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#MTEX2017

In-situ Mechanical Testing in the SEM

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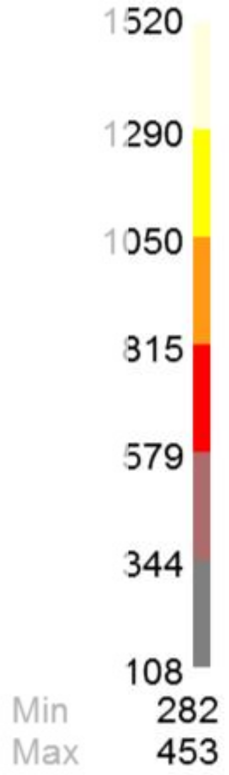
Content

A. <u>GUIs MTEX Experiment</u>
- dBSD / DICE GUI
- The experiment

B. <u>DIC</u>
- What is DIC
- Combining DIC with EBSD

C. <u>Change in orientation of grains</u>
- Crystal Plasticity models
- Orientation change in grains

D. <u>Martensite</u>
- Identifying variants
- Strain-induced martensite



Cons

- No user interface (but JQdaFonseca *'I dislike GUIs'*)
- Have to learn MTEX/Matlab and write out everything you want
  - **Can be difficult to get started**
- Can be slow
- *'object orientated approach is a pain to understand algorithm'* Ben Britton
- Need a Matlab license- can be a pain if your license needs internet

Other similar applications options

- Channel 5 (and other EBSD software houses) have their own EBSD analysis software
  - **Quick, user interface**
- Some similar open source packages, e.g. ATOM http://www.atom-software.eu/
- And some open source packages or code in other formats (??)

Pros

- For texture one of the best (*'MTEX is pretty good for texture'* B.B. again)
- Get the most from your EBSD data:
- & do things not possible in other commercial packages
  - **Or without the hassle and errors if you did it from 1st principles yourself**
- Good user community / support & help files
- Always improving code

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MTEX new user recommendations

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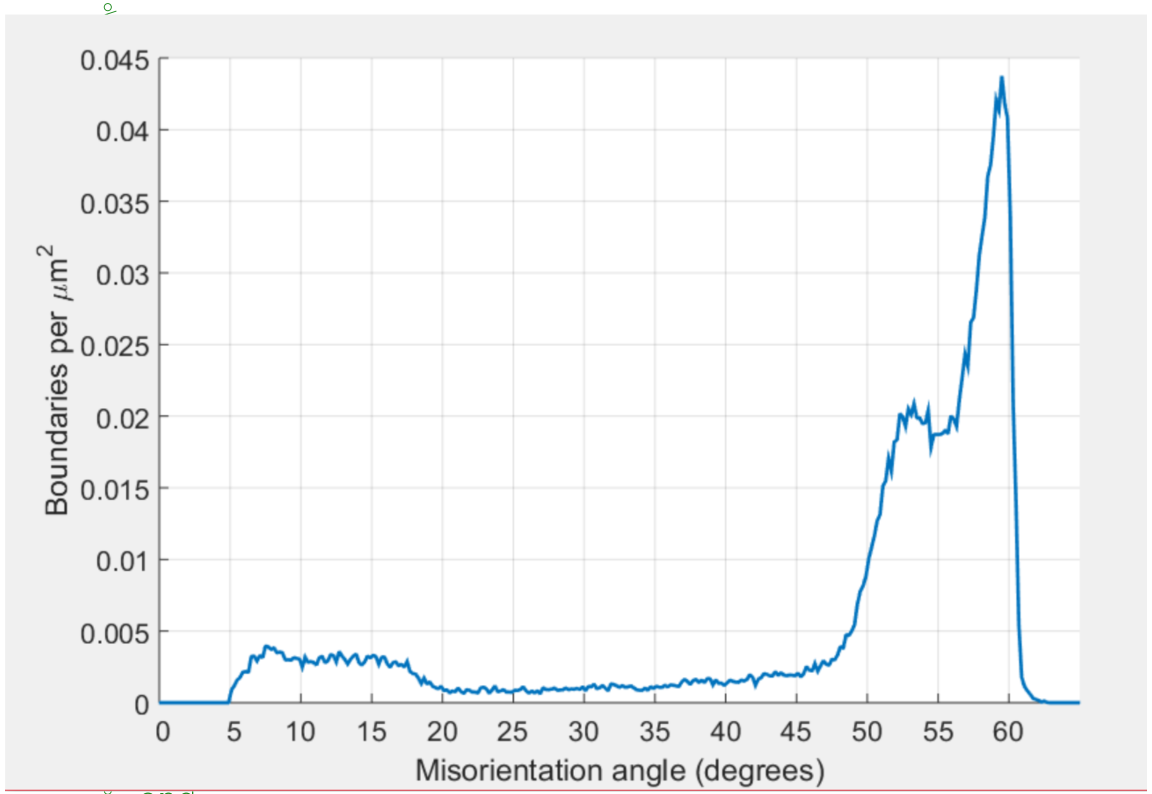
1. Use the help files in Matlab
   - **I often search 'MTEX + function'**
2. Not an obvious answer there, go to the google user group https://groups.google.com/forum/?fromgroups=#!forum/mtexmail
   - **Try a few keywords related to your problem in 'Search' of old posts first**
   - **If nothing comes up….**
3. Post a question on the group
   - **Be as detailed as possible**
   - **It may make sense to you, but write it so it would make sense to an Undergrad/ MSc / PhD in a related Science field**
4. If you get no response, but think the question is valid
   - **Try contacting someone on user group who has answered similar questions- maybe they've not checked the group for a while-> *they may ignore you but nothing to lose***
5. Be inquisitive, (when necessary or if you're bored) have a look at the code for a particular function or even put in code breaks and follow variables to see what it does
   - **E.g. >>> edit calcGrains (*gives Matlab code for this)***
6. Be prepared to be frustrated by the simplest of problems.
   - **It takes time, but the learning curve is worth it from the functionality you get**
7. When you get your MTEX skills share your knowledge with your group and the community

A

Modify MTEX code to do what you want


```
function OUT = plotAngleDistribution_adj(obj,varargin)
% plot axis distribution
%
% Syntax
%   plotAngleDistribution(mdf)
%   plotAngleDistribution(CS1,CS2)
%   plotAngleDistribution(grains.boundary.misorientation)
%
```




```
% end
```

```
% seach for existing bar plots and adjust bar center
% h = findobj(mtexFig.gca,'type','bar','-
or','type','hgGroup');
% h = flipud(h(:));

unit = '%';

    % bin size given?
    if max(obj.angle) < maxOmega/2, maxOmega =
max(obj.angle);end
    nbins =
round(maxOmega/get_option(varargin,'resolution',5*degree));

    % compute bins
    bins = -eps:varargin{1}*pi/180:65*pi/180;
%linspace(-eps,maxOmega+0.01,nbins);
    nbins=length(bins);
    density = zeros(nbins-1,1);
    lg = {};

% compute angle distribution

  d = histcounts(obj.angle,bins).';
  midPoints = 0.5*(bins(1:end-1) + bins(2:end));
  density(:,end) =  d(1:end) ;

OUT=[midPoints'/degree,density];
```

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dBSD – *digital back-scattered diffraction*

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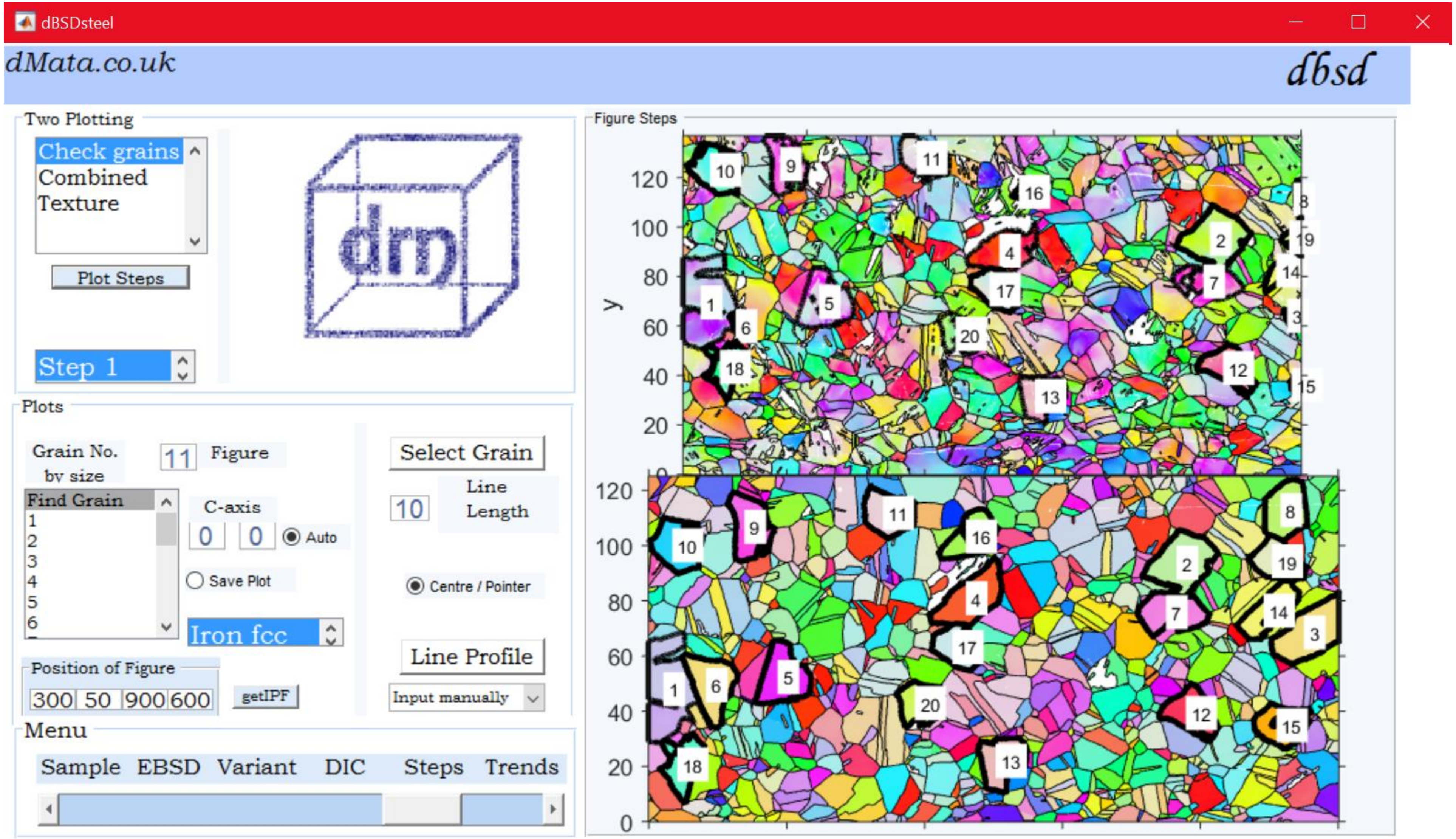

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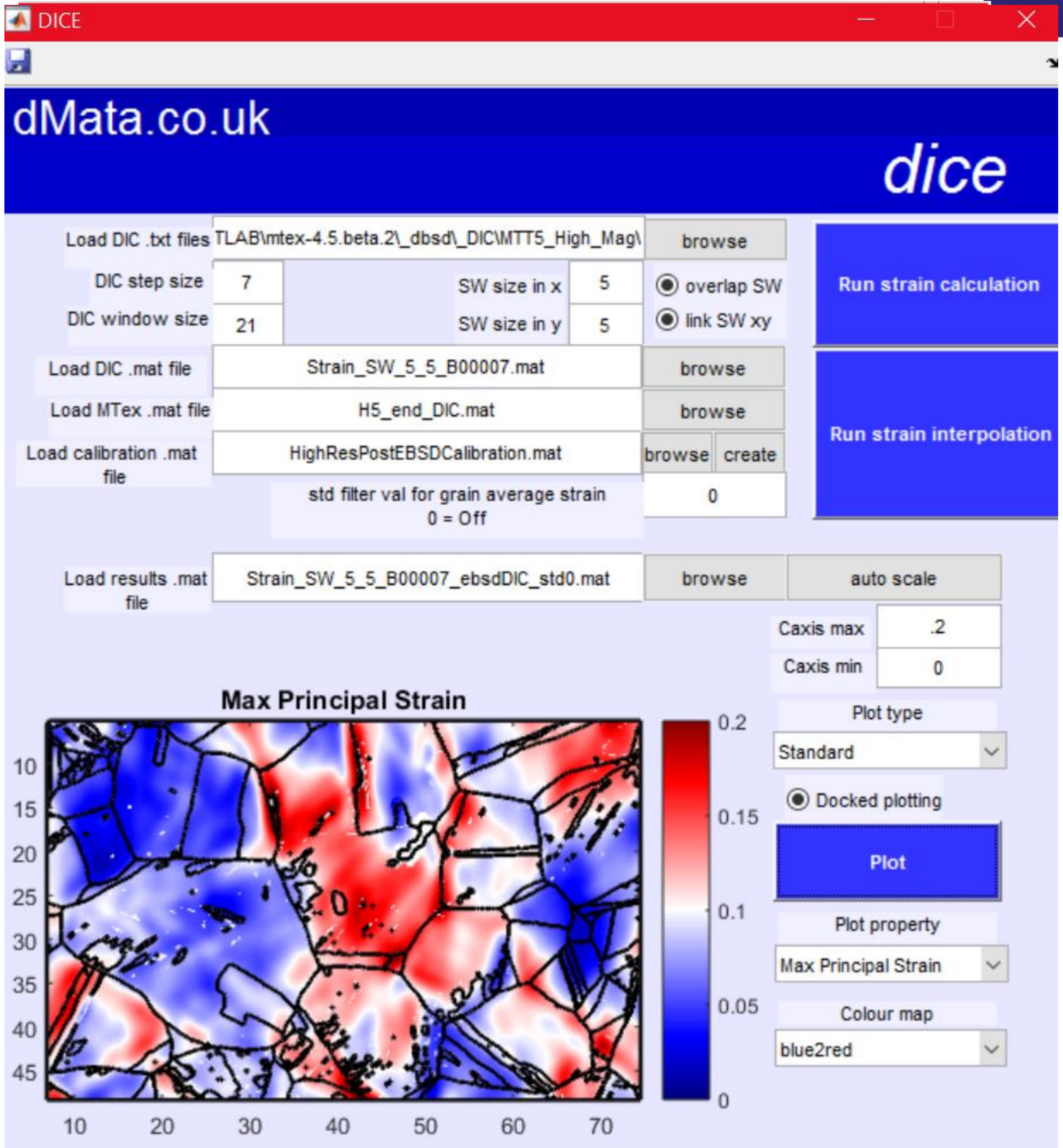
dice – *digital image correlation e*



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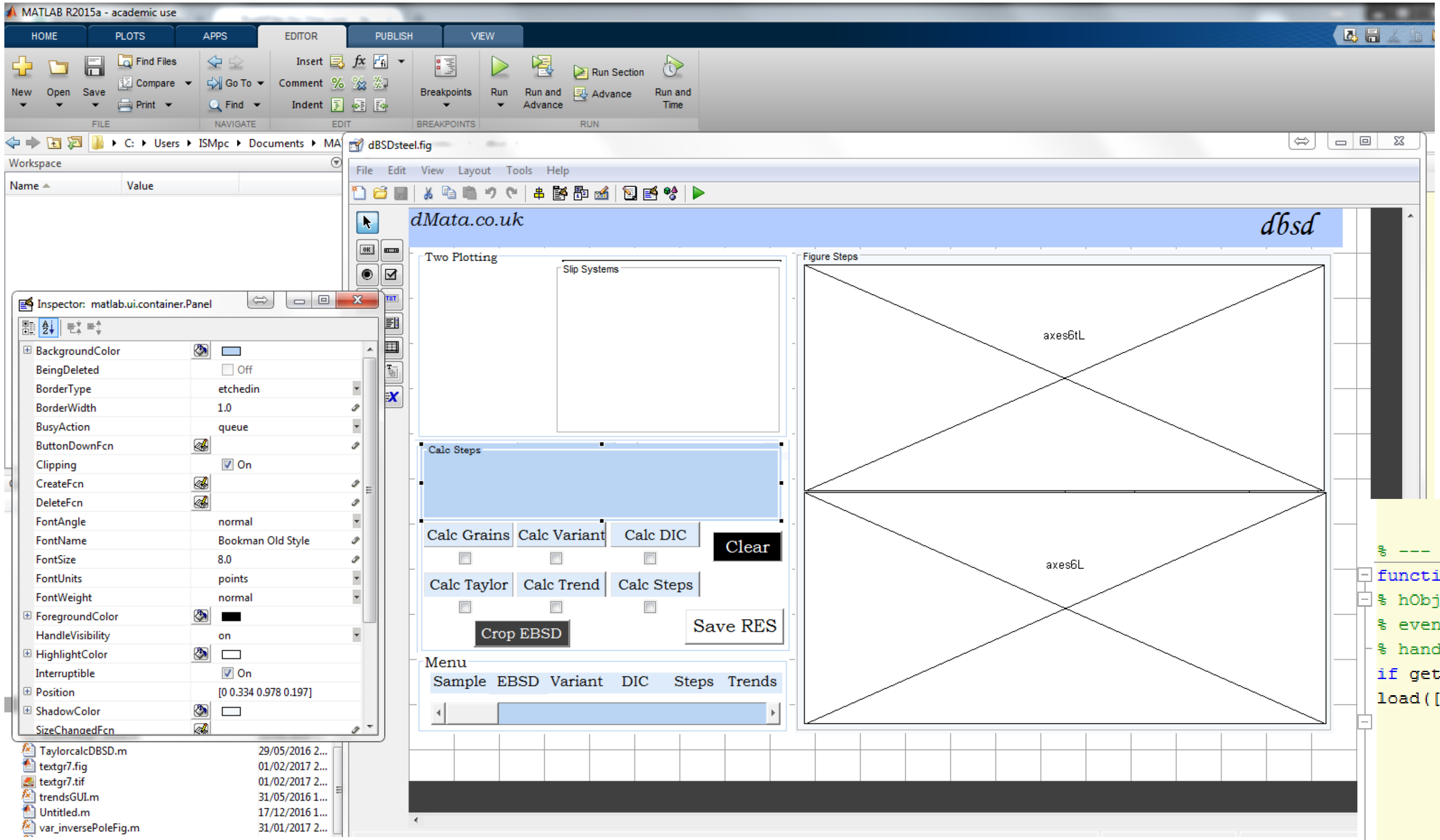
GUIs




```
% --- Executes on button press in mapgrains_b.
function mapgrains_b_Callback(hObject, eventdata, handles)
% hObject    handle to mapgrains_b (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)
if get(handles.exist_stepload_b,'value')==1
load([cd,'\variables\step_handle.mat'],'FN','PN')
        for n=1:length(PN)
            load([PN{n},FN{n}],'ebsd','grains','dbsd')
            CS=dbsd.CS;
            ebsd_{n}=ebsd;
            phasea=dbsd.phases{2};
            grains=grains(phasea);
            grains_{n}=grains;
            clear ebsd grains
        end

        save([cd,'\variables\ebsdstep'],'ebsd_','grains_','CS','phasea')
        mapgrains
        set(handles.existmapgr_b,'value',1)
else
    menu('create steps 1st','ok')
end
```

>>guide

A

GUIs: Graphical User Interfaces

GUIs can make working with data easier but can cause problems

- Cross-platform capabilities
  - Problems with different versions of Matlab (or PC type)
  - And even different screen resolutions
  - In theory within Matlab it is possible to create an executable of a GUI?
- Treatment of variables
  - MTEX uses some calculations that are slow, so good to store variables
  - Global variables
    - make life easy for simple GUIs
    - But cause problems with increased complexity, both memory issues and code confusion
  - getappdata
    - makes getting variables more explicit so less code confusion- but still memory issues
  - Saving larger variables as a file
    - Good solution for larger datasets (e.g. ebsd, grains, IPF color)
    - Issues with '/' vs '\'
    - I use local variables (saved in a folder 'variables') which can then be saved and loaded later-
      - but better options?
- Make GUIs that can be used without the GUI
  - Use the GUI to get input data and then call external functions

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GUIs: Graphical User Interfaces

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- Plot to a GUI can be problematic

```
handa=handles.axes6;
menuPlot(choi,handa,h);
```

- And within function menuPlot

```
plot(grains.boundary,'parent',hhan,'edgecolor','k','linewidth',1)
ylabel('Boundaries per \mum^2','parent',hhan);
```

- A change we had to make to plot.m

```
try axis(mP.ax,'tight'); end
% mP.micronBar.setOnTop <- had to get rid of this to enable plot
within GUI
```

- Or just plot externally

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The Experiment

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Transformation-Induced Plasticity (TRIP) Steel

- High energy absorption capacity & fatigue strength
- Due to a combination of the hard martensite phase (BCC) in the soft austenite matrix (FCC), analogous to a hard-particle-reinforced composite
- well suited for automotive structural and safety parts

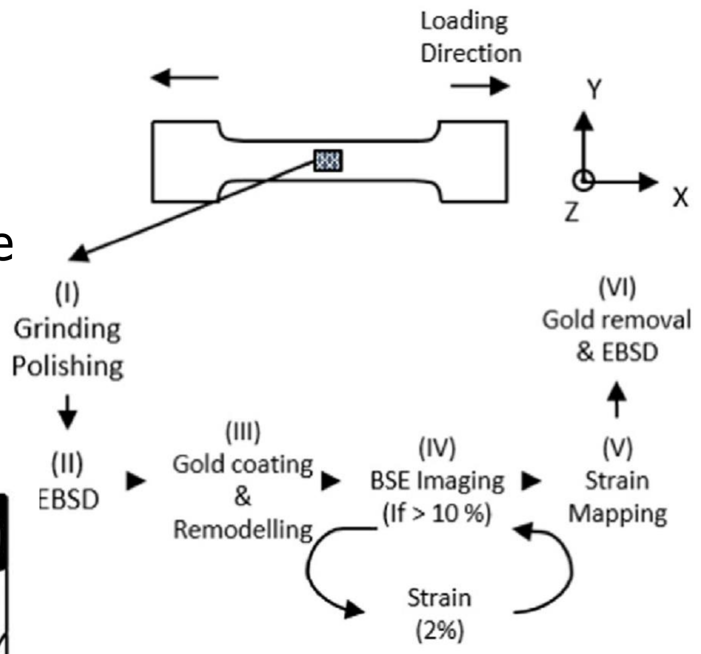
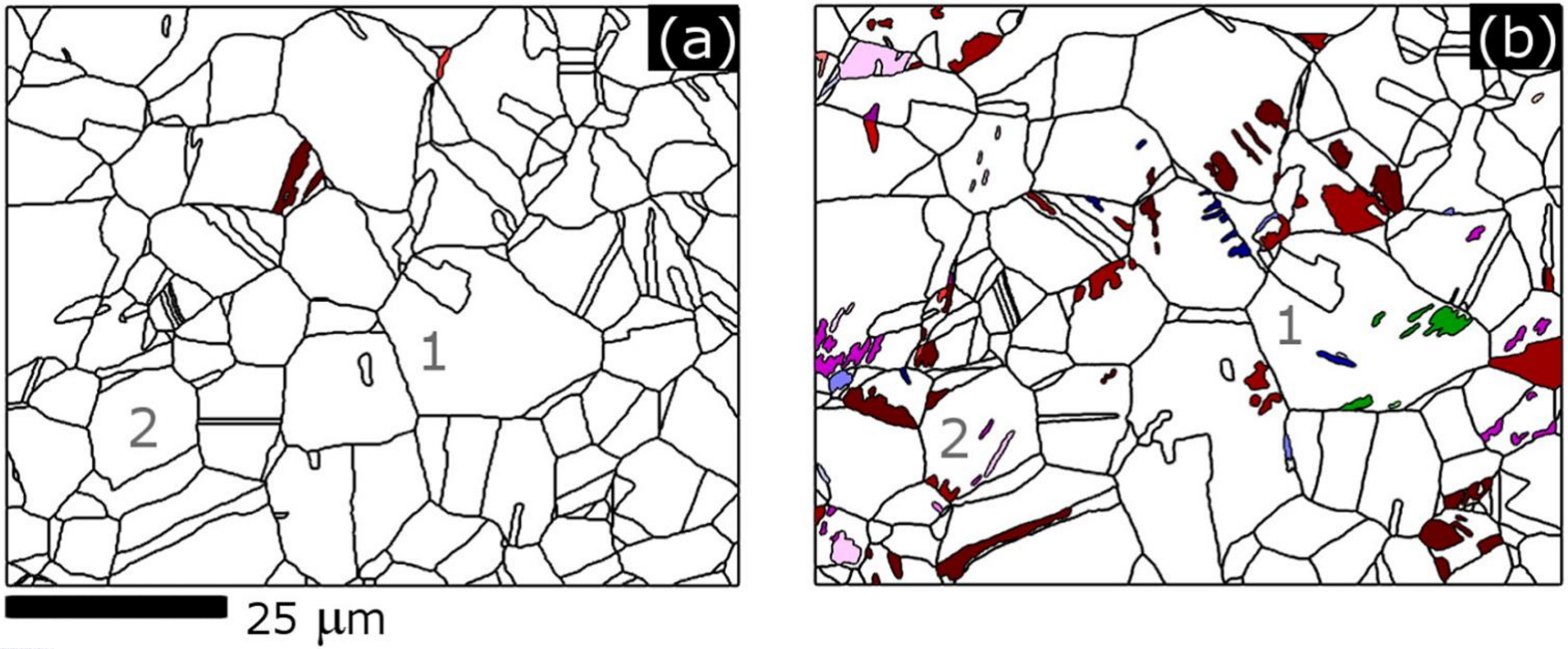


Fig. 2. Schematic of sample design and flowchart of experimental procedure.

Start **After Applied strain**



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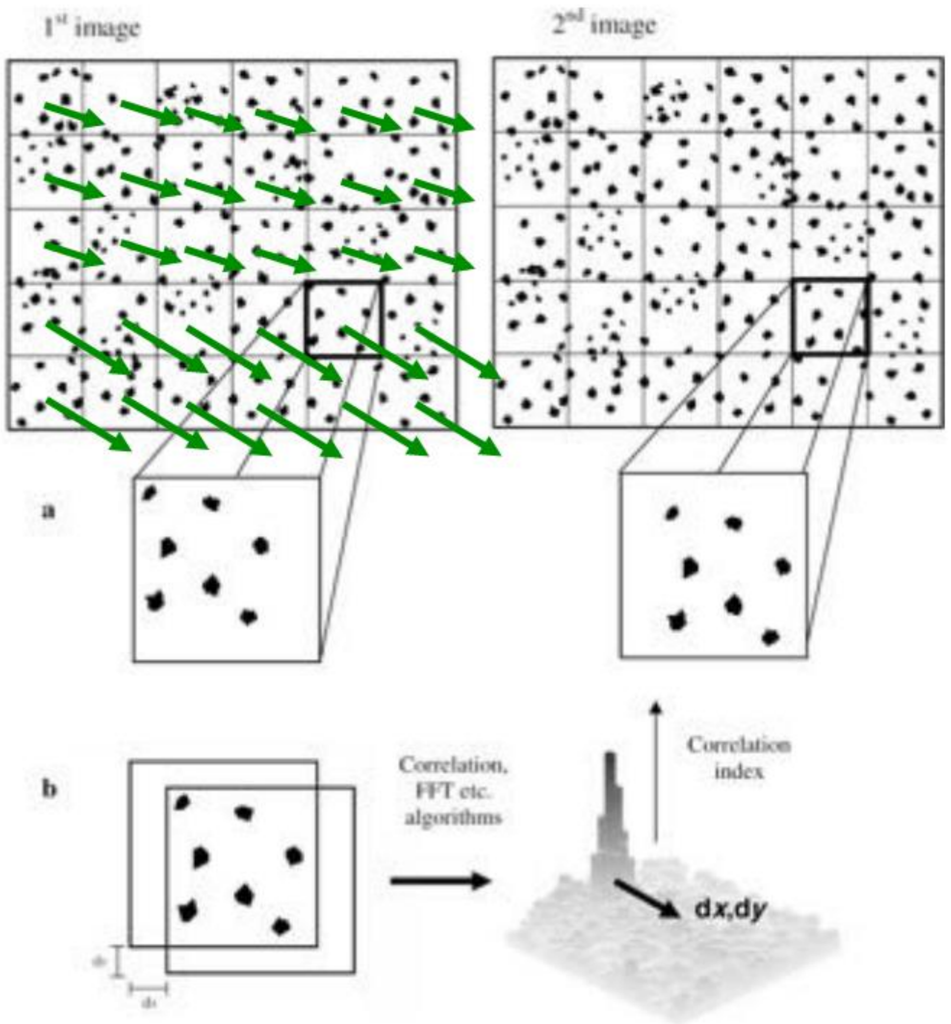
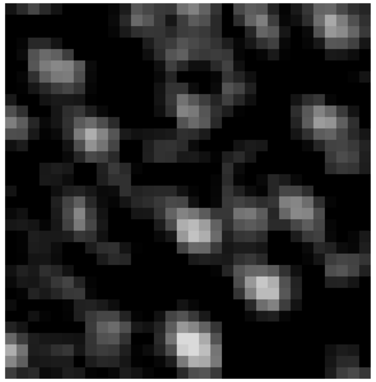
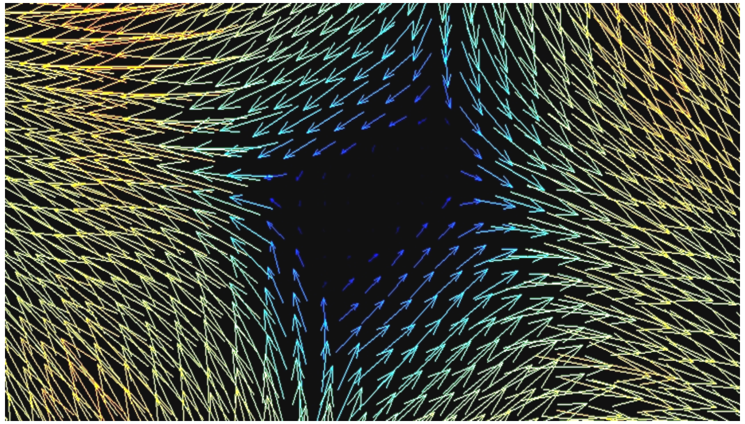
How DIC works





Features

Displacement Field

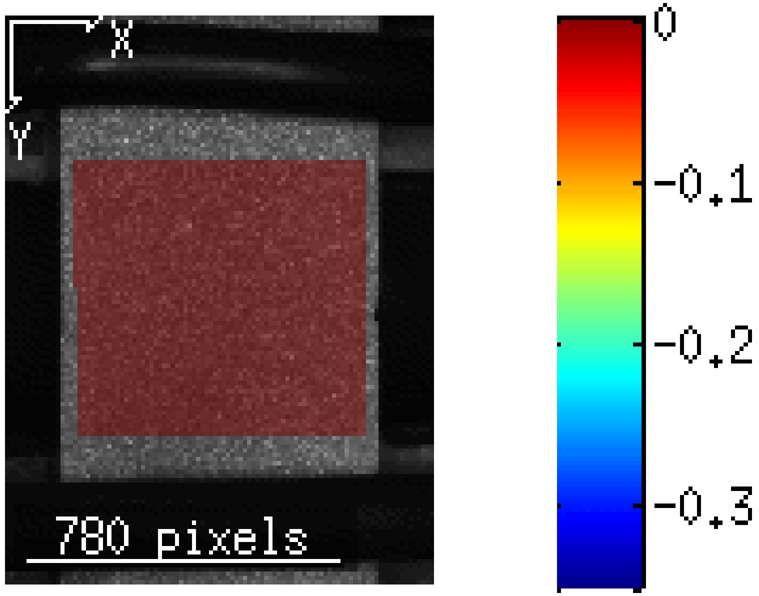


Get maps of strain tensor

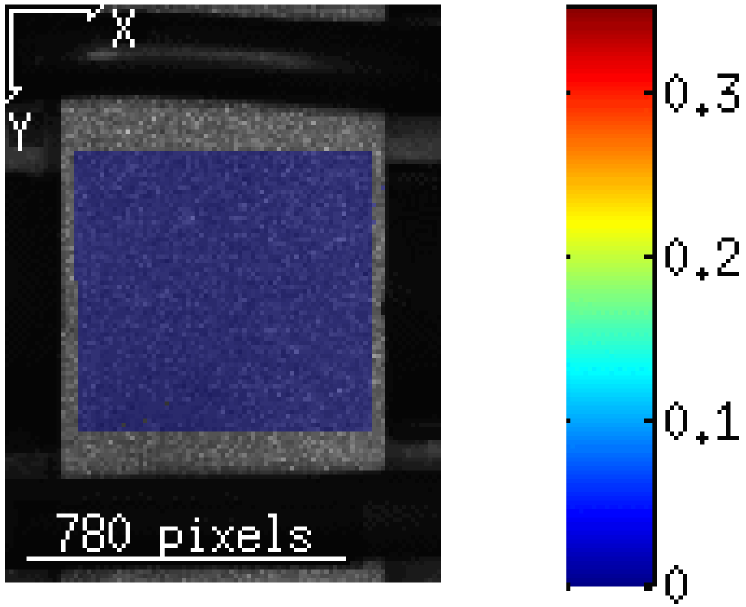
REF: J.Q. Da Fonseca, P.M. Mummery, P.J. Withers, J. Microsc. 218 (2005) 9–21

B

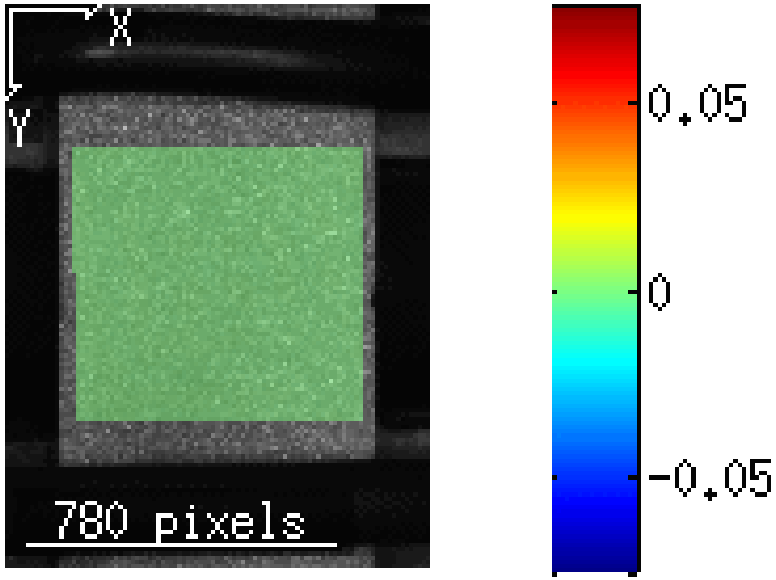
Example: Tensile test of a Weld



E_{xx}

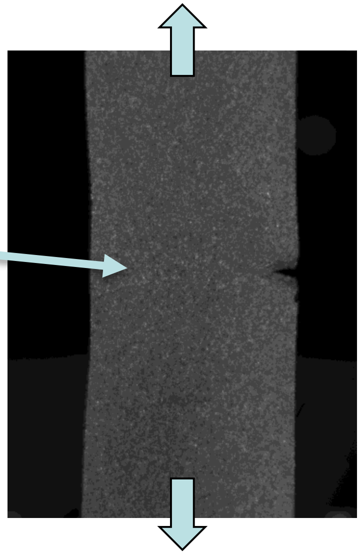


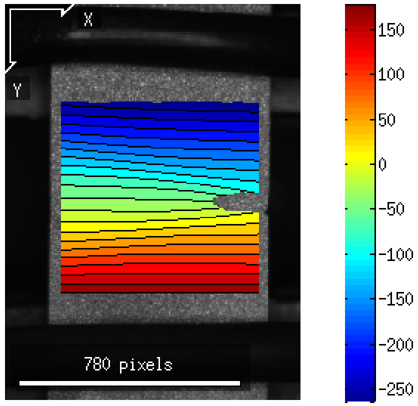
E_{yy}



E_{xy}

Weld in centre





REF: http://www.ncorr.com/index.php/sem-s-dic-challenge-weld

B

DIC Software Packages

We are using La Vision’s da Vis (http://www.lavision.com/en/products/davis-software/index.php)

- **Probably the best**
- **But License is Expensive**

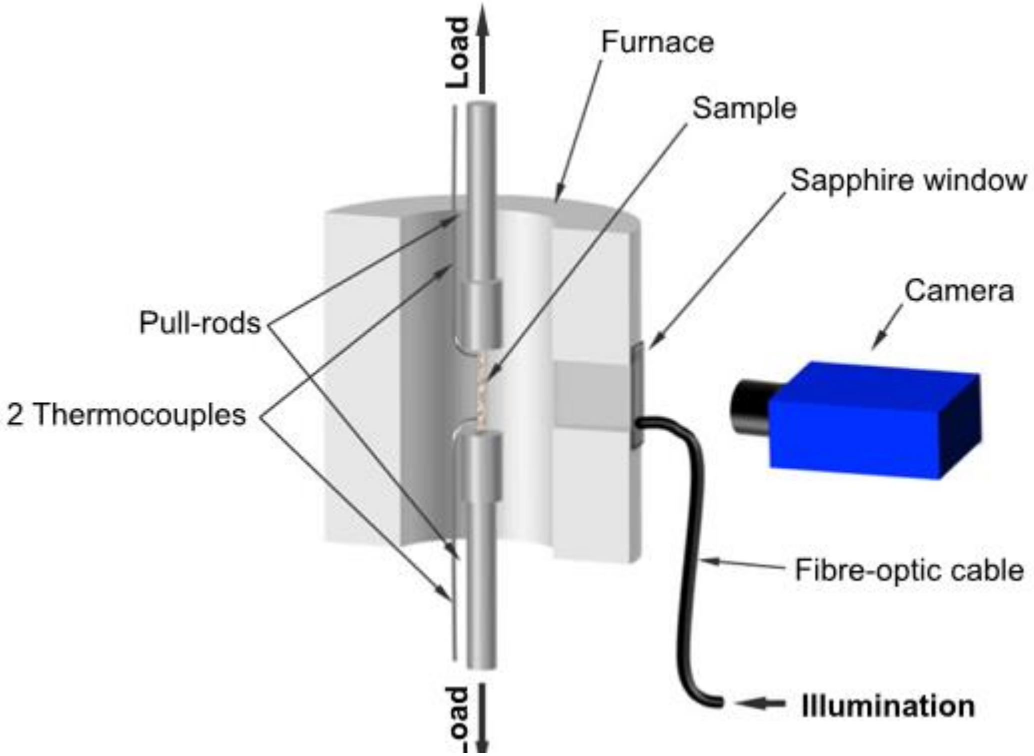
Other Options

- Ncorr – http://www.ncorr.com/
  - **J Blaber, B Adair, and A Antoniou, "Ncorr: Open-Source 2D Digital Image Correlation Matlab Software." Experimental Mechanics (2015)**
  - **Open source and runs with Matlab**
- VIC-2D by Correlated solutions http://correlatedsolutions.com/vic-2d/
  - **Commercial software**
  - **Cheaper than da Vis**
  - **Quicker and easier to use than Ncorr**
- *ARAMIS GOM http://www.gom.com/3d-software/download.html*
  - ***Open source software***
  - ***I don’t know a lot about this***

B

Macro-Meso Scales

Creep across a weld



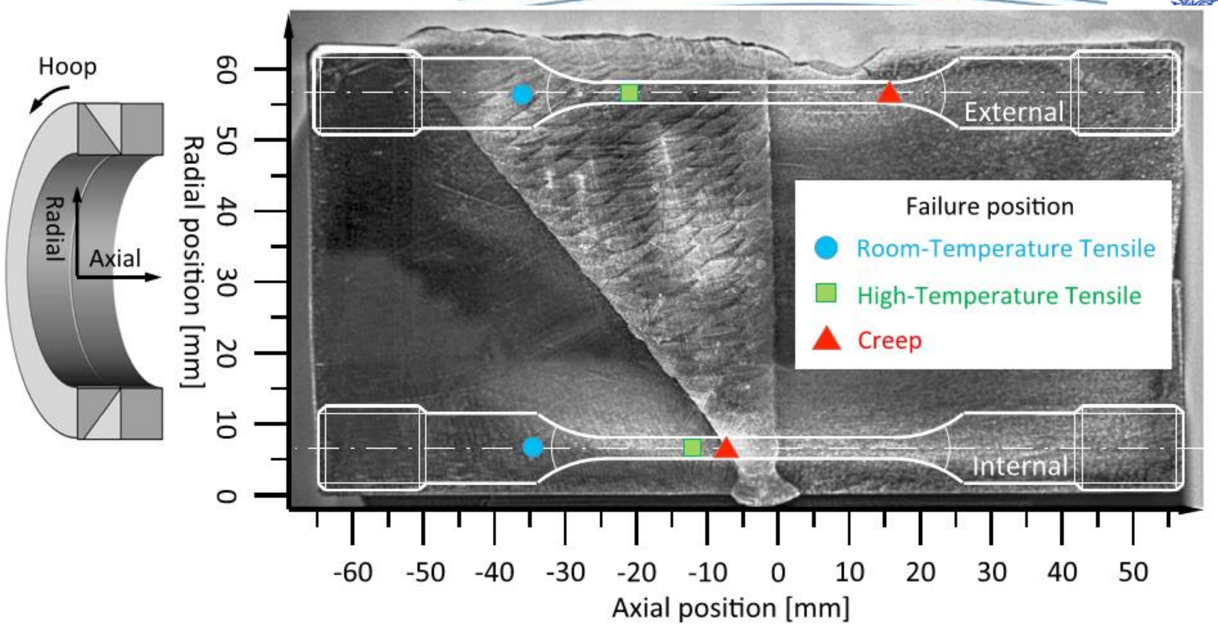


Fig. 1 Thick section (64 mm) austenitic stainless steel weldment showing creep test specimen extraction locations. Specimen rupture positions in cross-weld tensile tests and creep tests are also shown (note

Fig. 4 Photograph of small region of external sample surface after application and curing of paint layers showing the speckle pattern achieved

Sample etched

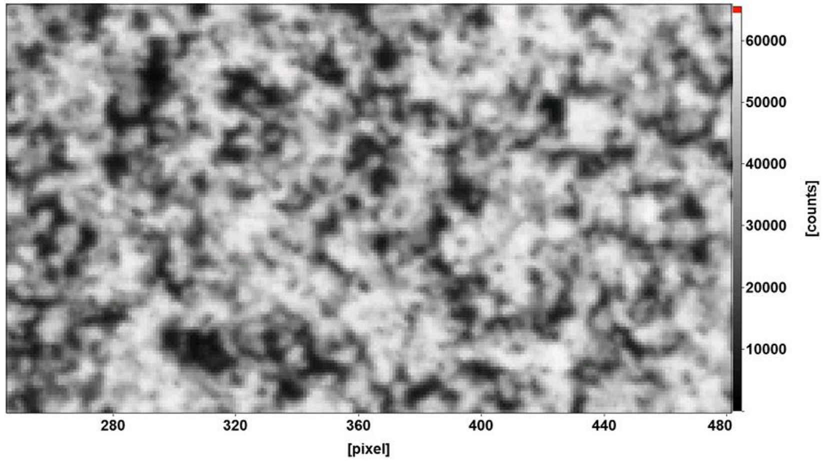


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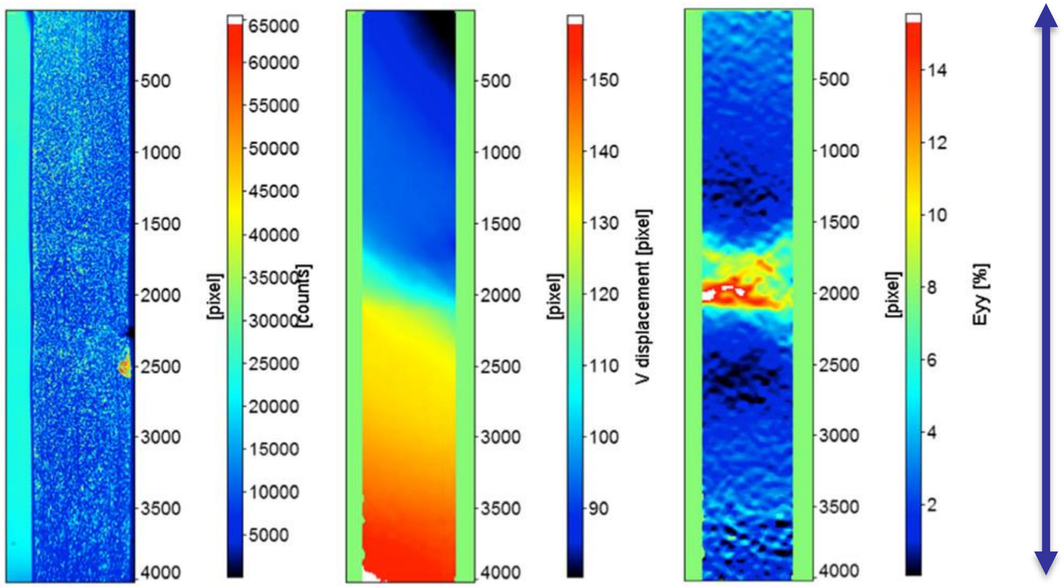
Fig. 8 DIC analysis of strain in the gauge section in the internal specimen from the stainless steel weldment at a creep life of 1000 h. On the left, the original image with pseudo colours, in the centre is the calculated displacement map and on the right is longitudinal local strain map. The 45° HAZ interface is at position 2485 pixels and the 90° HAZ interface is at 1678 pixels



35 mm

DIC as a strain gauge

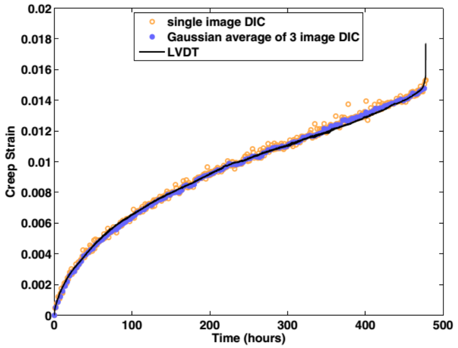


Fig. 7 Creep deformation-time curves for austenitic stainless steel at 550 °C under an applied stress of 350 MPa, comparing results based on strain measured by a conventional extensometer (LVDT) and DIC over the gauge length

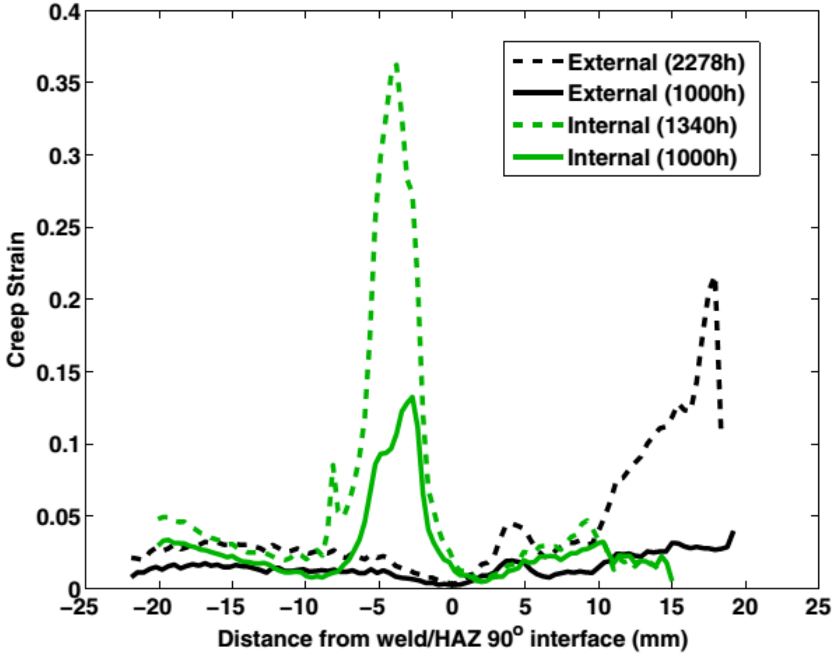


Fig. 9 Average strain across the width along both external and internal samples at 1000 h and at failure, with an applied stress of 315 MPa at 545 °C

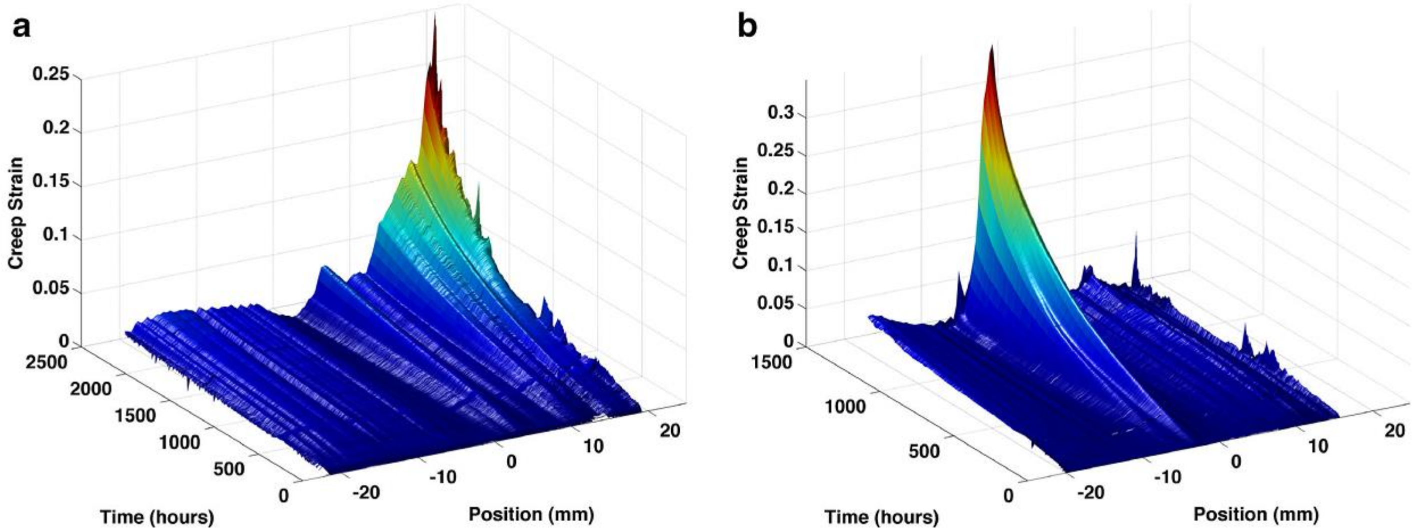


Fig. 10 3D surface plots showing the variation in measured creep strain along the gauge lengths relative to the weld/HAZ 90° interface of (**a**) the external, (**b**) the internal stainless steel cross-weld test specimens as a function of test duration for an applied stress of 315 MPa at 545 °C

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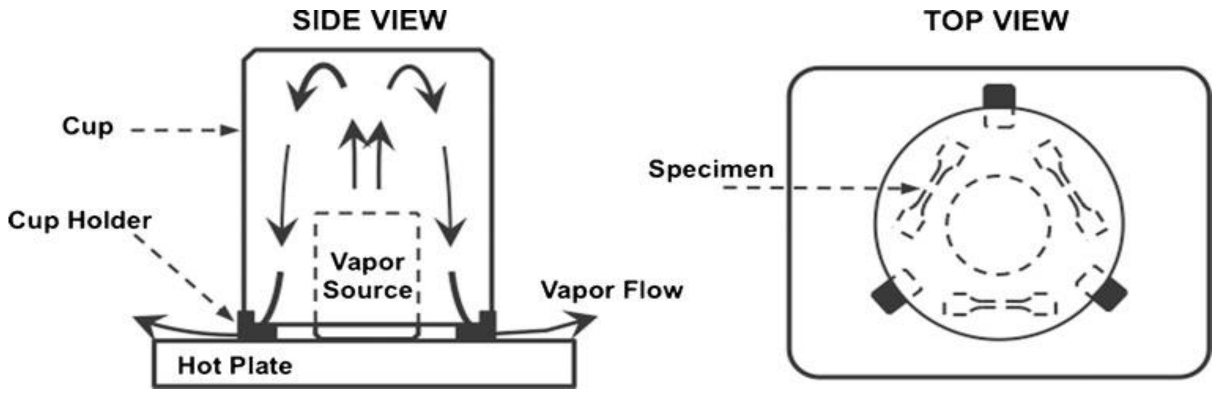
Other applications: - Young's Modulus or Flow Stress at different positions on a sample

B

Sub-micron resolution

- Sputter gold coating
- Remodel using water vapour or styrene at 100-150ºC



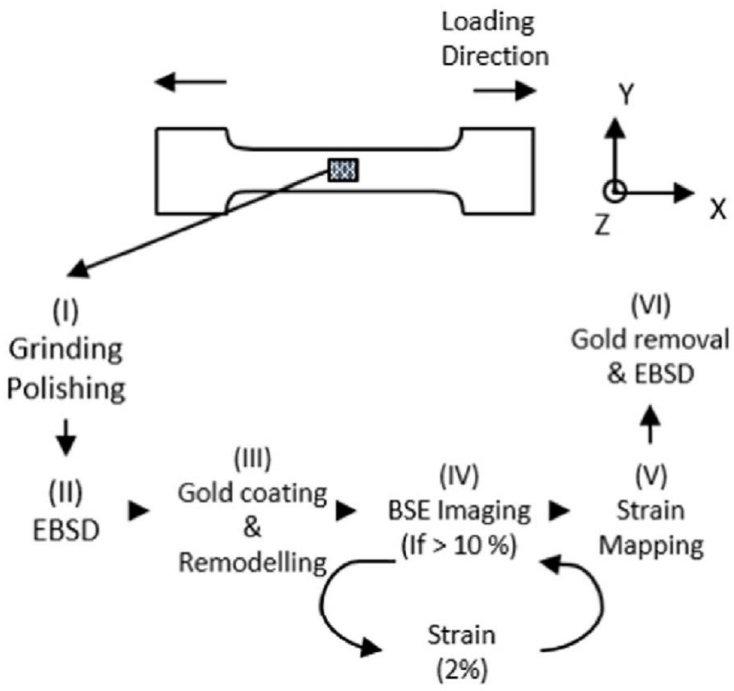
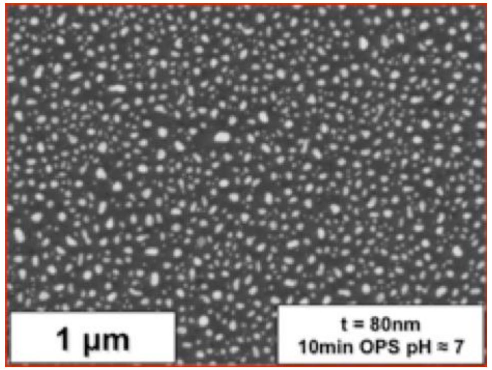
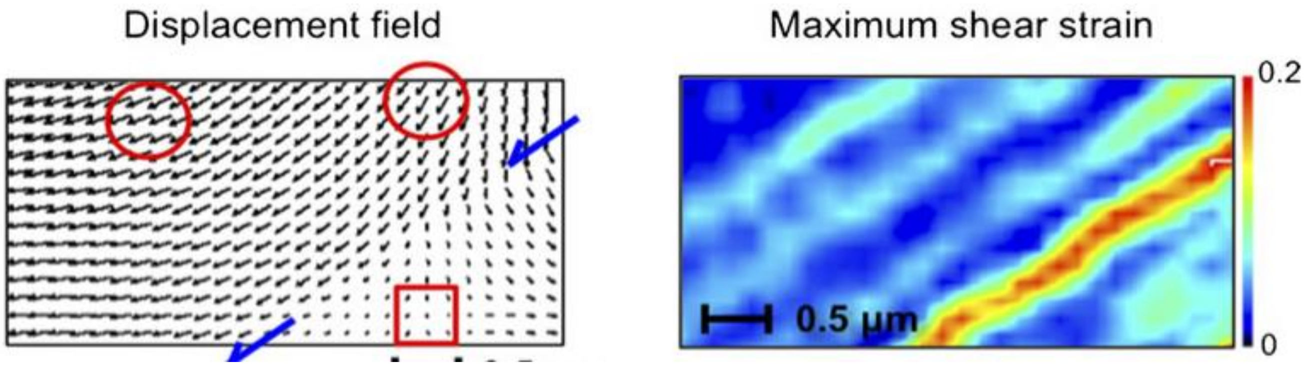


Fig. 2. Schematic of sample design and flowchart of experimental procedure.

Y.B. Das, A.N. Forsey, T.H. Simm, K.M. Perkins, M.E. Fitzpatrick, S. Gungor, R.J. Moat, JMADE. 112 (2016) 107–116.

- Speckle pattern image using a FEG SEM, BSE mode:
  - **Speckles are 10-100 nm, with equal spacing**





Di Gioacchino, Quinta da Fonseca, Exp. Mech., 2012

B

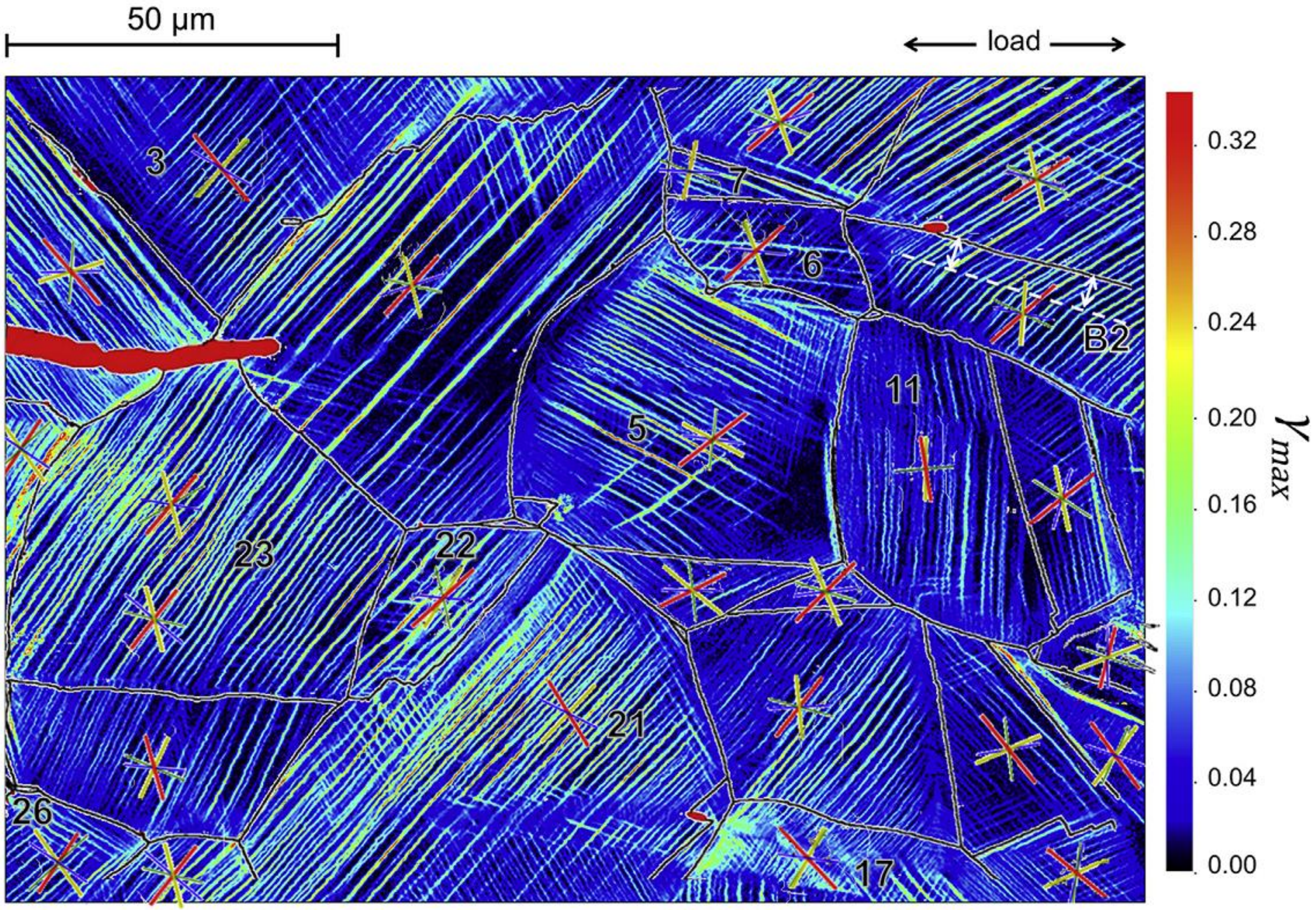
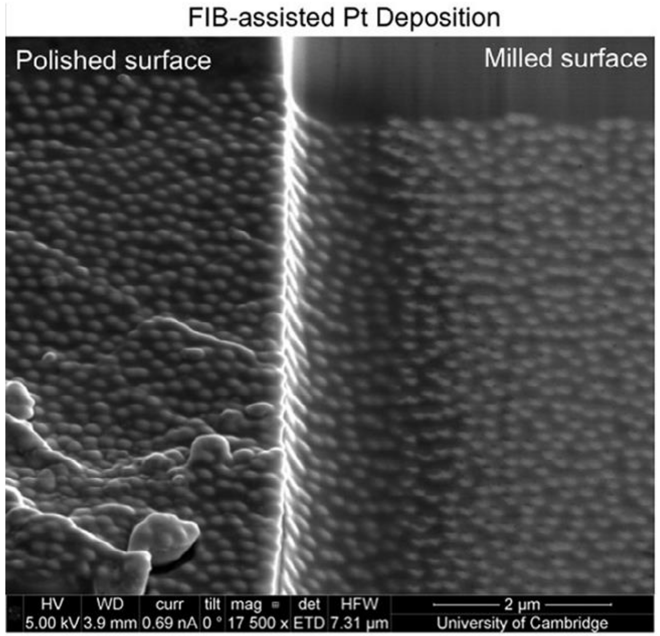


Fig. 4. Approximate positions of grain boundaries in Fig. 3. Deformation twin boundaries and transgranular ferrite stringers are removed for improved visibility. {111} plane traces are also superimposed. Traces are coloured (blue, green, yellow, red) according to increasing values of Schmid factor, see Table 3. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Di Gioacchino, Quinta da Fonseca,
International Journal of Plasticity 74 2015

Smaller Scale

- Fine speckle patterns can be made using either electron beam or focused ion beam (FIB) assisted deposition



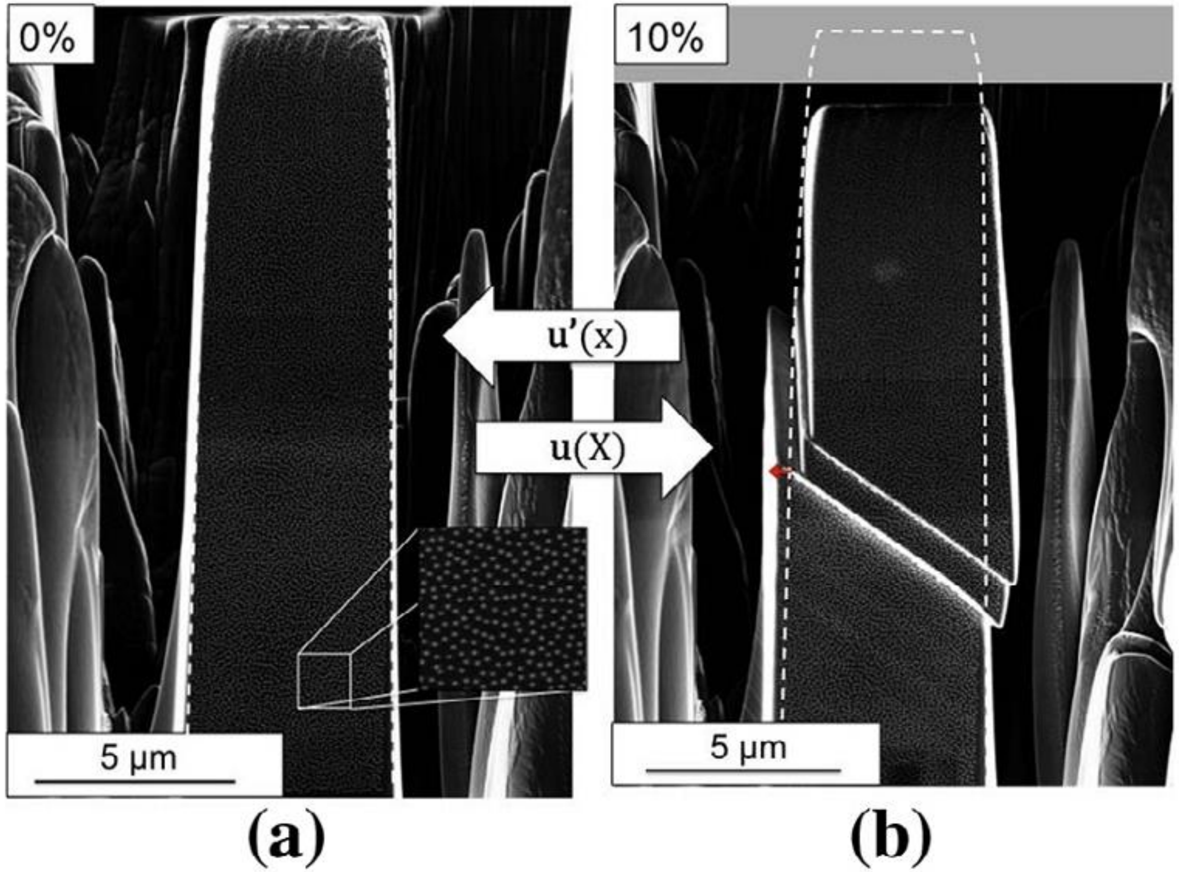


Fig. 3. SEM images acquired (a) before and (b) after deformation. The dashed line is the contour of the undeformed pillar, whilst the red arrow in (b) highlights the displacement of the bottom part of the pillar. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

REF: Di Gioacchino & Clegg Acta Materialia 78 (2014)

B

Comparison of rotations

Copper
single crystal

EBSD

$$m = q_1^* q_2$$

$$\vartheta_i = m_i \frac{2 \cdot \arccos(m^0)}{\sqrt{1 - (m^0)^2}}$$

DIC

$$\vartheta_3 = F_{21}/F_{11} \quad (\text{with } X_1 \equiv s)$$

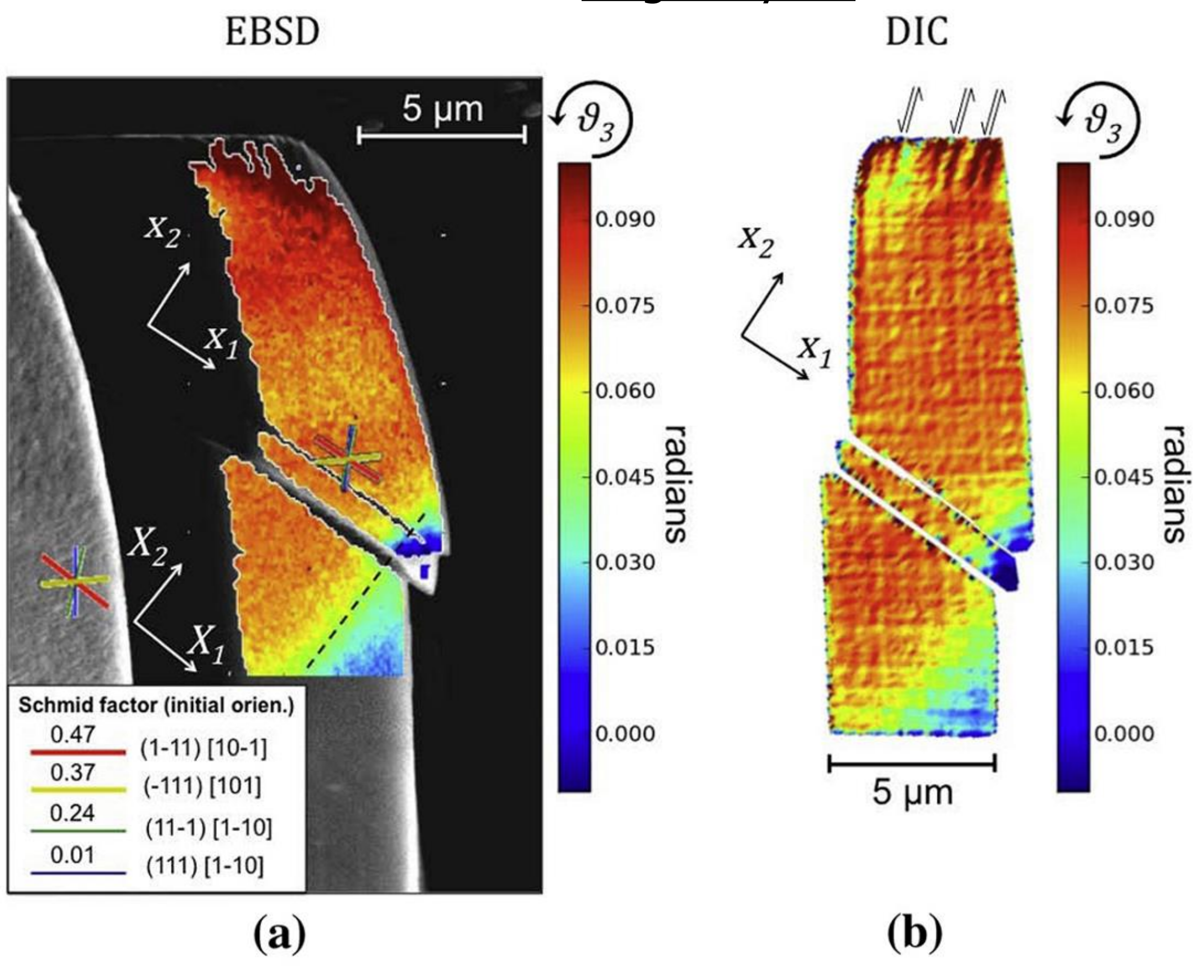


Fig. 6. In-plane lattice rotation ϑ_3 (a) as measured using EBSD, with overlap of traces of (1 1 1) planes; (b) as measured using DIC. The coordinate system (x_1, x_2, x_3) in (a), where x_3 is the out-of-plane axis, was used to calculate values in (b).

REF: Di Gioacchino & Clegg
Acta Materialia 78 (2014)

B

Practical Issues of in-situ DIC + EBSD

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Di Gioacchino, Clegg, 2014

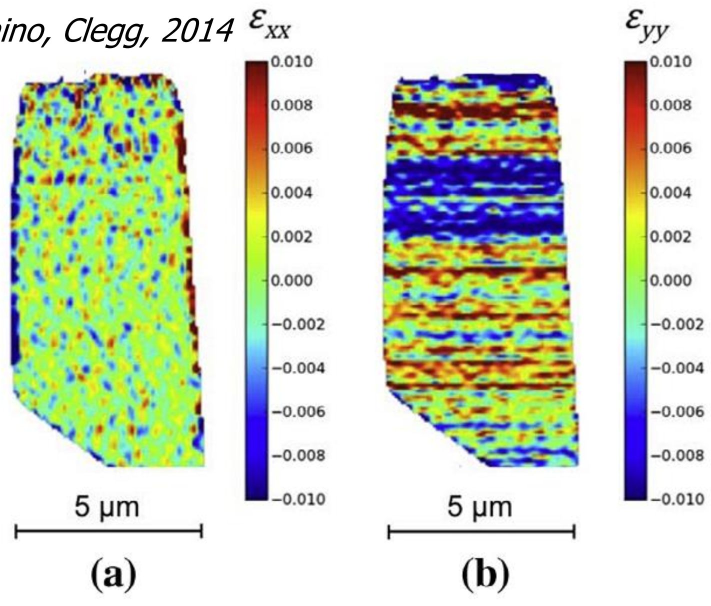

Fig. 4. Noise in the SEM scanning: (a) horizontal perturbation due to fluctuation in scan speed; (b) vertical perturbation due to error in the repositioning of the beam.

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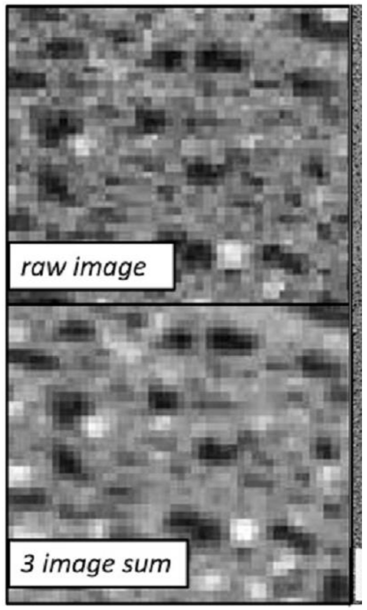
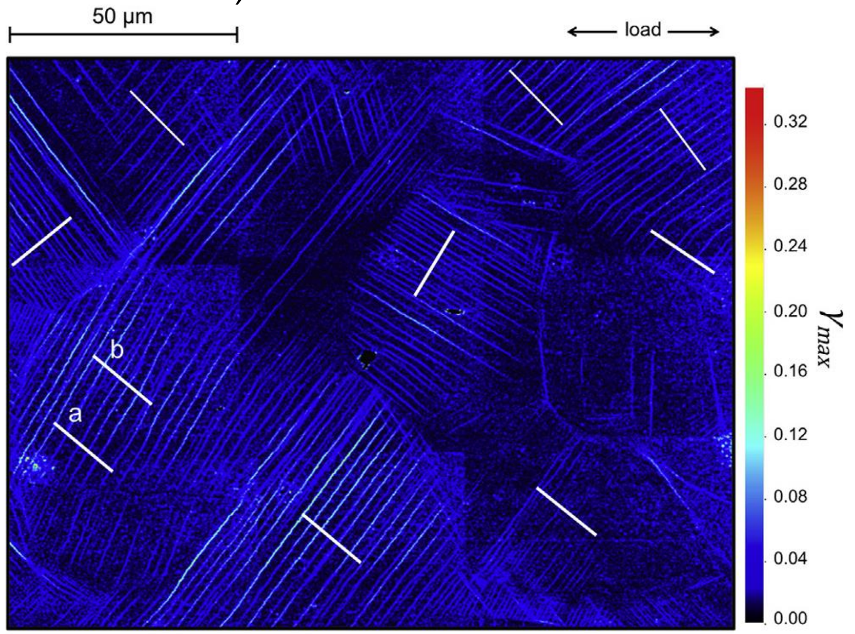


Di Gioacchino, Quinta da Fonseca, 2015



(a)

- Need features on surface
  - Three-stage procedure: EBSD -> DIC -> EBSD
  - Problems for transmission
- SEM can produce raster errors-
  - reduce by taking more than one image and summing
- Higher Mag. and combining multiple maps best for resolution
  - SEM with automated focus change helps (Manchester 80 maps overnight)
  - Normally better to do DIC on each map then combine vector maps
- Correction may be needed for drift
- Ex-situ can get closer WD and resolution but may lose some details (e.g. martensite)

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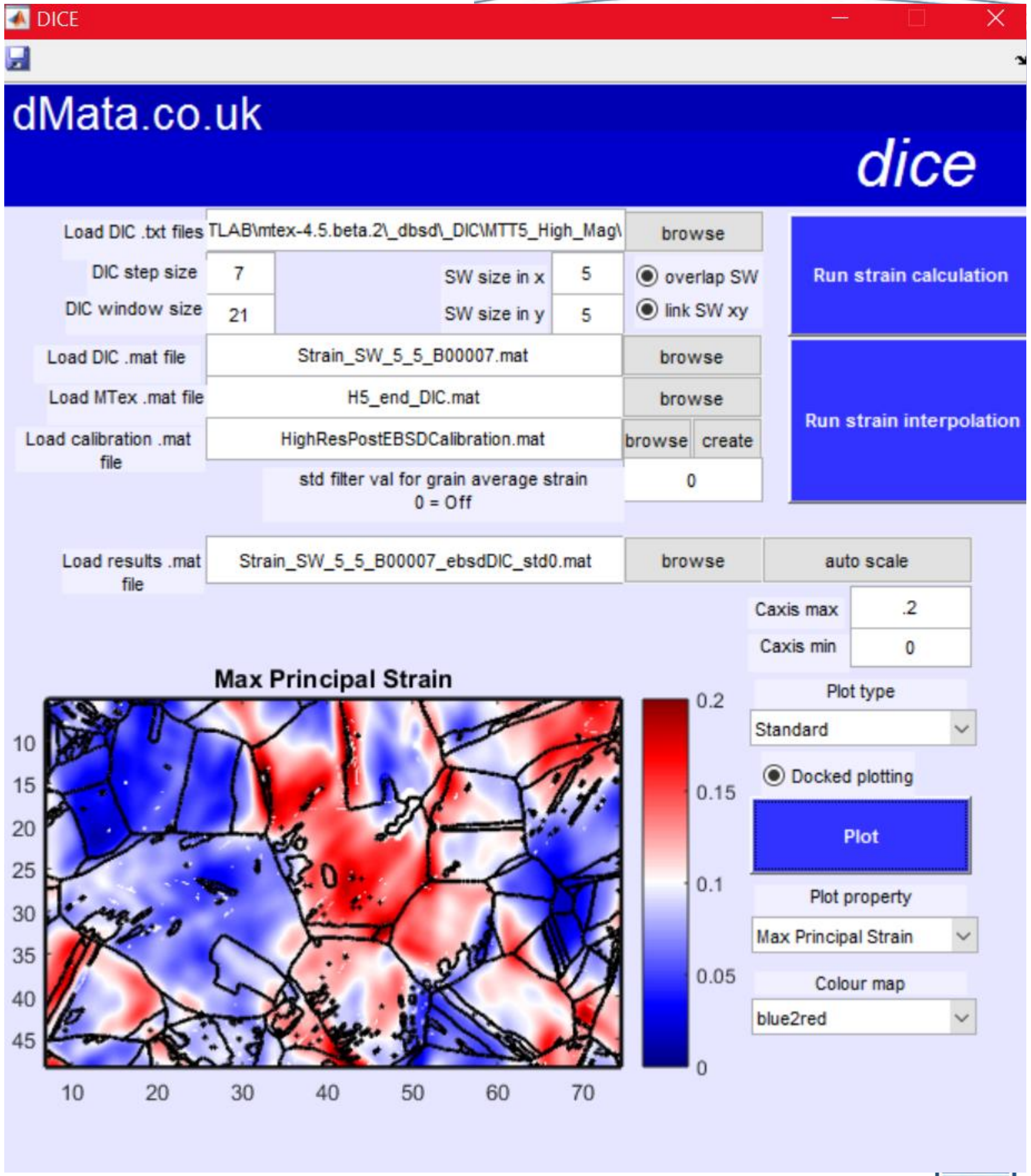
B

How we do DIC

- Do image analysis with DIC software
- Input vector maps
- Strain is calculated from a number of adjoining vectors (see next)
- Can change different parameters to suit the situation (next slide)
- EBSD data matched to DIC data visually
  - **Then DIC data interpolated so for each EBSD point we have strain components**
    - E.g. ebsd.Exx
  - **Displacement vectors rather than strain is used**



B

Getting the strain tensor

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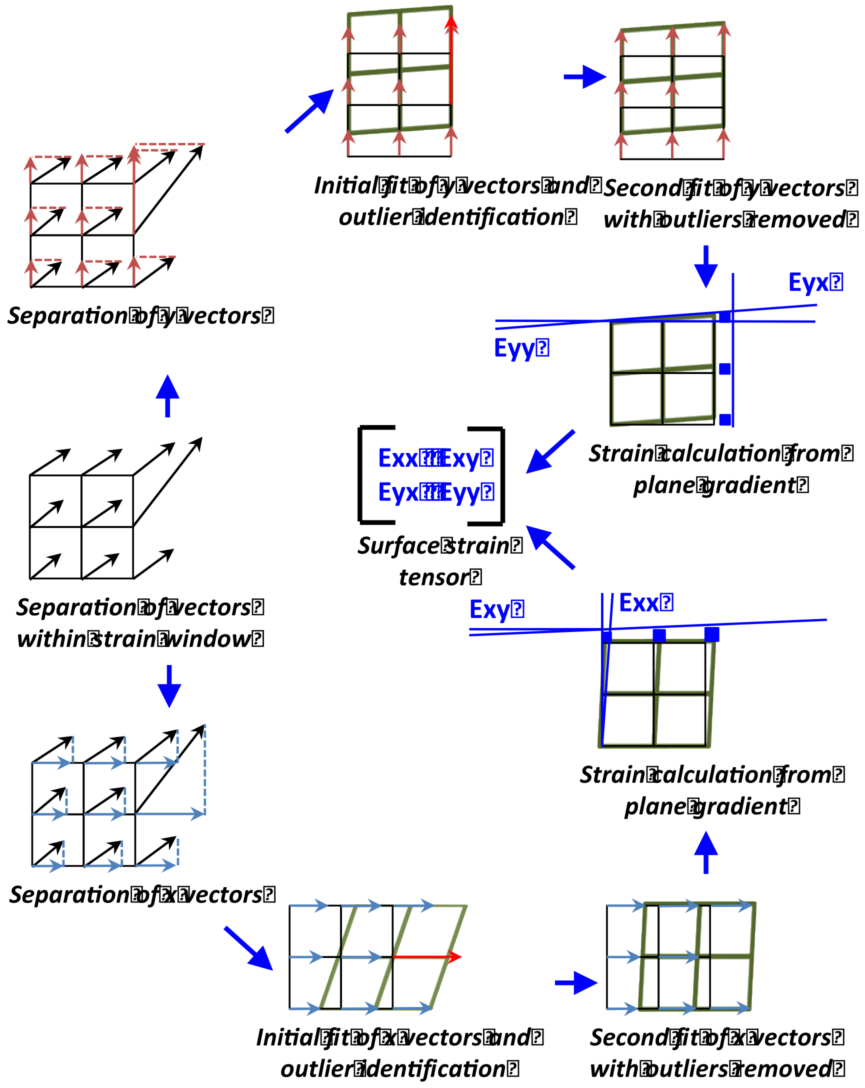
Local strains

- Example for a 3x3 strain window >>>>
- Strain is calculated by fitting a plane to the displacement vectors, values greater than a threshold std from mean displacement are removed and the fit performed again
- Increasing the strain window size increases the differentiation length of the strain calculation
- Rectangular strain windows can be used for highly directional strain fields
- Strain is calculated for each vector position
- This is then interpolated onto the ebsd grid
  - **E.g. ebsd.Exx**



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B

Getting the strain tensor

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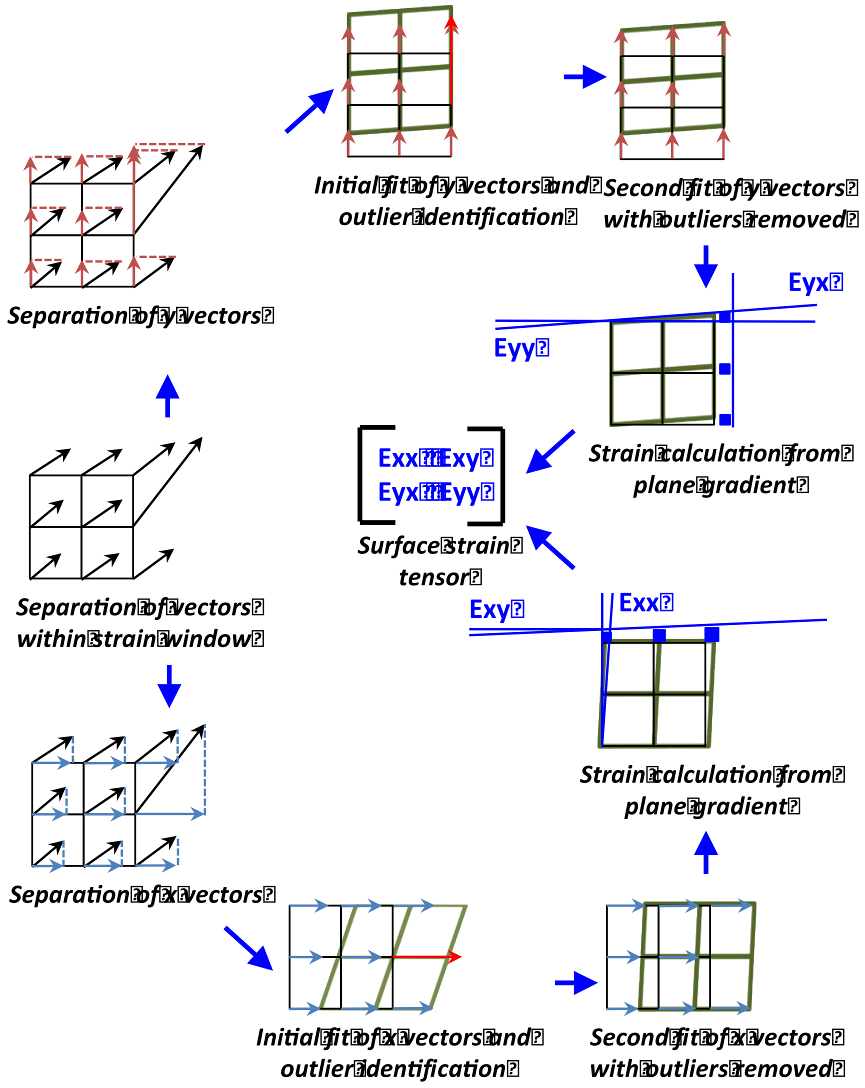
Grain strains

- Grain strains are calculated in the same way as local strains, but using all displacement vectors within the grain for the fit
- It is particularly important to set a reasonable value for the std filter in this case as spurious vectors at the grain boundaries can disproportionately affect the result unless removed
  - **Can also be used to remove gb regions**
- These strains are saved in ebsd and grains
  - **E.g. grains.Exx**
    - ebsd.Eyx



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B

DICE GUI

(a) Load DIC files = DIC output .txt file input

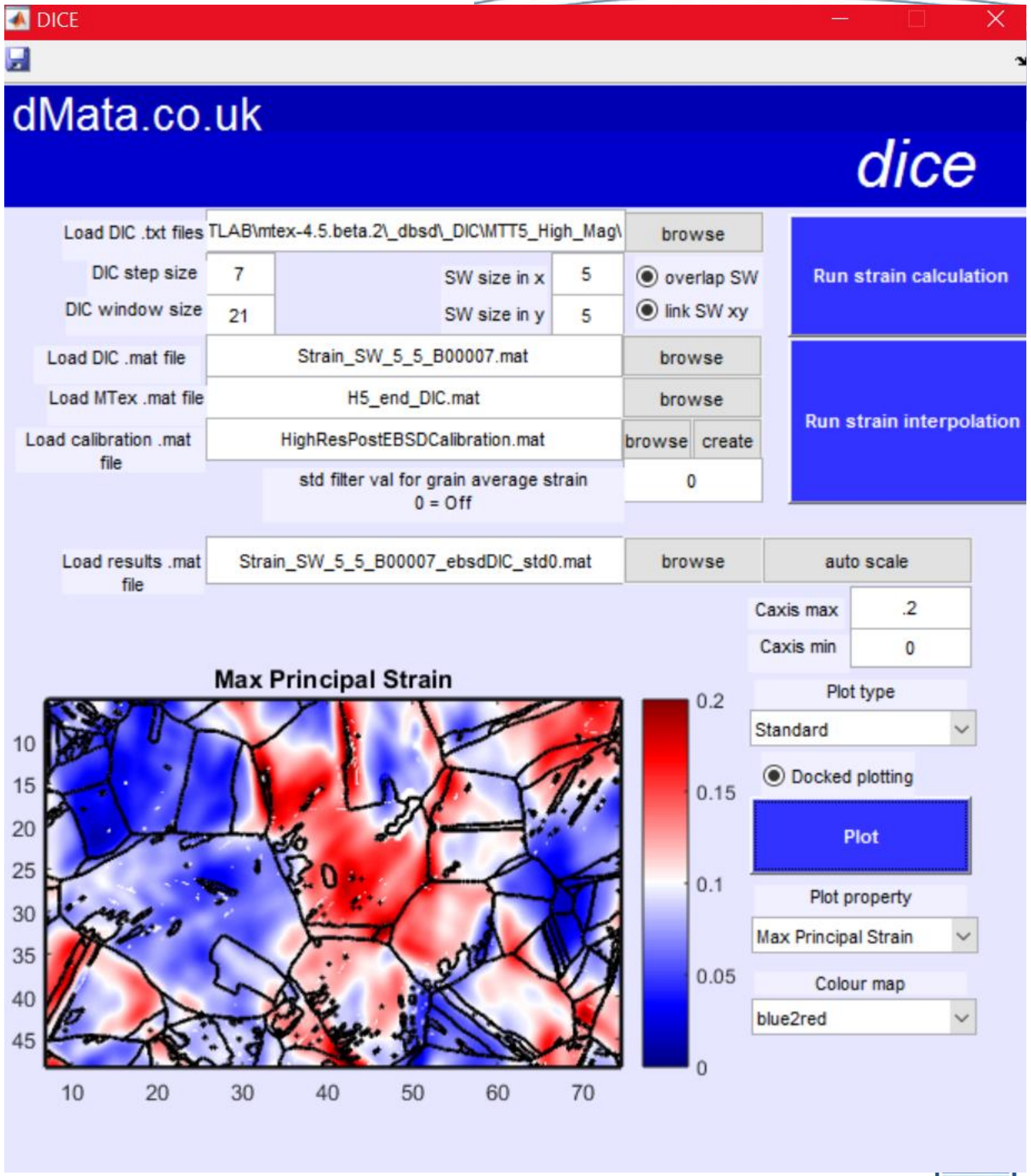
- DIC step size and DIC window size are not used in the calculation, rather they are stored so the size of the region affecting the strain calculation can be determined
- SW size = is the number of vectors in each direction are used to calculate local strain

(b) Load DIC .mat file = saved once (a) above has run

(c) Load calibration .mat file = created separately

- Std filter = outlier filter for average grain strain calculation

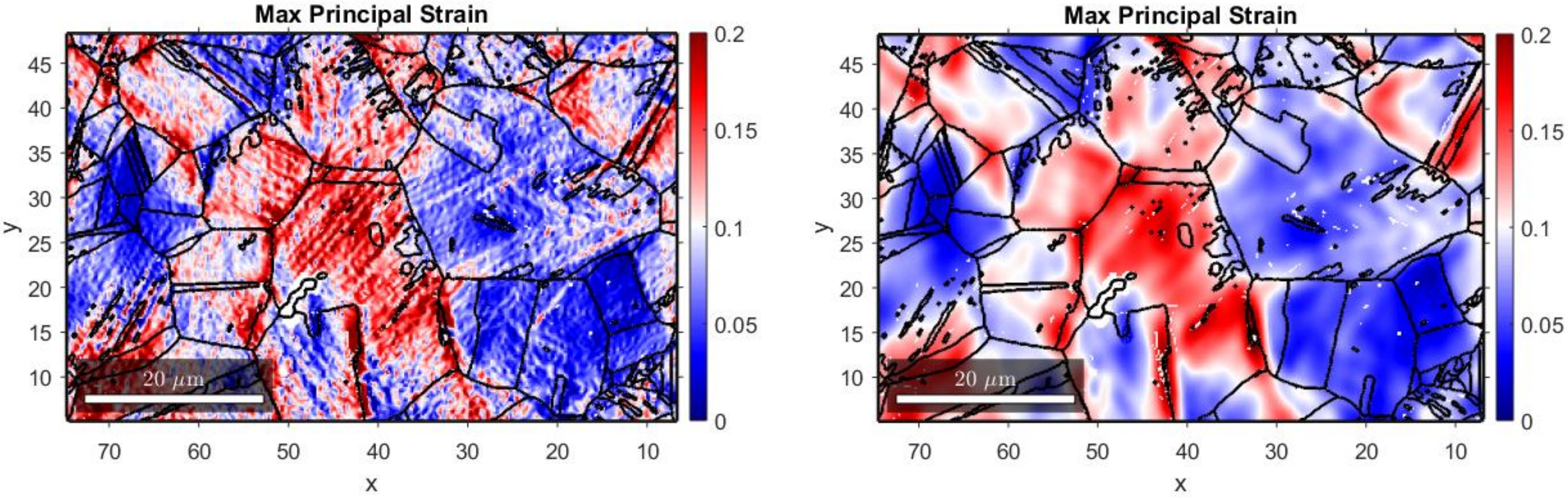
(d) Load results .mat file = load result from step (b)



B

Different Strain Windows

SW = 3 : 3 **SW = 5 : 5**



B

Experiment: DIC Strain Heterogeneity

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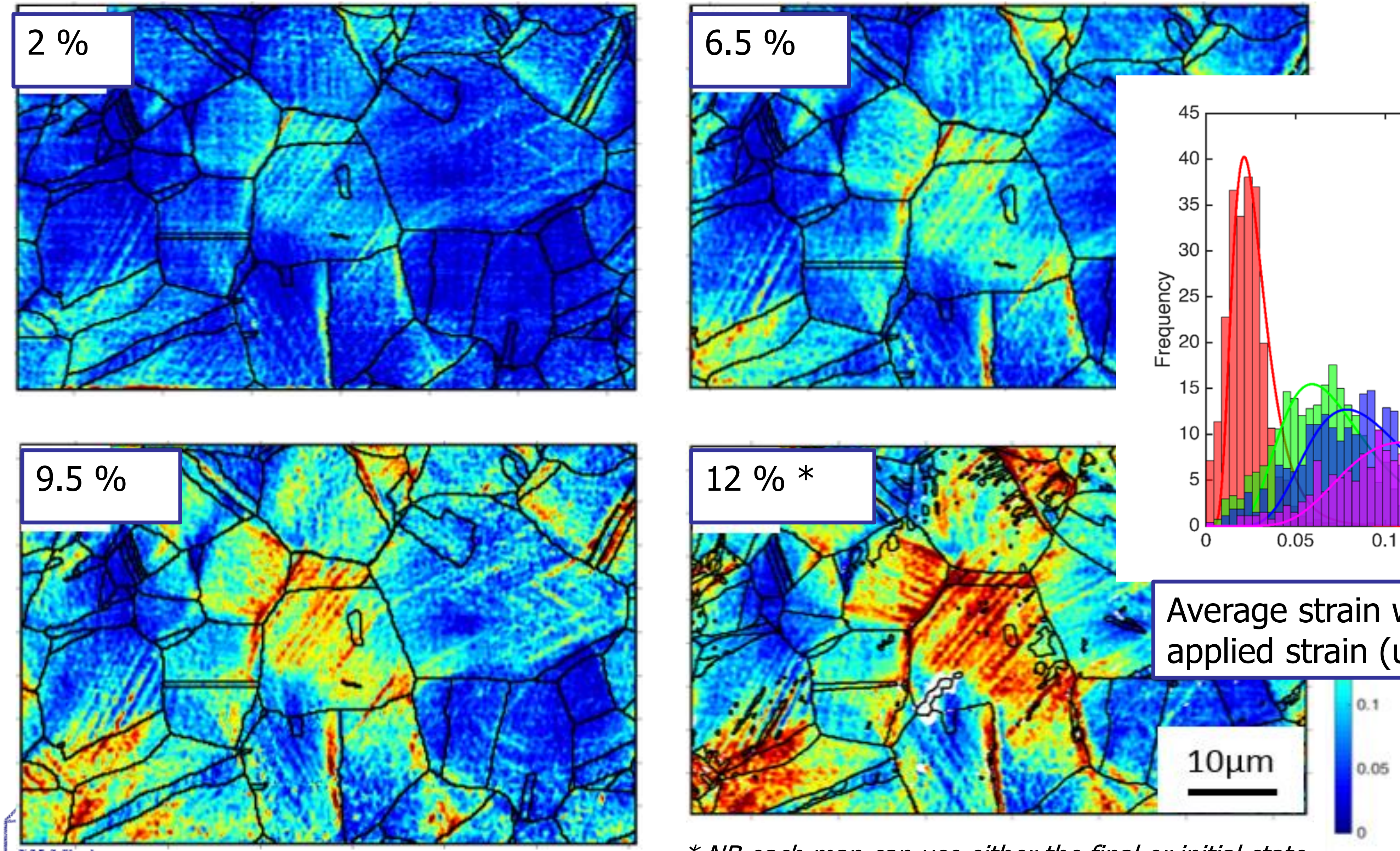

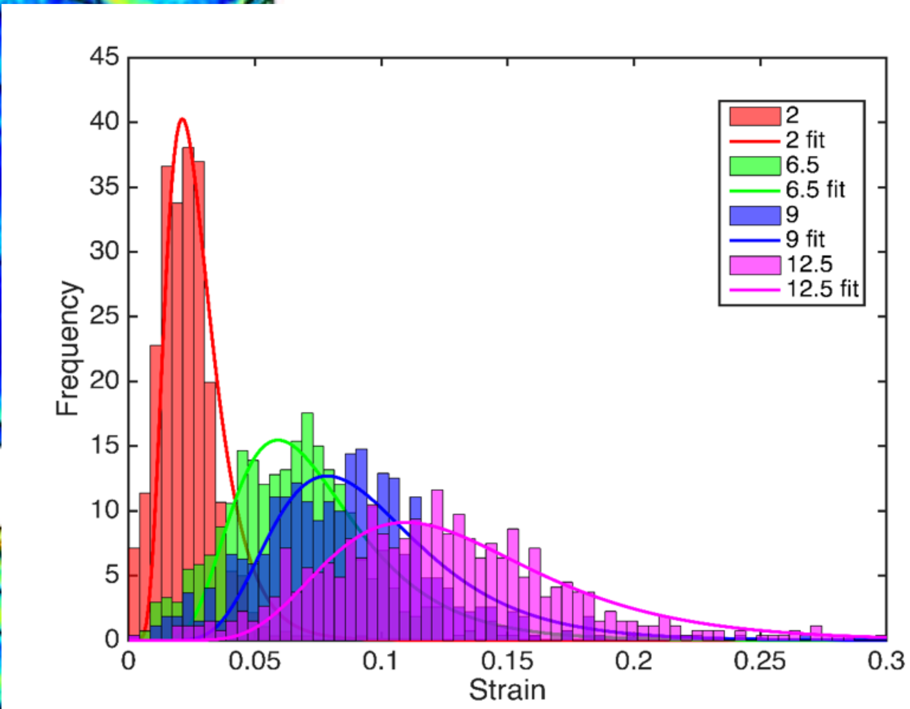

Average strain within grains at different applied strain (using low mag. Images)

** NB each map can use either the final or initial state*

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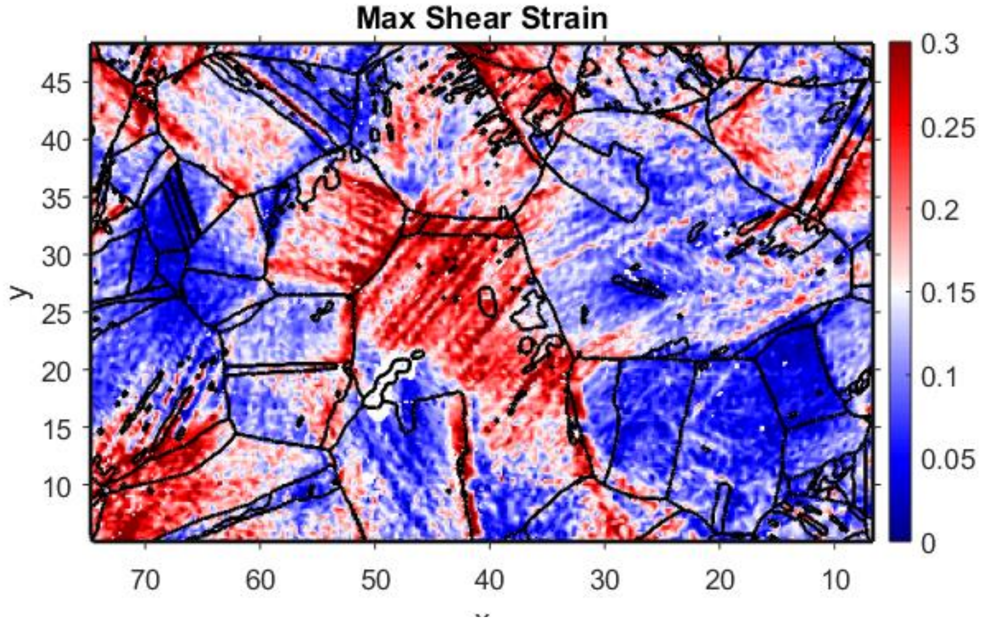
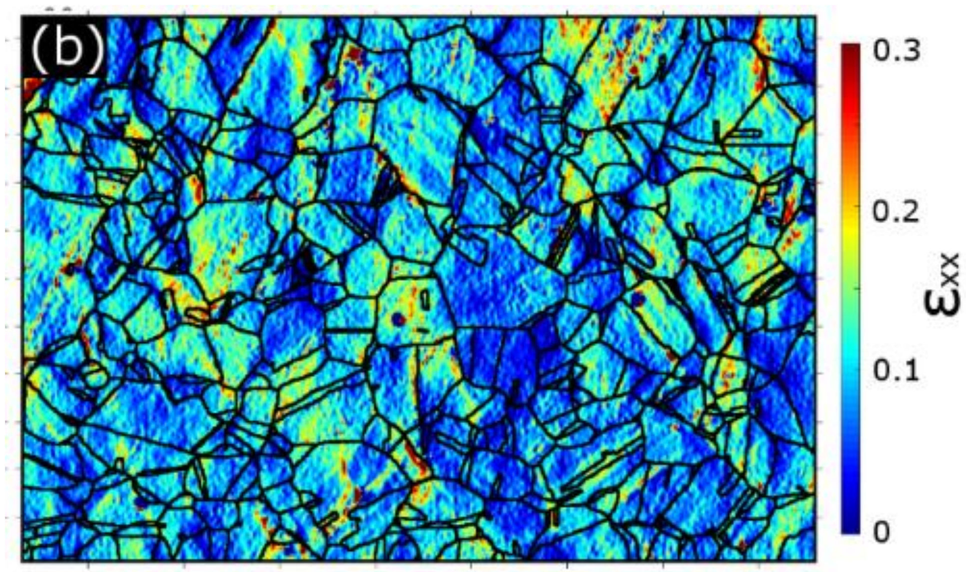
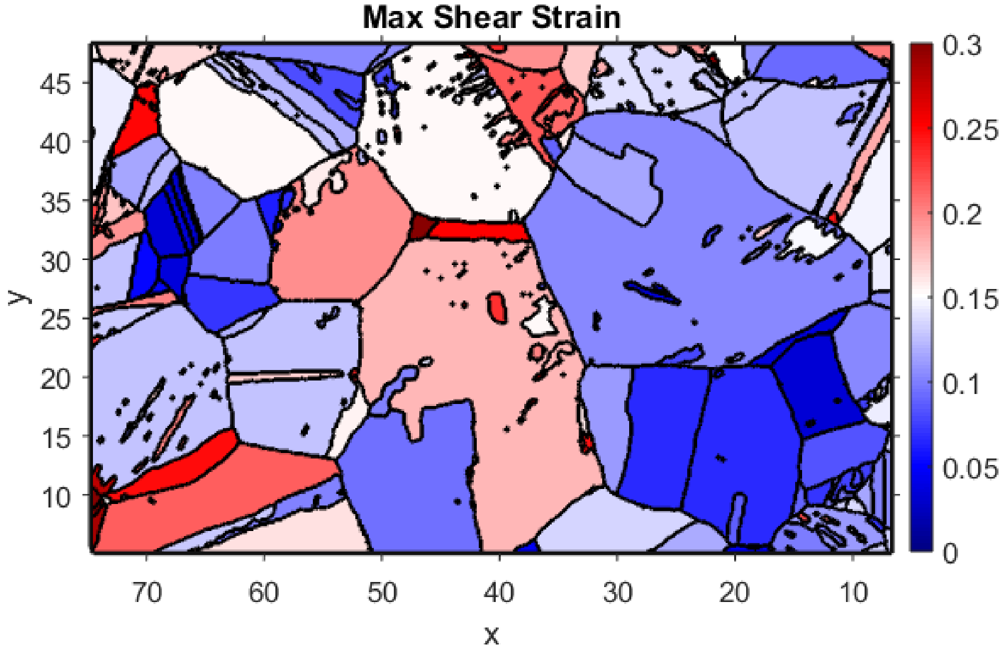
B

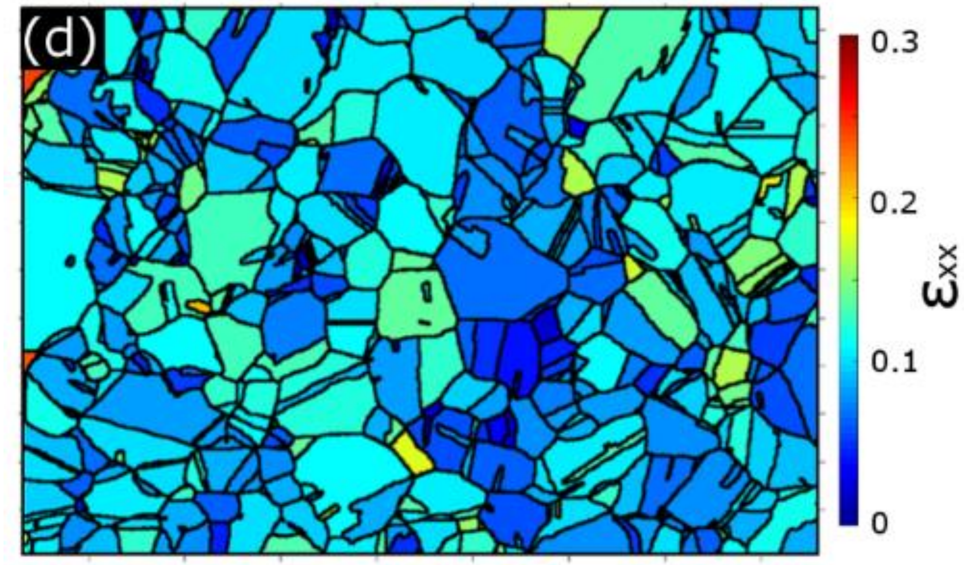
Local Strain vs Strain in grains





Local strain





Average grain strain

B

DIC vs EBSD

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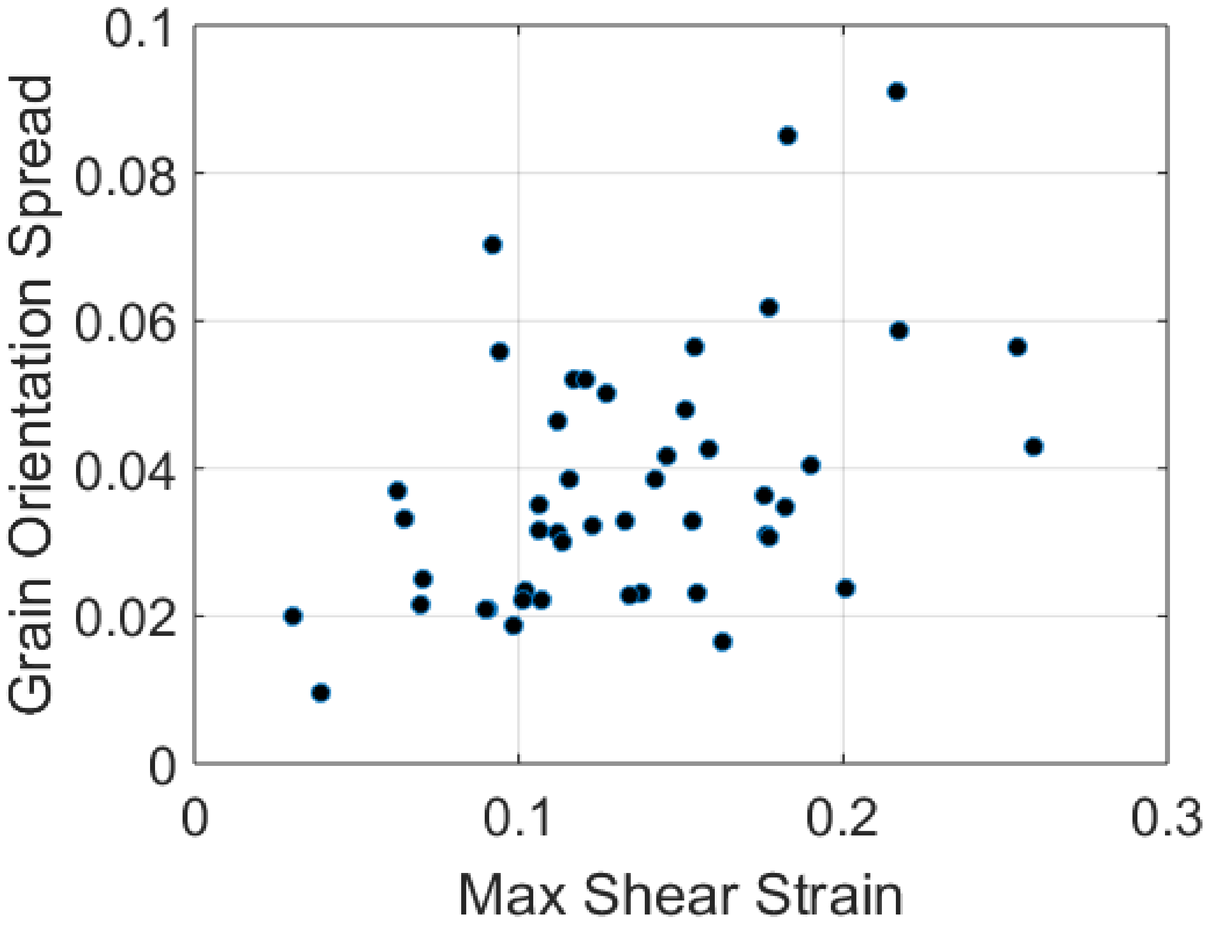
Swansea University

EBSD



DIC

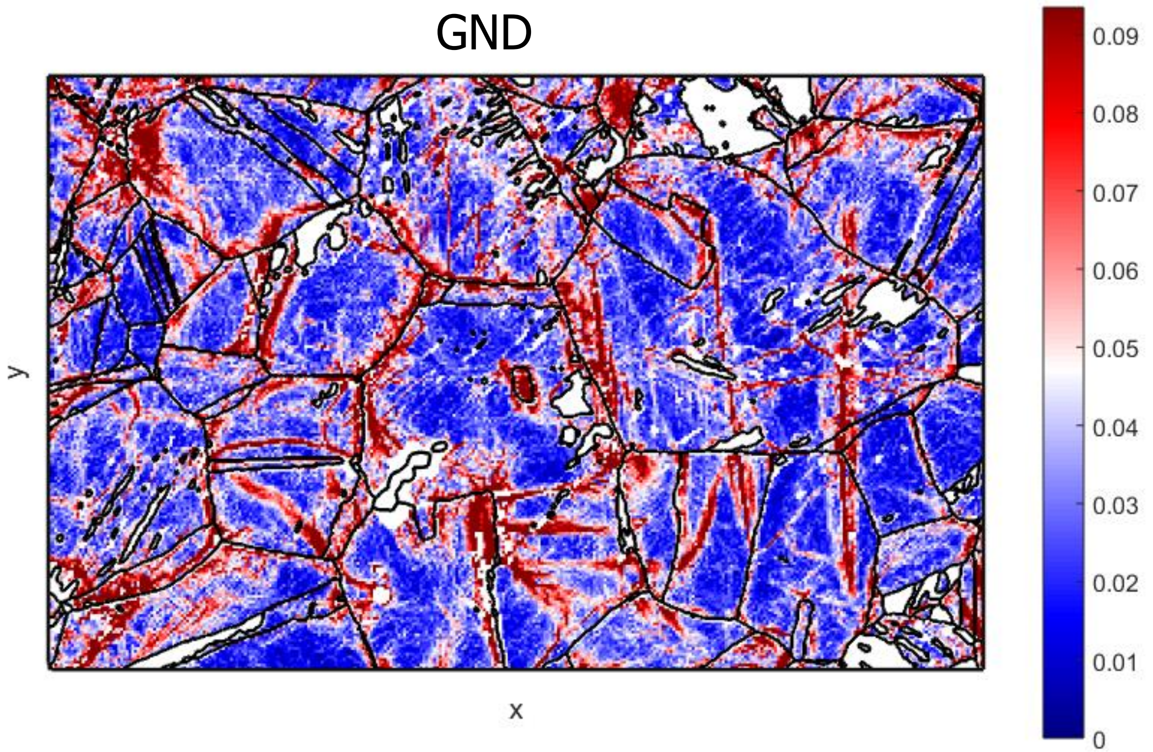
grains =grains(grains.area>10);
plot(grains.EpMax, grains.GOS, 'o')

Uses high mag image and SW = 5, 5

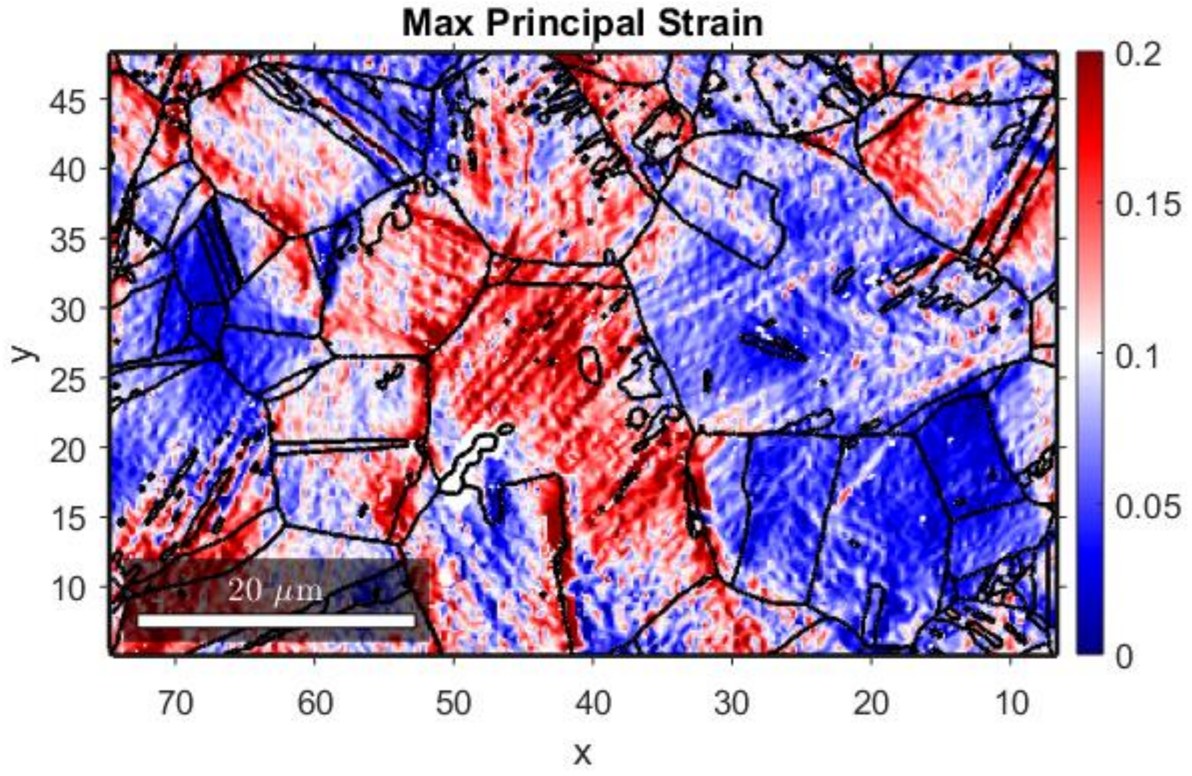
B

DIC vs EBSD

EBSD



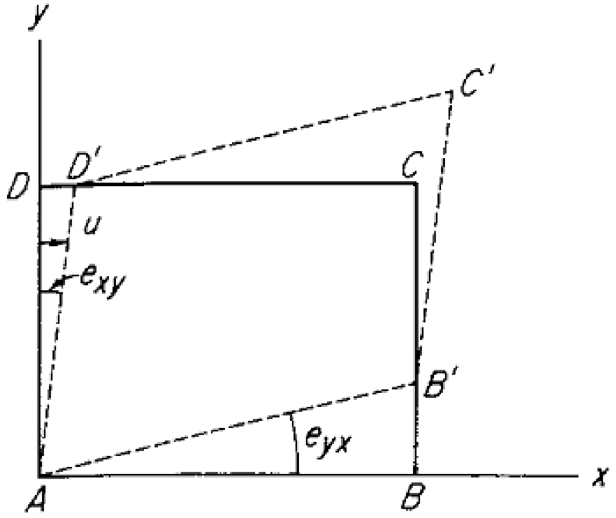
DIC



Some scratches

B

Strain tensor



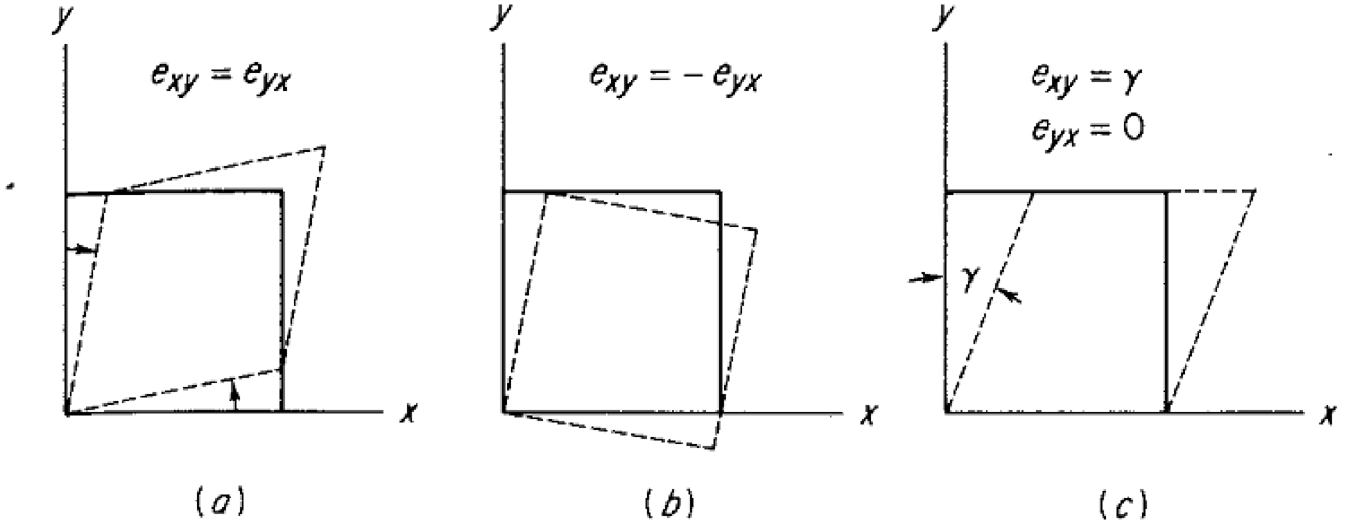


Figure 2-15 Some examples of displacement with shear and rotation. (*a*) Pure shear without rotation; (*b*) pure rotation without shear; (*c*) simple shear. Simple shear involves a shape change produced by displacements along a single set of parallel planes. Pure shear involves a shape change produced by equal shear displacements on two sets of perpendicular planes.

$$\omega_3 = \frac{1}{2}(F_{12} - F_{21})$$

Rigid Body Rotation

1=x
2=y

$$\vartheta_3 = F_{21}/F_{11} \quad (\text{with } X_1 \equiv s)$$

Lattice Rotation

REF: Dieter 1986

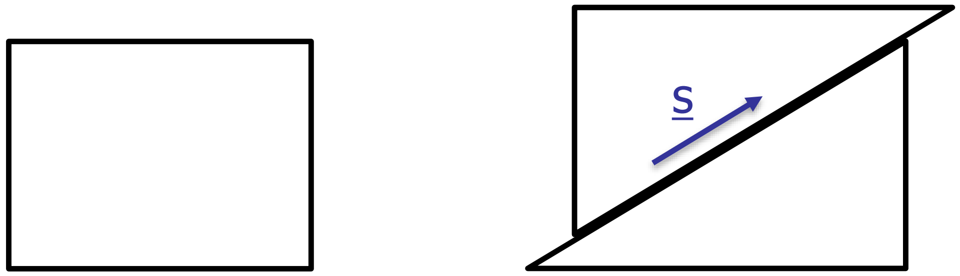
EBSD and DIC rotations

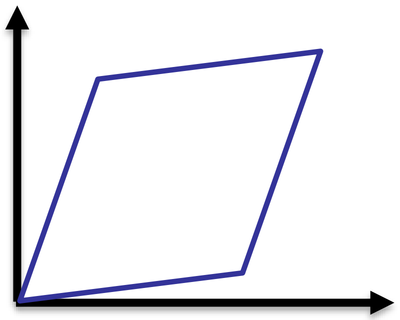
$$F = R^e F^p$$

F = deformation tensor *DIC*
R^e = lattice rotations & *elastic strains* *EBSD*
F^p = plastic deformation by dislocations movement through lattice

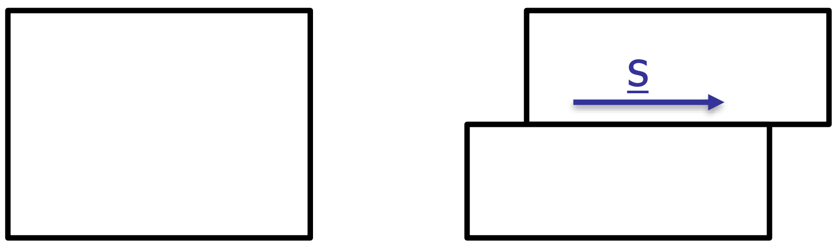
$Single\ slip\ for\ R^e = 0$

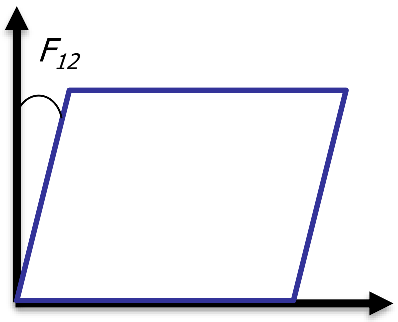
Wrt our axes





Shear along x-axis + Rotation





Simple Shear (along x-axis)
$F_{12} = F^p$

B

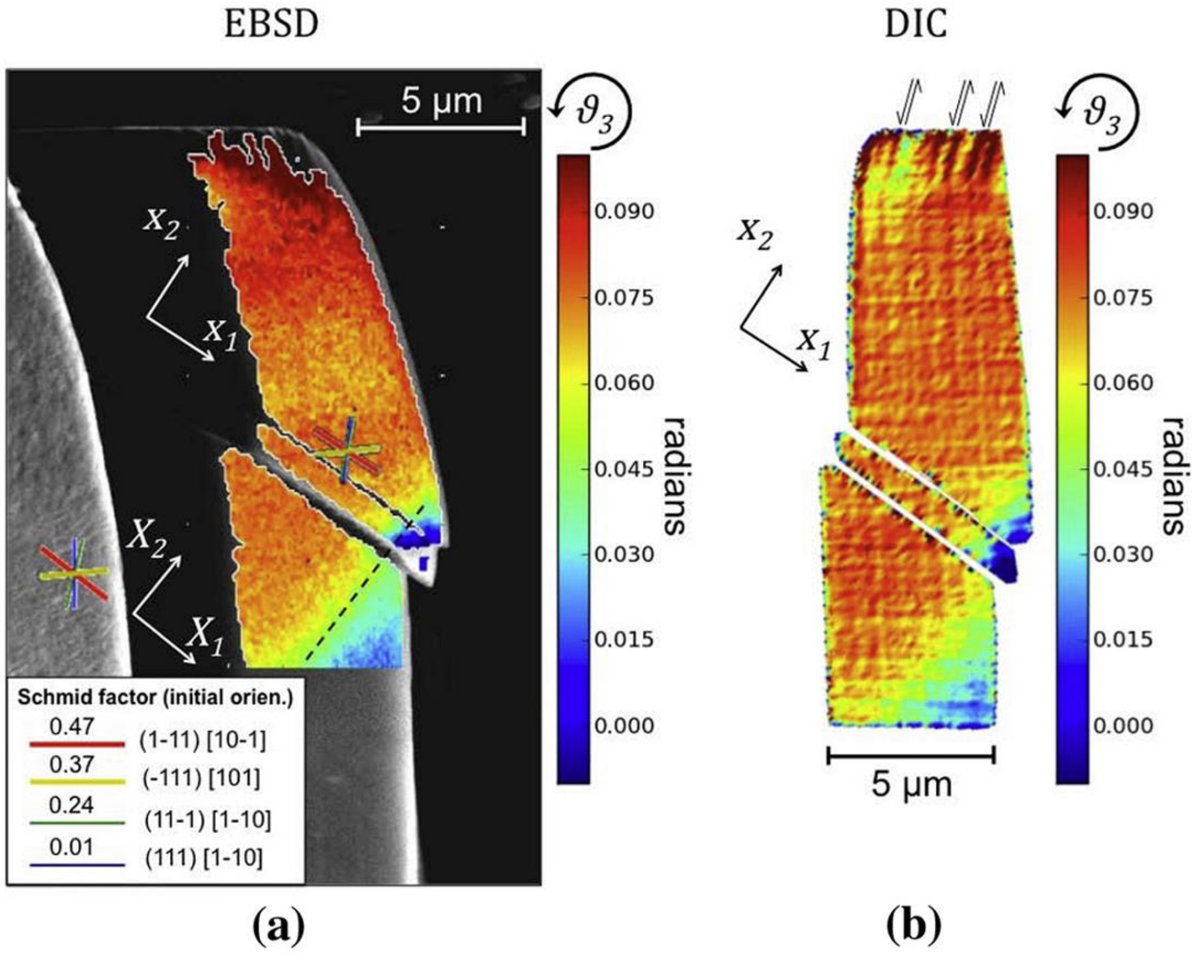
Comparison of rotations

Copper
single crystal

EBSD

$$m = q_1^* q_2$$

$$\vartheta_i = m_i \frac{2 \cdot \arccos(m^0)}{\sqrt{1 - (m^0)^2}}$$



DIC

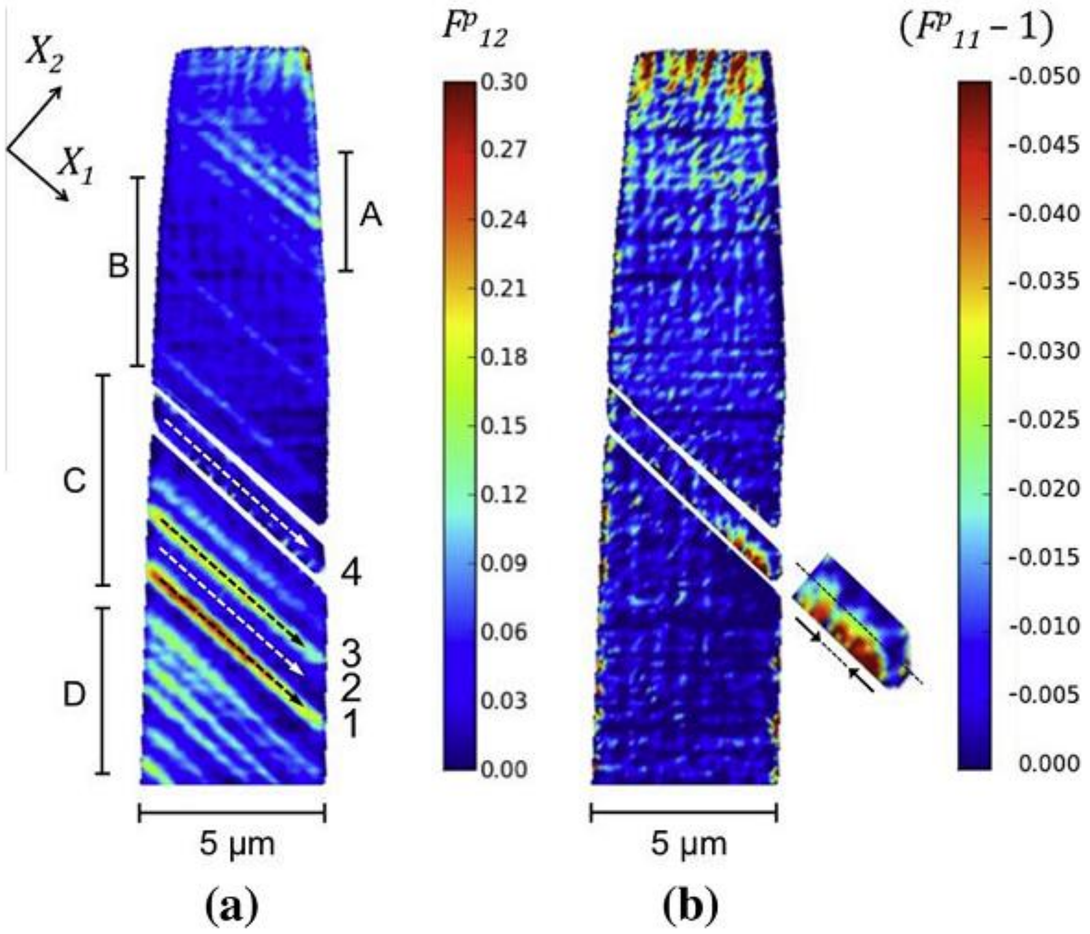
$$\vartheta_3 = F_{21}/F_{11} \quad (\text{with } X_1 \equiv s)$$

Fig. 6. In-plane lattice rotation ϑ_3 (a) as measured using EBSD, with overlap of traces of (1 1 1) planes; (b) as measured using DIC. The coordinate system (x_1, x_2, x_3) in (a), where x_3 is the out-of-plane axis, was used to calculate values in (b).

REF: Di Gioacchino & Clegg
Acta Materialia 78 (2014)

B

Plastic deformation F^p



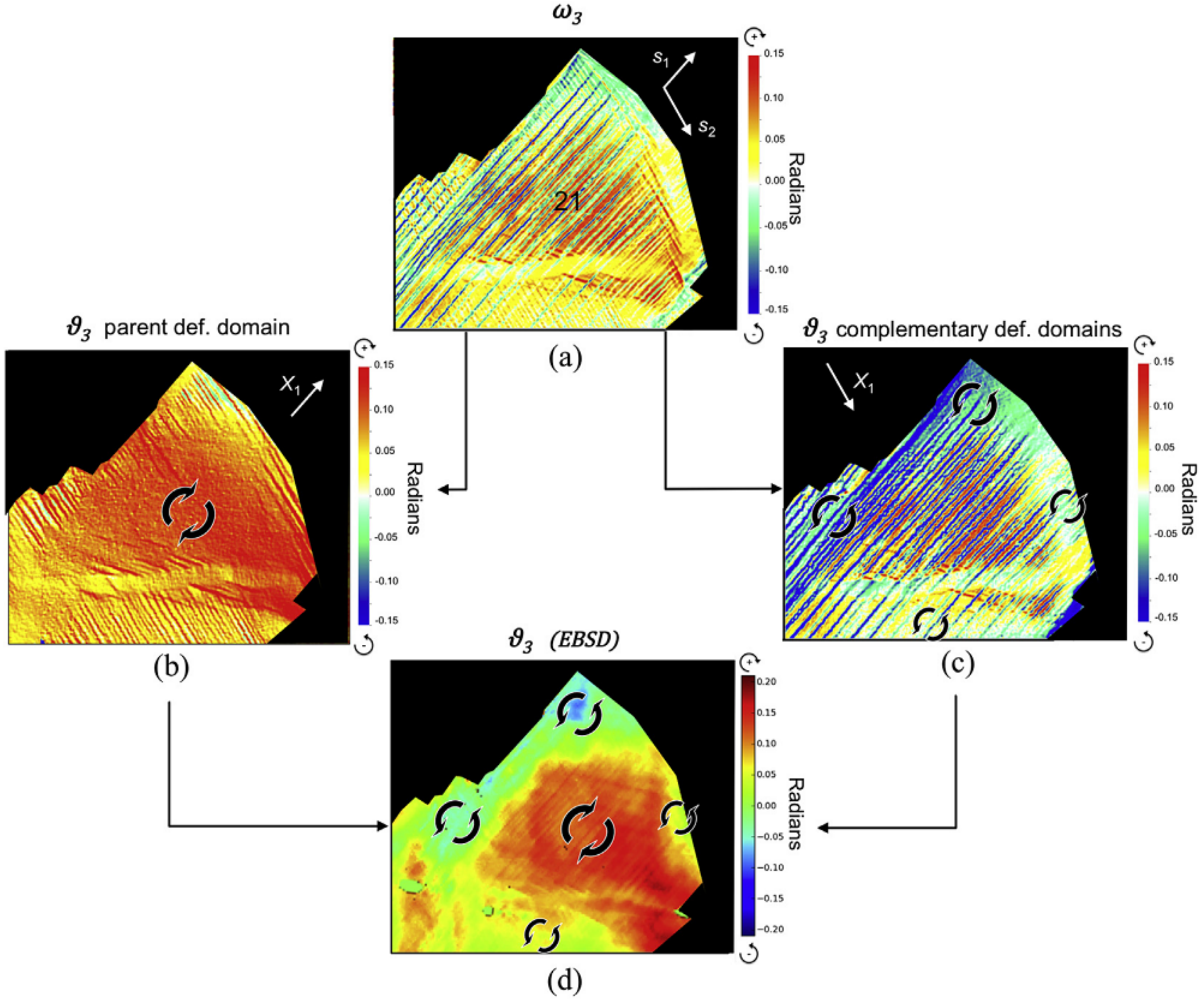
$$F = R^e \boldsymbol{F}^p$$

Fig. 7. Maps of (a) slip along X_1, F^p_{12}, and (b) of $F^p_{11} - 1$. The coordinate system. (X_1, X_2, X_3) Fig. 6(a) was used, where X_3 is the out-of-plane axis.

REF: Di Gioacchino & Clegg
Acta Materialia 78 (2014)

B

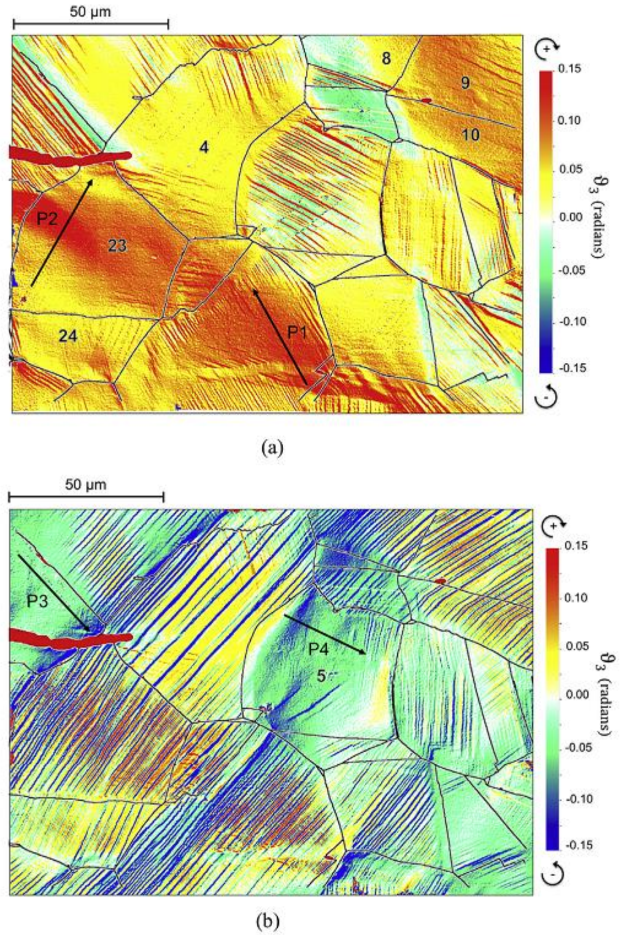
Crystal within a polycrystal



Di Gioacchino, Quinta da Fonseca,
International Journal of Plasticity 74 2015

B

Comparing EBSD and DIC



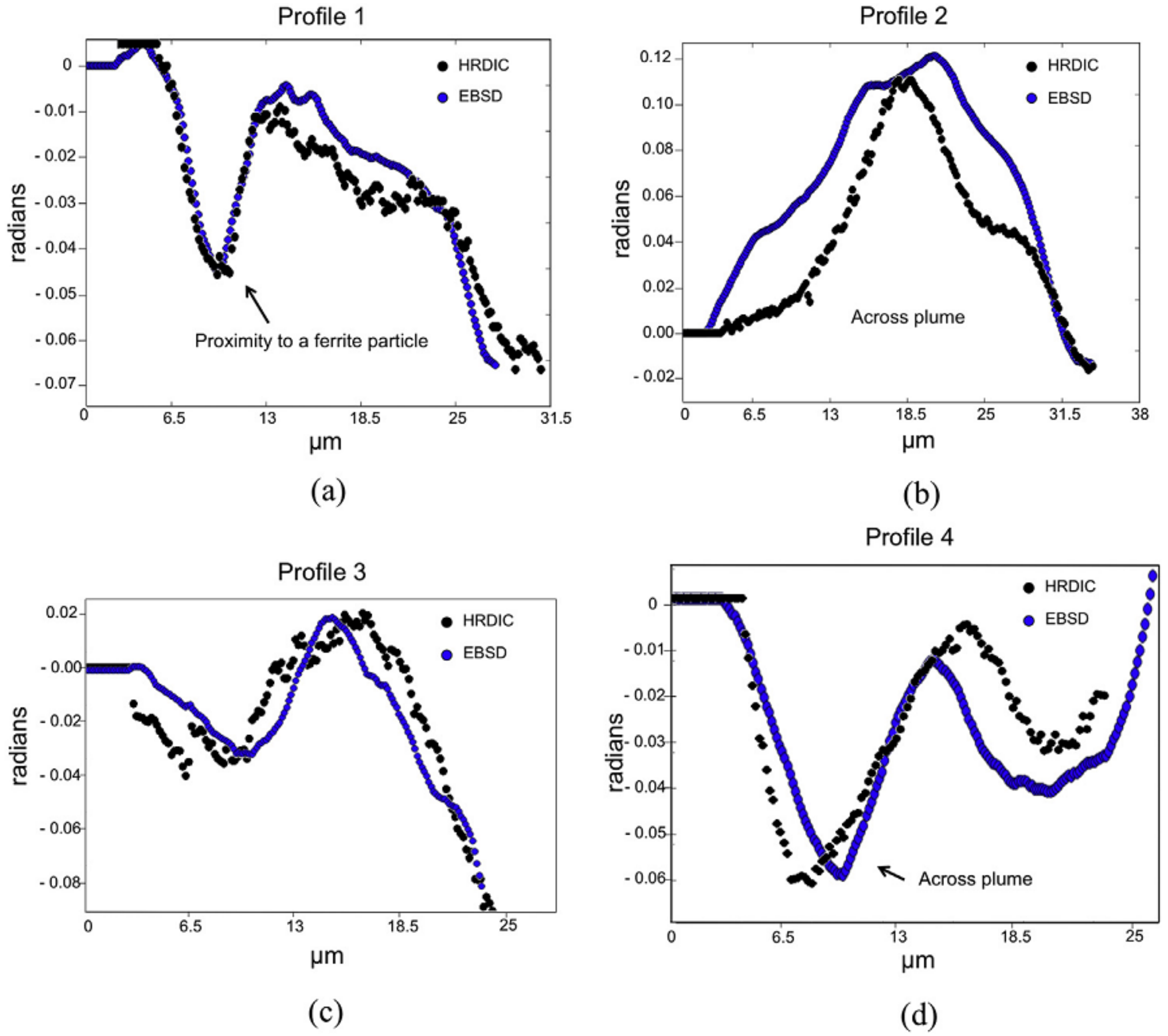


Fig. 7. Plots showing the variation of HRDIC and EBSD measured values of ϑ_3 for the profiles 1–in Figs. 3a and 6.

NB lines are along slip lines (P1?)

Di Gioacchino, Quinta da Fonseca, International Journal of Plasticity 74 2015

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EBSD line profile

```
%% get points along the line
[xx ,yy]=ginput(2);
%% find which grain it is
single_grain = findByLocation(grains,[xx(1)  yy(1)]);
%% create a line segment
lineSec =  [xx(1)   yy(1); xx(2) yy(2)];
%% get spatial orientation details along the lines
ebsd_line = spatialProfile(ebsd(grainSL),lineSec);

oroL=ebsd_line_.orientations;%orientation along line
oro1=ebsd_line_(1).orientations;%orientation at start point
mis2=inv(oroL)*oro1;%misorientation relative to start
mis2q=quaternion(mis2);%in quaternions
m0=real(mis2q);% [ m0 m1 m2 m3]
%rotation around z-axis
theta3_(:,:)=(180/pi)*mis2q.d.*(2*(acos(m0)))./sqrt(1-m0.^2);%%fabios
formula
```

DIC line profile

```
%% get strain tensor components
Exx(1,1,:) = ebsd_line_{nn}.Exx;    Exy(1,1,:) = ebsd_line_{nn}.Exy;
Eyx(1,1,:) = ebsd_line_{nn}.Eyx;    Eyy(1,1,:) = ebsd_line_{nn}.Eyy;
Ezeros = zeros(1,1,length(Exx));
%% create strain tensor - assume no volume change and no shear in z
F_DIC_=[Exx, Exy, Ezeros; …
      Eyx, Eyy, Ezeros;…
      Ezeros , Ezeros, Ezeros-Exx-Eyy];
 %% rotate the data so x-direction is parallel to slip direction
F_DIC_Rb = rotate_DIC_data(F_DIC_,slip_angle);
%% put data back into ebsd
    ebsd_line.Exx = F_DIC_Rb(1,1,:);
    ebsd_line.Eyy = F_DIC_Rb(2,2,:);
    ebsd_line.Exy = F_DIC_Rb(1,2,:);
    ebsd_line.Eyx = F_DIC_Rb(2,1,:);
```

DIC rotation to slip plane

```
function F_DIC_Rb = rotate_DIC_data(F_DIC_,slipangle)

if nargin==1
   slipangle=45;
end
%% create rotation about z-axis
r = rotation('axis',vector3d([0 0 1]),'angle',slipangle*pi/180);

%% rotate for each ebsd point within grain using matrix form- other options exist
rm = r.matrix;
F_DIC_Rb = zeros(size(F_DIC_,1),size(F_DIC_,2),size(F_DIC_,3));
for nj = 1:size(F_DIC_Rb,3)
   F_DIC_Rb(:,:,nj) = rm*F_DIC_(:,:,nj)*rm';
end
end
```

B

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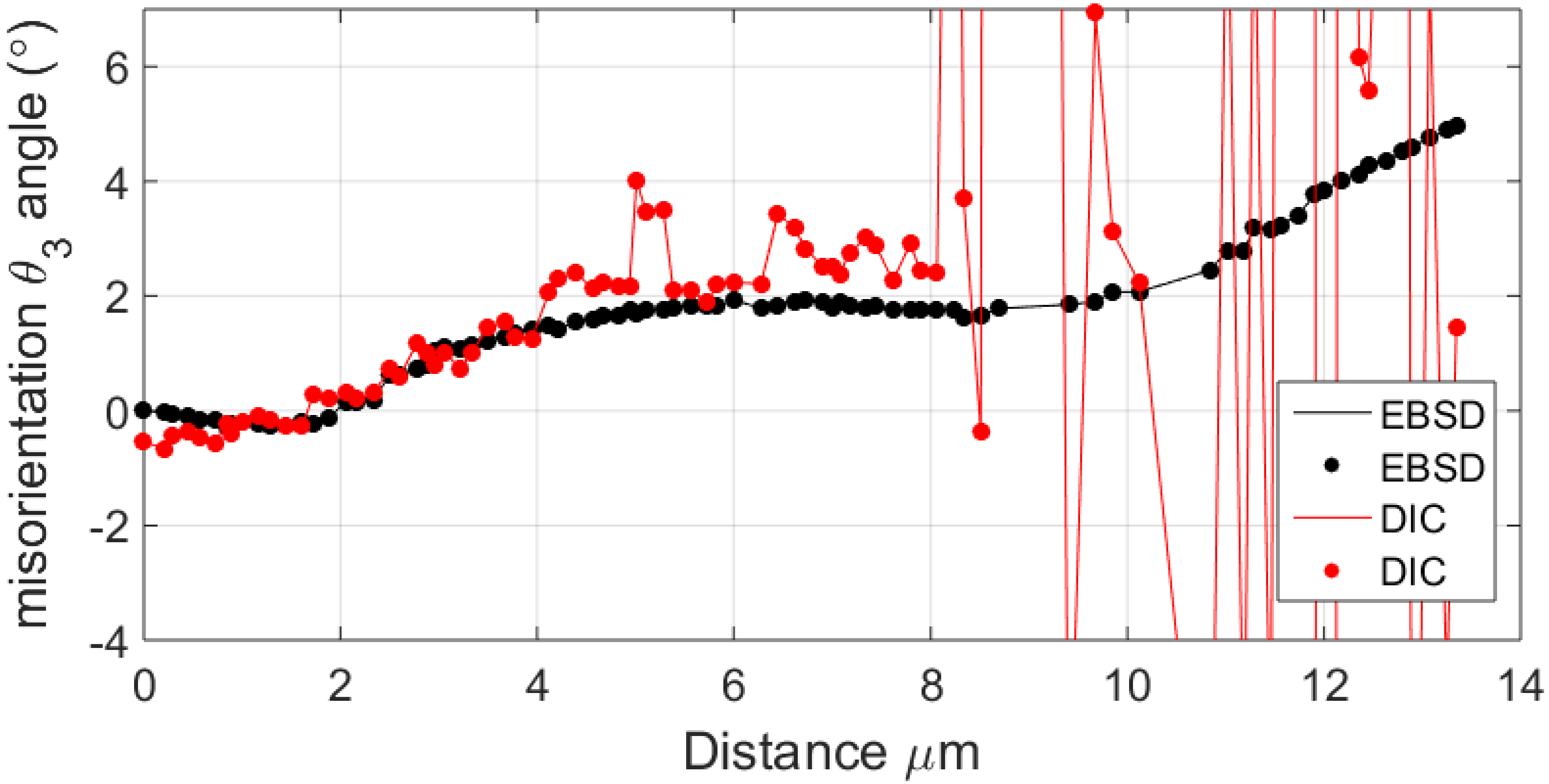
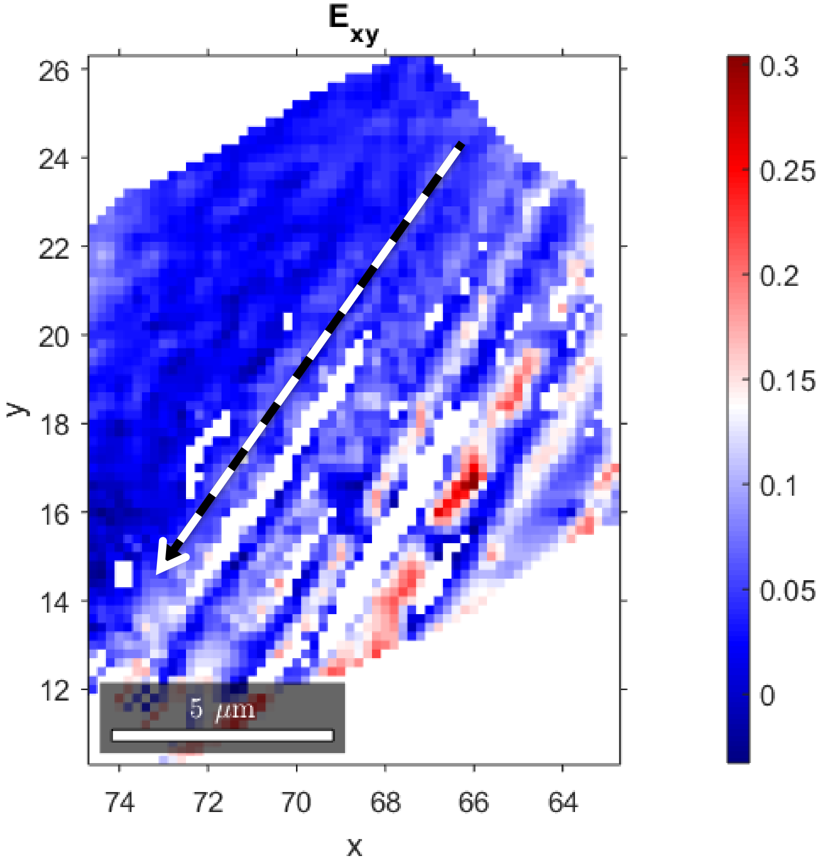
Swansea University





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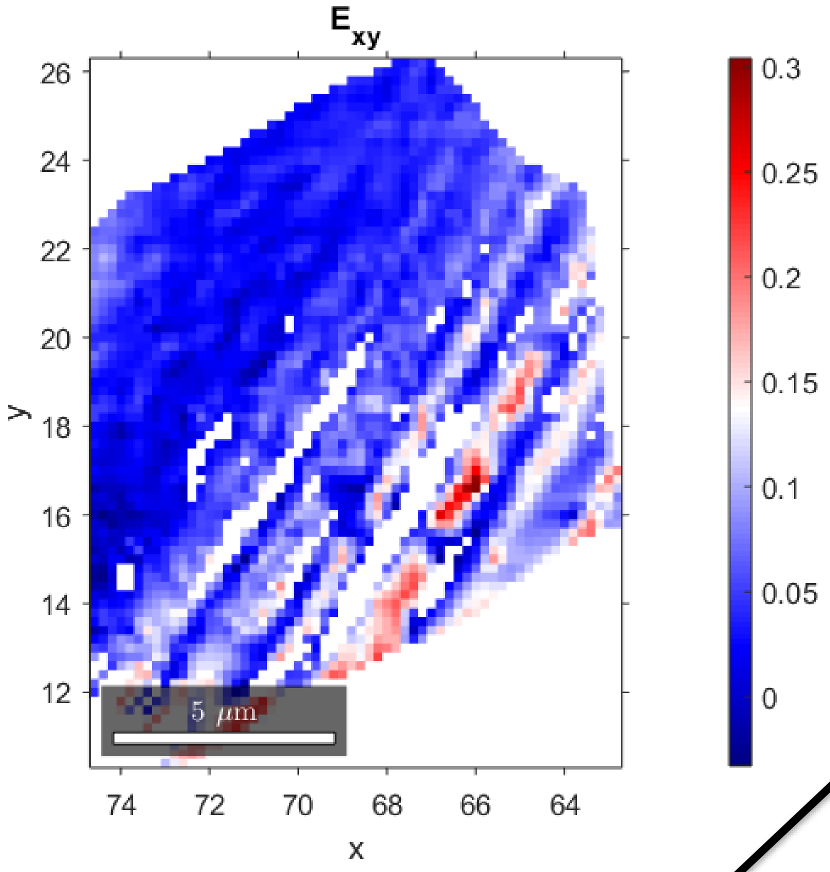
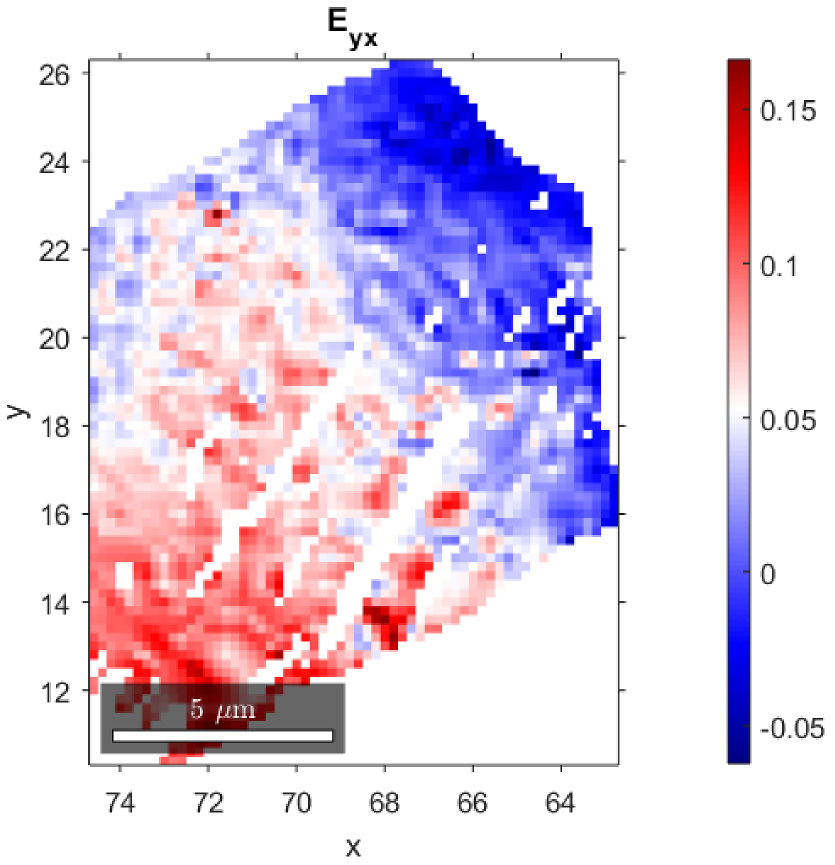
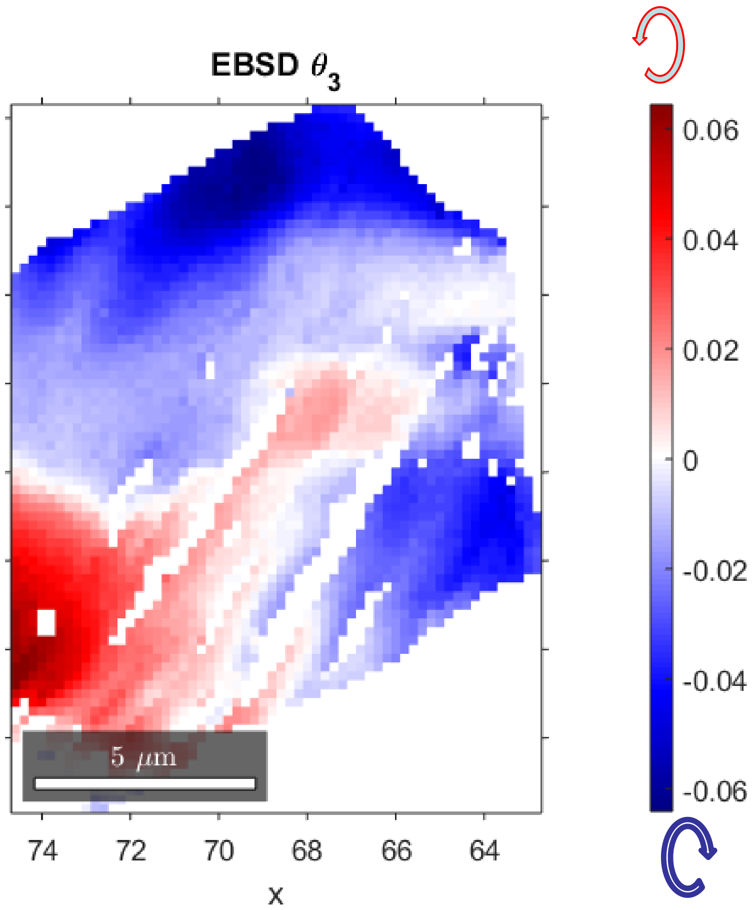
B

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

$$\vartheta_3 = F_{21}/F_{11} \quad (\text{with } X_1 \equiv s)$$



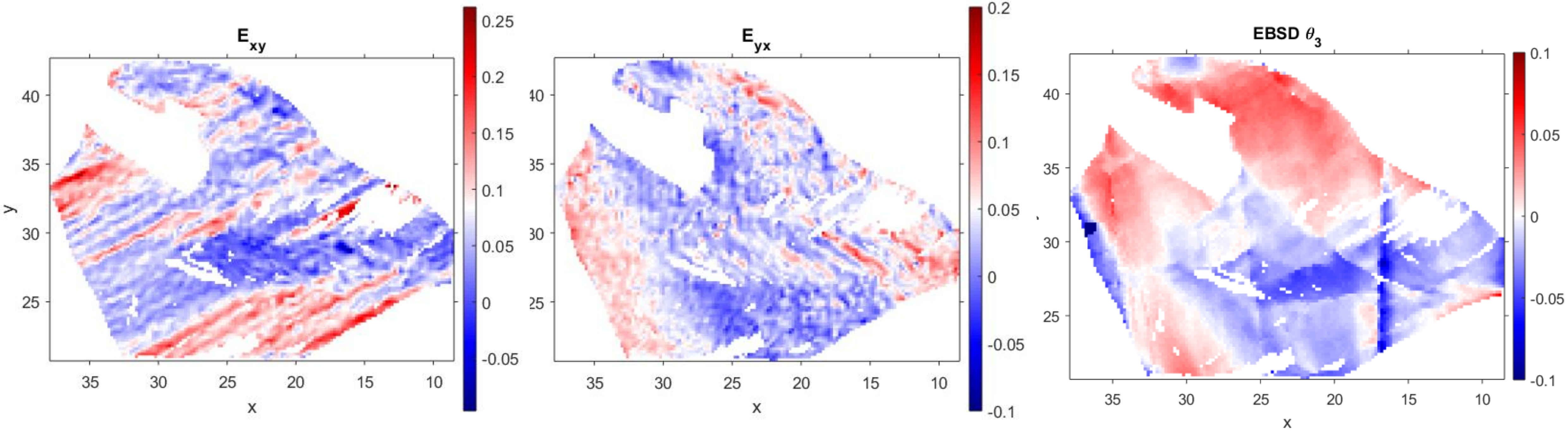




$$\vartheta_i = m_i \frac{2 \cdot \arccos(m^0)}{\sqrt{1 - (m^0)^2}}$$

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

$$\vartheta_3 = F_{21}/F_{11} \quad (\text{with } X_1 \equiv s)$$

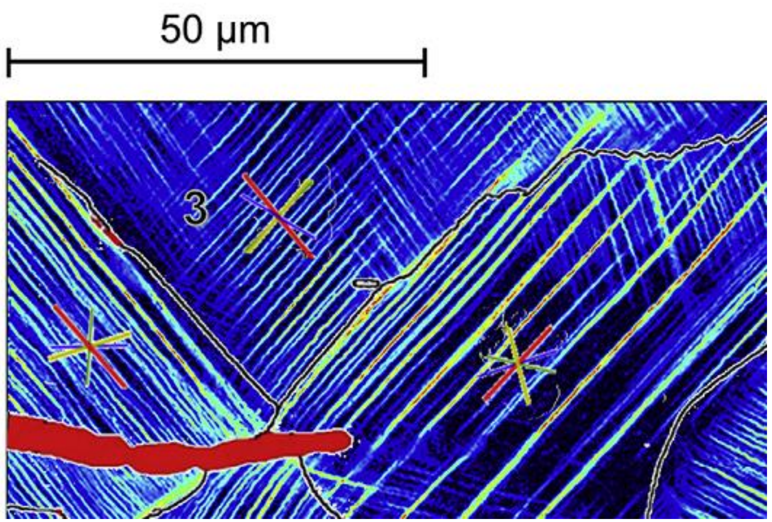


$$\vartheta_i = m_i \frac{2 \cdot \arccos(m^0)}{\sqrt{1-(m^0)^2}}$$

Image Analysis

Slip lines represent an image analysis problem
- Radon transform
- Hough transform
- Fourier transform

Get information on:
- Closeness of slip lines to slip planes
- Number/spacing of lines in different grains
- Pick out certain regions in maps
  - E.g. not on slip lines



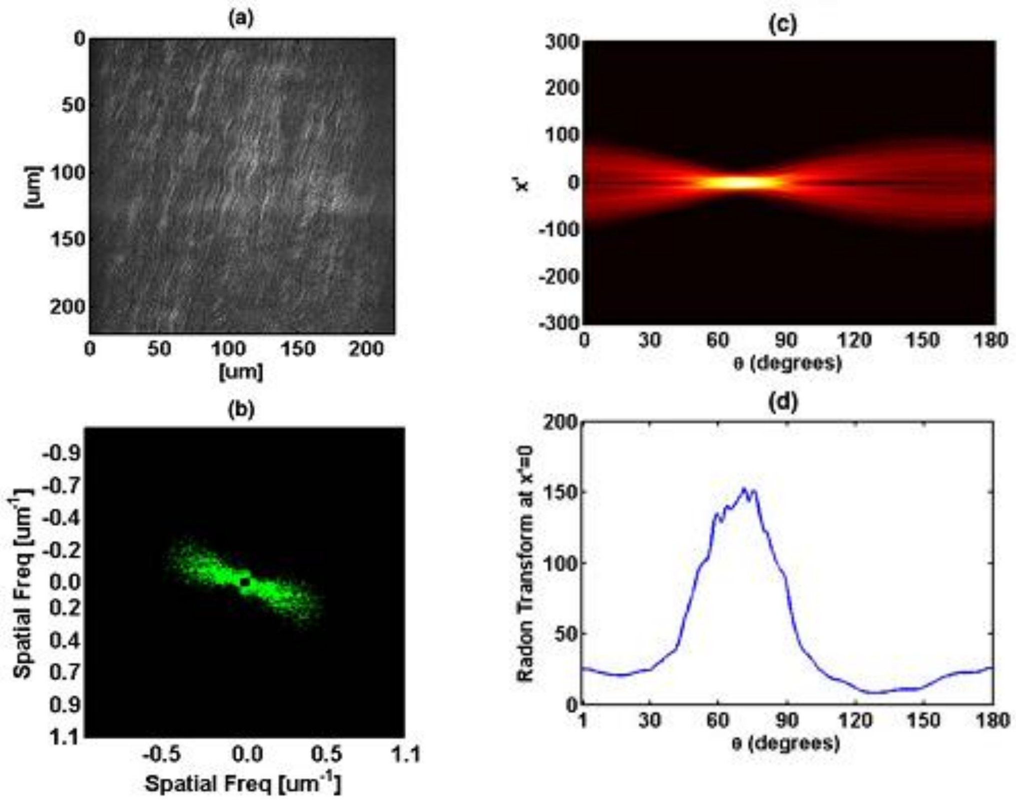


Fig. 1.
(Color online) Steps of the process performed in order to retrieve the orientation of fibers in cornea lamella. (a) Original second harmonic generation (SHG) image; (b) Filtered FFT image using a band pass filter (BPF) and processed using histogram adjustment and median filter; (c) Radon transform of the FFT transform showing peak at dominant orientation; (d) Plot of $x = 0$ of the Radon transform.

[1] Y. Mega, M. Robitaille, R. Zareian, J. Mclean, J. Ruberti, C. Dimarzio, Second Harmonic Generation Images, PMC. 37 (2013) 3312–3314.

Crystal Plasticity Models

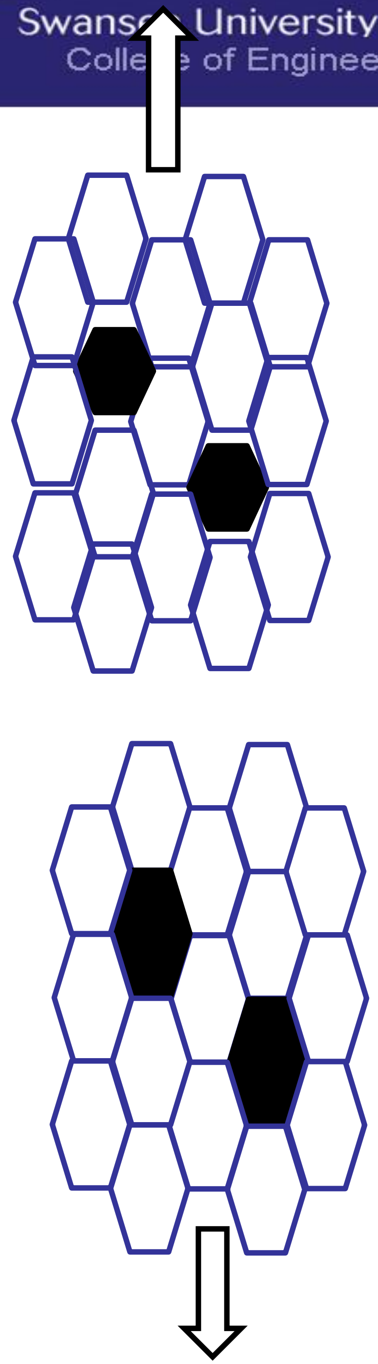
In crystal plasticity models we have two extremes

A. Assume all grains have the same stress state

- Schmid factor / Sachs model
- Best use:
  - single crystals
  - when we can define stress state of a grain
  - HCP (anisotropic alloys)

B. Assume all grains have the same strain state

- Taylor model
- Best use:
  - Averaging over many grains
  - Predicted texture changes sharper than reality
  - For isotropic crystal symmetries (e.g. not great for HCPs)



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Prifysgol Abertawe Swansea University

Slip systems

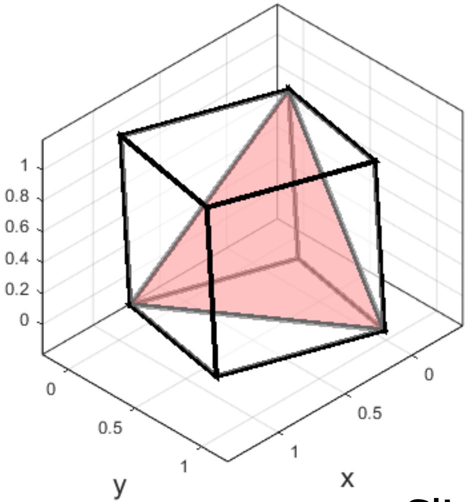
Table 1
The glide systems in f.c.c. crystals

Glide plane	Glide direction		
(111)	1 [1$\bar{1}$0]	2 [10$\bar{1}$]	3 [01$\bar{1}$]
($\bar{1}$11)	4 [110]	5 [101]	6 [01$\bar{1}$]
(1$\bar{1}$1)	7 [110]	8 [10$\bar{1}$]	9 [011]
(11$\bar{1}$)	10 [1$\bar{1}$0]	11 [101]	12 [011]

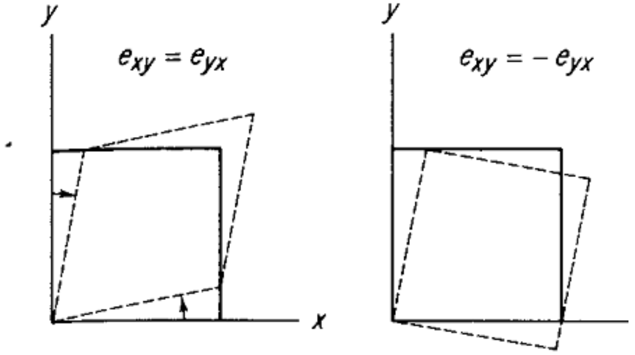
Table 2
The coefficients $e_{ij,n}$ for the twelve glide systems of f.c.c. crystals given in Table 1

ij \ n	1	2	3	4	5	6	7	8	9	10	11	12
11	1	1	0	$\bar{1}$	$\bar{1}$	0	1	1	0	1	1	0
12	1	1	0	1	1	0	$\bar{1}$	$\bar{1}$	0	1	1	0
13	1	1	0	1	1	0	1	1	0	$\bar{1}$	$\bar{1}$	0
21	$\bar{1}$	0	1	$\bar{1}$	0	$\bar{1}$	1	0	1	$\bar{1}$	0	1
22	$\bar{1}$	0	1	1	0	1	$\bar{1}$	0	$\bar{1}$	$\bar{1}$	0	1
23	$\bar{1}$	0	1	1	0	1	1	0	1	1	0	$\bar{1}$
31	0	$\bar{1}$	$\bar{1}$	0	$\bar{1}$	1	0	$\bar{1}$	1	0	1	1
32	0	$\bar{1}$	$\bar{1}$	0	1	$\bar{1}$	0	1	$\bar{1}$	0	1	1
33	0	$\bar{1}$	$\bar{1}$	0	1	1	0	$\bar{1}$	1	0	$\bar{1}$	$\bar{1}$

$\cdot \frac{1}{\sqrt{6}}$



REF: Dieter 1986



$$\begin{Bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{Bmatrix}$$

Slip system deformation tensor

$$\begin{bmatrix} 1 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \end{bmatrix}$$

Pure strain component

$$\begin{bmatrix} 1 & 0 & 0.5 \\ 0 & \bar{1} & \overline{0.5} \\ 0.5 & \overline{0.5} & 0 \end{bmatrix}$$

Pure rotation component

$$\begin{bmatrix} 0 & 1 & \overline{0.5} \\ \bar{1} & 0 & 0.5 \\ 0.5 & \overline{0.5} & 0 \end{bmatrix}$$

REF: H.J. Bunge, Some applications of the Taylor theory of polycrystal plasticity, Krist. Und Tech. 5 (1970) 145–175.

Sachs model

$$\tau_R = \frac{P\cos\lambda}{A/\cos\phi} = \frac{P}{A}\cos\phi\cos\lambda$$

Only slip system(s) with max Schmid factor are active

$$\dot{\sigma}_{11}\mu_{11}^{i} = \dot{\tau}^{i} = \sum_{j} h^{ij}\dot{\gamma}^{j}$$

Hardening component, slip activity

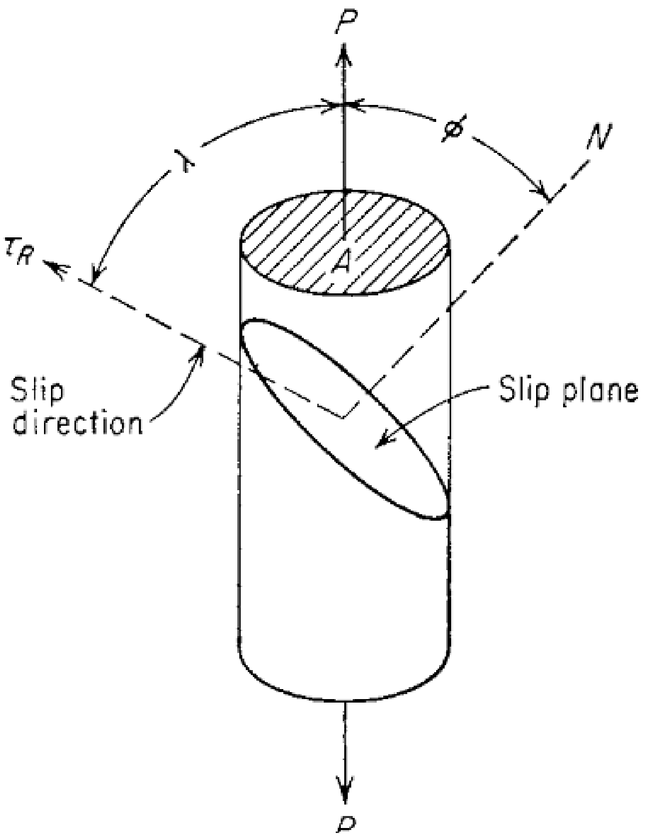


Figure 4-18 Diagram for calculating critical resolved shear stress.

REF: Bjorn Clausen, Characterisation of Polycrystal Deformation by Numerical Modelling and Poly crystal Deformation by Modelling, Numerical Measurements, Neutron Diffraction, Riso National Laboratory, 1997.

REF: Dieter 1986

c

Taylor Model

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Slip system strain tensor — Macroscopic strain tensor

$$\sum_{s=1}^{12} b_s \begin{bmatrix} \varepsilon_{11}^{c\prime} & \varepsilon_{12}^{c\prime} & \varepsilon_{13}^{c\prime} \\ \varepsilon_{21}^{c\prime} & \varepsilon_{22}^{c\prime} & \varepsilon_{23}^{c\prime} \\ \varepsilon_{31}^{c\prime} & \varepsilon_{32}^{c\prime} & \varepsilon_{33}^{c\prime} \end{bmatrix} = \begin{bmatrix} E_{11}^{c\prime} & E_{12}^{c\prime} & E_{13}^{c\prime} \\ E_{21}^{c\prime} & E_{22}^{c\prime} & E_{23}^{c\prime} \\ E_{31}^{c\prime} & E_{32}^{c\prime} & E_{33}^{c\prime} \end{bmatrix}$$

e.g. for tension

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \overline{0.5} & 0 \\ 0 & 0 & \overline{0.5} \end{bmatrix}$$

Slip activity

$$\min \sum_{s=1}^{12} b_s$$

Rotation

$$r_k = \sum_{s=1}^{12} b_s \begin{bmatrix} \omega_{11}^{c\prime} & \omega_{12}^{c\prime} & \omega_{13}^{c\prime} \\ \omega_{21}^{c\prime} & \omega_{22}^{c\prime} & \omega_{23}^{c\prime} \\ \omega_{31}^{c\prime} & \omega_{32}^{c\prime} & \omega_{33}^{c\prime} \end{bmatrix}$$

Table 2

The coefficients $e_{ij,n}$ for the twelve glide systems of f.c.c. crystals given in Table 1

ij \ n	1	2	3	4	5	6	7	8	9	10	11	12
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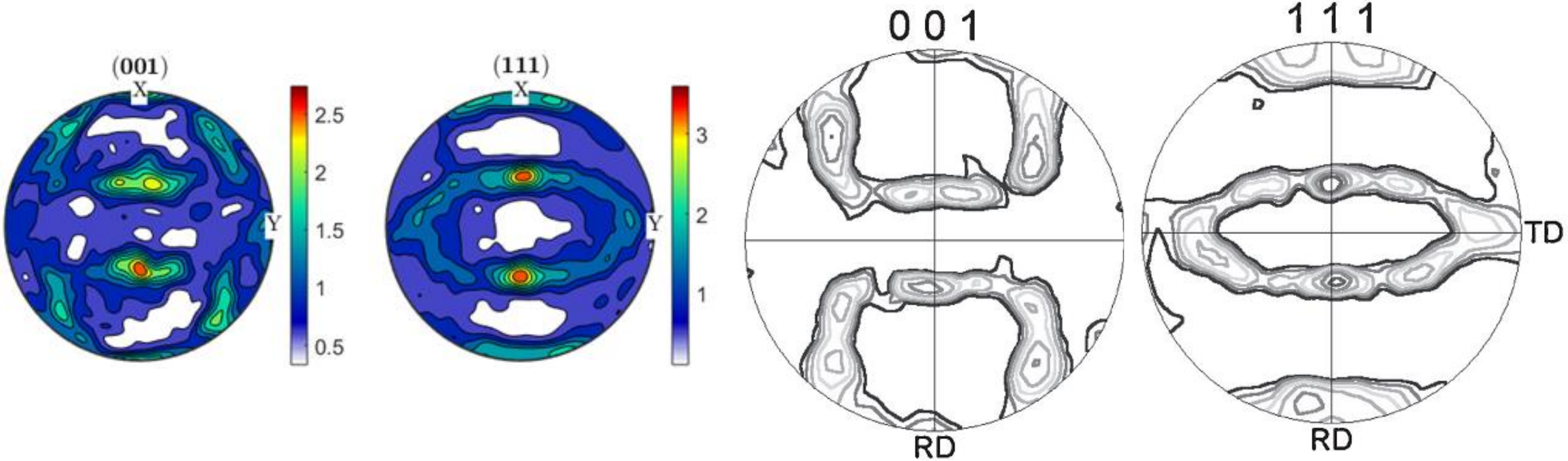
12	1	1	0	1	1	0	$\bar{1}$	$\bar{1}$	0	1	1	0
13	1	1	0	1	1	0	1	1	0	$\bar{1}$	$\bar{1}$	0
21	$\bar{1}$	0	1	$\bar{1}$	0	$\bar{1}$	1	0	1	$\bar{1}$	0	1
22	$\bar{1}$	0	1	1	0	1	$\bar{1}$	0	$\bar{1}$	$\bar{1}$	0	1
23	$\bar{1}$	0	1	1	0	1	1	0	1	1	0	$\bar{1}$
31	0	$\bar{1}$	$\bar{1}$	0	$\bar{1}$	1	0	$\bar{1}$	1	0	1	1
32	0	$\bar{1}$	$\bar{1}$	0	1	$\bar{1}$	0	1	$\bar{1}$	0	1	1
33	0	$\bar{1}$	$\bar{1}$	0	1	1	0	$\bar{1}$	1	0	$\bar{1}$	$\bar{1}$

$\cdot \frac{1}{\sqrt{6}}$

Pure strain component

$$\begin{bmatrix} 1 & 0 & 0.5 \\ 0 & \bar{1} & \overline{0.5} \\ 0.5 & \overline{0.5} & 0 \end{bmatrix}$$

FCC rolling example Texture Predictions



Jung, K.-H., Kim, D.-K., Im, Y.-T., & Lee, Y.-S. (2013). Metal. Materials Transactions, 54(5), 769–775.

BCC rolling example Texture Predictions

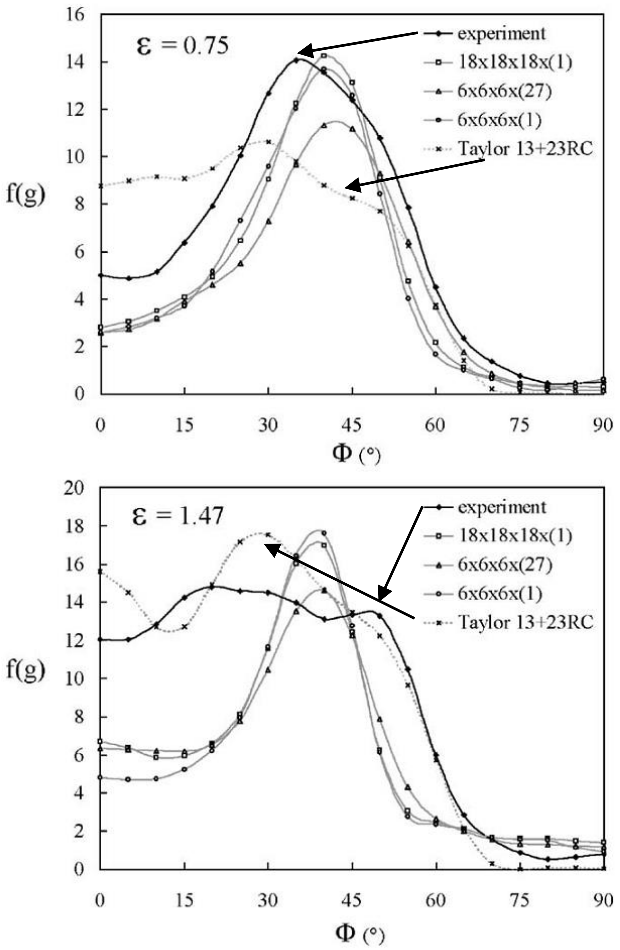
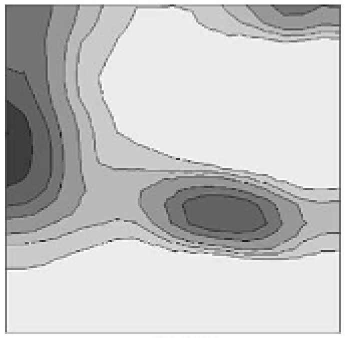


Fig. 12. Experimental and predicted orientation densities along the α fibre. The results for the Taylor RC model have been subject to the additional Gaussian spread which gives best correlation with the relevant experimental texture.

Experimental



0.75

Models

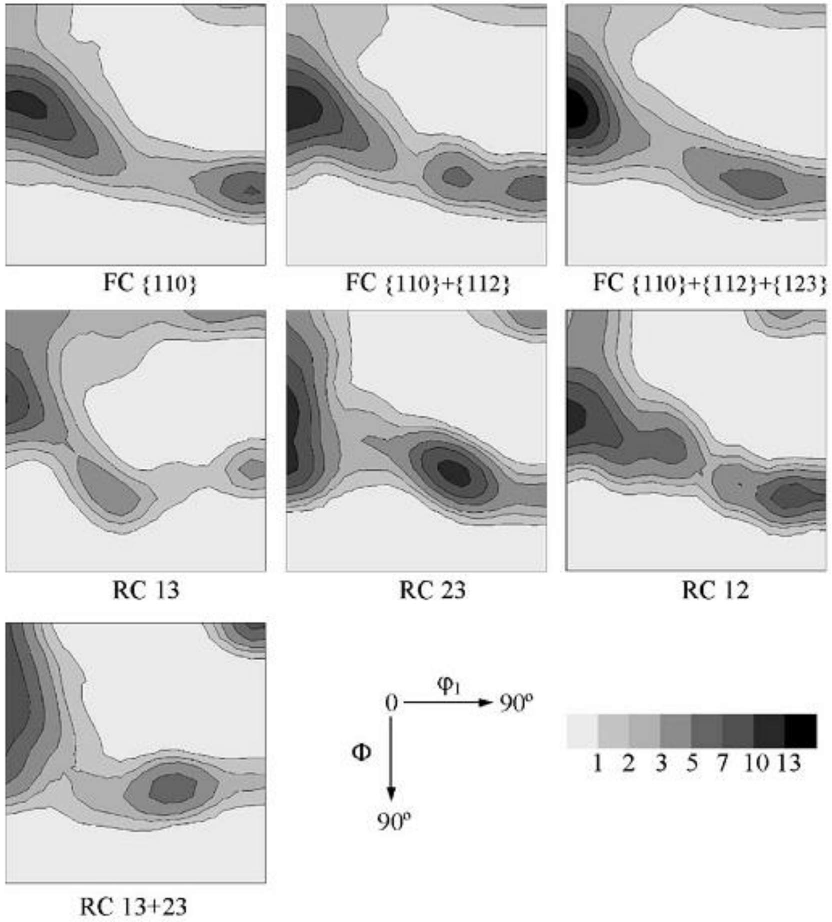


Fig. 4. Sections through ODFs at Euler angle $\varphi_2 = 45°$ of textures calculated using Taylor modelling at a strain of 0.75, which have been convoluted with a Gaussian of 8° spread. The contour levels shown are multiples of random density, note that these are significantly greater than used for the experimental results. The top row shows the effect of slip planes on FC prediction, the lower four show the effect of relaxed constraints.

Taylor Model Variations
RC = Relaxed Constraints
FC = Full Constraints
18x18x18 = CPFEM

P.S. Bate, J. Quinta da Fonseca, Texture development in the cold rolling of IF steel, Mater. Sci. Eng. A. 380 (2004) 365–377. doi:10.1016/j.msea.2004.04.007.

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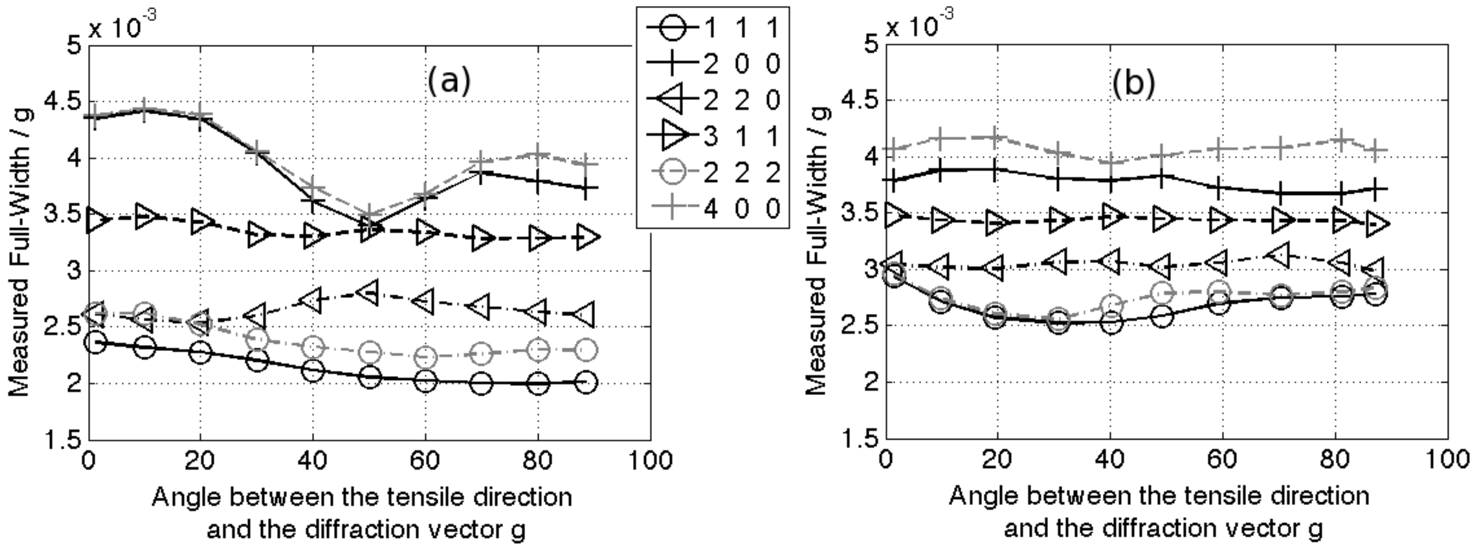
Extra Parameters

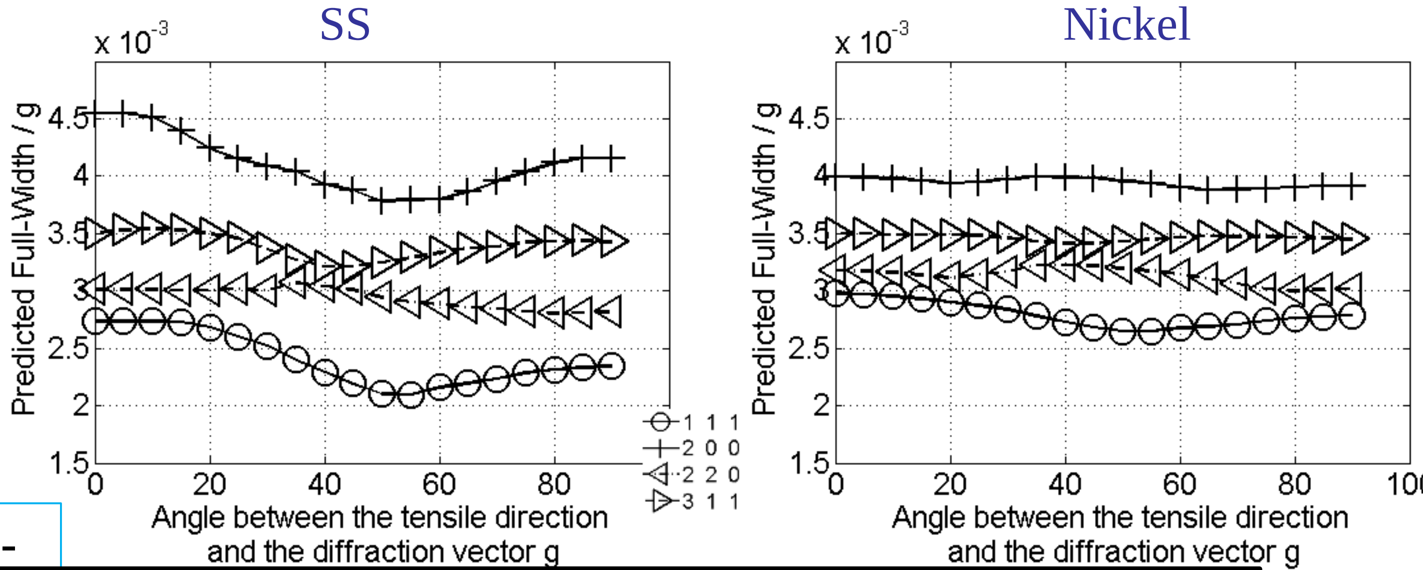
	Strain	Edge Percentage % (k_3)	Dislocation density variation % (k_1)	Mobile Dislocation % (k_2)
Stainless Steel	Fatigue *	53%	33%	100%
	10%	49%	0%	33%
	16%	56%	0%	50%
	30%	52%	0%	24%
Nickel	10%	100%	33%	23%
	30%	94%	24%	15%

More edge for Ni- expected

Ni has broadening related to Taylor factor to account for arrangement changes

Ni has less mobile dislocation e.g. from cross-slip (e.g. a flatter change of FW)

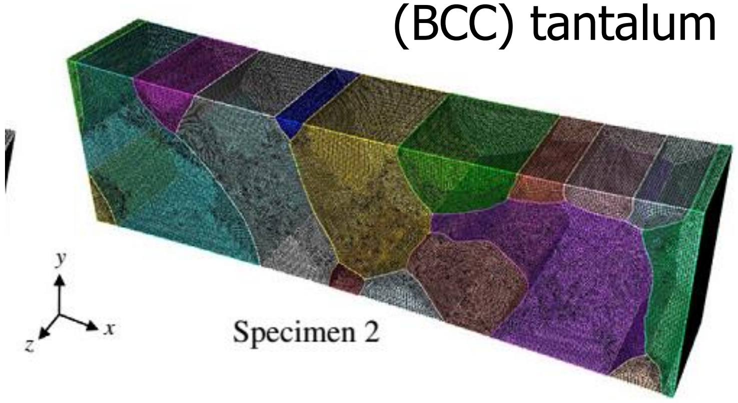


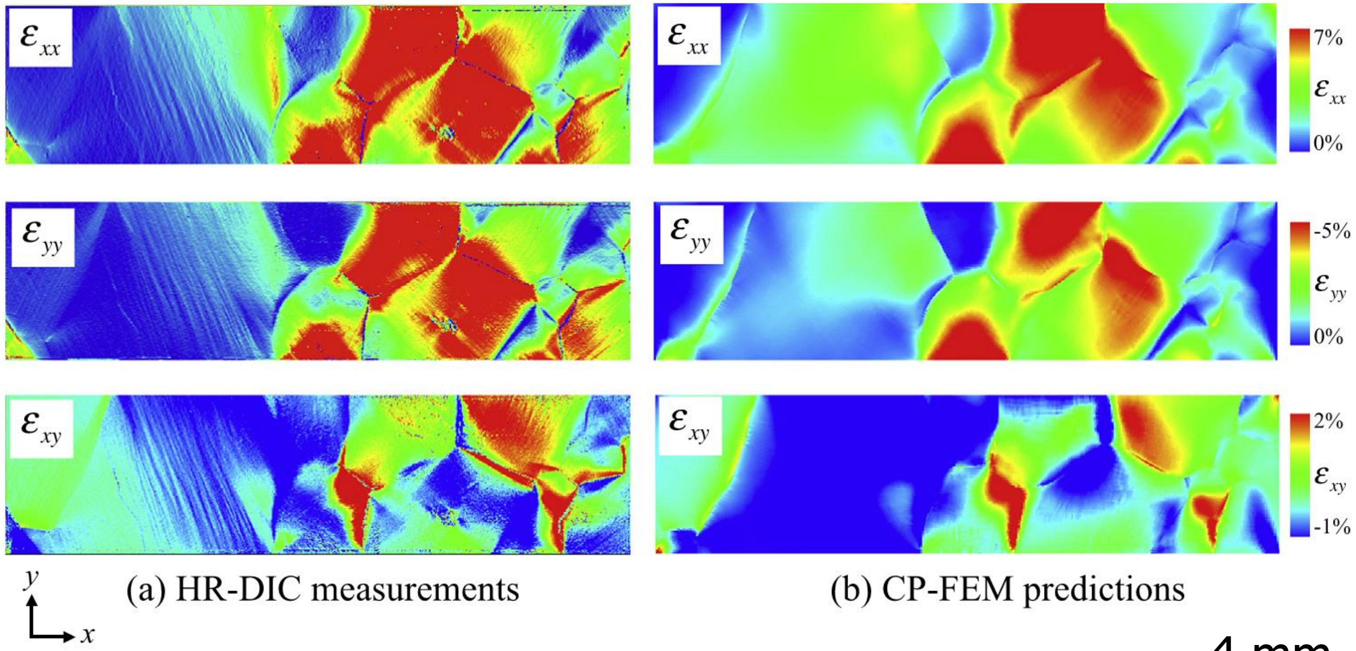


T.H. Simm, P.J. Withers, J. Quinta Da Fonseca, Peak broadening anisotropy in deformed face-centred cubic and hexagonal close-packed alloys, J. Appl. Crystallogr. 47 (2014) 1535–1551.

Crystal Plasticity Modelling

(BCC) tantalum





4 mm

Fig. 6. A comparison of measured and predicted surface strain … (Points B–C in Fig. 4(b)).

A reasonable correlation for this situation.
- Large columnar grains

BUT in most cases it is very difficult to model changes at the grain scale
- We don't know orientation details below surface
- Chaotic system (small changes big effects)
- Length scale issues- CPFEM often smoother than DIC / EBSD even when we match cell sizes

So currently looking at selected grains / orientations maybe a better idea

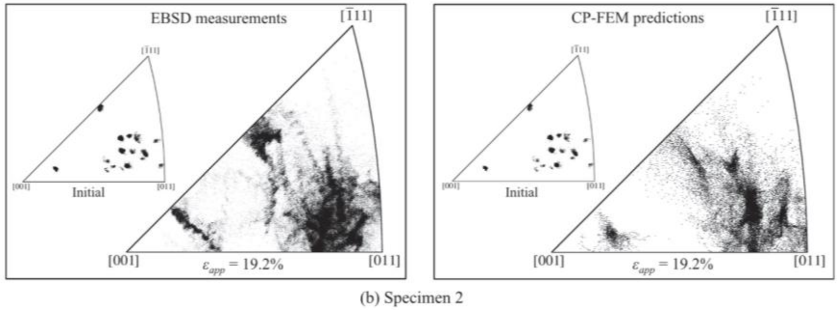


Fig. 10. EBSD measurements and CP-FEM predictions of deformed textures. (a) Specimen 1 (ε_{app} = 6.8%) and (b) Specimen 2 (ε_{app} = 19.2%).

REF: H. Lim, J.D. Carroll, C.C. Battaile, T.E. Buchheit, B.L. Boyce, C.R. Weinberger, Int. J. Plast. 60 (2014) 2014.

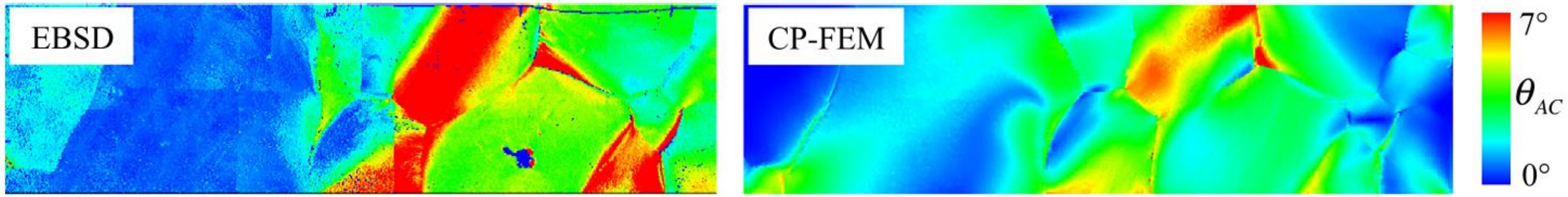


Fig. 13. A comparison of misorientation angles obtained from EBSD measurements and the CP-FEM simulation at 4.2% applied strain for specimen 1 (Point C in Fig. 4) relative to the initial crystal orientation (Point A).

Schmid factor & Taylor factor vs DIC

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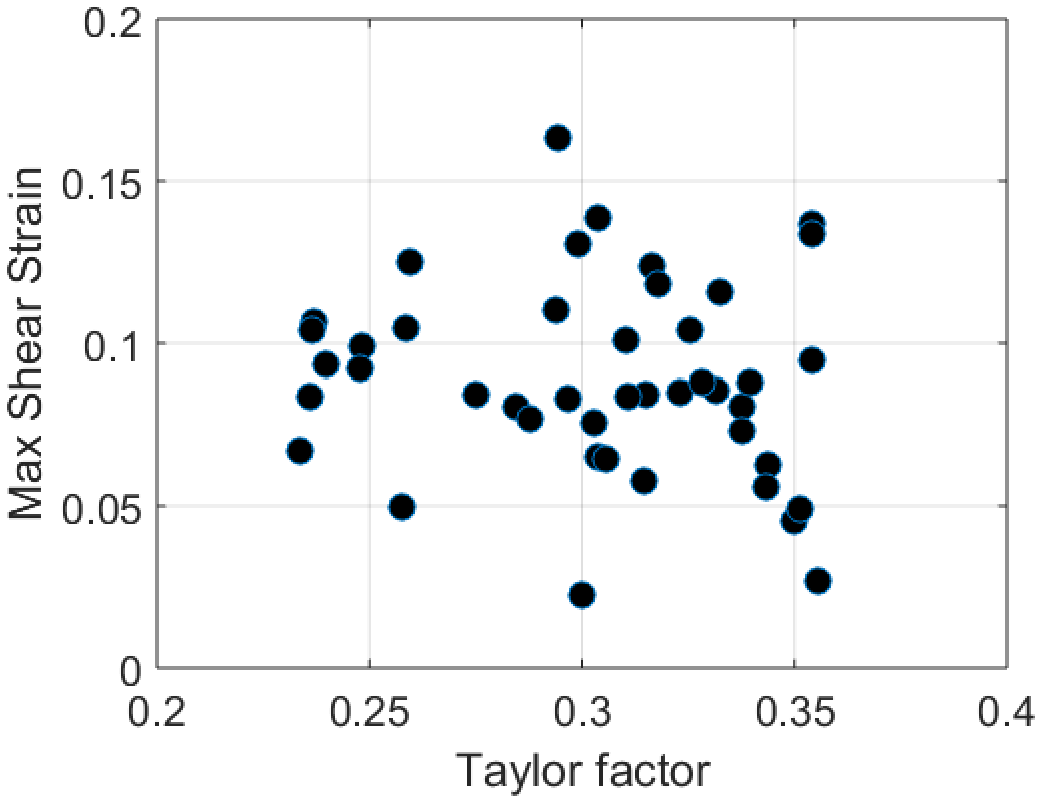

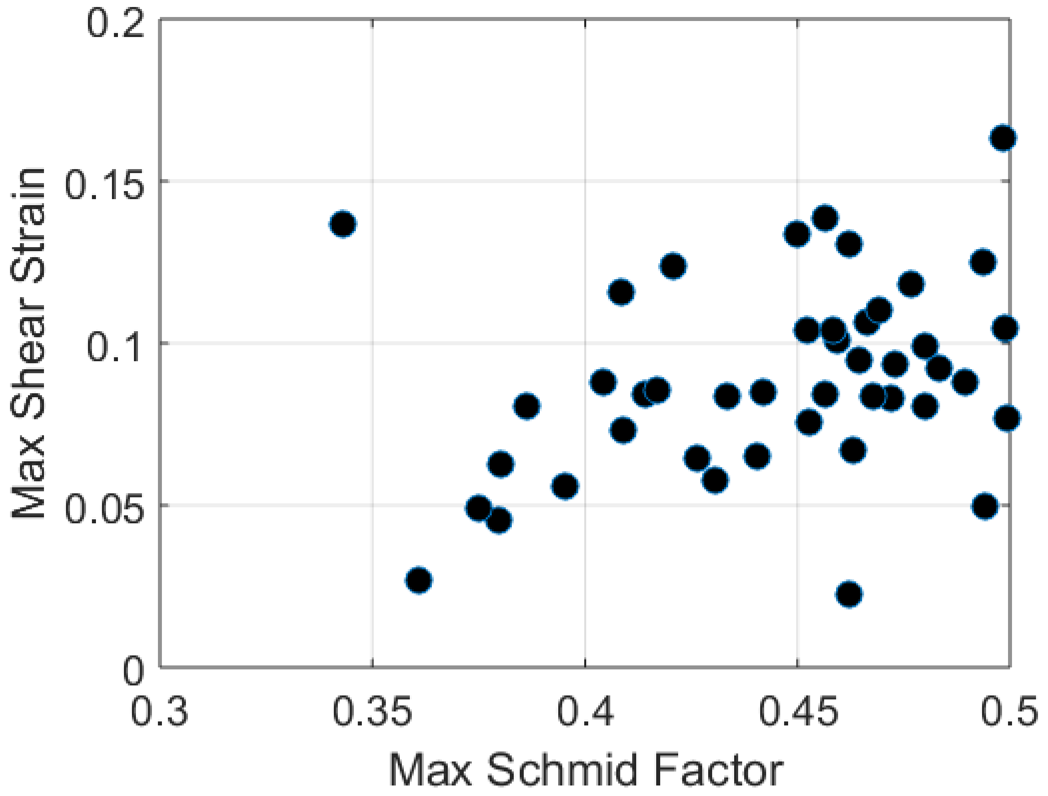

Is there a better variable to compare EBSD with DIC?

- Orientation change from Taylor
- When multiple slip systems have high Schmid factor?
- Find a better way to ignore strain close to grain boundaries?

Uses high mag map and 3 x 3

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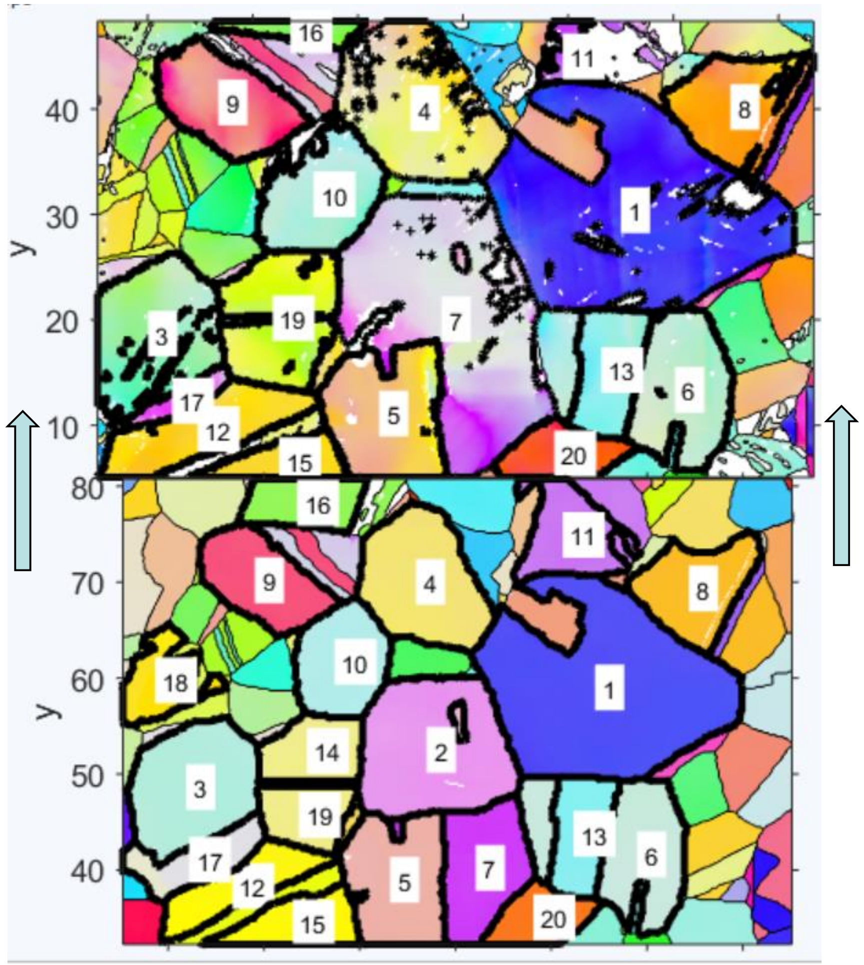
c

Steps



grains2
ebsd2

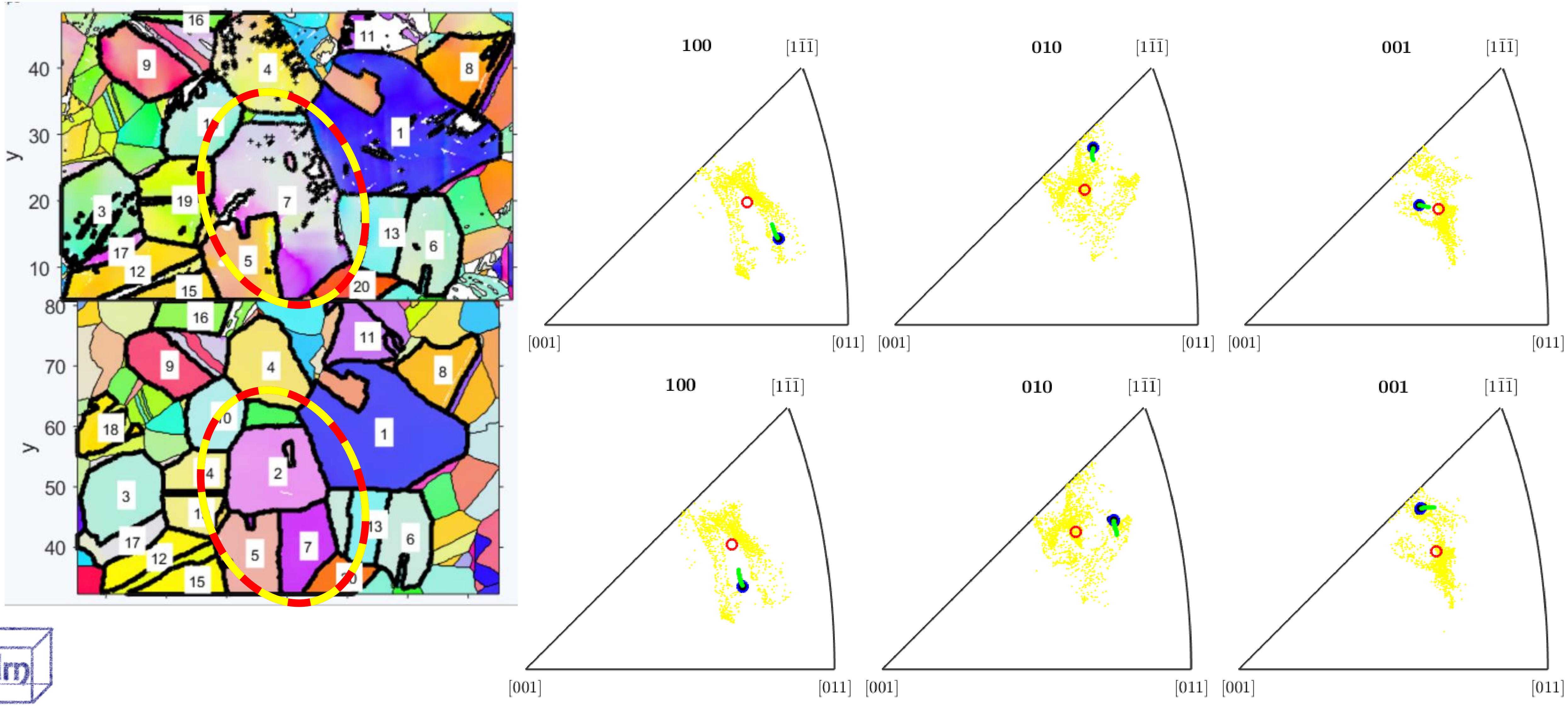
grains1
ebsd1

```
figure(1)
plot(grains1.boundary)
[x1_ y1_]=ginput(1);
figure(2)
[x2_ y2_]=ginput(1);
plot(grains2.boundary)

x=x+xadj;y=y+yadj;

figure(2)
posmax2=grains2.findByLocation([x,y]);
```

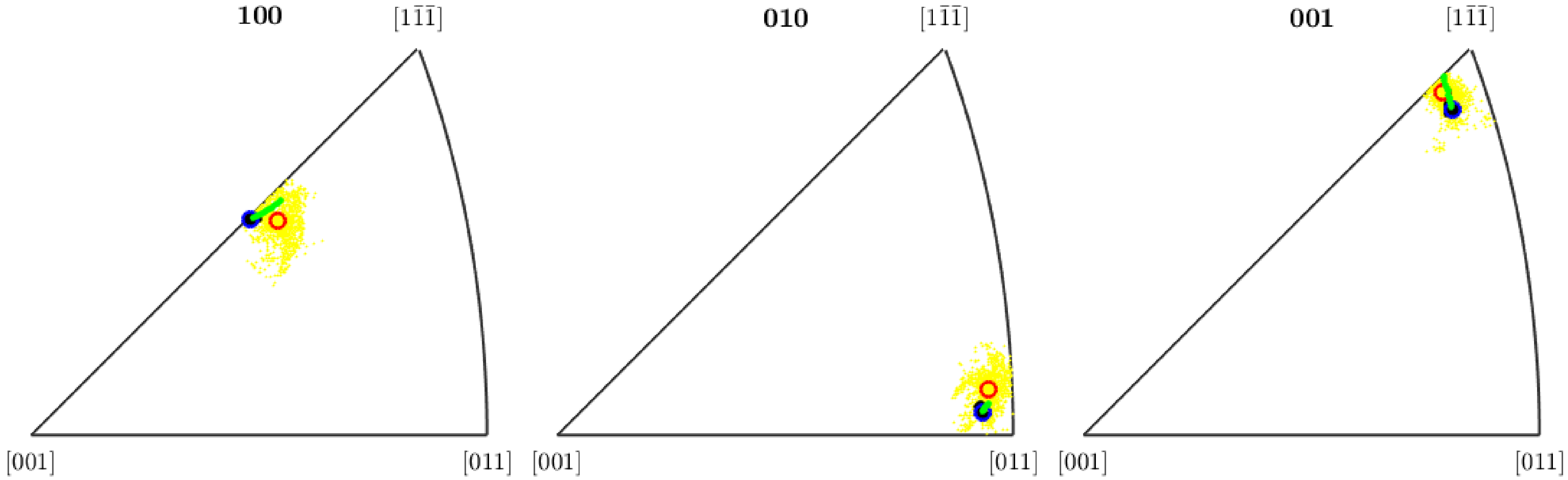
(may want to add component to grains)

c

Local Orientation changes



Taylor orientation predictions of grains



D

Martensite: identify variants

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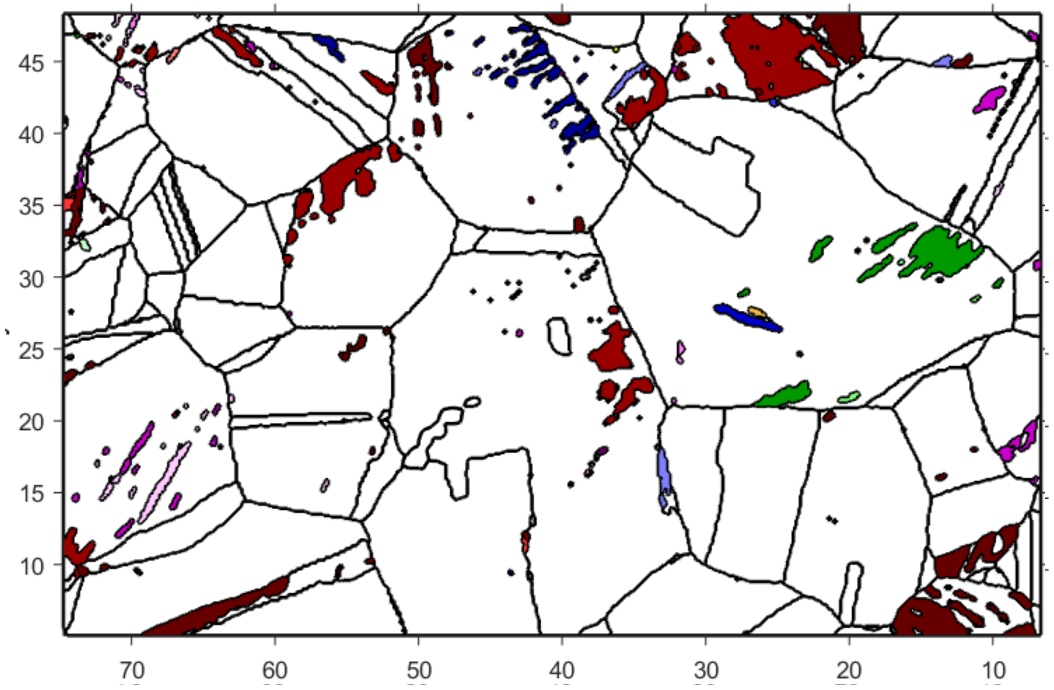
Identify martensite boundaries by type

```
MO=gB(phases{2},phases{3}(1:7)).misorientation;%the gb misorientation of boundaries between bcc and fcc,
ind_5deg{n} =angle(KCO(n)*inv(MO))<5*degree;%find boundaries that are
%define vectors of KS variants then use map to define misorientation
KCO(n)=orientation('map', DFCC(n), DBCC(n), PFCC(n), PBCC(n));
ind_5deg{n} =angle(KCO(n)*inv(MO))<5*degree;%find boundaries that are within 5degrees of a particular variant - output is logical for boundaries in gB_
```



Convoluted way to plot colors

```
indKS=ind_5deg{varno};
    % the grain boundaries of the particular variants
    gBKS=gB_(indKS);
    % and their grain IDs
    id_KS=gBKS.grainId;
idBCC=unique(id_KS(:,2));
% create new grains for each variant
grains2('iron b').color=col{n};
grains3_{n}=grains2(idBCC);
```

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Martensite: quantify variants


```
indKS=ind_5deg{varno};
    % the grain boundaries of the particular variants
gBKS=gB_(indKS);
    % and their grain IDs
id_KS=gBKS.grainId;
    % id of bcc grains for the particular variant
idBCC=unique(id_KS(:,2));
    % unique pairs of FCC + BCC
[idFCCBCC, ~, i2]=unique(id_KS,'rows');
% length of each pair so idFCCBCC = [idFCC idBCC lengthofGB]
used to differentiate when martensite has two parents
for nn=1:length(idFCCBCC)
        idFCCBCC(nn,3) =  sum(i2==nn);
         % create a variable idFCC that has parentID of each martensite
        xpos = find(idBCC(nn)==idFCCBCC(:,2));
        idFCC(nn) = idFCCBCC(xpos(find(idFCCBCC(xpos,3)== max(idFCCBCC(xpos,3)))),1);
end
```

Martensite grain may be represented by >1 KS variant. So pick one with the longest boundary

D


```matlab
%% add properties about variants to parent grains
IDss2 =sortrows(IDss_,4);
idfccs = unique(IDss2(:,4));
%IDss=[ varID , var no. , length boundary , parentID]
for nn=1:length(idfccs)
    posx = find( IDss2(:,4) == idfccs(nn) );
    varIDsC{ nn } = IDss2(posx,1);
    grains(idfccs(nn)).prop.varSum = length(posx);%number of variants
    area1 = sum( grains( varIDsC{ nn } ).area );%area of variants
    areaT = area1 + grains(idfccs(nn)).area;%area of FCC grain + variants
    grains(idfccs(nn)).prop.varAreaPC =100* area1 / areaT;
    grains(idfccs(nn)).prop.varArea = area1;
end
if length(varIDsC)<length(grains)
   varIDsC( length(grains) )={[]};
end
grains.prop.varIDs =  varIDsC;
```

```matlab
%% add properties about variants to daughter (variant) grains

idbccs = unique(IDss2(:,1));
for nn=1:length(idbccs)
    posx = find( IDss2(:,1) == idbccs(nn) );
    grains(idbccs(nn)).prop.parentID = IDss2(posx,4);
    grains(idbccs(nn)).prop.varNo = IDss2(posx,2);
    varColorC{ idbccs(nn) } = col{ IDss2(posx,2) };
end
%%
for nn=1:length(grains)
    varArea(nn) = grains(nn).varArea;
    varNo(nn) = grains(nn).varNo;
    grArea(nn) = grains(nn).area;
end

totArea = sum( grArea );
for n=1:24
   pos = n == varNo;
   varAreaAll(n) = sum( grArea(pos) ) / totArea;
   varSumAll(n) = sum( (pos) );
end
```

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Can do a similar thing using merge, but we don't have the variant info

```
[grains_merged,parentId] = merge(grains, gBKS);
hw = waitbar(0,'Updating Variant info. Please wait...');

% scroll through each FCC grain above ECD of 1
% find the position of the grain that matches x,y of merged_grain
% gbM2_ID=[];
% grains_merged2 = grains;
for n=1:length(grains_merged)

    if grains_merged(n).phase==2%is BCC
        daughters{n} = find(n==parentId);
        if length(daughters{n})==1%% BCC phase with no FCC
            grains_merged(n).phase = 0;
            grains_merged(n).prop.BCCpc = 100;
            grains_merged(n).prop.daughterNo = 1;
            grains_merged(n).prop.daughterArea = grains_merged(n).area;
            grains_merged(n).prop.daughterAreapc = 100;
        else %%transformed grains
            grains_merged(n).prop.BCCpc = 0;
            grains_merged(n).prop.daughterNo = length(daughters{n});

            bccBinary =grains(daughters{n}).phase==2;%find which daughters are bcc
            fccBinary =grains(daughters{n}).phase==1;%find which daughters are fcc
            bCCgrainNo{n} = daughters{n}(bccBinary);%%the bcc grain nos
            fCCgrainNo{n} = daughters{n}(fccBinary);%%the fcc grain nos
```

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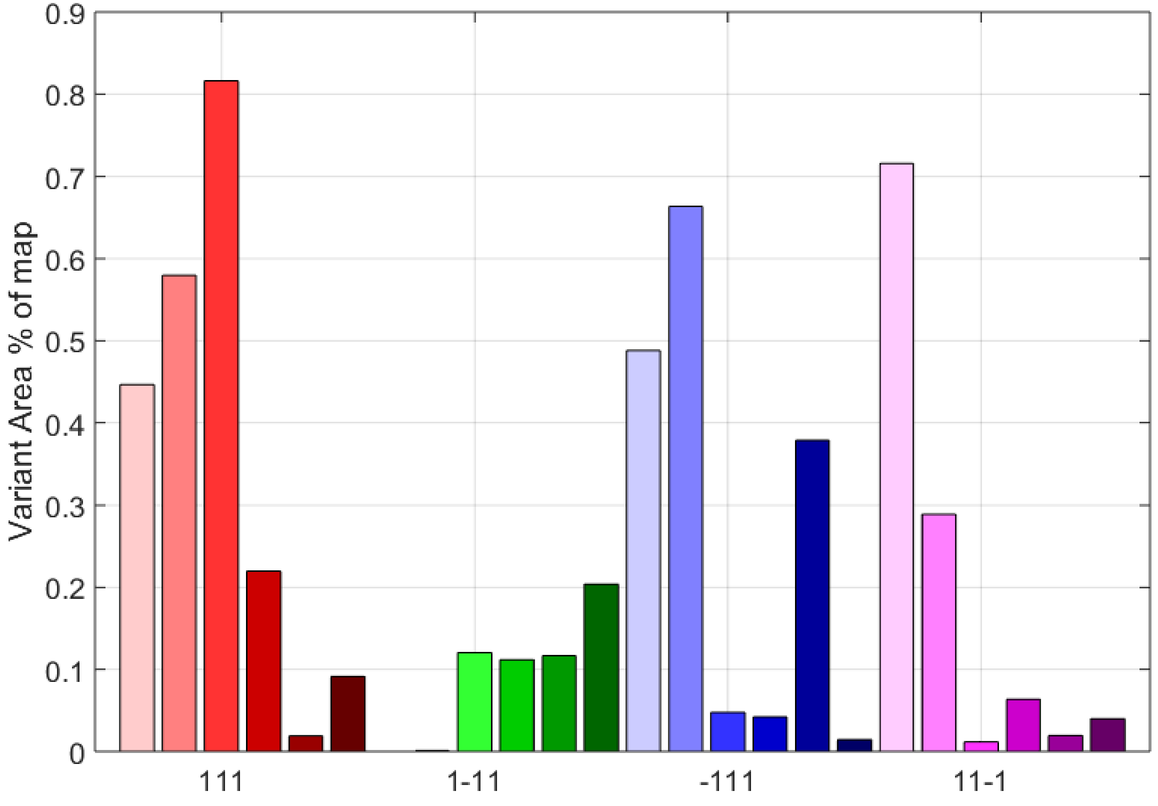
```
            grains_merged(n).prop.daughterArea = sum(grains(bCCgrainNo).area);
            grains_merged(n).prop.daughterAreapc =100* sum(grains(bCCgrainNo).area) / sum(grains(daughters{n}).area);
            grains_merged(n).prop.GOS = mean( grains(fCCgrainNo{n}).GOS );
        end
    else%not transformed grains
        daughters{n} = [];
        grains_merged(n).prop.BCCpc = 0;
        grains_merged(n).prop.daughterNo = 0;
        grains_merged(n).prop.daughterArea = 0;
        grains_merged(n).prop.daughterAreapc = 0;

        bccBinary =grains(daughters{n}).phase==2;%find which daughters are bcc
        fccBinary =grains(daughters{n}).phase==1;%find which daughters are fcc
        bCCgrainNo{n} = daughters{n}(bccBinary);%%the bcc grain nos
        fCCgrainNo{n} = daughters{n}(fccBinary);%%the fcc grain nos
        grains_merged(n).prop.GOS = mean( grains(fCCgrainNo{n}).GOS );
    end

end
grains_merged.prop.daughters=daughters;
grains_merged.prop.graindaughters=bCCgrainNo;
grains_merged.prop.grainparent=fCCgrainNo;
close(hw)
```

D

Martensite

Quantification of martensite types



After 10% strain

Red

	$\gamma \,||\, \alpha'$
	$(111) \,||\, (011)$
V1	$[\bar{1}01] \parallel [\bar{1}\bar{1}1]$
V2	$[\bar{1}01] \parallel [\bar{1}1\bar{1}]$
V3	$[01\bar{1}] \parallel [\bar{1}\bar{1}1]$
V4	$[01\bar{1}] \parallel [\bar{1}1\bar{1}]$
V5	$[1\bar{1}0] \parallel [\bar{1}\bar{1}1]$
V6	$[1\bar{1}0] \parallel [\bar{1}1\bar{1}]$

Blue

	$\gamma \,||\, \alpha'$
	$(\bar{1}11) \,||\, (011)$
V13	$[0\bar{1}1] \parallel [\bar{1}\bar{1}1]$
V14	$[0\bar{1}1] \parallel [\bar{1}1\bar{1}]$
V15	$[\bar{1}0\bar{1}] \parallel [\bar{1}\bar{1}1]$
V16	$[\bar{1}0\bar{1}] \parallel [\bar{1}1\bar{1}]$
V17	$[110] \parallel [\bar{1}\bar{1}1]$
V18	$[110] \parallel [\bar{1}1\bar{1}]$

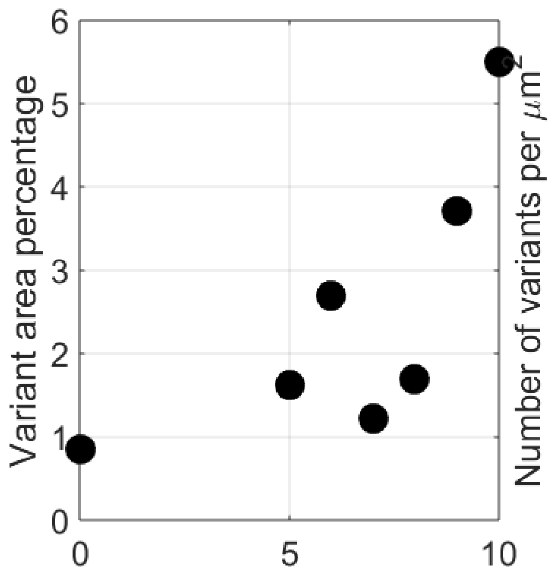
Green

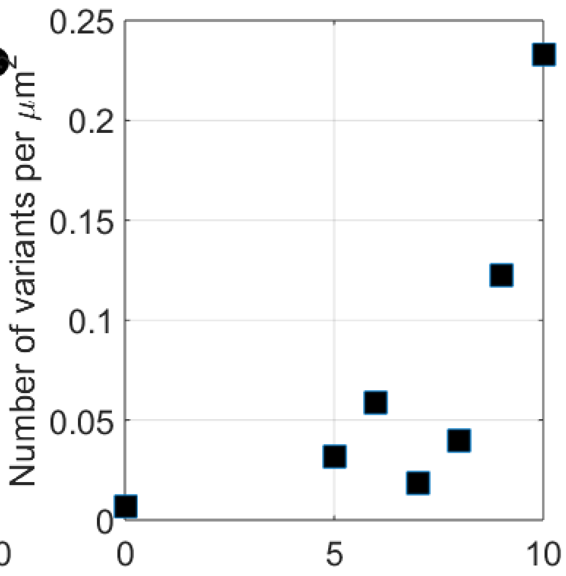
	$\gamma \,||\, \alpha'$
	$(11\bar{1}) \,||\, (011)$
V7	$[\bar{1}10] \parallel [\bar{1}\bar{1}1]$
V8	$[\bar{1}10] \parallel [\bar{1}1\bar{1}]$
V9	$[0\bar{1}\bar{1}] \parallel [\bar{1}\bar{1}1]$
V10	$[0\bar{1}\bar{1}] \parallel [\bar{1}1\bar{1}]$
V11	$[101] \parallel [\bar{1}\bar{1}1]$
V12	$[101] \parallel [\bar{1}1\bar{1}]$

Pink

	$\gamma \,||\, \alpha'$
	$(1\bar{1}1) \,||\, (011)$
V19	$[10\bar{1}] \parallel [\bar{1}\bar{1}1]$
V20	$[10\bar{1}] \parallel [\bar{1}1\bar{1}]$
V21	$[\bar{1}\bar{1}0] \parallel [\bar{1}\bar{1}1]$
V22	$[\bar{1}\bar{1}0] \parallel [\bar{1}1\bar{1}]$
V23	$[011] \parallel [\bar{1}\bar{1}1]$
V24	$[011] \parallel [\bar{1}1\bar{1}]$

D

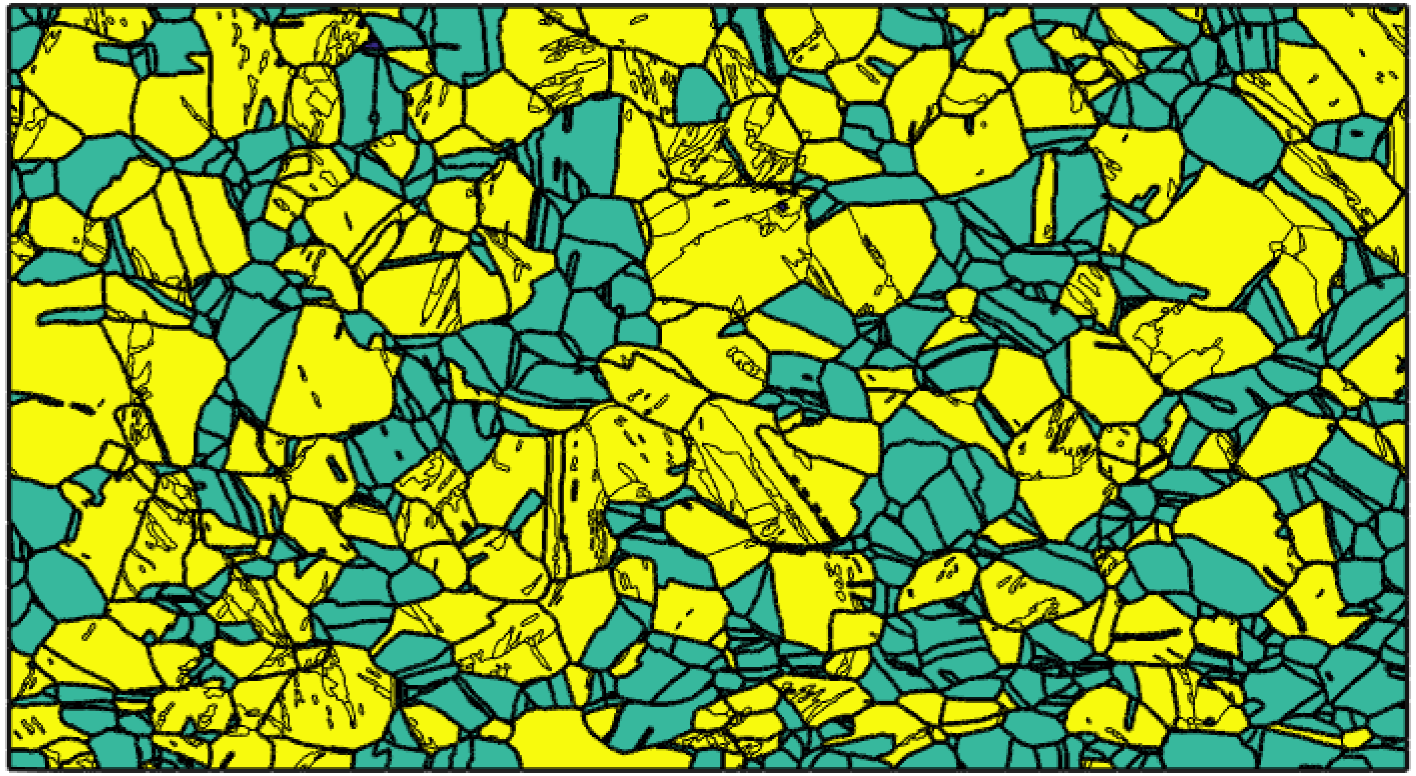




10 %

Austenite transformed: 59.7367 %

Martensite Area: 5.5411 %



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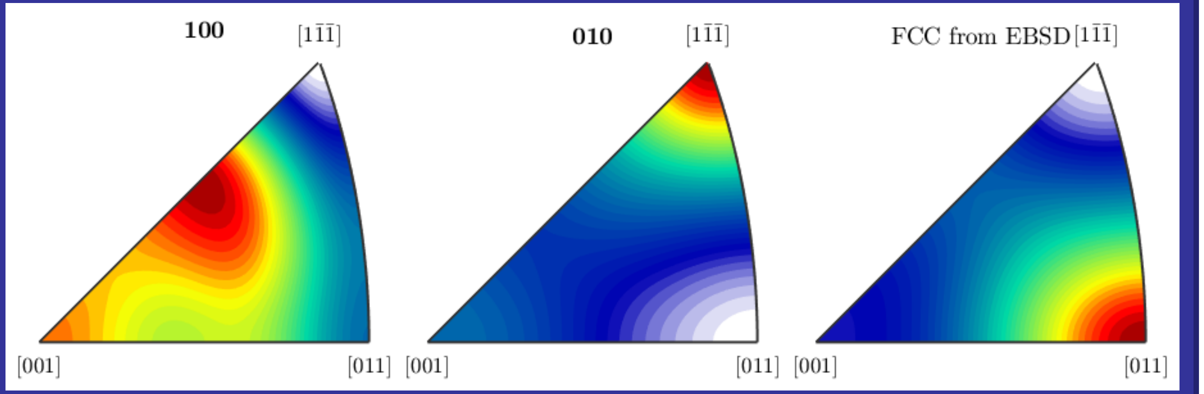
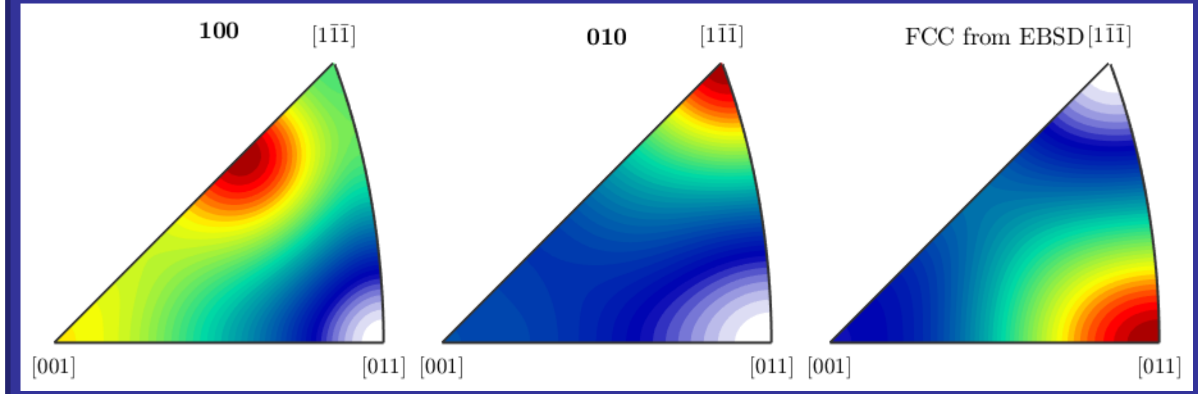
Texture of sample- inverse pole figures

8% strain

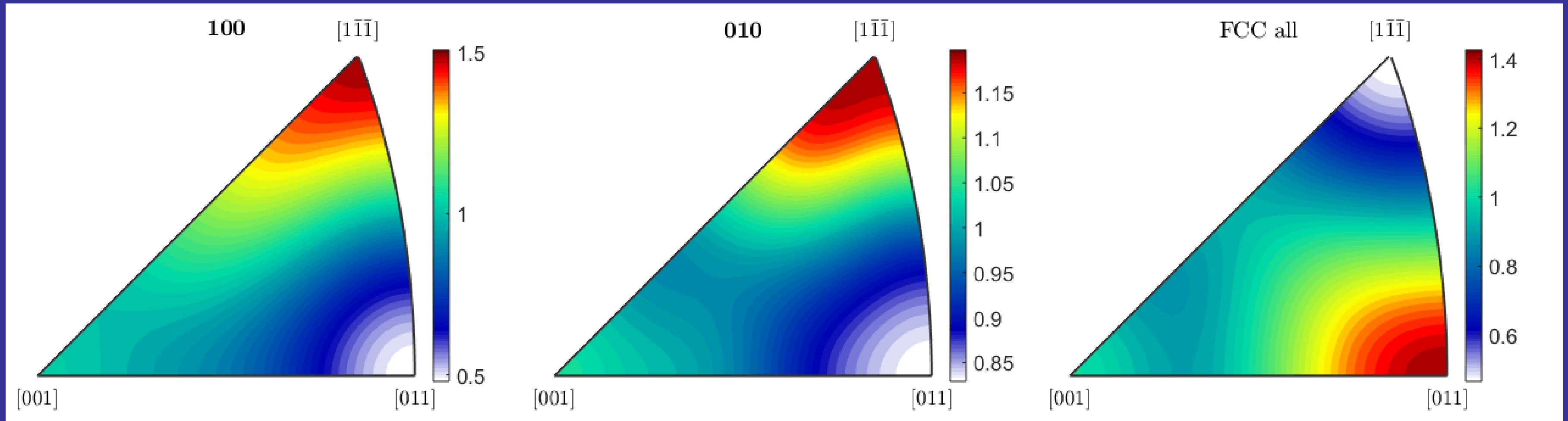
Before test



After test

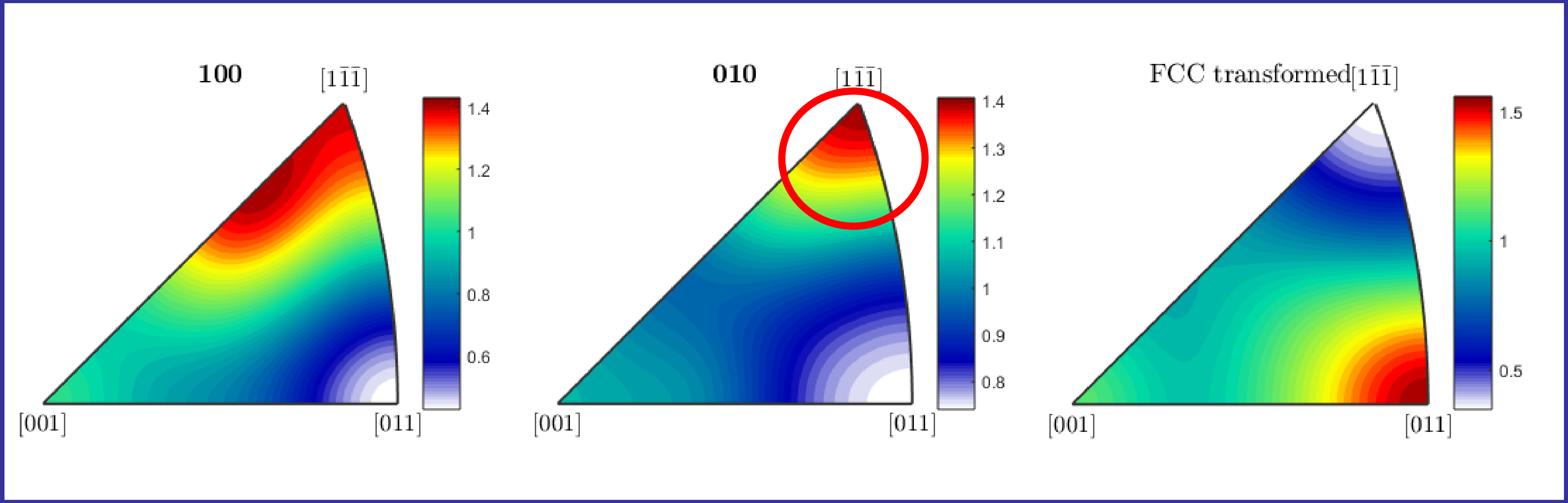


10% strain



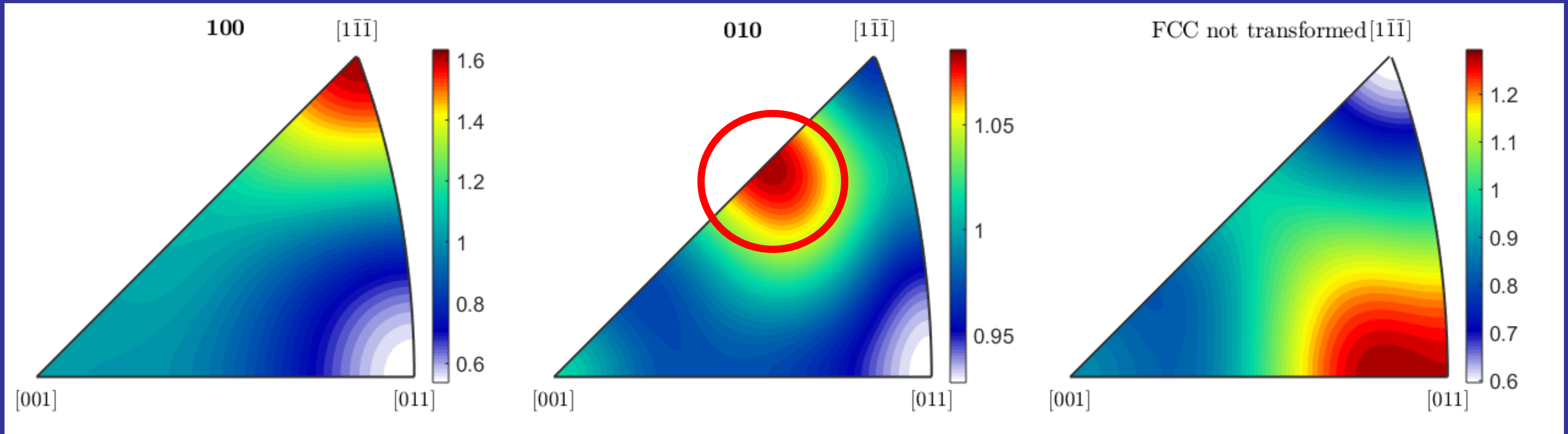
Orientation of FCC grains by variant transformation

FCC transformed



10 % strain

FCC, not transformed

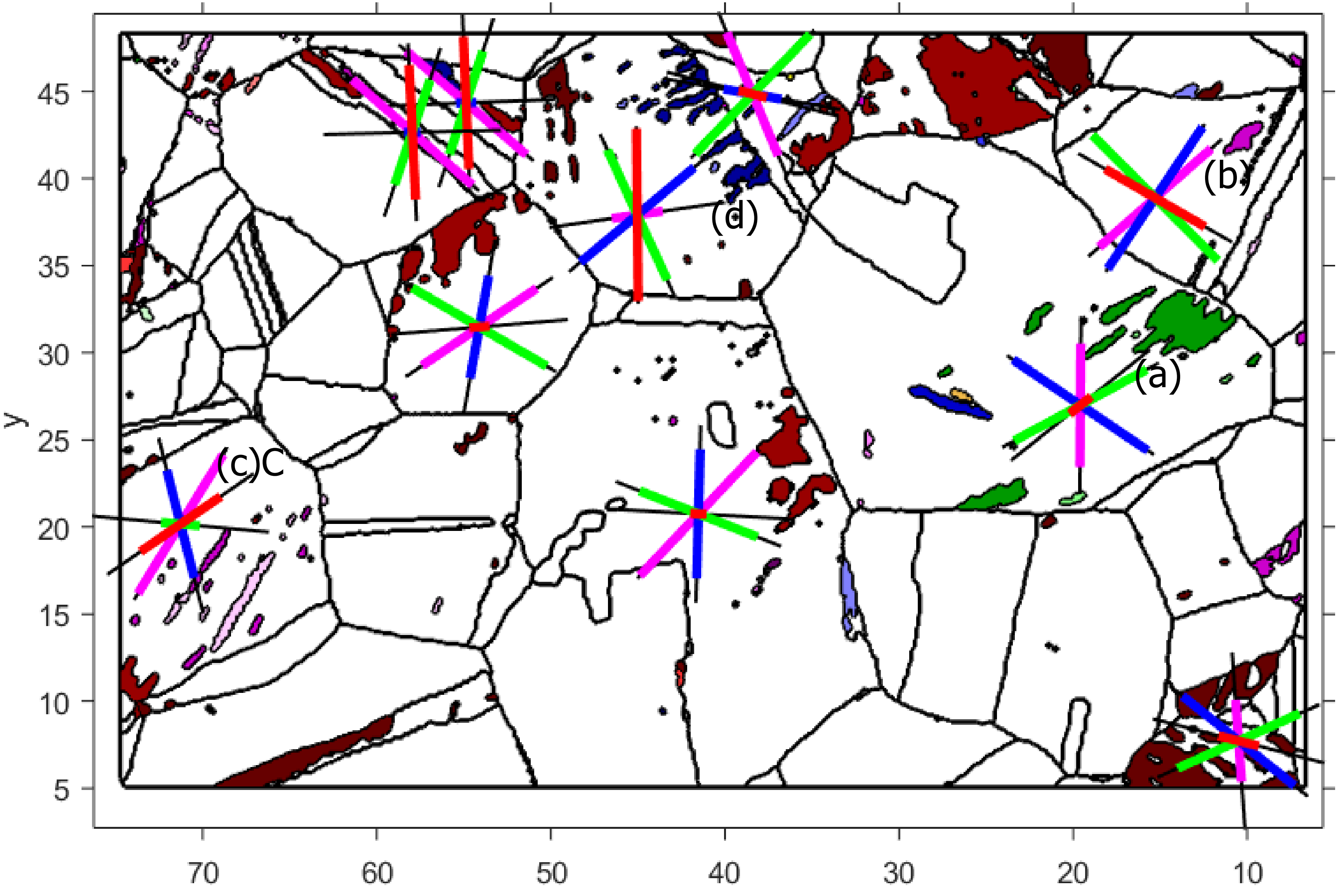


D

KS variants- FCC planes

- The variant with slip system with max Schmid factor often form (a->d)
    - i.e same {111} plane
- But not always
    - Red variants (111)
    - Or Smaller grains

A statistical analysis of the maps is needed



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KS variants- BCC planes

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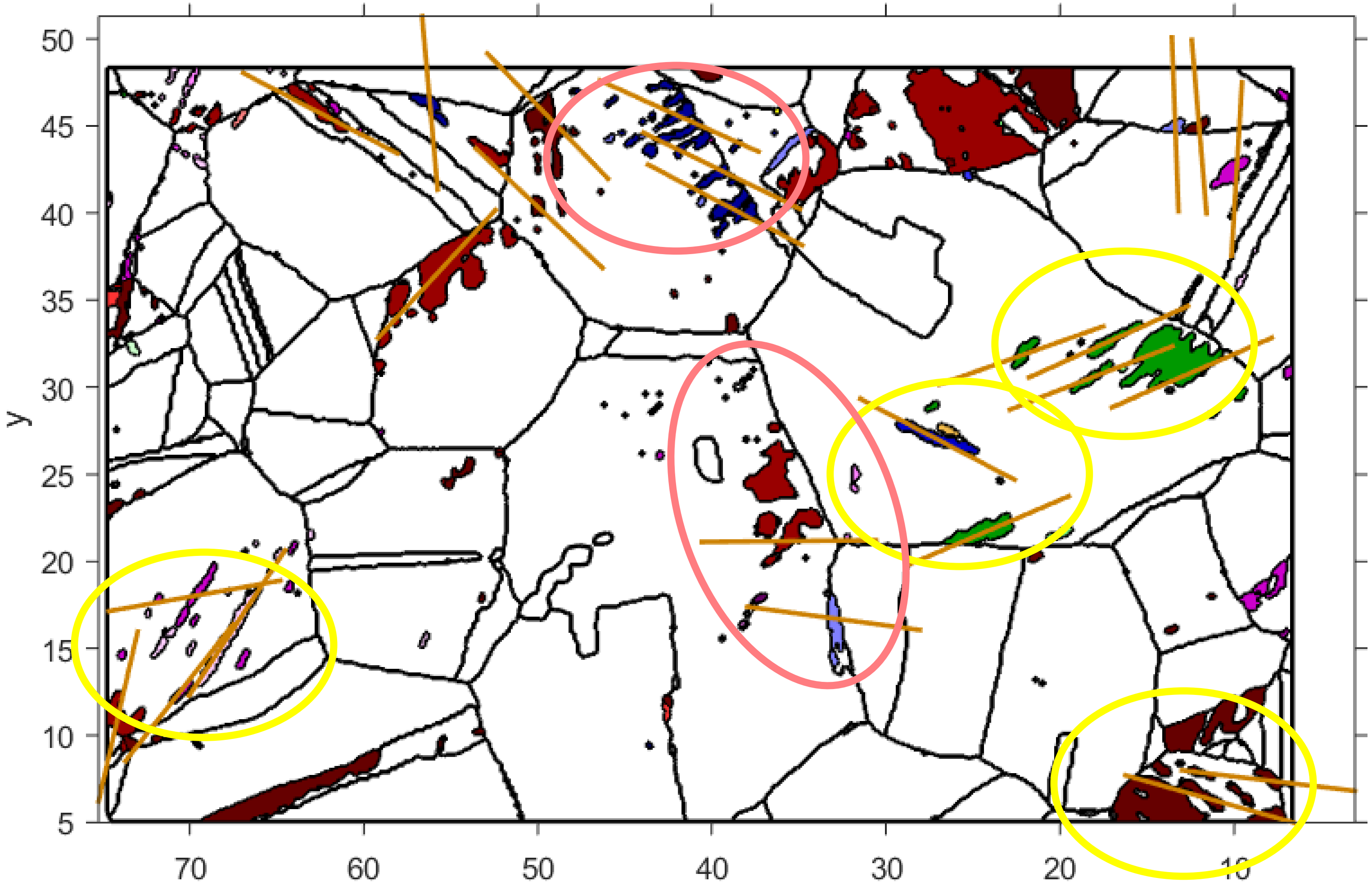
- The variant often forms along the (011) plane
- But again not always

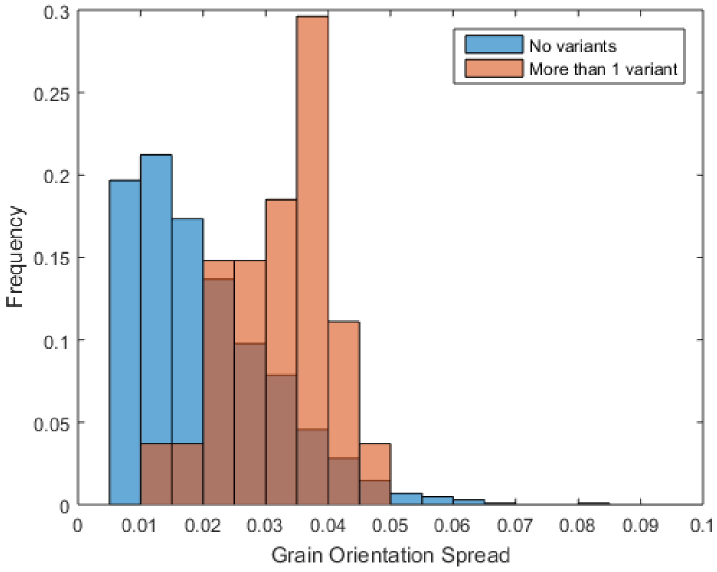


D

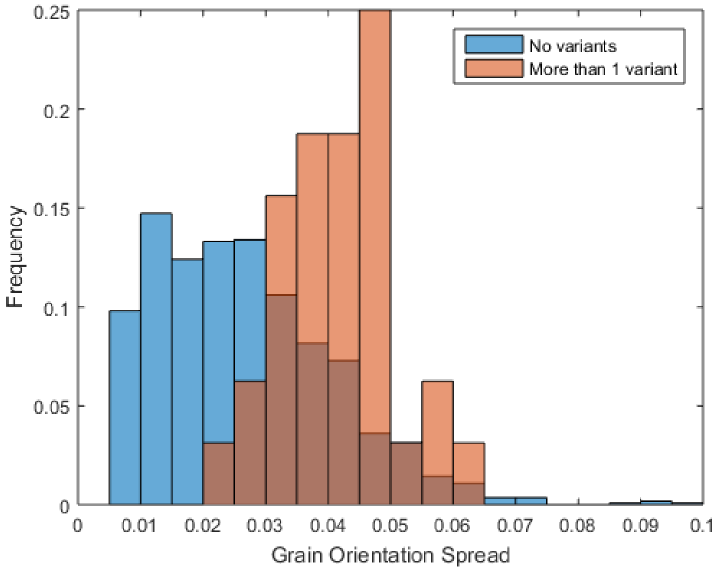
Misorientation

FCC grains with martensite have greater misorientation
- Is this the cause of variant formation?

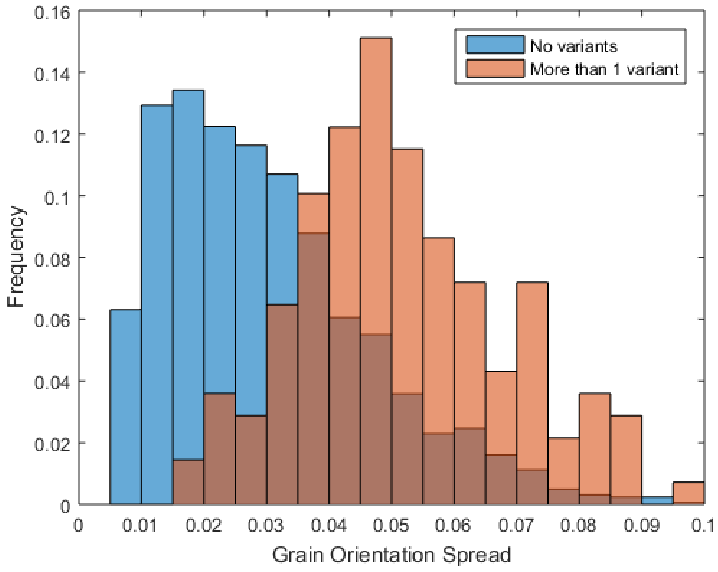
6 %



8 %



10 %



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Strain-induced Martensite

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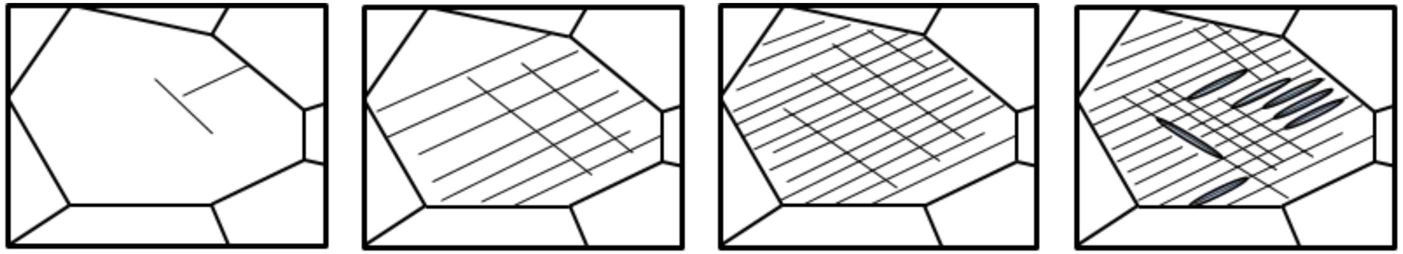
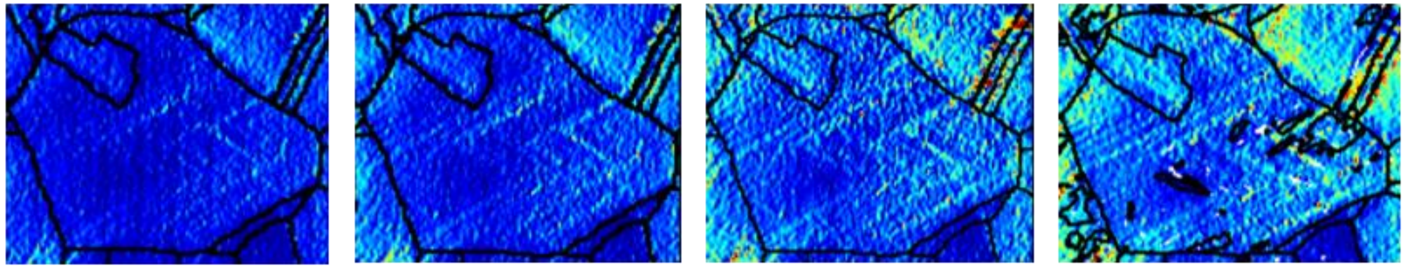
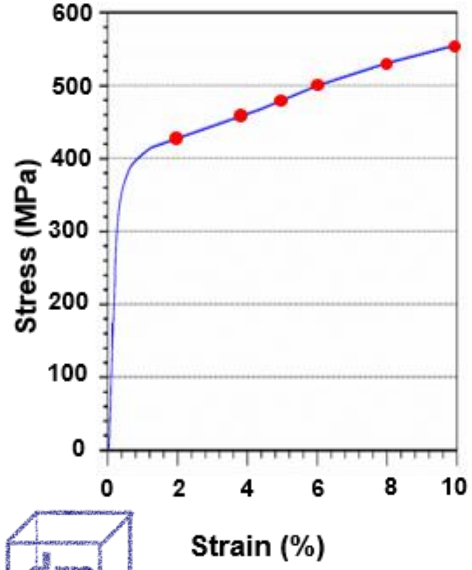
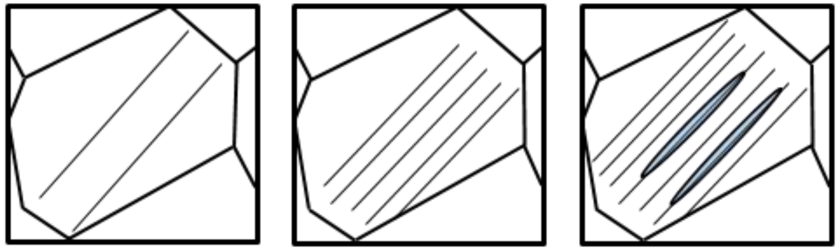


{111} Slip planes — New {111} Slip planes — α′ on {111} slip planes

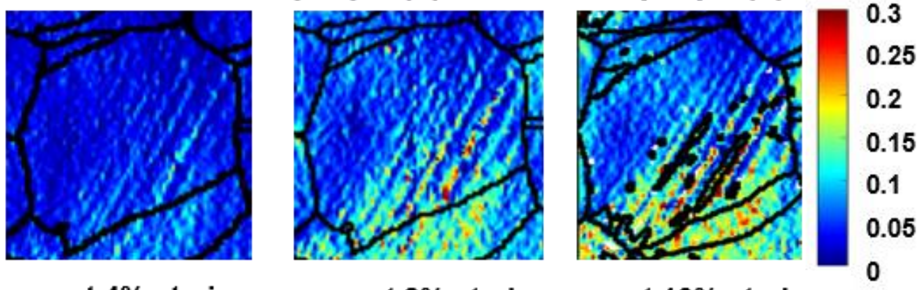


ε_{xx} at 2% strain — ε_{xx} at 4% strain — ε_{xx} at 8% strain — ε_{xx} at 10% strain

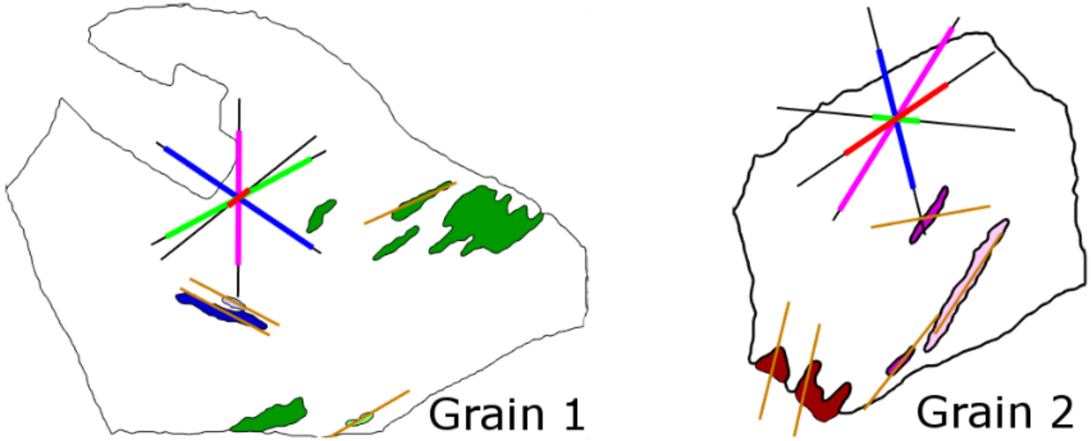




{111} Slip planes — α′ on {111} slip planes



ε_{xx} at 4% strain — ε_{xx} at 8% strain — ε_{xx} at 10% strain



Red

	$\gamma \parallel \alpha'$ $(111) \parallel (011)$
V1	$[\bar{1}01] \parallel [\bar{1}\bar{1}1]$
V2	$[\bar{1}01] \parallel [\bar{1}1\bar{1}]$
V3	$[01\bar{1}] \parallel [\bar{1}\bar{1}1]$
V4	$[01\bar{1}] \parallel [\bar{1}1\bar{1}]$
V5	$[1\bar{1}0] \parallel [\bar{1}\bar{1}1]$
V6	$[1\bar{1}0] \parallel [\bar{1}1\bar{1}]$

Blue

	$\gamma \parallel \alpha'$ $(\bar{1}11) \parallel (011)$
V13	$[0\bar{1}1] \parallel [\bar{1}\bar{1}1]$
V14	$[0\bar{1}1] \parallel [\bar{1}1\bar{1}]$
V15	$[\bar{1}0\bar{1}] \parallel [\bar{1}\bar{1}1]$
V16	$[\bar{1}0\bar{1}] \parallel [\bar{1}1\bar{1}]$
V17	$[110] \parallel [\bar{1}\bar{1}1]$
V18	$[110] \parallel [\bar{1}1\bar{1}]$

Green

	$\gamma \parallel \alpha'$ $(11\bar{1}) \parallel (011)$
V7	$[\bar{1}10] \parallel [\bar{1}\bar{1}1]$
V8	$[\bar{1}10] \parallel [\bar{1}1\bar{1}]$
V9	$[0\bar{1}\bar{1}] \parallel [\bar{1}\bar{1}1]$
V10	$[0\bar{1}\bar{1}] \parallel [\bar{1}1\bar{1}]$
V11	$[101] \parallel [\bar{1}\bar{1}1]$
V12	$[101] \parallel [\bar{1}1\bar{1}]$

Pink

	$\gamma \parallel \alpha'$ $(1\bar{1}1) \parallel (011)$
V19	$[10\bar{1}] \parallel [\bar{1}\bar{1}1]$
V20	$[10\bar{1}] \parallel [\bar{1}1\bar{1}]$
V21	$[\bar{1}\bar{1}0] \parallel [\bar{1}\bar{1}1]$
V22	$[\bar{1}\bar{1}0] \parallel [\bar{1}1\bar{1}]$
V23	$[011] \parallel [\bar{1}\bar{1}1]$
V24	$[011] \parallel [\bar{1}1\bar{1}]$

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Conclude

#MTEX2017

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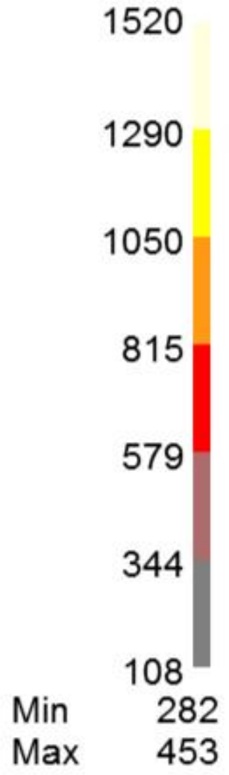

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