Parent BOR Code: QuickStart Guide

About

The Parent BOR code is designed to reconstruct the parent β microstructure from the α phase EBSD data for Zr alloys.

More details can be found in:

<Paper details>

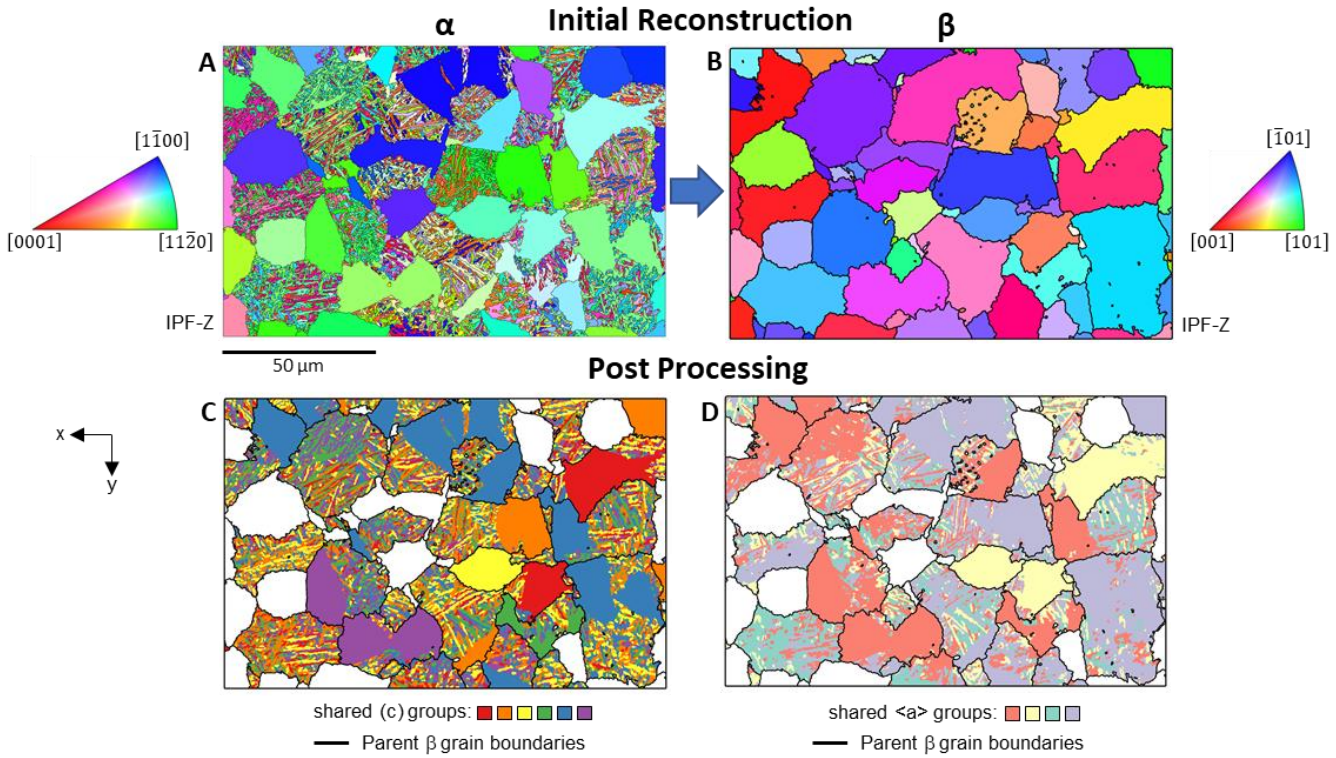


Figure 1 – Burgers Orientation Relationship based reconstruction and analysis of a duplex Zircaloy-4 microstructure. (A) input α phase (HCP) map. (B) output β phase (BCC) map of the prior β structure. (C) shared basal plane analysis with respect to each prior β grain, based upon the new post processing routines. (D) shared <a> direction analysis, with the same post processor.

Before you start….

- **MTEX:** To run this code, you will need to have MTEX [1] installed – the code is currently designed to work with version: **5.4.** MTEX can be downloaded from: https://mtex-toolbox.github.io/download.
- **Input File:** The code is setup to work with a .h5 file as an input and follow Bruker conventions (x axis = west & z axis = out of plane). An alternative input option is included to allow use of the simulated dataset which should be saved as a .mat file and loaded as per the instructions in the 'Load EBSD data' section.

Setting up the code

To run the code, you will need to update Reconstruct_Main.m (suggestion: save a copy and edit this):

- General Setup (lines 15-26)

```
15      %% General Setup
16      % load MTEX and add relevant folders to the path
17
18      % Setup MTEX (default = Bruker setup)
19 -    run('C:\Users\ruthb\Documents\MTEX\mtex-5.4.0\startup.m'); %start MTEX [change file location]
20 -    setMTEXpref('xAxisDirection','west');
21 -    setMTEXpref('zAxisDirection','outOfPlane');
22
23      % Add folders
24 -    settings.file.mainFolder=['C:\Users\ruthb\Documents\GitHub1\ParentBOR'];%full code location
25 -    addpath('Functions','h5','Results')% Folders to add
26
```

  - *Line 19:* Update the location of your MTEX start up file
  - *Lines 20-21:* Update the MTEX preferences – the default is the Bruker setup
  - *Line 24:* Update the location of the main folder

- Load EBSD data (lines 27-40)

```
27      %% Load EBSD data
28      % name the dataset and load a h5 file or stored ebsd variable
29
30      % EBSD file name
31      % [If using a simulated dataset use the filename and add .h5]
32 -    settings.file.fname=('2ai_3(bottom)_re.h5');%file name including file type
33
34      % load the EBSD data (h5 version)
35 -    [ebsd, header] = loadEBSD_h5(settings.file.fname);
36
37      % For simulated dataset: [comment out line 35 & uncomment lines 38-39]
38      % load PaperSimulatedDataset.mat; %load the ebsd data
39      % ebsd=alpha_ebsd; %rename the alpha phase data
40
```

  - *Line 32:* Update file name – this will be used to label the results folder, so needs to be filled in whether you use the h5 loading version or not (add .h5 to the end of your file name to ensure the code works).
  - h5 version (*line 35*): no changes required
  - Alternative version (*lines 38-39*): use these lines if loading a pre-saved EBSD variable, e.g. one from the simulated dataset. The .mat file name will need to be changed on *line 38*. *Line 39* need only be used if the α phase EBSD variable is not named 'ebsd'.

- Reconstruction Setup (lines 41-59)

```
41      %% Reconstruction Setup
42      % Setup and store the grain processing and reconstruction settings
43
44      % Phases
45 -    settings.phases.phase1=('Zirconium - alpha'); %phase1 - HCP
46 -    settings.phases.phase2=('Zirconium - beta'); %phase2 - BCC
47
48      % Grain processing
49 -    settings.grains.gbThreshold = 4*degree;% grain boundary threshold angle
50 -    settings.grains.smallGrains = 5; % threshold grain size below which the grains will be removed
51 -    settings.grains.smoothGrains = 2;% smoothing value (0 = off) Note: smoothed grains not used in calculations
52
53      % Reconstruction settings
54 -    settings.reconstruct.cutoff = 4; % Threshold value for matching GB misorientations (degrees)
55 -    settings.reconstruct.inflationPower = 1.6; % controls MCL alorithm
56
57      % Implement settings
58 -    [settings,ebsd] = Setup(settings,ebsd); %run Setup function
59
```

  - *Lines 45-46:* If your phases are labelled differently, update the phase names. The β phase will be created if not already in the dataset (ignore the warning about the phase not existing when the code runs).

- [IMPORTANT] The next few lines control how the reconstruction works:
  - Grain processing settings:
    - *Line 49:* misorientation angle required to recognise a grain boundary
    - *Line 50:* grains with less than this number of pixels will be removed
    - *Line 51:* smoothing value for grain processing (only affects output plots)
  - Reconstruction settings:
    - *Line 54:* cutoff value – controls the identification of grain boundary types (i.e. parent grain boundaries vs. α/α grain boundaries). Note: this is more for visual identification rather than impacting the reconstruction.
    - *Line 55:* inflation power – controls the MCL[1] algorithm and therefore the reconstruction quality (see paper for more details). 1.6 is set as default however you may need to experiment with this value to suit your dataset (particularly for smaller datasets).
- *Line 58:* Implement chosen settings – no changes required.

- Plotting setup

```
%% Plotting Setup
% Plotting options & which plots to output
% Note: 1 = ON & 0 = OFF

% General
PlotOpt.general.SaveOn     = 1;       %Save figures
PlotOpt.general.Scalebar   = 'Off';    %Include scalebar: 'On' or 'Off'

% Part 1 plots - Reconstruction
PlotOpt.IPFs.dir           = zvector; %IPF direction
PlotOpt.IPFs.HCP.initial   = 0;       %Alpha phase IPF map (no smoothing)
PlotOpt.IPFs.HCP.smoothed  = 1;       %Alpha phase IPF map (smoothed gBs)
PlotOpt.IPFs.BCC.raw       = 1;       %Initial output for beta phase IPF map
PlotOpt.IPFs.BCC.processed = 0;       %Reprocessed beta phase IPF map (no smoothing)
PlotOpt.IPFs.BCC.smoothed  = 1;       %Reprocessed beta phase IPF map (smoothed gBs)

% Part 2 plots - Post Processing
PlotOpt.Quality.devis      = 0;       %Reconstruction quality (devis)
PlotOpt.Quality.min_angle  = 0;       %Reconstruction quality (min_angle)
PlotOpt.AlphaVar.all       = 0;       %Alpha variants plot - all 12 variants (12 colours)
PlotOpt.AlphaVar.dir       = 0;       %Alpha variants plot - shared direction (4 colours)
PlotOpt.AlphaVar.planes    = 0;       %Alpha variants plot - shared planes (6 colours)
PlotOpt.AlphaVar.combo     = 1;       %Combined plot - alpha variants (the 3 plots above)
PlotOpt.BetaCert.noOfVar   = 0;       %Beta certainty - no of unique alpha variants per beta grain
PlotOpt.BetaCert.betaOpt   = 0;       %Beta certainty - no of unique beta options for each beta grain

% Part 3 plots - Analysis (Interactive plots & pole figures)
PlotOpt.Interactive.HCP    = 0;       %Interactive IPF map to select an alpha grain
PlotOpt.Interactive.BCC    = 1;       %Interactive IPF map to select a beta grain
PlotOpt.BetaOpt_PF.g_sel   = [];      %Grain selected for PF analysis (option to manually enter or updated through beta interactive plot)
PlotOpt.BetaOpt_PF.basic   = 0;       %For selected beta grain - PF for current beta option with alpha grain orientations(1 polefig, 2 colours)
PlotOpt.BetaOpt_PF.colour  = 1;       %For selected beta grain - PFs for all beta options + alpha grain ori(1-6 polefigs, alpha var colouring)

% Part 4 plots - Alternative beta options
PlotOpt.altBeta.combo      = 1;       %Combo plot for each of the altenative beta options for the grains (1 plot, 6 subplots)
PlotOpt.altBeta.alphaVar   = 0;       %Alpha variants (12 variants/shared (c)/shared <a>) - Combined plots x6 (numbered)

```

  - *Line 65:* Choose whether to save the output plots (1 = On; 0 = Off). If saving is selected, these plots will save at 600 dpi in the results folder in a folder called 'Results_(file name)'.
  - *Line 66:* Option to turn scale bars on or off for all plots
  - Lines 69-95: This part contains the ability to turn the plotting on or off for all potential plots. The default setup outputs:
    - Initial α microstructure – IPFZ (smoothed grains)
    - Initial reconstruction output (β phase) - IPFZ
    - Reprocessed reconstruction output (β phase) – IPFZ
    - Combined plot of α variant analysis: all 12 variants/shared directions/shared planes
    - Interactive (β phase) plot to select a β grain for further analysis (takes a mouse click)
    - Pole figure plot for selected β grain and the α grains contains within that grain (colour version – α grain dots coloured by variant number)
    - Alternative β orientation combo plot – 6x IPFZ maps with the alternative parent β orientations selected (defaults to first option for each β grain if there are no further β options to be selected)

[1] MCL algorithm = Markov Clustering algorithm – for more details see: https://micans.org/mcl/ or [2], [3]

Running the Code

Once the settings have been updated, the code can be run either in one go or stepped through.

If the code reaches the end, the workspace will be saved in the results file enabling it to be returned to.

Example Output

File: 'Example.h5'

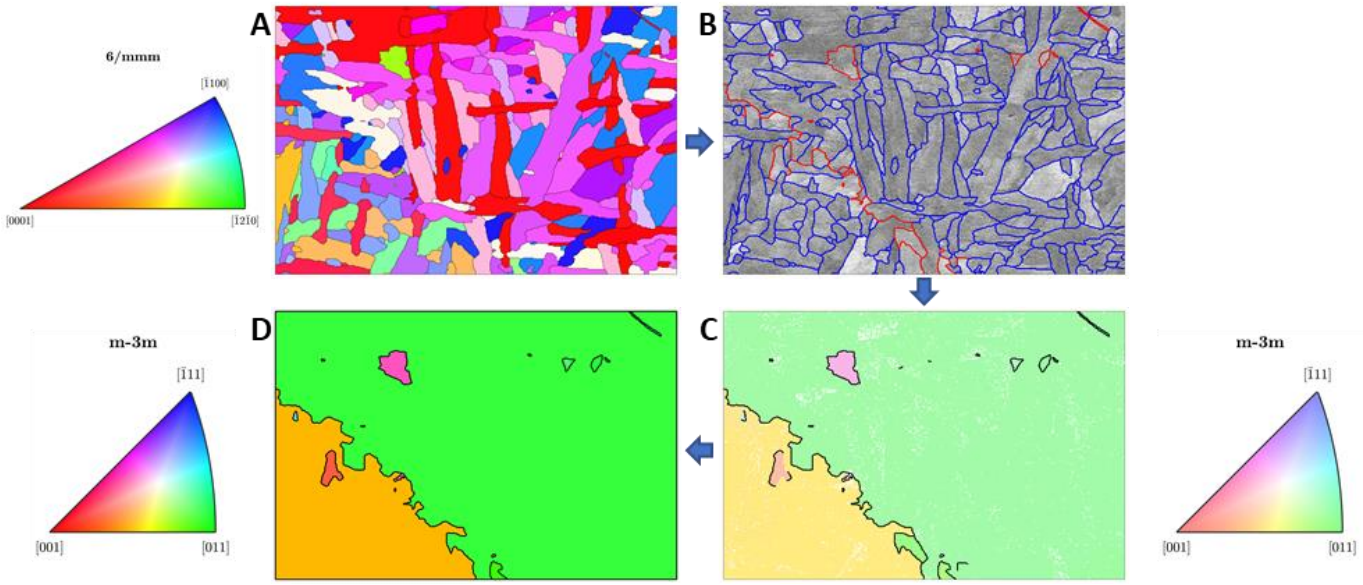
Settings:

- Grain Processing Settings:
  - Grain boundary threshold: 4.0 degrees
  - Small grains threshold: 5 pixels
  - Smoothing value: 2
- Reconstruction Settings:
  - Cutoff: 4.0
  - Inflation power: 1.6

Outputs:

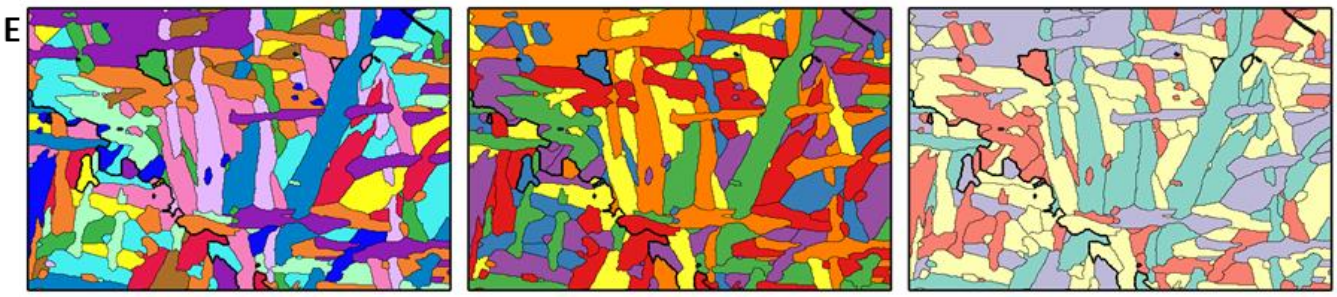
- Reconstruction Section Outputs:
  - No of alpha grains: 262
  - Total BOR gB (%): 87.77
  - Total non-BOR gB (%): 12.23
  - No of discrete clusters (MCL): 24
  - Average angular deviation from BOR: 1.16
  - No of beta grains: 17

Plotting - Part 1



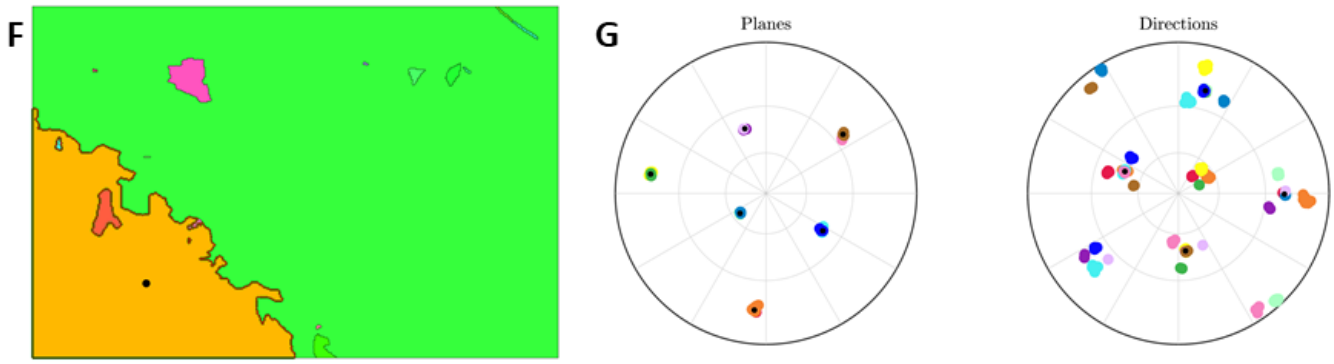
(A) Initial α microstructure – IPFZ (smoothed grains)
(B) Grain boundary type plot – Red = parent grain boundary; Blue = α/α grain boundary
(C) Initial reconstruction output (β phase) – IPFZ
(D) Reprocessed reconstruction output (β phase) – IPFZ

Plotting – Part 2



(E) Combined plot of α variant analysis: all 12 variants/shared directions/shared planes

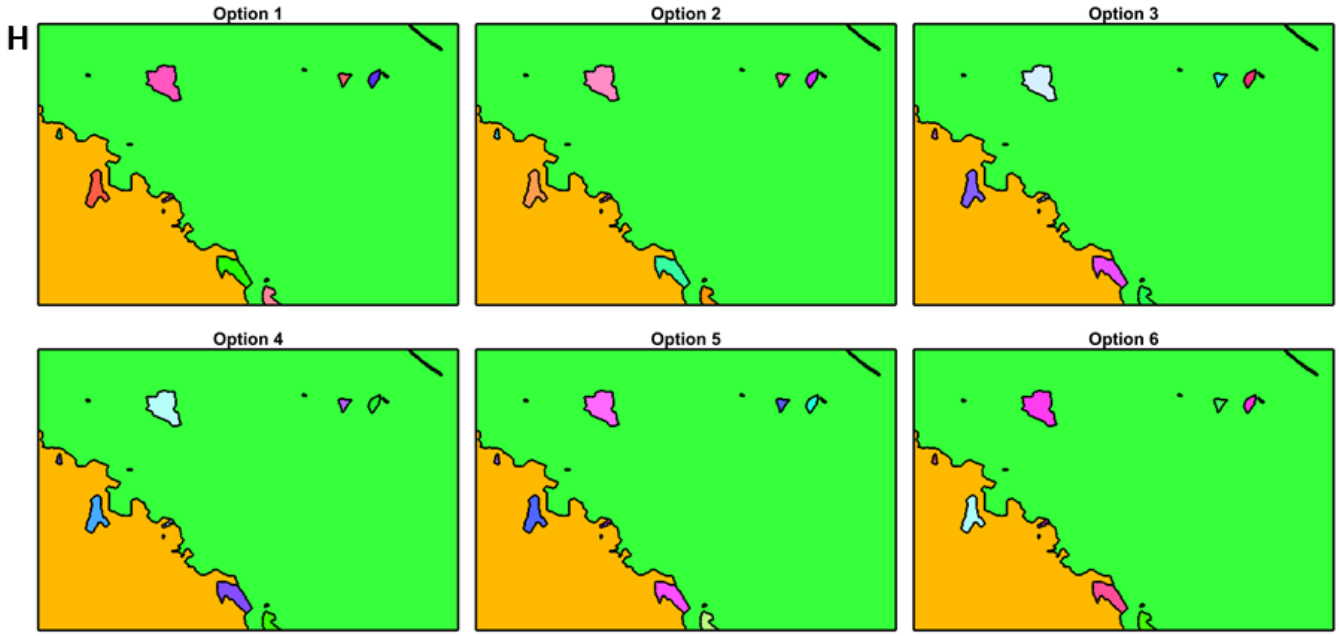
Plotting – Part 3



(F) Interactive (β phase) plot to select a β grain for further analysis (takes a mouse click)

(G) Pole figure plot for selected β grain and the α grains contains within that grain (colour version – α grain dots coloured by variant number)

Plotting – Part 4



(H) Alternative β orientation combo plot – 6x IPFZ maps with the alternative parent β orientations selected (defaults to first option for each β grain if there are no further β options to be selected)

References

[1] F. Bachmann, R. Hielscher, and H. Schaeben, "Texture analysis with MTEX- Free and open source software toolbox," *Solid State Phenom.*, vol. 160, pp. 63–68, 2010.

[2] S. van Dongen, "PhD Thesis," University of Utrecht, 2000.

[3] T. Nyyssönen, P. Peura, and V. T. Kuokkala, "Crystallography, Morphology, and Martensite Transformation of Prior Austenite in Intercritically Annealed High-Aluminum Steel," *Metall. Mater. Trans. A Phys. Metall. Mater. Sci.*, vol. 49, no. 12, pp. 6426–6441, 2018.