

COE-C2004 - Materials Science and Engineering
2021-2022 Autumn II

Assignment 1, 01.11.2021

Task 1. (25 points, Lecture1)

Open solution.

Task 2. Atomic structure and interatomic bonding (10 points, Lecture1)

2.1 Calculate the energy (in J) and force (in N) of attraction between a cation with a valence of +2 and an anion with a valence of -1, the centers of which are separated by a distance of 5.3 nm. (Please give the detailed calculation process, and explain your choices or equations and numbers.) **(6 points)**

Solution:

The attractive energy between positive and negative ions can be calculated using Eq.1:

$$E_A = -\frac{A}{r} \quad (\text{Eq. 1}) \quad (0.5 \text{ points})$$

Herein, $r = 5.3 \text{ nm} = 5.3 \times 10^{-9} \text{ m}$, and A represents lattice energy and its value could be given in Eq. 2 as:

$$A = \frac{1}{4\pi\epsilon_0} (|Z_1 e|)(|Z_2 e|) \quad (\text{Eq. 2}) \quad (0.5 \text{ points})$$

where ϵ_0 is the vacuum permittivity constant ($8.85 \times 10^{-12} \text{ F/m}$), e is the elementary charge ($1.602 \times 10^{-19} \text{ C}$), Z is the chemical valence of ion. Combining Eq. 1 and Eq. 2:

$$E_A = -\frac{1}{4\pi\left(8.85 \times 10^{-12} \frac{\text{C}^2}{\text{N}\cdot\text{m}^2}\right)(5.3 \times 10^{-9} \text{ m})} [|+2|(1.602 \times 10^{-19} \text{ C})][|-1|(1.602 \times 10^{-19} \text{ C})] =$$

$$-8.7082 \times 10^{-20} \text{ J} \quad (2 \text{ points})$$

Mathematically, energy (E) and force (F) are related as:

$$E = \int F \, dr \quad (\text{Eq. 3}) \quad (0.5 \text{ points})$$

The force of attraction between two ions can be driven as Eq. 4:

$$F_A = \frac{A}{r^2} \quad (\text{Eq. 4}) \quad (0.5 \text{ points})$$

if we take ion 1 to be the cation that has a charge of +2 and ion 2 to be the anion with charge -1; also, from the problem statement. Thus, we compute the force of attraction between these two ions as follows:

$$F_A = \frac{A}{r^2} = \frac{1}{4\pi\left(8.85 \times 10^{-12} \frac{\text{C}^2}{\text{N}\cdot\text{m}^2}\right)(5.3 \times 10^{-9} \text{ m})^2} [|+2|(1.602 \times 10^{-19} \text{ C})][|-1|(1.602 \times 10^{-19} \text{ C})] =$$

$$1.6430 \times 10^{-11} \text{ N} \quad (2 \text{ points})$$

Task 3. Crystal structure (40 points, Lecture2)

3.1 Explain the lattice and unit cell of the crystal structure (please use figures and illustrations and make a proper citation of the figures if they are not created by you). (4 points)

Solution:

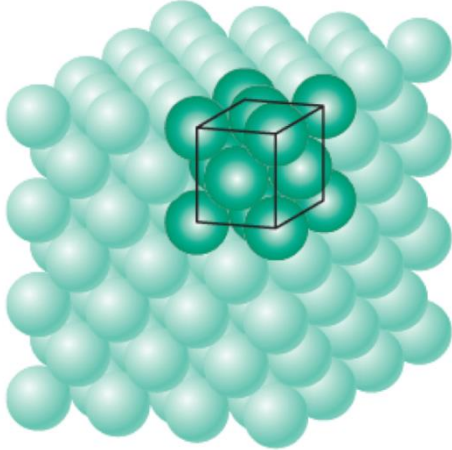


Figure 2 Lattice and unit cell illustration: green balls mean the hard-sphere atoms, black cube means the smallest unit cell. [1]

(a) Lattice (2 points)

The term lattice is used in the context of crystal structures. When describing crystalline structures, atoms (or ions) are thought of as being solid spheres having well-defined diameters. This is termed as the atomic hard-sphere model in which spheres representing nearest-neighbor atoms touch one another. Generally, lattice means a three-dimensional array of points coinciding with atom positions (or sphere centers), as the arrangement of green balls shown in Figure 2.

(b) Unit cell (2 points)

The atomic order in crystalline solids indicates that small groups of atoms form a repetitive pattern. Thus, in describing crystal structures, it is often convenient to subdivide the structure into small repeat entities called unit cells. Thus, the unit cell is the basic structural unit or building block of the crystal structure and defines the crystal structure by virtue of its geometry and the atom positions within, as the black cube marked in Figure 2.

3.2 For four types of crystal structure:

- (a) Primitive cubic;
- (b) Body-centered cubic (BCC);
- (c) Face-centered cubic (FCC);
- (d) ideal Hexagonal close-packed (HCP),

finish the following tasks:

- Draw the unit cell with the coordinate system (Please create it on your own, copy/paste from textbook/slides is not accepted!); (1 points*4)
- Mark the most closely packed planes and directions and list their Miller indices; (4 points*4)
- Determine the number of nearest neighbors; (2 points*4)
- Calculate the atomic packing factor (Please give the detailed calculation process.). (2 points*4)

Solution:

Figure 3 shows the unit cell of the required crystal structure in the coordinate system. The most closely packed planes are marked with blue shaded areas and the most closely packed directions are marked with red arrows. Table 1 listed the corresponding Miller indices and the nearest neighbors' number for each structure. It shall be noted that the single unit cell for HCP is the cell marked with black solid lines. The atomic packing factor can be calculated as follows:

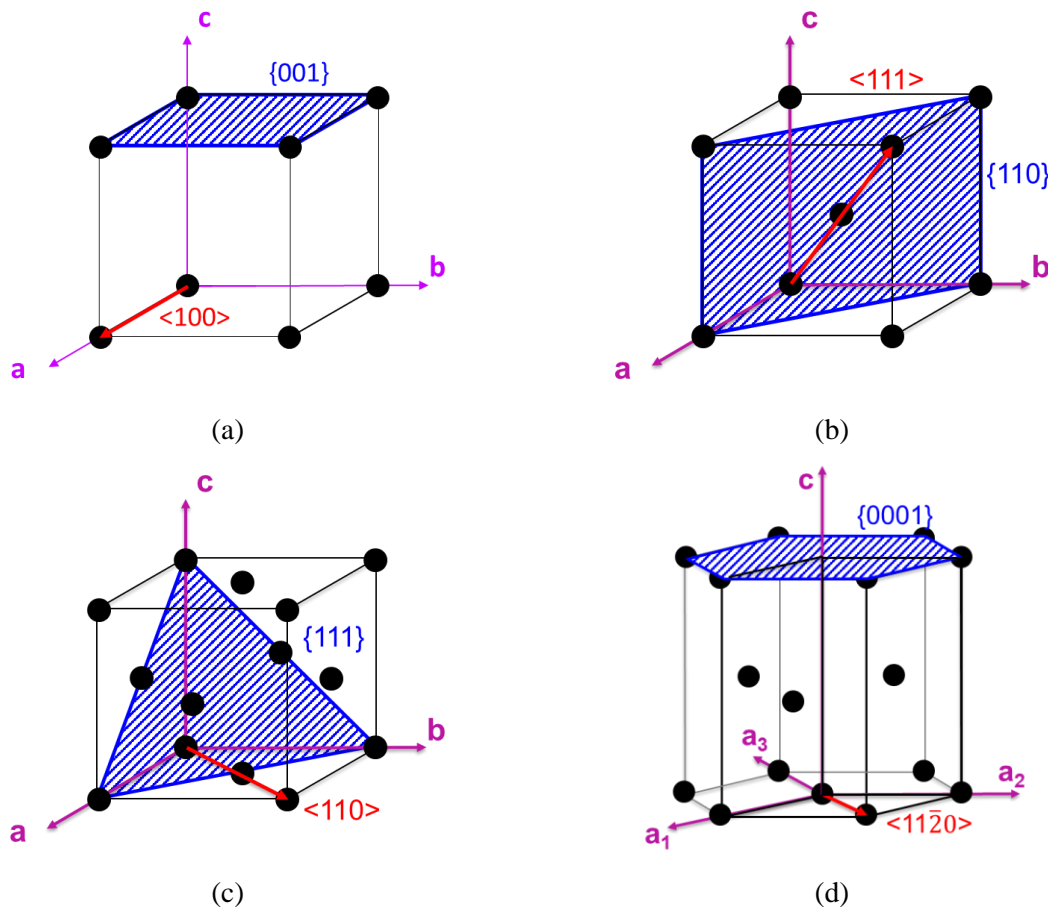


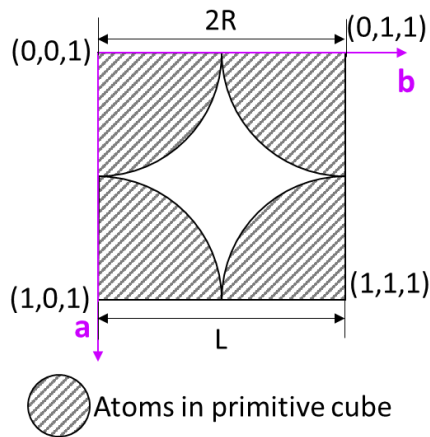
Figure 3 The schematic diagram of unit cells (cell with black solid lines) of (a) Primitive cubic, (b) BCC, (c) FCC, and (d) HCP crystal structure in the coordinate system. Their most closely packed planes are marked as the blue shaded areas and the most closely packed directions are marked with the red arrows.

Table 1 Summary of the crystal structure information.

	Primitive cubic	BCC	FCC	HCP
Most closely packed planes	{100}	{110}	{111}	{0001}
Most closely packed directions	$\langle 100 \rangle$	$\langle 111 \rangle$	$\langle 110 \rangle$	$\langle 11\bar{2}0 \rangle$
Number of nearest neighbors	6	8	12	12
Atomic packing factor	0.52	0.68	0.74	0.74

(a) Primitive cubic:

As the (001) plane in unit cell illustrated, the atoms touch one another across an axial direction, and the length of which is $2R$. Because the unit cell is a cube, its volume is L^3 , where L is the cell edge length.



Atom radius: $R = \frac{L}{2}$,

Number of atoms in a unit cell: $N = \frac{1}{8} \times 8 = 1$,

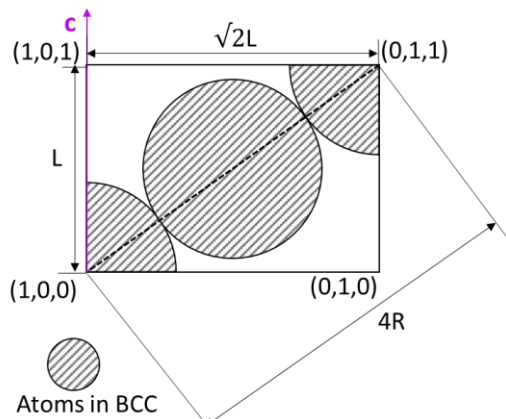
Atoms' volume in a unit cell: $V_a = \frac{4}{3} \pi R^3 \cdot N$,

Unit cell's volume: $V_c = L^3$,

Atomic packing factor: $APF = \frac{V_a}{V_c} = \frac{\frac{4}{3} \pi (\frac{L}{2})^3 \cdot 1}{L^3} = \frac{\pi}{6} \approx 0.52$.

(b) BCC:

As the unit cell illustrated, the atoms touch one another along the body diagonal direction on the diagonal plane (110) in BCC, and the length of which is $4R$. Because the unit cell is a cube, its volume is L^3 , where L is the cell edge length.



Atom radius: $R = \frac{\sqrt{3}L}{4}$,

Number of atoms in a unit cell:

$$N = \frac{1}{8} \times 8(\text{corner}) + 1(\text{body center}) = 2,$$

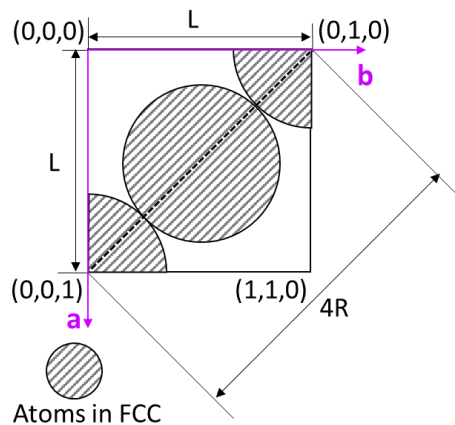
Atoms' volume in a unit cell: $V_a = \frac{4}{3} \pi R^3 \cdot N$,

Unit cell's volume: $V_c = L^3$,

Atomic packing factor: $APF = \frac{V_a}{V_c} = \frac{\frac{4}{3} \pi (\frac{\sqrt{3}L}{4})^3 \cdot 2}{L^3} = \frac{\sqrt{3}\pi}{8} \approx 0.68$.

(c) FCC:

As the unit cell illustrated, the atoms touch one another across a face diagonal on the base plane in FCC, and the length of which is $4R$. Because the unit cell is a cube, its volume is L^3 , where L is the cell edge length.



Atom radius: $R = \frac{\sqrt{2}L}{4}$,

Number of atoms in a unit cell:

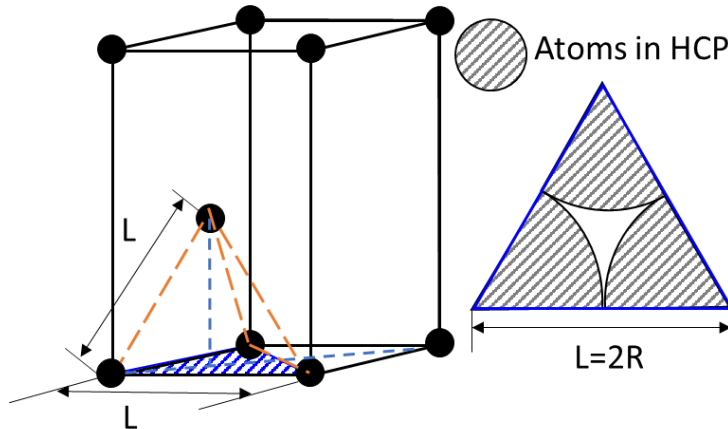
$$N = \frac{1}{8} \times 8(\text{corner}) + \frac{1}{2} \times 6(\text{face-center}) = 4,$$

Atoms' volume in a unit cell: $V_a = \frac{4}{3} \pi R^3 \cdot N$,

Unit cell's volume: $V_c = L^3$,

Atomic packing factor: $APF = \frac{V_a}{V_c} = \frac{\frac{4}{3} \pi (\frac{\sqrt{2}L}{4})^3 \cdot 4}{L^3} = \frac{\sqrt{2}\pi}{6} \approx 0.74$.

(d) Ideal HCP with $L_c/L_a=1.6333$.



As the unit cell illustrated, the atoms touch one another across a pyramid line and the length of which is $2R$, the pyramid structure is composed by three atoms in the bottom plane and one atom in the mid-plane. For ideal HCP ($L_c/L_a=1.6333$), the length of the pyramid is the HCP cell edge length L . The blue shaded area shown in the unit cell is chosen to illustrate the relationship of atom radius and edge length.

Atom radius: $R = \frac{L}{2}$,

Number of atoms in a unit cell:

$$N = \frac{1}{6} \times 12(\text{corner}) + \frac{1}{2} \times 2(\text{top and bottom plane center}) + 3(\text{mid-plane}) = 6,$$

Atoms' volume in a unit cell: $V_a = \frac{4}{3}\pi R^3 \cdot N$,

Unit cell's volume: $V_c = 3 \cdot \left(\frac{\sqrt{3}}{2} \cdot r_{c/a} \cdot L^3\right)$,

Atomic packing factor:

$$APF = \frac{V_a}{V_c} = \frac{\frac{4}{3}\pi\left(\frac{L}{2}\right)^3 \cdot 6}{3 \cdot \left(\frac{\sqrt{3}}{2} \cdot r_{c/a} \cdot L^3\right)} = \frac{2\pi}{3\sqrt{3} \cdot r_{c/a}} \approx 0.74.$$

Task 4. Polycrystal structure (25 points, Lecture2&Exercise1)

- 4.1 (a) Describe briefly, what the dislocation is and the types of dislocations.
(b) Describe briefly, what the crystallographic orientation is.
(c) Explain, how the grain size distribution of polycrystals can be determined and represented.

Solution:

(a): Definition and types of dislocations (2 points)

Dislocations are perturbations of the perfect crystal along a line. The type of dislocation most easy to visualize is a line where a crystallographic plane terminates in a crystal (Figure 4 a). This terminal line of the partial crystallographic plane in the crystal is also referred to as an edge dislocation. Alternatively, such an edge dislocation can be considered to be generated by cutting a crystal perpendicular to the terminal line of the cut and subsequent reattaching both parts of the crystal. Another type of dislocation is obtained if both parts of the crystal are not displaced perpendicular but parallel to the terminal line of the cut. This generates a screw dislocation (Figure 5). If one makes a circuit on a plane perpendicular to the line of and encircling the screw dislocation, one never returns to the starting points but rather one moves on a spiral around the dislocation line. The displacement to the separated crystallites in the plane of cut can be at any angle to the dislocation line, neither perpendicular nor parallel (Figure 6). Such a mixed dislocation can be considered as composed of the two basic types, i. e. edge dislocation and screw dislocation.

A dislocation is characterized by its line element \mathbf{s} and its Burgers vector \mathbf{b} . The line element is the unit vector tangential to the dislocation line. If the dislocation line is curved, \mathbf{s} will change along the dislocation line. The Burgers vector has the length and direction of the vector by which the two parts of the crystal above and below the plane of motion of the dislocation are displaced with respect to each other. It can be defined exactly by the Burgers circuit (Figure 4 b, c). For this, the arrangement of lattice sites in a plane perpendicular to the dislocation line is drawn for the perfect and the dislocated crystal. After defining the direction of the dislocation line, a closed circuit around the dislocation line clockwise (right-hand screw) around the positive direction of the dislocation line (Figure 4 b) is created. If the same circuit is drawn in the perfect crystal, the start and finish points of the circuit are not identical (Figure 4 c). The difference vector between finish and start is the Burgers vector. The Burgers vector does not change along a dislocation line. For edge dislocations, the Burgers vectors are perpendicular to the dislocation line whereas for screw dislocations the Burgers vectors and line elements are parallel to each other.

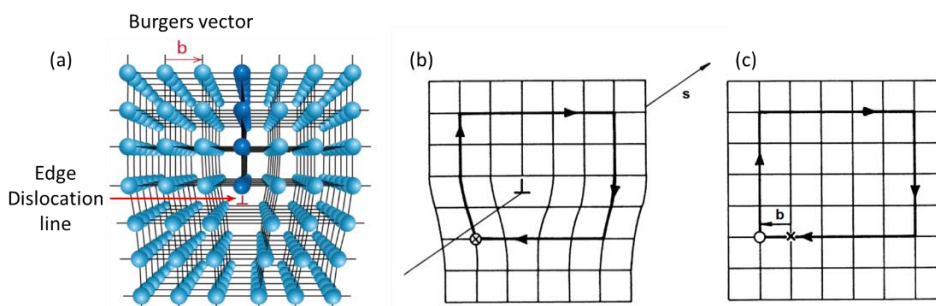


Figure 4 Schematic drawings of dislocation. (a) Atom configuration at an edge dislocation. (b) Edge dislocation, extra half-plane of atoms inserted in a crystal structure. (c) Definition of the Burgers vector \mathbf{b} by a Burgers circuit. \mathbf{s} indicates the direction of the dislocation line. Circle and cross indicate start and finish of the circuit. [2]

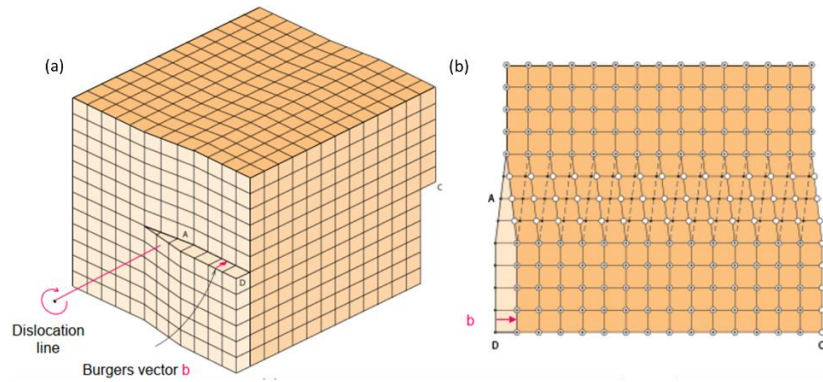


Figure 5 Screw dislocation, spiral planar ramp resulting from shear deformation. (a) Schematic of screw dislocation in a crystal. (b) Top view of screw dislocation in (a). [3]

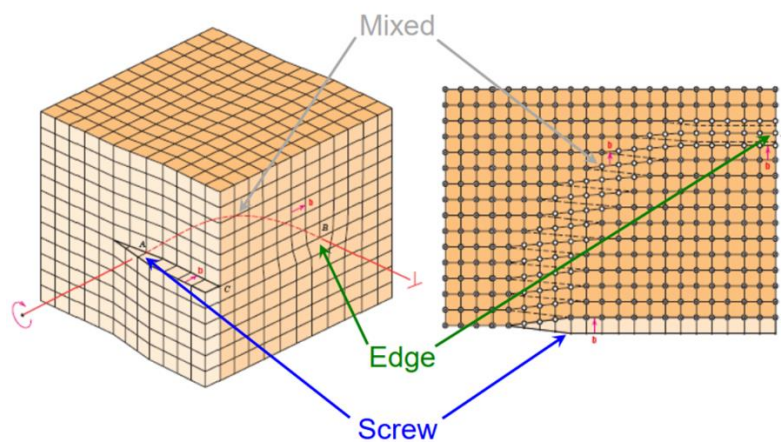


Figure 6 Edge, Screw, and Mixed dislocations. [3]

(b): Definition of crystallographic orientation (2 points)

The crystallographic orientation describes the relationship between the crystal coordinate system and the sample coordinate system of a single crystal/grain. It can be defined by a mathematical 3*3 rotation matrix \mathbf{g} , which transforms the sample frame $\{\mathbf{S}\}$ into the crystal frame $\{\mathbf{C}\}$: $\{\mathbf{C}\} = \mathbf{g} \cdot \{\mathbf{S}\}$.

Representation of crystallographic orientation

The crystallographic orientation can be represented by the rotation matrix, Miller indices, Euler angles, rotation axis/angle methods, and so on.

(1) Rotation matrix

The rotation matrix \mathbf{g} is a 3×3 matrix, in terms of a rolled specimen with the cubic crystal symmetry,

$$\mathbf{g} = \begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix} = \begin{pmatrix} \cos\alpha_1 & \cos\beta_1 & \cos\gamma_1 \\ \cos\alpha_2 & \cos\beta_2 & \cos\gamma_2 \\ \cos\alpha_3 & \cos\beta_3 & \cos\gamma_3 \end{pmatrix} \quad (\text{Eq. 7})$$

As shown in Figure 7, α_1 , β_1 , and γ_1 are the angles between the first crystal axis [100] and the three sample axes X, Y, Z, respectively; α_2 , β_2 , and γ_2 are the angles between the second crystal axis [010] and the three sample axes X, Y, Z, respectively; α_3 , β_3 , and γ_3 are the angles between the third crystal axis [001] and the three sample axes X, Y, Z, respectively.

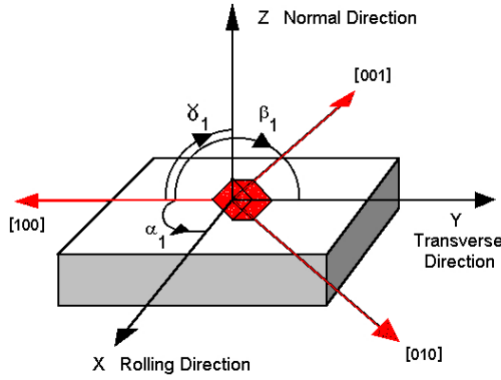


Figure 7 Relationship of the specimen and crystal coordinate system: the rotation matrix g . [4]

(2) Miller indices method

Miller or Miller-Bravais (for HCP) indices method is a method to express the sample axes in the crystal coordinates, which is conventionally written as $(hkl)[uvw]$ or $\{hkl\}\langle uvw \rangle$. The indices (hkl) and $[uvw]$ are used to measure the sample axes Z and X in the crystal coordinate respectively, i.e. for a rolled sample, ND and RD axes. An example is given in Figure 8, Goss orientation can be expressed as $(110)[001]$, that means, the normal direction of crystal plane (110) is parallel to the specimen ND (Z -axis), and the crystal direction $[001]$ is parallel to the specimen RD (X -axis). The rotation matrix g and Miller indices $(hkl)[uvw]$ are related through:

$$g = \begin{pmatrix} u/N_1 & q/N_2 & h/N_3 \\ v/N_1 & r/N_2 & k/N_3 \\ w/N_1 & s/N_2 & l/N_3 \end{pmatrix} \quad (\text{Eq. 8})$$

The indices $[qrs]$ corresponds to the specimen Y direction, i.e. TD axis in a rolled sample, and $[qrs] = (hkl) \times [uvw]$. The parameters $N_1 N_2 N_3$ are required to normalize the three columns of the matrix to unity:

$$\begin{aligned} N_1 &= \sqrt{u^2 + v^2 + w^2} \\ N_2 &= \sqrt{q^2 + r^2 + s^2} \\ N_3 &= \sqrt{h^2 + k^2 + l^2} \end{aligned} \quad (\text{Eq. 9})$$

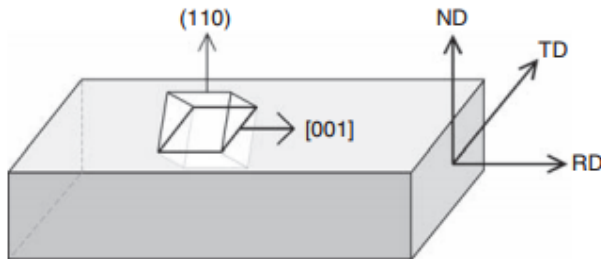


Figure 8 Schematic illustration of the relationship between the crystal and specimen axes for the $(110)[001]$ Goss orientation. [4]

(3) Euler angle method

The Euler angle method is the most concise way to represent an orientation since it only uses three rotation orientations, ϕ_1 , Φ , ϕ_2 . There are several conventions to define the Euler angles, here the Bunge definition [5] is applied (Figure 9):

1. rotation by ϕ_1 about the ND, transforming the rolling direction RD into RD', on (001) plane of the crystal frame;
2. rotation by Φ about the axis RD' (in its new orientation), transforming the normal direction ND into direction $[001]$ of the crystal frame and bringing TD into the (001) plane in the crystal frame;

3. rotation by φ_2 about ND'' (in its new orientation, i.e. [001] direction).

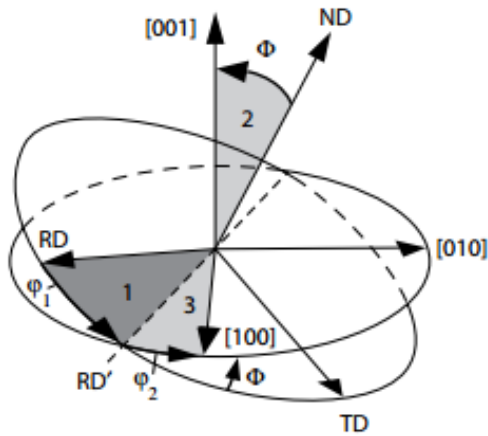


Figure 9 Schematic presentation showing the Bunge definition of the Euler angles. [4]

Mathematically, these three rotations can be expressed as:

$$g_{\varphi_1} = \begin{pmatrix} \cos\varphi_1 & \sin\varphi_1 & 0 \\ -\sin\varphi_1 & \cos\varphi_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$g_{\Phi} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\Phi & -\sin\Phi \\ 0 & \sin\Phi & \cos\Phi \end{pmatrix} \quad (\text{Eq. 10})$$

$$g_{\varphi_2} = \begin{pmatrix} \cos\varphi_2 & \sin\varphi_2 & 0 \\ -\sin\varphi_2 & \cos\varphi_2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Therefore, the relationship between the rotation matrix g and the Euler angles is:

$$g = g_{\varphi_2} \cdot g_{\Phi} \cdot g_{\varphi_1} \quad (\text{Eq. 11})$$

(4) Rotation axis/angle parameters method and misorientation

The rotation axis/angle parameter $[uvw]/\theta$ method is the transformation between the crystal coordinate system and the specimen coordinate system via a rotation through an angle θ about a specific axis $[uvw]$, as shown in Figure 10. The rotation matrix g and rotation axis/angle parameter $[uvw]/\theta$ are related through:

$$\begin{aligned} 2\cos\theta &= g_{11} + g_{22} + g_{33} - 1 \\ u \cdot 2\sin\theta &= g_{23} - g_{32} \\ v \cdot 2\sin\theta &= g_{31} - g_{13} \\ w \cdot 2\sin\theta &= g_{12} - g_{21} \end{aligned} \quad (\text{Eq. 12})$$

common axis
[uvw] = [001]

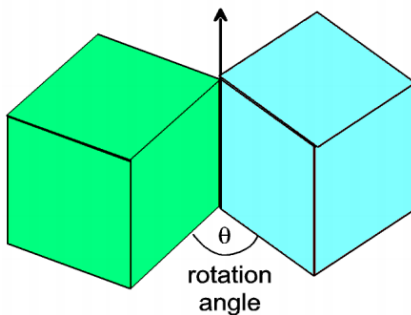


Figure 10 The angle/axis of rotation between two cubes. [4]

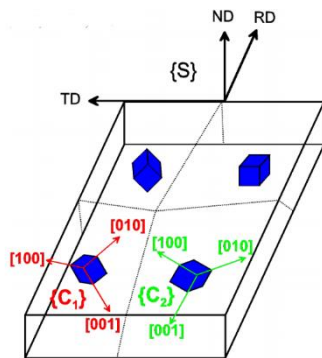


Figure 11 Schematic diagram for grain misorientation definition. [4]

The rotation axis/angle method is useful in the misorientation description. The misorientation between two grains is the rotation matrix \mathbf{g}^M to transform crystal frame $\{C_1\}$ of grain 1 into the crystal frame $\{C_2\}$ of grain 2: $\{C_2\} = \mathbf{g}^M \cdot \{C_1\}$ or $\mathbf{g}^M = \mathbf{g}_1^{-1} \cdot \mathbf{g}_2$ (Figure 11). The misorientation matrix \mathbf{g}^M is analogous to the rotation matrix \mathbf{g} , and it can be expressed in the rotation axis/angle parameter $[uvw]/\theta$ method. In general, only the misorientation angle θ is considered in misorientation distribution.

(c): Definition and characterization of grain size (2 points)

The grain structure can be observed with several advanced stereological methods, e.g. the light optical microscopy (LOM), SEM, or coupling EBSD methods. After the imaging of grain structure, the grain size can be calculated according to the standard DIN EN ISO 643 by counting the intersections of grain boundaries with overlaid special geometrical curves in the micrograph, like with a straight line or with spirals. With advanced numerical software, e.g. ImageJ or Mtex toolbox in Matlab, a more accurate way can be employed to determine the grain size. A grain region can be fitted with a circle in 2D or a sphere in 3D, which has the same area or volume as the grain region. Consequently, their diameter can be defined as the grain equivalent diameter, which is used for the grain size representation. The grain size distribution or the statistical frequency of specific grain sizes can be presented in a histogram, which generally follows the log-normal distribution.

4.2 Analyze the grain size and grain shape of the attached EBSD data (ebsd2.ctf). (Hint: Do grain reconstruction, plot the grain map, give the total grain number and finally inner grain number, draw the distribution figures, and calculate the characteristic parameters of the distribution. It is better to use the log-normal distribution for grain size and Beta distribution for grain shape.)

Solution:

Commands: See the attached pages.

Results:

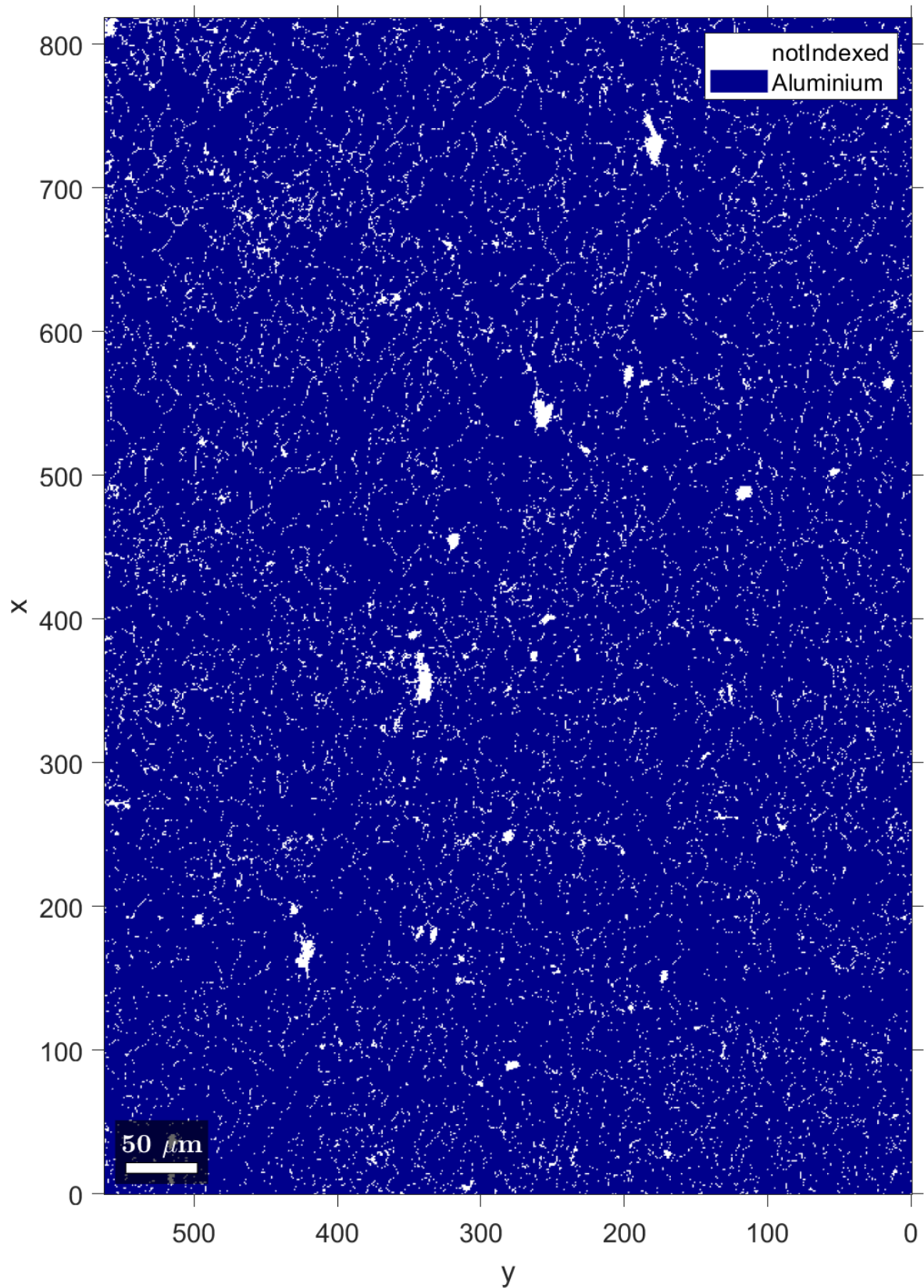


Figure 12 Phase map.

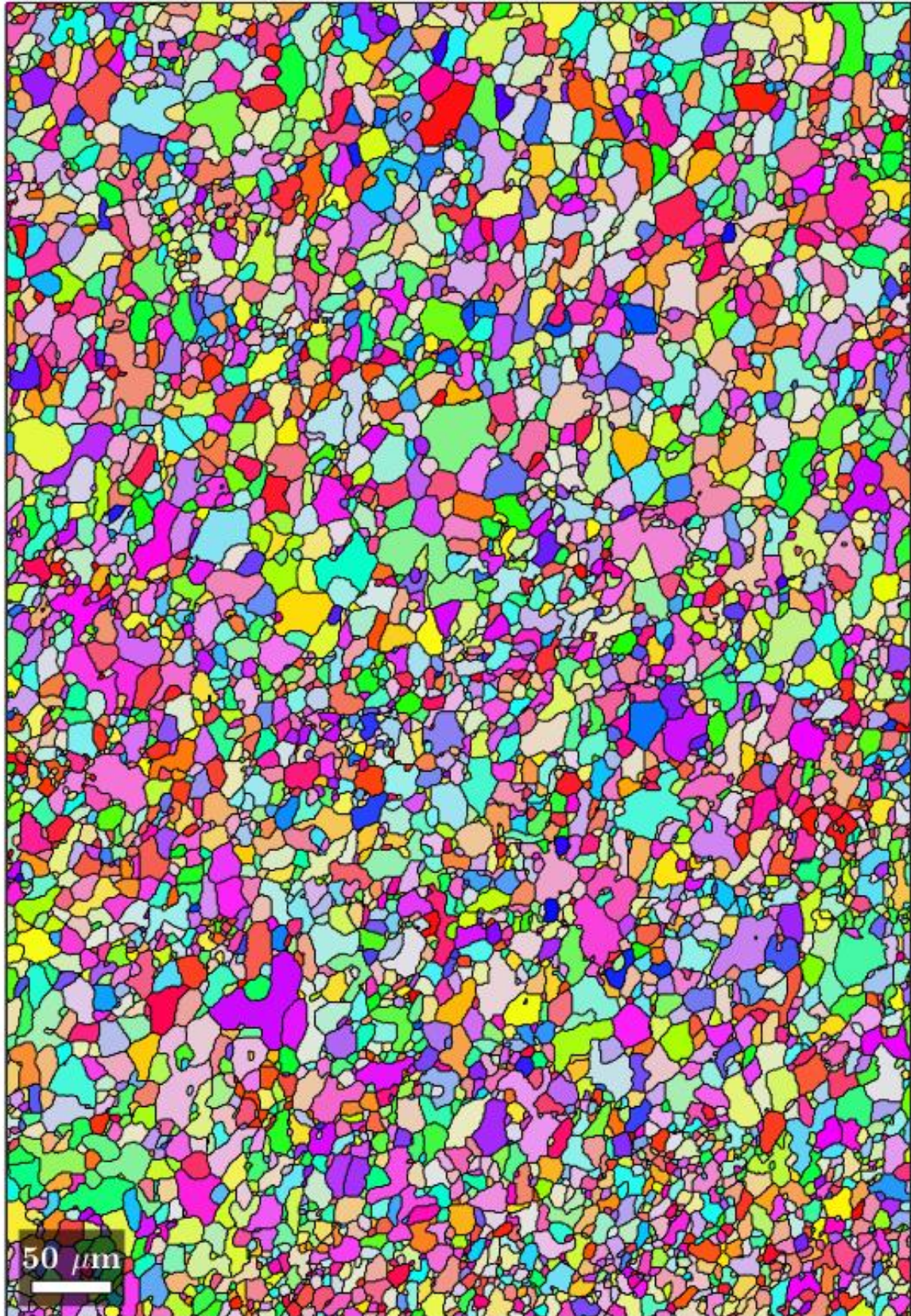


Figure 13 Grain mean orientation map.

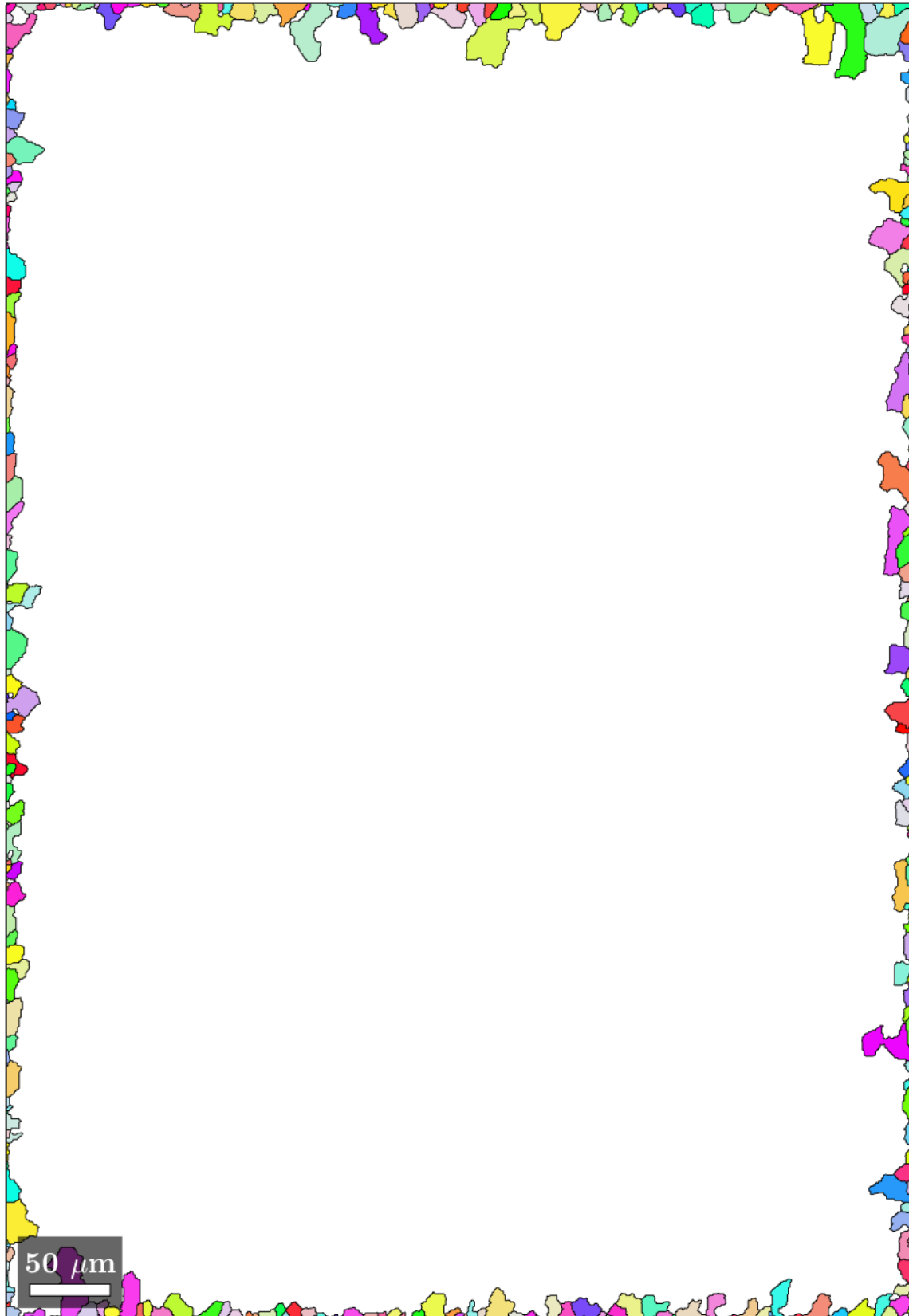


Figure 14 Boundary grain mean orientation map.

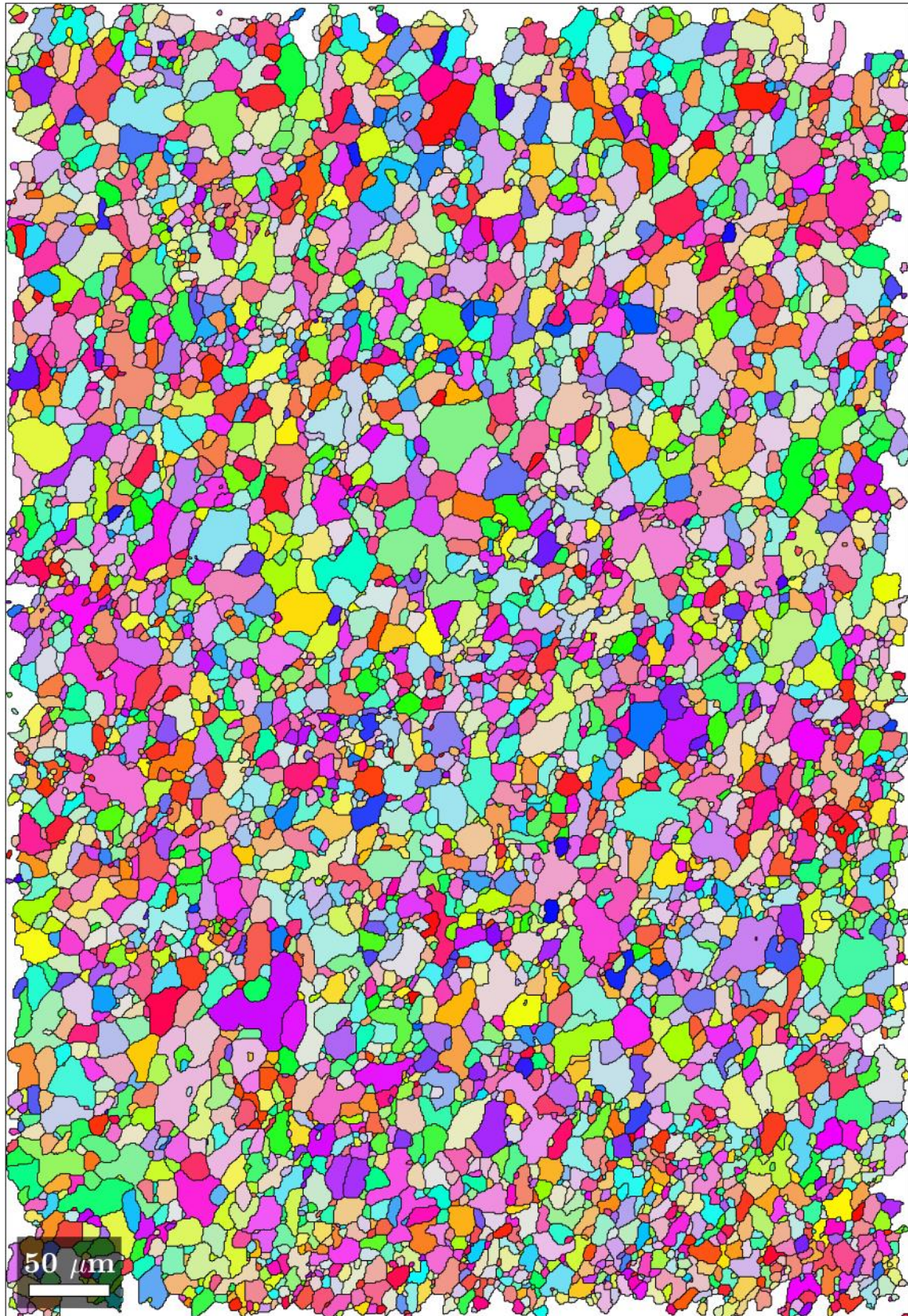


Figure 15 Inner grain mean orientation map.

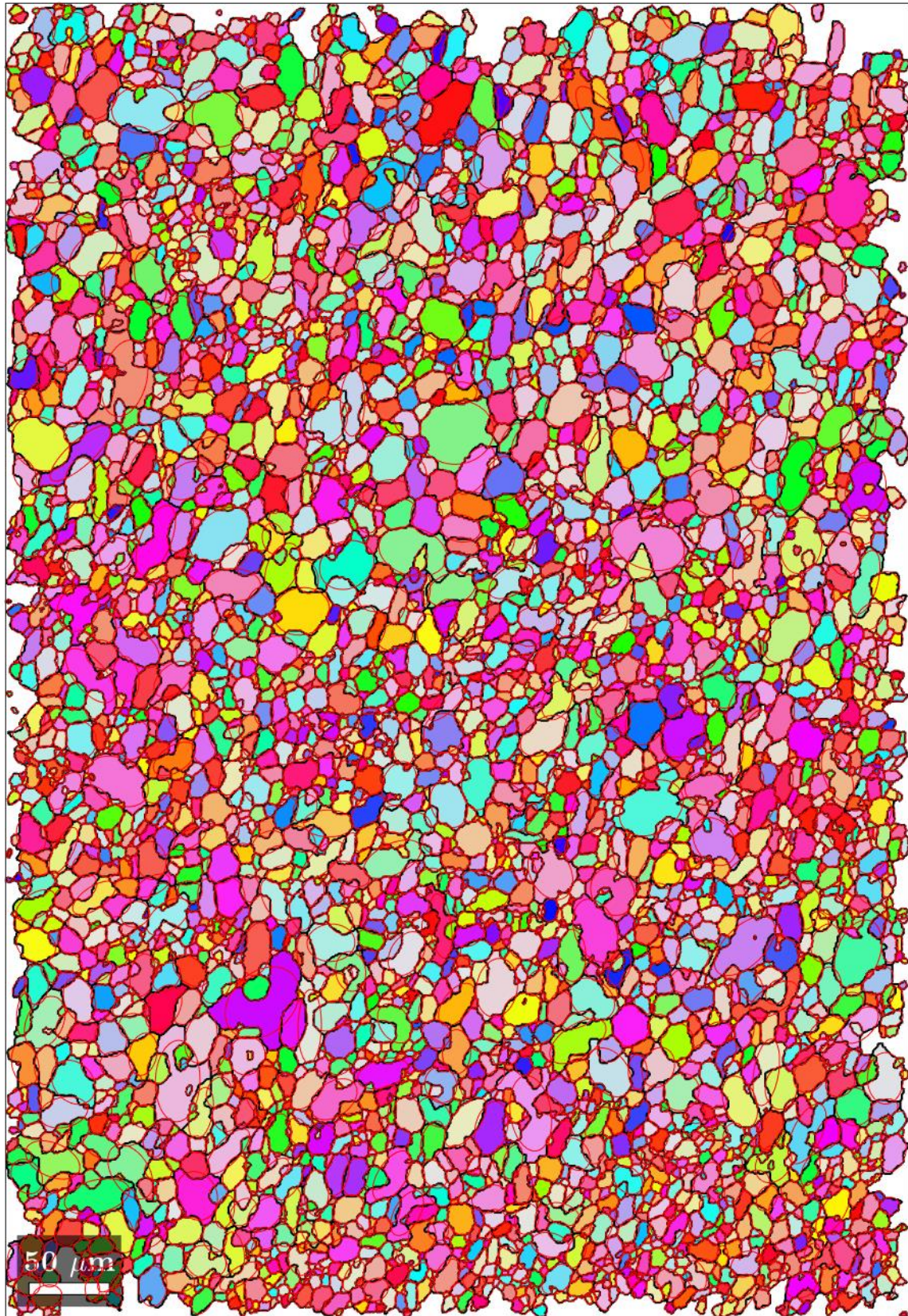


Figure 16 Inner grain mean orientation map with fitted ellipses.

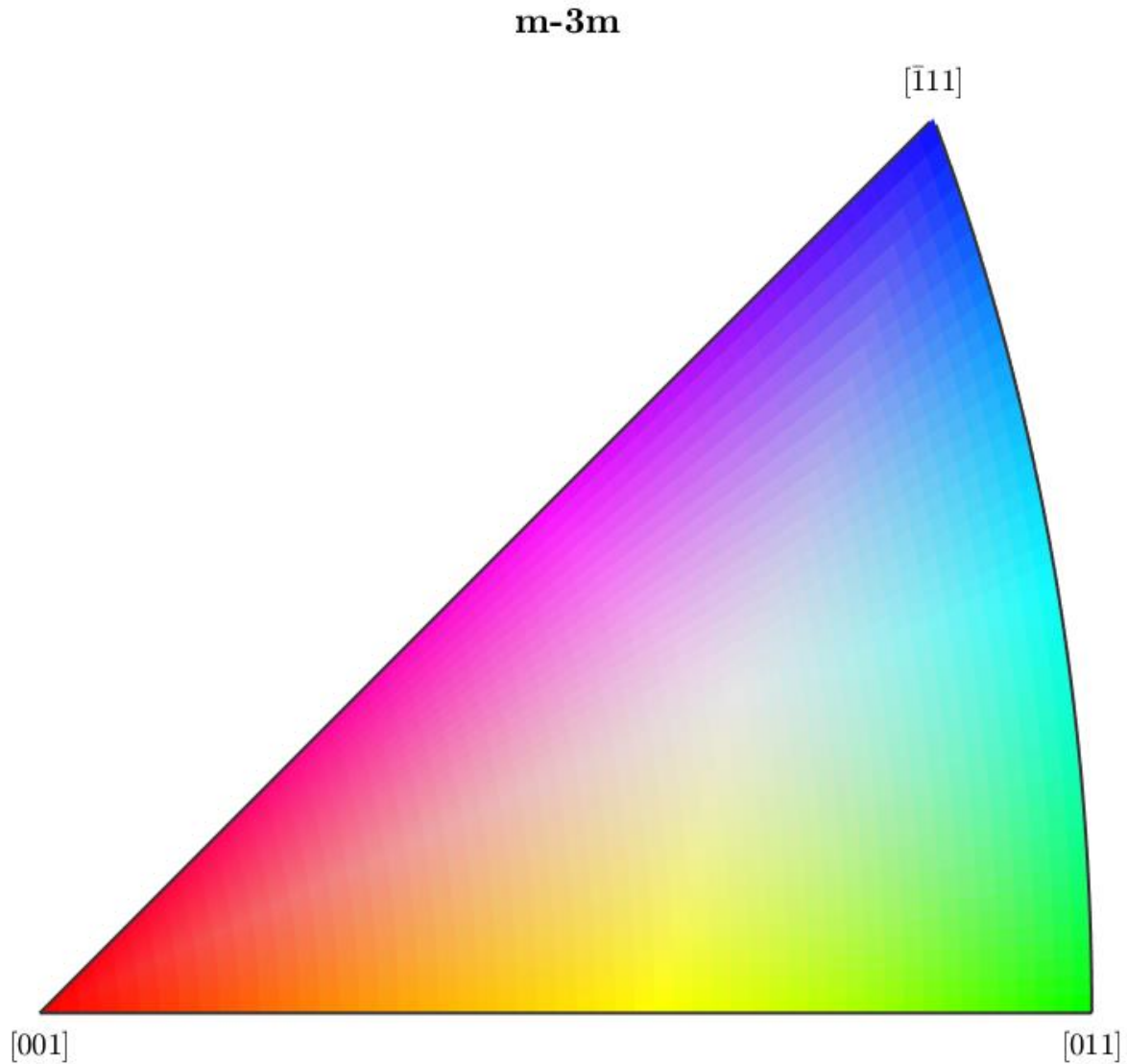


Figure 17 IPF color bar for orientation maps in Figures 13-16.

After grain reconstruction with the misorientation as 15° for grain boundaries, the grain mean orientation map is shown in Figure 13. The initial grain number is 5580. After correction for $MAD < 1$ and deleting very small grains, the total grain number for the focused phase is 5323. The inner grain number is 4977. The grain size and shape distribution are shown in Figure 18, and the fitted parameters are listed in Table 2. The average grain size is $8.9304 \mu\text{m}$ and the average grain shape aspect ratio is 0.6978.

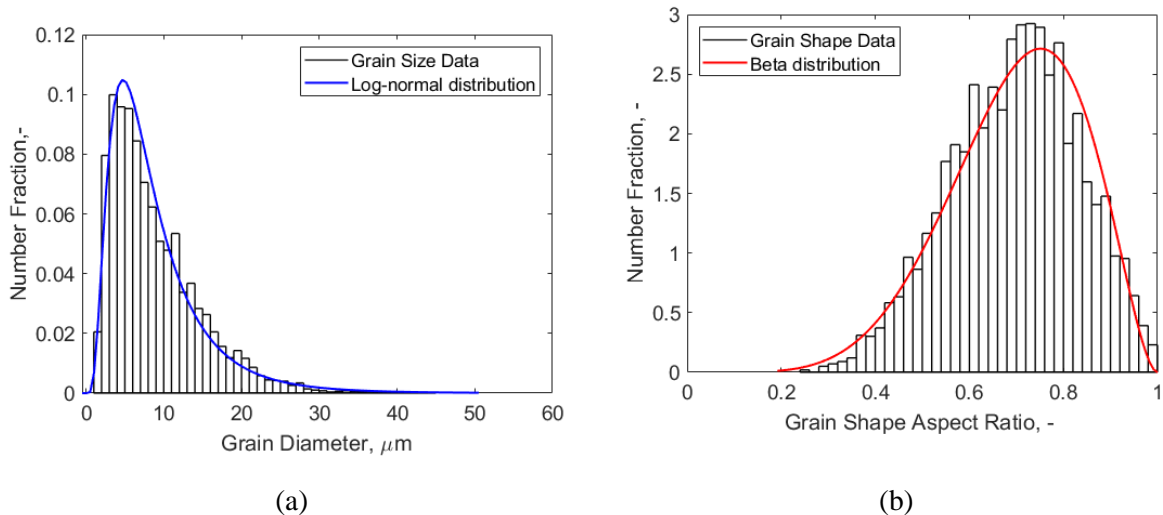


Figure 18 (a) Grain size distribution with log-normal function fitting and (b) Grain shape distribution with Beta function fitting.

Table 2 Grain size and shape distribution parameters.

Grain size distribution			Grain shape distribution		
μ	σ	mean	α	β	mean
1.9787	0.6492	8.9304 μm	6.5559	2.8397	0.6978

(Grain reconstruction + any phase/grain/orientation map after grain reconstruction – 5 points;
Grain number information – 2 points;
Grain size and shape distribution figures with fitting curves – (2+1)*2=6 points;
Grain size and shape distribution parameters and mean values– 3*2=6 points;)

Reference:

1. Callister W. D., Rethwisch D. G., *Materials Science and Engineering: An Introduction*, 8th Edition. 2009: Wiley.
2. Gottstein G., *Physical foundations of materials science*. 2004, Berlin ; New York: Springer. xiv, 502 p.
3. Read W. T., *Dislocations in crystals*. International series in pure and applied physics. 1953, New York,: McGraw-Hill. 228 p.
4. Engler O., Randle V., *Introduction to Texture Analysis: Macrotexture, Microtexture, and Orientation Mapping*. 2nd ed. 2010, Boca Raton: CRC Press. 488.
5. Bunge H. J., 2 - Orientation of individual crystallites, in *Texture Analysis in Materials Science*, Bunge H. J., Editor. 1982, Butterworth-Heinemann. p. 3-41.

Due date: 18:00, 07.11.2021.

Contact: MyCourses ‘General discussion’ channel,

Q&A: every Tuesday at 16:30-18:00 (via Zoom: <https://aalto.zoom.us/j/62428835336>).

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%% Script for EBSD Data analysis
% Purpose: EBSD analysis with Matlab-MTEX toolbox
% Functions: Import EBSD data
%             EBSD plotting & initial analyses
%             Grain reconstruction
%             Grain Size & Shape analysis
%
% Record of revision:
%   Date           Programmer           Description of change
%   =====
%   01-11-2021     Wenqi Liu            Original code for MTEX 5.4.0
%
%----- General Comments END-----
%% Import the Data.
% Specify crystal symmetry.
CS = {...
    'notIndexed',...
    crystalSymmetry('6/mmm', [5.8 5.8 4.6], 'X||a*', 'Y||b', 'Z||c', 'mineral', 'Ti3Al -
alpha2', 'color', [0.53 0.81 0.98]),...
    crystalSymmetry('4/mmm', [4 4 4.1], 'mineral', 'TiAl - gamma', 'color', [0.56 0.74
0.56]),...
    crystalSymmetry('m-3m', [3.3 3.3 3.3], 'mineral', 'Titanium-Cubic', 'color', [0.85
0.65 0.13]),...
    crystalSymmetry('m-3m', [4 4 4], 'mineral', 'Aluminium', 'color', [0.94 0.5 0.5]),...
    crystalSymmetry('m-3m', [4 4 4], 'mineral', 'Aluminium', 'color', [0 0 0.55])};
% plotting convention
setMTExpref('xAxisDirection','north');
setMTExpref('zAxisDirection','outOfPlane');
% path to files
pname = 'Z:\Documents\MATLAB\MSEcourse2020';
% which files to be imported
fname = [pname '\ebd2.ctf'];
% create an EBSD variable containing the data
ebd = EBSD.load(fname,CS,'interface','ctf',...
    'convertEuler2SpatialReferenceFrame');

%% Initial analyses - Phase Map.
% Index/Phase analysis.
figure;plot(ebd,'coordinates','on');
saveas(gcf, 'A1Task4_PhaseMap.png')

%% Grain reconstruction.
% Consider only indexed & corrected data.
ebd_corrected = ebd(ebd.mad<1);
ebdcorri=ebd_corrected('indexed');
% Reconstruct the grain structure.
[grains,ebdcorri.grainId,ebdcorri.mis2mean] =
calcGrains(ebdcorri,'angle',15*degree);
initialGrainNr=length(grains);
% Delete the very small grains which might be caused by the measurement error.
ebdcorri(grains(grains.grainSize<2)) = [];
% Redo grain segmentation.
[grains,ebdcorri.grainId] = calcGrains(ebdcorri,'angle',15*degree);
% Pick up the focused phase.
grainsAl=grains('Aluminium');
totalGrainNr=length(grainsAl);
% Plotting grain mean orientation maps.
figure;
ipfKey = ipfColorKey(ebd('Aluminium'));
ipfKey.inversePoleFigureDirection = vector3d.Z;
colors = ipfKey.orientation2color(grainsAl.meanOrientation);
plot(grainsAl,colors);
saveas(gcf, 'A1Task4_TotalGrainMap.png')

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%% Grain Size & Shape Data Analysis.
% Find the boundary grains.
outerBoundary_id = any(grainsAl.boundary.grainId==0,2);
grain_id = grainsAl.boundary(outerBoundary_id).grainId;
grain_id(grain_id==0) = [];
% Plot the boundary grains with their mean orientations.
figure;
plot(grainsAl(grain_id),grainsAl(grain_id).meanOrientation);
saveas(gcf, 'A1Task4_BoundaryGrainMap.png')
% Remove the boundary grains.
grainsAl(grain_id) = [];
innerGrainNr=length(grainsAl);
% Plot the inner grains with their mean orientations.
figure;plot(grainsAl,grainsAl.meanOrientation);
saveas(gcf, 'A1Task4_InnerGrainMap.png')
% Fit the equivalent ellipses of grains.
[GrainfitEangle,GrainfitElongA,GrainfitEshortb] = fitEllipse(grainsAl);
% Extract Grain Data.
Grainarea=grainsAl.area;
GraineqR=grainsAl.equivalentRadius;
GraineqD=GraineqR*2;
Grainasp=1./grainsAl.aspectRatio;
% Plot fitted ellipses
figure;
plot(grainsAl,grainsAl.meanOrientation,'linewidth',1);
hold on;
plotEllipse(grainsAl.centroid,GrainfitElongA,GrainfitEshortb,GrainfitEangle,'lineColor'
,'r');
hold off;
saveas(gcf, 'A1Task4_InnerGrainMap+FitE.png')

%% Grain size - number fraction distribution
% Plot data originally in dataset "diameter data".
[CdfF,CdfX] = ecdf(GraineqD,'Function','cdf');% compute empirical cdf
BinInfo.rule = 5;
BinInfo.width = 1;
BinInfo.placementRule = 1;
[~,BinEdge] = internal.stats.histbins(GraineqD,[],[],BinInfo,CdfF,CdfX);
[BinHeight,BinCenter] = ecdfhist(CdfF,CdfX,'edges',BinEdge);
figure;
hLine = bar(BinCenter,BinHeight,'hist');
set(hLine,'DisplayName','Grain Size
Data','FaceColor','none','EdgeColor','k','LineStyle','-','LineWidth',1);
xlabel('Grain Diameter, {\mu}m','fontsize',15);
ylabel('Number Fraction,-','fontsize',15);
% Create grid where function will be computed.
hold on;
XLim = get(gca,'XLim');
XLim = XLim + [-1 1] * 0.01 * diff(XLim);
XGrid = linspace(XLim(1),XLim(2),100);
% Fit this distribution to get parameter values.
pdnum = fitdist(GraineqD,'lognormal');
mu_n=pdnum.mu;
sigma_n=pdnum.sigma;
mean_n = mean(pdnum);
median_n = median(pdnum);
v_n = std(pdnum);
mode_n=exp(mu_n-sigma_n.^2);
YPlot = pdf(pdnum,XGrid);
hLine = plot(XGrid,YPlot,'Color','b','LineStyle','-','
'LineWidth',1.5,'DisplayName','Log-normal distribution');
legend('show','Location','northeast')
hold off;
saveas(gcf, 'A1Task4_GrainSizeDis.png')

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%% Grain shape aspect ratio - number fraction distribution
% Plot data originally in dataset "shape data".
[CdfF,CdfX] = ecdf(Grainasp,'Function','cdf'); % compute empirical cdf
BinInfo.rule = 5;
BinInfo.width = 0.02;
BinInfo.placementRule = 1;
[~,BinEdge] = internal.stats.histbins(Grainasp,[],[],BinInfo,CdfF,CdfX);
[BinHeight,BinCenter] = ecdfhist(CdfF,CdfX,'edges',BinEdge);
figure;
hLine = bar(BinCenter,BinHeight,'hist');
set(hLine,'DisplayName','Grain Shape
Data','FaceColor','none','EdgeColor','k','LineStyle','-','LineWidth',1);
hold on
% Create grid where function will be computed.
XLim = get(gca,'XLim');
XLim = XLim + [-1 1] * 0.01 * diff(XLim);
XGrid = linspace(XLim(1),XLim(2),100);
% Fit this distribution to get parameter values - Beta.
pdaspBeta = fitdist(Grainasp,'Beta');
a_aspBeta = pdaspBeta.a;
b_aspBeta = pdaspBeta.b;
mean_aspBeta = mean(pdaspBeta);
v_aspBeta = std(pdaspBeta);
median_aspBeta = median(pdaspBeta);
YPlot = pdf(pdaspBeta,XGrid);
hLine = plot(XGrid,YPlot,'Color','r','LineStyle','-','
'LineWidth',1.5,'DisplayName','Beta distribution');
legend('show','Location','northwest')
xlabel('Grain Shape Aspect Ratio, -','fontsize',15);
ylabel('Number Fraction, -','fontsize',15)
xlim([0 1]);
hold off;
saveas(gcf,'A1Task4_GrainShapeDis.png')

```