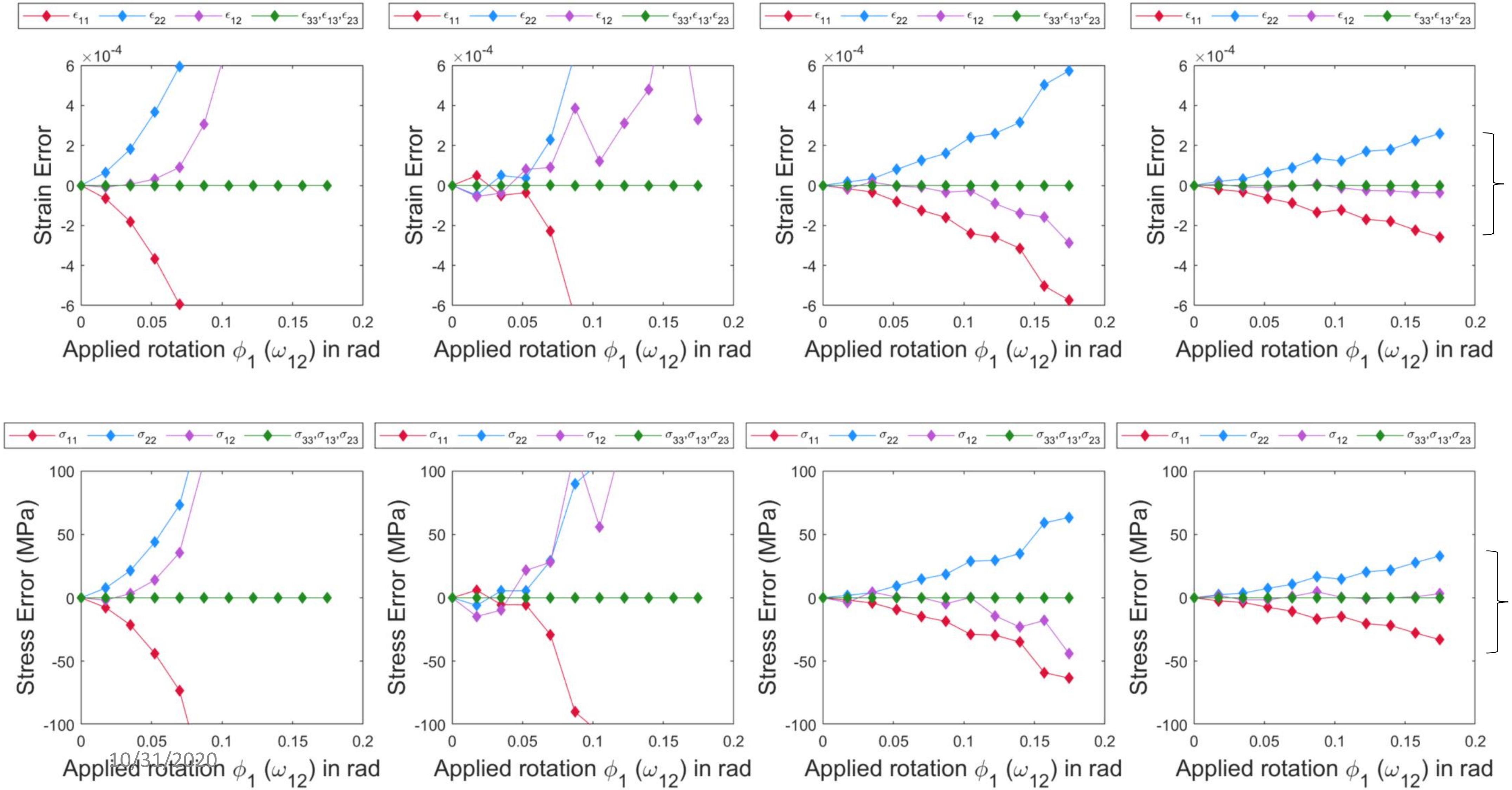
(c) 1[st] pass cross-correlation for remapping + 2[nd] pass cross-correlation for infinitesimal deformation

(d) 1[st] pass image registration for remapping + 2[nd] pass cross-correlation for infinitesimal deformation

- image registration (b) can not be used alone for accuracy.
- Method (d) outperforms (a) and (b).
- (d) slightly improves angular resolution compared to (c).

Phantom strain and stress

Cross-Correlation | Image Registration | Cross-Correlation Remap | Image Registration Remap

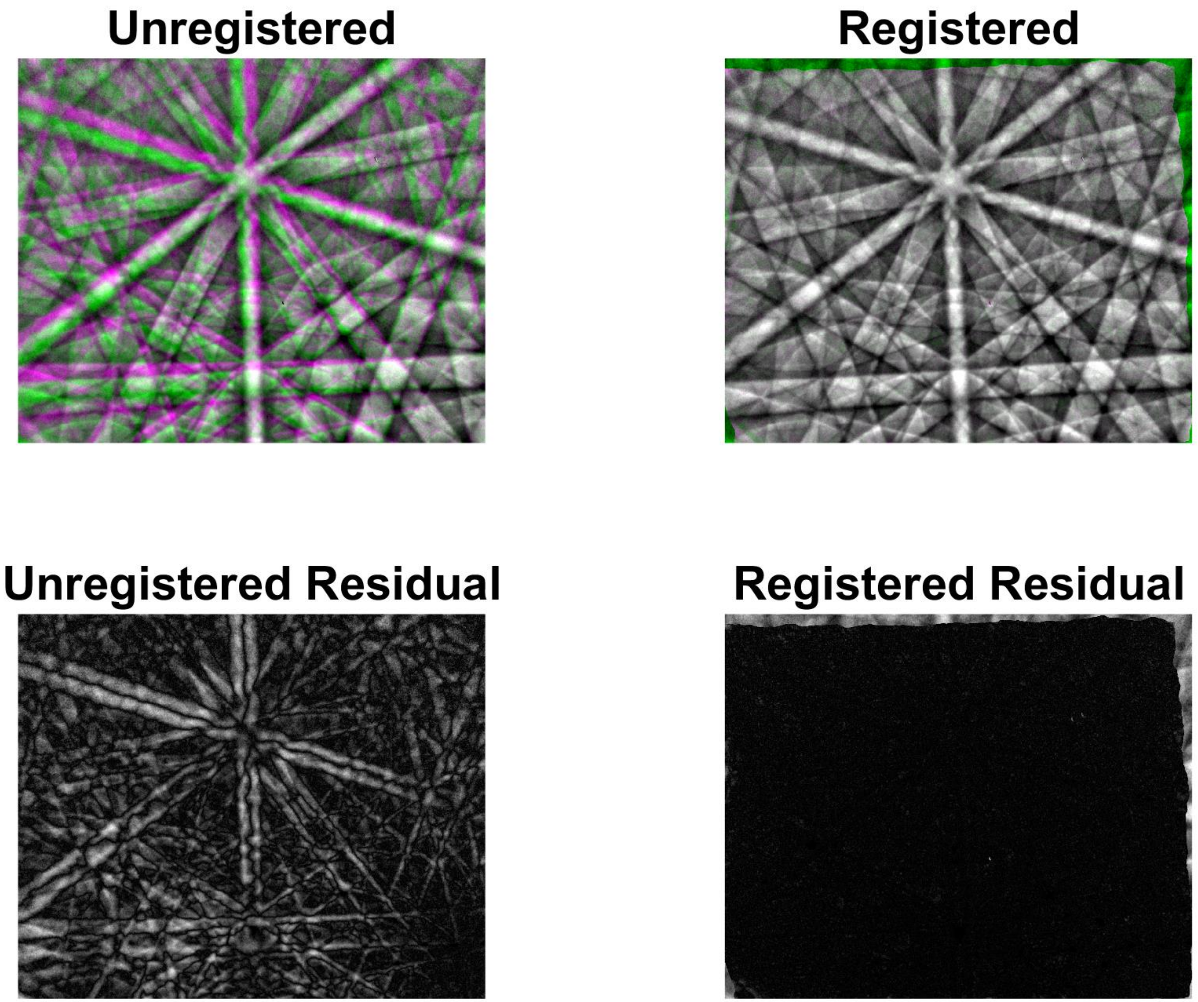


Phantom strain $<2\times10^{-4}$

Phantom stress <30 MPa

Zhu et al, 2020

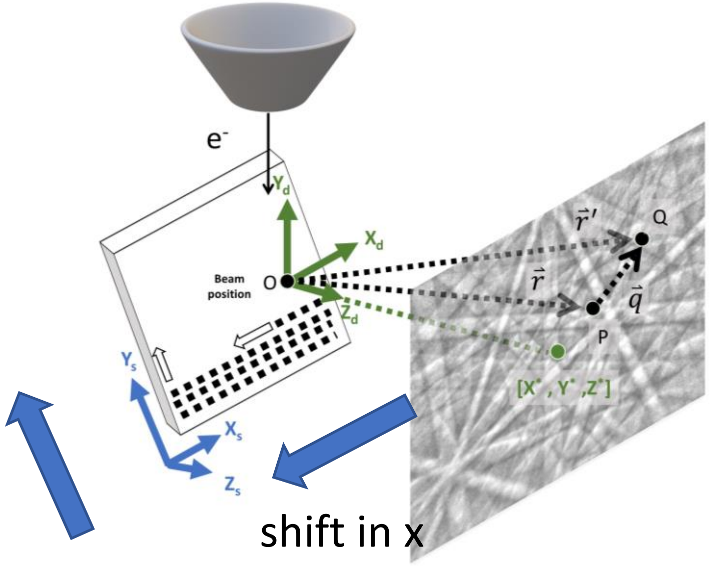
Registration with Experimental Pattern



Zhu et al, 2020

Zoom and Shift Correction

Zoom & shift in y



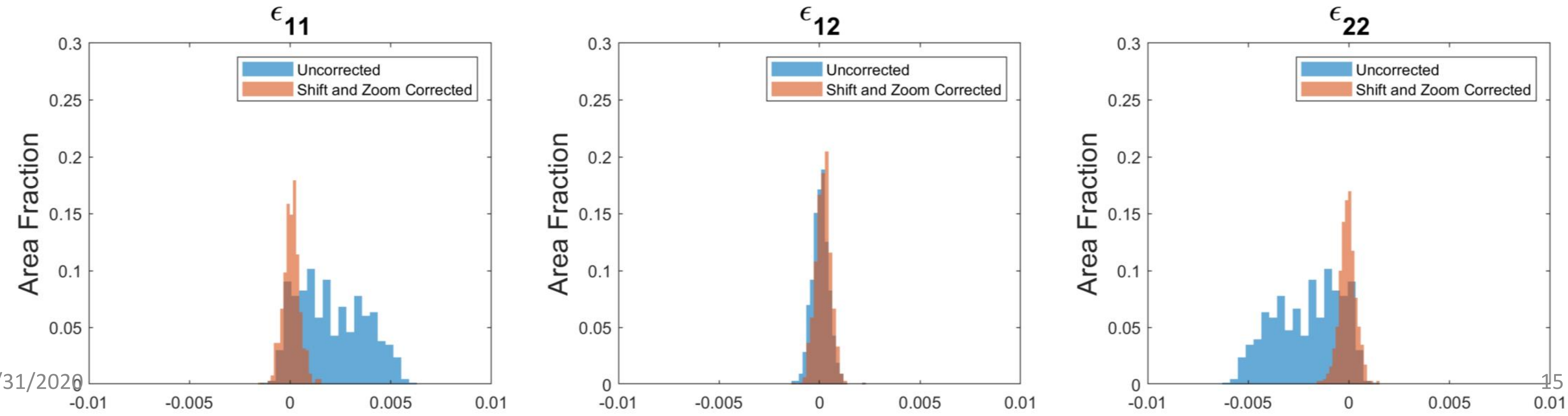
shift in x

Zoom or Shrinkage Correction: ratio between detector distance (DD) between the reference and test patterns.

Shift Correction: difference in beam position on the sample.

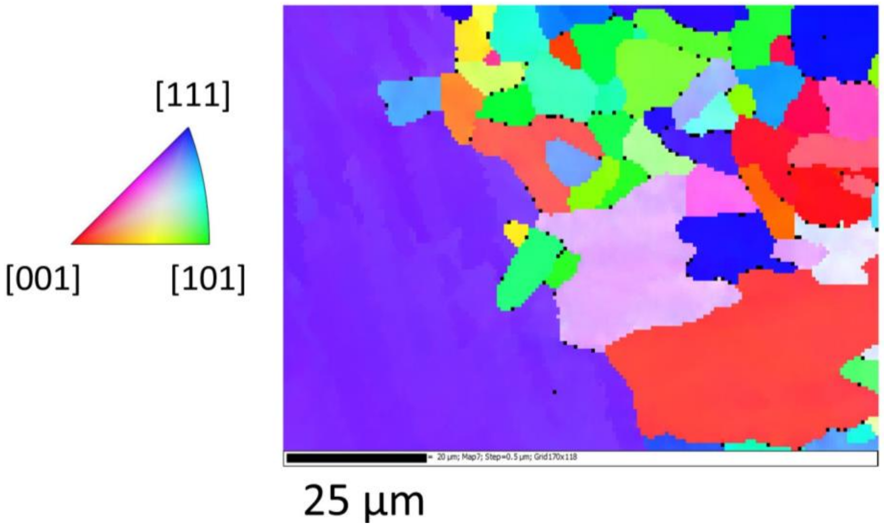
Britton *et al*, Ultramicroscopy 2011

Test Sample: Single crystal Silicon (200 μm by 200 μm)

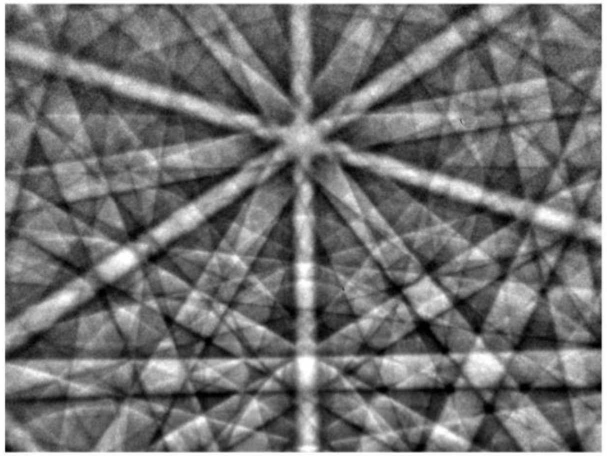


Additively Manufactured Inconel 625

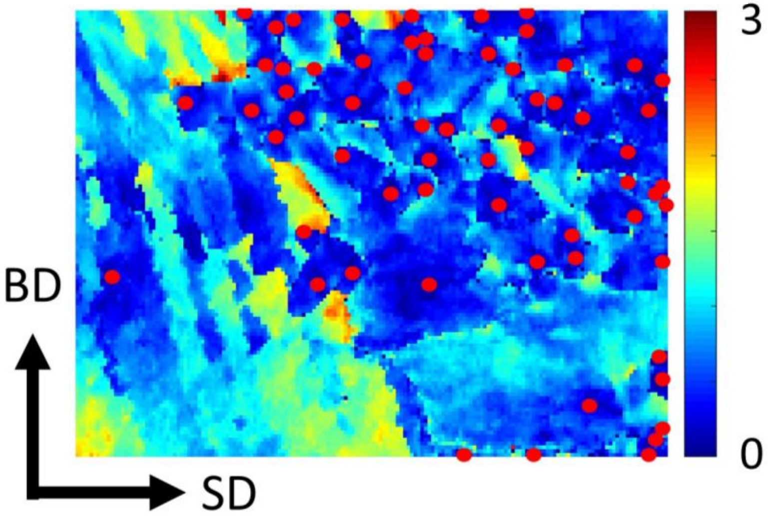
IPFY



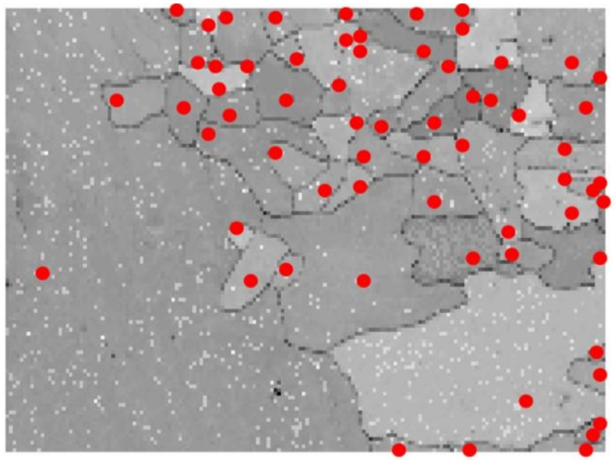
EBSP



Reference Misorientation



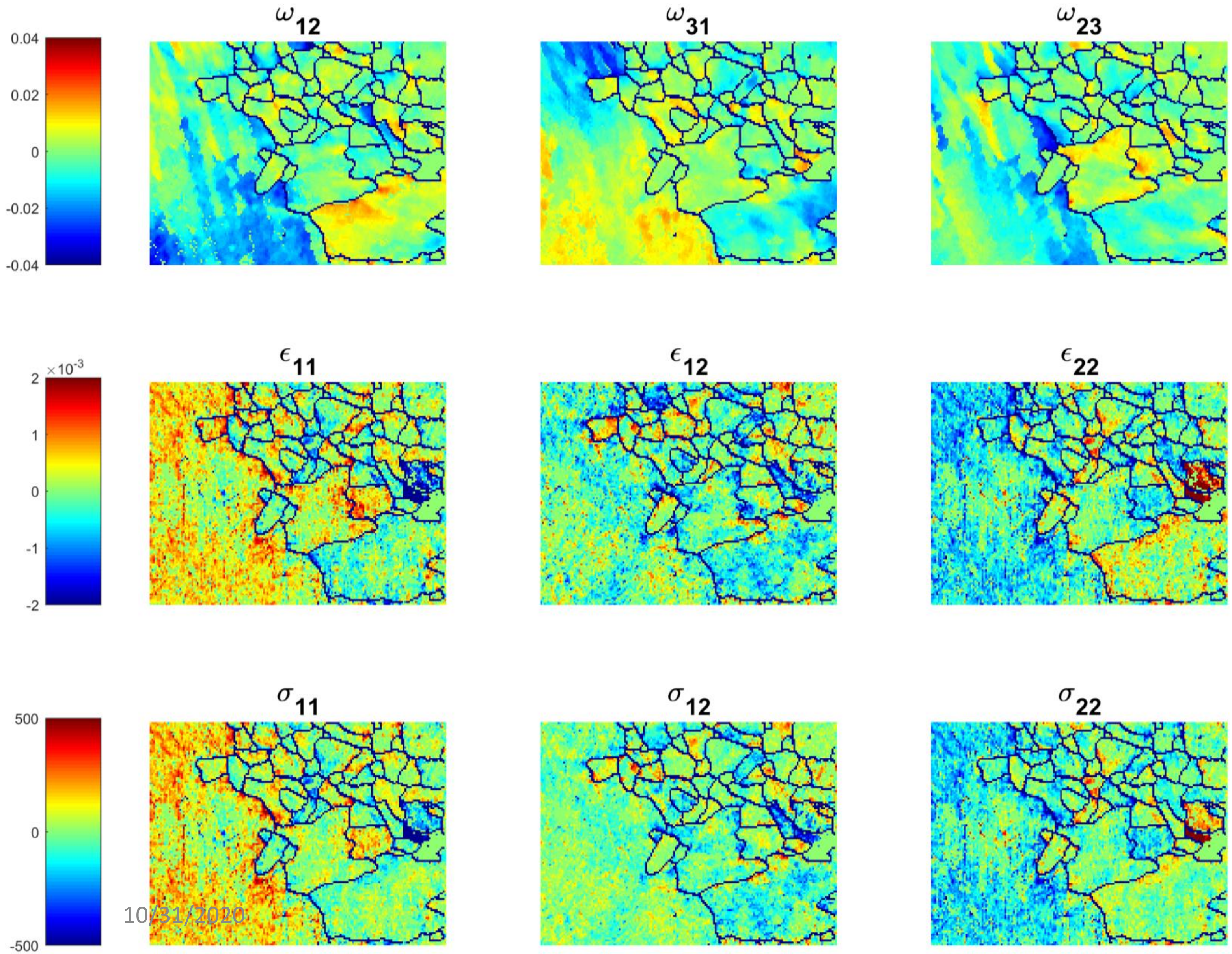
Band Contrast



Reference points obtained based on:

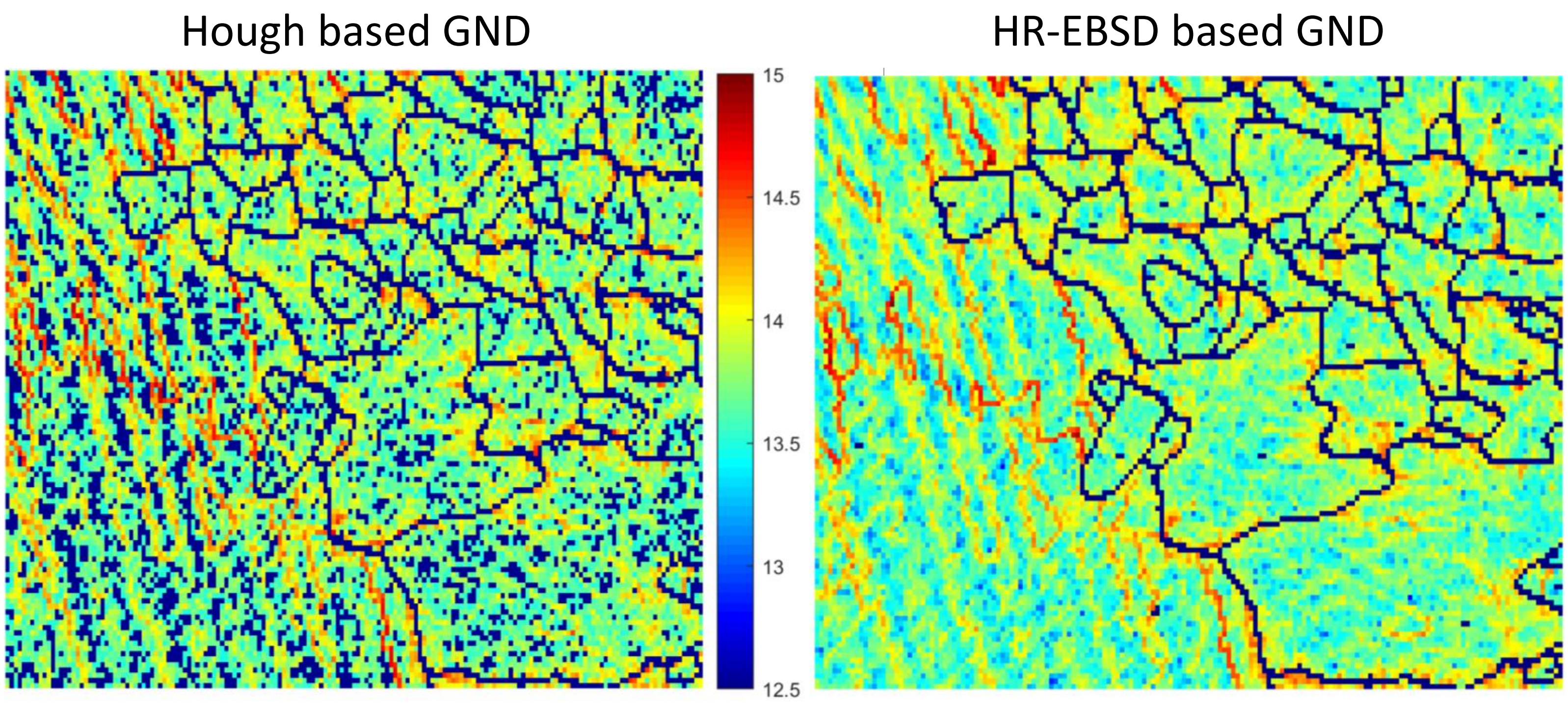
$$\frac{\text{band contrast}}{\text{mean angular deviation}}$$

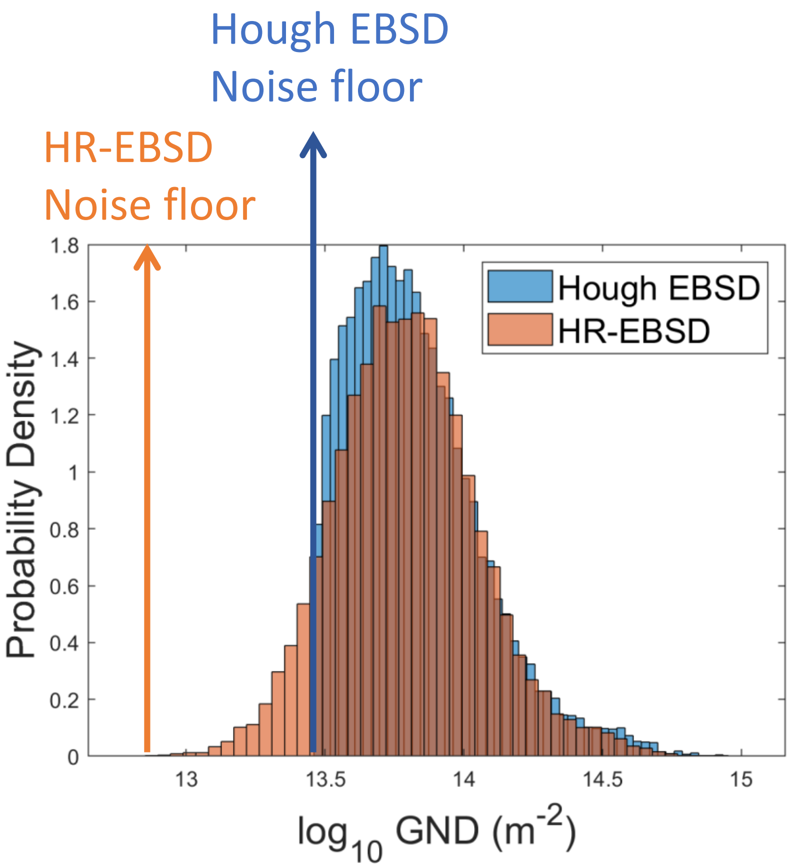
Lattice Rotation, Strain, Stress



- Columnar growth in the large grain (sub-grain structure)
- Large compressive or tensile residual stresses in the columnar grain.
- Stress concentration near triple junctions and high angle grain boundaries (strain compatibility).

Hough vs HR-EBSD based GND Density





- High density dislocation structures are very similar between the two
- Low density dislocation structures are more clearly revealed in HR-EBSD based GND map

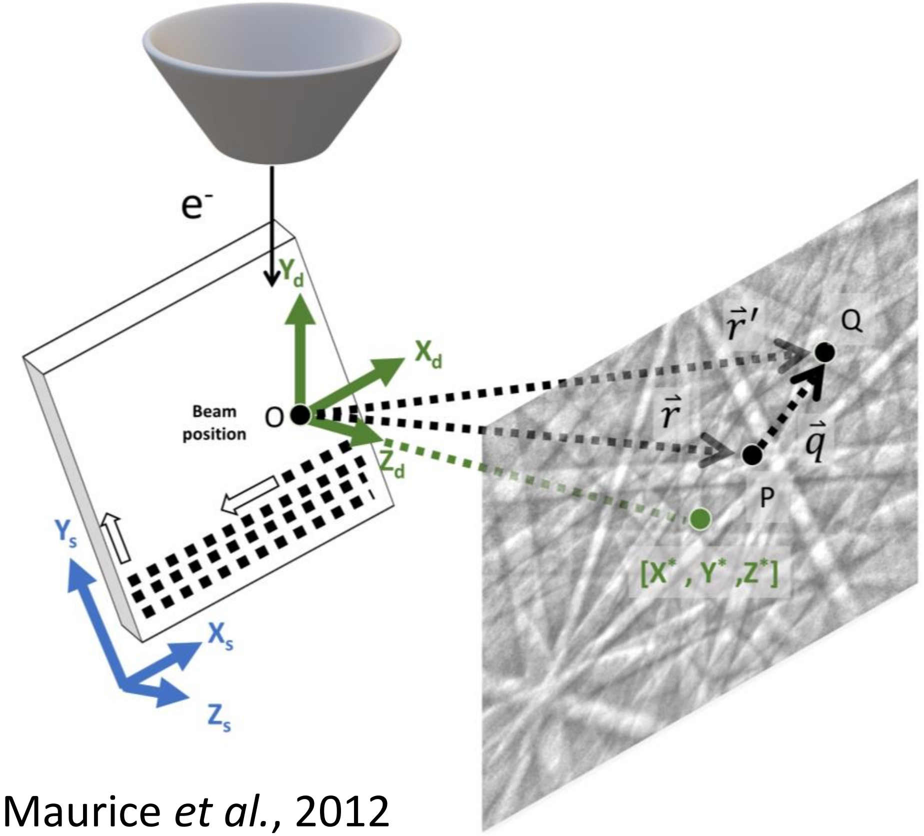
Summary

- Multiresolution image registration is a fast and accurate remapping for HR-EBSD.
- Phantom strain < 2×10^{-4} and phantom stress <30 MPa.
- Lower GND noise floor ($\Delta\rho \approx 2 \times 10^{12}$ lines/m^2)
- Additively manufactured Inconel 625 shows significant residual stress build-up in the columnar grain region/ stress concentration near grain boundaries and triple junctions (strain compatibility).

Zhu, C., Kaufmann, K. and Vecchio, K., 2020. Novel Remapping Approach for HR-EBSD based on Demons Registration, Ultramicroscopy

zchaoyi@andrew.cmu.edu

HR-EBSD (Essentials)



Maurice *et al.*, 2012

Deformation gradient tensor F between two images can be calculated from shifts measured between many regions of interest (ROIs).

Non-linear minimization method to obtain deformation gradient tensor:

$$min f(F) = \sum_{\{ROI\}} \frac{1}{2} \left| \frac{Z^*}{(F \cdot \vec{r}) \cdot \vec{k}} F \cdot \vec{r} - (\vec{r} + \vec{q}) \right|^2 \quad \text{(Levenberg–Marquardt)}$$

$$*F_{\text{sample}} = R_{\theta_{tilt}} \, F \, R_{\theta_{tilt}}{}^T \quad \text{(Coordinate Transformation)}$$

$$F_{sample} = PDQ^T \quad \text{(SVD)}$$

$$R_{sample} = PQ^T \quad \text{(Rotation Matrix)}$$

ω can then be obtained through parametrizing R_{sample} using Rodrigues vector i.e. axis-angle pair (m_k, θ)

$$\omega_{ij} = -\varepsilon_{ijk} m_k \theta = -\varepsilon_{ijk} \theta_k \quad \text{(Lattice Rotation Tensor)}$$

$$\varepsilon_{sample} \approx \frac{1}{2}\left(F_{sample} + F_{sample}{}^T\right) - I \quad \text{(Residual Strain Tensor)}$$

$$\sigma_{sample} = C : \varepsilon_{sample} \; (t = \sigma_{sample} Z_s = [0,0,0]) \quad \text{(Residual Stress Tensor)}$$

*Coordinate transformation is required to bring it from detector frame (X_d,Y_d,Z_d) to sample frame (X_s,Y_s,Z_s)

High Resolution-EBSD: Motivation

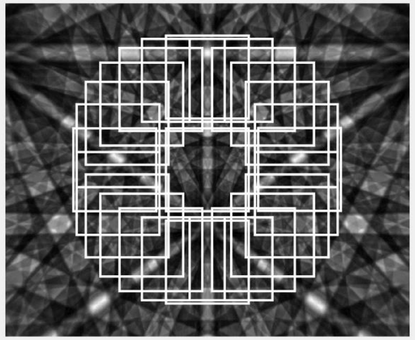
Higher level of sensitivity:

- Rotation: whole diffraction pattern moving ($1x10^{-4}$ rad)
- Elastic stretch: change interplanar angles and lattice spacing ($1x10^{-4}$)
- GND lower limit:
  - $\Delta\theta = 0.5^\circ$ (Hough based) → $\Delta\rho \approx 2 \times 10^{14}$ lines/m^2
  - $\Delta\theta = 10^{-4}$ rads (XCF based) → $\Delta\rho \approx 2 \times 10^{12}$ lines/m^2

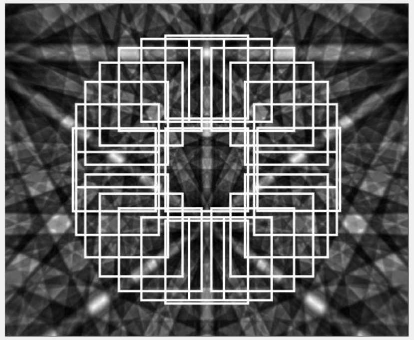
Obtaining the total shift vectors

$$F_f = F_i \cdot R_f$$

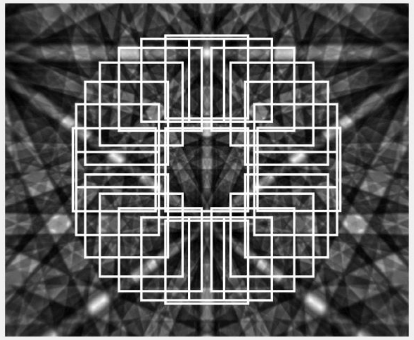
Reference Pattern

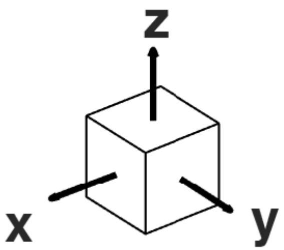


Remapped Reference Pattern



Test Pattern

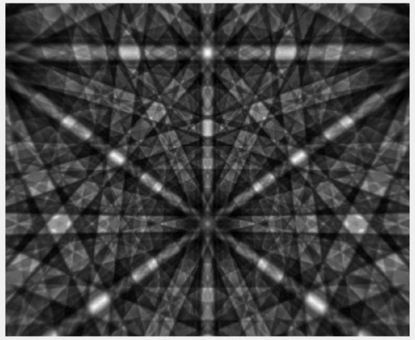




$$\min f(F) = \sum_{\{ROI\}} \frac{1}{2} \left| \frac{Z^*}{(F \cdot \vec{r}) \cdot \vec{k}} F \cdot \vec{r} - (\vec{r} + \vec{q}) \right|^2$$

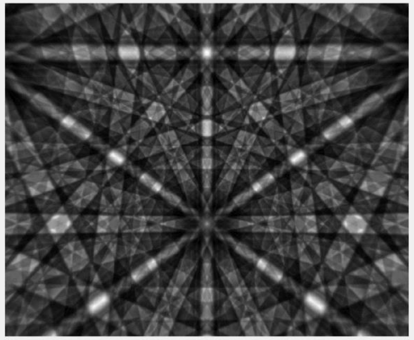
q_f

Finite Shift



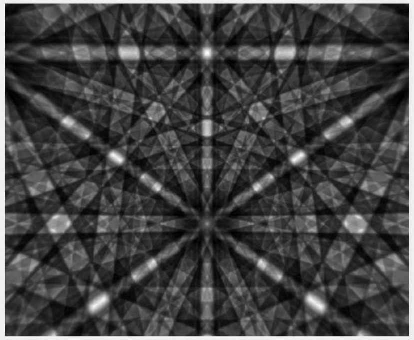
q_i

Infinitesimal Shift

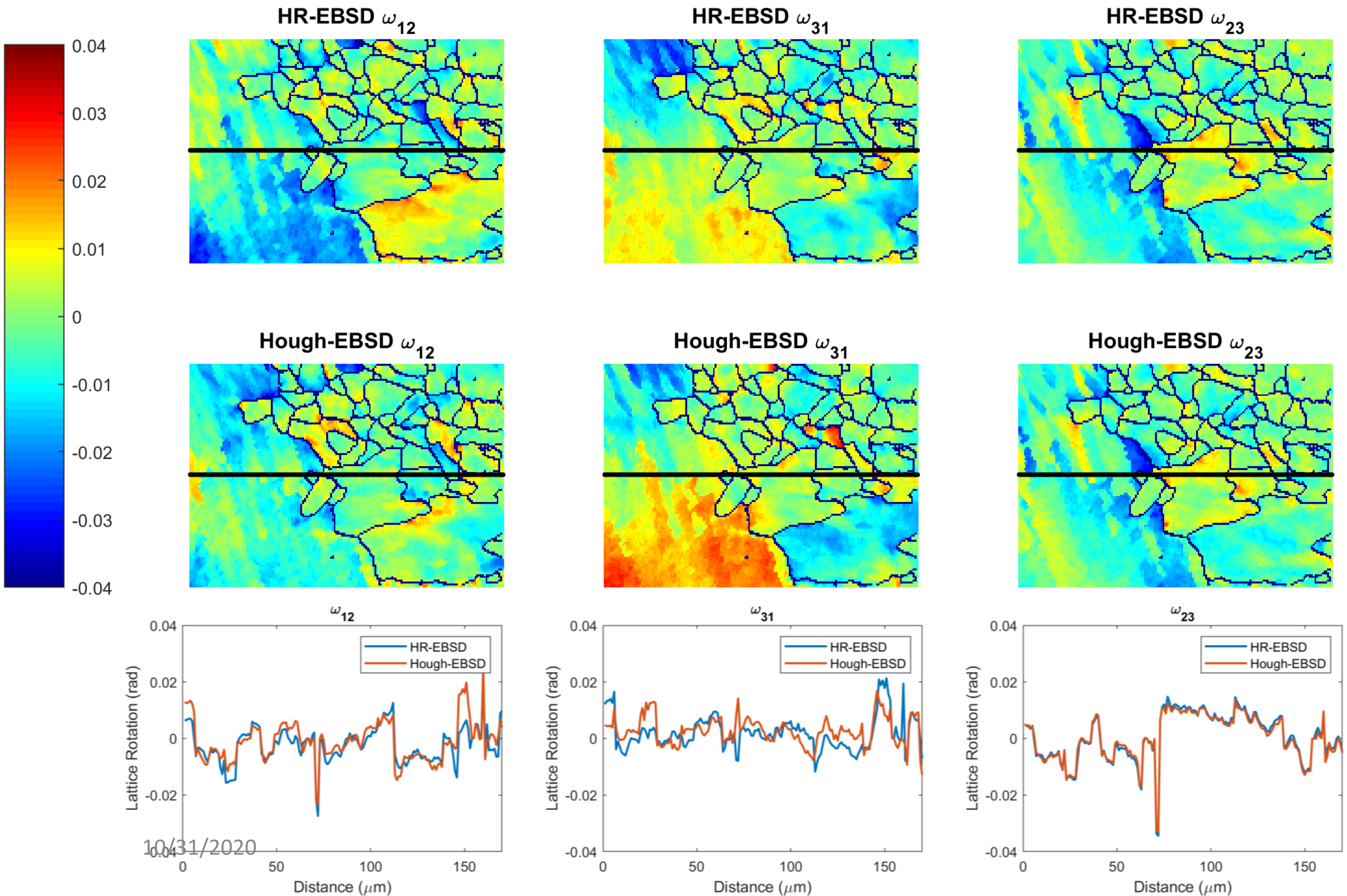


$q = q_f + q_i$

Total Shift



Hough vs HR-EBSD based Lattice Rotation



Hough-EBSD lattice rotation tensor

$$\omega_{23} \approx \frac{1}{2}(g_{23} - g_{32})$$

$$\omega_{31} \approx \frac{1}{2}(g_{31} - g_{13})$$

$$\omega_{12} \approx \frac{1}{2}(g_{12} - g_{21})$$

- Nominally similar values and trend, especially ω_{23}
- Hough based lattice rotation tensor can be used as a quick check

Hough Indexing