Deformation structure vs. grain structure

1. Overview over files

WAnalysisORCHIDMTEX

Main script for analysis of differently processed tungsten plate material

Contains Part A to E

Part A	Definition of files and conventions, loading of EBSD file
	A1 Loading of EBSD data
	A2 Display of orientation map
Part B	Preparation of data analysis
	B1 reshaping EBSD data on grid, selecting a particular phase, setting all other NaN
	B2 creation of random arrangement of same orientations
Part C	Numerical data analysis
	C1 calculation of distant disorientations along horizontal and vertical directions (including calculating absolute frequencies)
	C2 calculation of distant disorientations along diagonal directions (including calculating absolute frequencies)
	C3 calculation of disorientations with randomly selected neighbors (requires B2)
	C4 fitting of the dependence of mean disorientation angle on step distance (requires C1)
	X1 Fraction of low angle boundaries as function of step distance
	X2 Boundary density and mean chord length as function of step distance (boundaries defined by threshold angle)
Part D	Mean chord length
	D1 Mean chord length as function of threshold angle
	D2 Mean chord length as function of step distance – empirical data (without fixed threshold angle for boundaries)
	X3 Anisotropy of mean chord length distribution in dependence of step distance (qualitative)
	D3 Mean chord length as function of step distance – grain boundaries only (grain boundaries defined by lost orientation correlation)

D4 Mean chord length as function of step distance – two types of boundaries (grain boundaries defined by lost orientation correlation, deformation boundaries preserve orientation correlation)

X4 Relevant and irrelevant fractions

Part E Disorientation angle distributions

E1 Disorientation angle distributions for selected step distances

E2 Separation of distributions from deformation boundaries and grain boundaries

X5 Separation by selecting two distributions of different step distances

X6 Anisotropy of mean chord length distribution in dependence of step distance (quantitative)

Subroutines (called from main script or a subroutine)

misorientation	misorientation(P1,P2,P3,P4,Q1,Q2,Q3,Q4) calculates the misorientation $\Delta Q = PQ^{-1}$ between orientations P and Q in the crystallographic system of Q
disorientation	disorientation(ΔQ1, ΔQ2, ΔQ3, ΔQ4) finds the minimum disorientation angle from all equivalent misorientations taking into account cubic symmetry
distantdisorientation	distantdisorientation(Q1,Q2,Q3,Q4,ddx,ddy) calculates all disorientation angles (and the mean disorientation angle) between points of the selected phase in different distances along a particular direction [ddx, ddy] in the map
cl1Rayleigh	cl1Rayleigh(param1,x) double integrated Rayleigh function
cl2Rayleigh	cl2Rayleigh(param2,x) double integrated superposition of two Rayleigh functions

References (for the background behind the analysis)

1. W. Pantleon, Unbiased evaluation of chord length distributions from orientation maps, Mater. Sci. Forum 495-497 (2005) 219-224
2. W. Pantleon, Deformation structure versus grain structure after severe plastic deformation, Probl. Mater. Sci. 52 (2007) 13-23.

2. Exercises

X0 Preparation

Open the main script "WAnalysisORCHIDMTEX". Chose in header, the proper casename "Wasreceived" and update the paths to the ORCHID scripts and the provided data files. Execute all parts A1 to C4 individually.

The material under consideration is warm-rolled tungsten, the investigated surface is a longitudinal section with the rolling direction horizontally and the normal direction vertically. The microstructure (as e.g. seen from A2) reflects the rolling geometry with elongated features along the horizontal direction.

X1 Fraction of low angle boundaries as function of step distance

Boundaries are usually assumed to be present, if the disorientation angle determined between to neighboring measuring points is above a certain threshold value (1°) which takes into account the limited angular accuracy of the orientation determination by the EBSD acquisition system. Low angle boundaries (LABs) with disorientation angle below 15° are distinguished from high angle boundaries (HABs) with disorientation angle of 15° and above.

Find the fraction of low angle boundaries of all boundaries (!) for different step sizes along the horizontal and the vertical direction in the orientation map. Use the absolute frequencies of the disorientation angles determined (in C1) for bins of width 1° where e.g. bin 1 accounts for the disorientation angles below 1°, bin 15 for disorientation angles equal or larger than 14° but lower than 15° and bin 63 to all disorientation angles equal or above 62°.

X2 Boundary density and mean chord length of high angle boundaries as function of step distance

High angle boundaries are in general identified, if the disorientation angle determined between to neighboring measuring points is above 15°. Find the density of intercepts N_L = NHAB / NPhasesel / stepsize along horizontal and vertical testing lines with high angle boundaries, from the number of high angle boundaries NHAB (given by the absolute frequencies obtained in C1), the total number of pixels in the selected phase (NPhasesel) and the step size (stepsize) of the map.

Calculate the mean chord length $l=1/N_L$ in dependence on step size from the intercept density N_L.

X3 Anisotropy of the mean disorientation angle dependence

Execute C2 and observe the difference between the different directions: Displaying the dependence of the mean disorientation angle on the step distances reveals larger differences between the horizontal and the vertical direction (This is related to the anisotropy of the microstructure induced by rolling). The dependence for the analyzed diagonal direction falls in between the two extreme cases.

Explore the anisotropy (directional dependence) of the behavior for different directions by selecting a different direction diagdir=[ddx, ddy] in C2 and repeating the plot of D2. (Executing parts C3-D1 is not necessary.)

X4 Relevant and irrelevant fractions

Execute parts D3-D4. The fitting with a single type of (uncorrelated) boundaries (D3) does not lead to a satisfying description of the data, where a nice description can be obtained (D4) by taking into account two different types of boundaries, deformation and grain boundaries (where the orientations on both sides of deformation boundaries are still correlated, any orientation correlation is lost across grain boundaries).

Calculate the relevant fractions of all boundaries, grain boundaries and deformation boundaries as well as the irrelevant fraction in dependence on step distance for the horizontal and the vertical direction by using the obtained fit parameters.

X5 Disorientation angle distributions and separation according to boundary type

Execute E1 and observe the difference of the distributions depending on the step distance: For small step distances the distributions are bimodal and clearly reveal two different contributions, one at low angles, and the other at high angles. With increasing step distance the low angle contribution becomes less and less pronounced and finally disappears. The disorientation angle distributions converge to the uncorrelated disorientation distribution obtained from random arrangement of the same orientations. Obviously the convergence is faster in vertical direction than in horizontal direction, reflecting the anisotropy.

The two contributions from deformation boundaries preserving an orientation correlation and grain boundaries with uncorrelated orientations can be separated based on the individual weights of the different contributions obtained by the fits in D4 for disorientation distributions of two different step distances. Execute E2 based on two different step distances and observe the two separated distributions. The disorientation angle distribution of boundaries with uncorrelated orientations is indeed quite similar to the completely uncorrelated disorientation angle distribution obtained from random arrangement of the same orientations and contains only a small, but non-vanishing fraction with low disorientation angles below 15°. The distribution of disorientation angles across boundaries preserving an orientation correlation, however, consists mainly of low disorientation angles, but has fraction of disorientation angles of 15° and above. It becomes apparent that the distinction between both types of boundaries using a threshold angle of 15° is entirely arbitrary.

For the separation of the distributions along the vertical direction, two specific distributions were selected in the above evaluation corresponding to step distance of 4 µm (8 times step size) and 32 µm (64 times step size) or ilistsely1 = 6 and ilistsely2 = 12, respectively. Explore the effect of the selected distributions on the separation result by choosing different values for ilistsely1 and ilistsely2 for gaining confidence in the procedure of E2.

X6 Anisotropy of the mean disorientation angle dependence (quantitatively)

The anisotropy of the mean disorientation angle dependence was investigated qualitatively in X3. Repeat the exercise and explore the anisotropy (directional dependence) of the obtained mean chord lengths for different directions by selecting a different direction diagdir=[ddx, ddy] in C2 and adapting the fitting procedure of D4 to obtain the mean chord length in dependence of the direction.