COE-C2004 - Materials Science and Engineering
2020-2021 Autumn II

Assignment 1, 26.10.2020

Task 1. <u>Open solution.</u>

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 –3, the centers of which are separated by a distance of 6.8 nm. (Please give the detailed calculation process, and explain your choices or equations and numbers.)

<u>Solution:</u>

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

$$E_A = -\frac{A}{r} \tag{Eq. 1}$$

Herein, r = 6.8 nm = 6.8×10^{-9} m, and **A** represents lattice energy and its value could be given in Eq. 2 as:

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

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

$$E_A = -\frac{1}{4\pi\left(8.85\times10^{-12}\frac{C^2}{N\cdot m^2}\right)(6.8\times10^{-9}m)}[|+2|(1.602 \times 10^{-19} \, C)][|-3|(1.602 \times 10^{-19} \, C)] =$$

$$-2.0362 \times 10^{-19} \, J$$

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

$$E = \int F \, dr \tag{Eq. 3}$$

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

$$F_A = \frac{A}{r^2} \tag{Eq. 4}$$

if we take ion 1 to be the cation that has a charge of +2 and ion 2 to be the anion with charge –3; also, from the problem statement. Thus, we compute the force of attraction between these two ions as follows:

$$F_A = \frac{A}{r^2} = \frac{1}{4\pi\left(8.85\times10^{-12}\frac{C^2}{N\cdot m^2}\right)(6.8\times10^{-9}m)^2}[|+2|(1.602 \times 10^{-19} \, C)][|-3|(1.602 \times 10^{-19} \, C)] =$$

$$2.9944 \times 10^{-11} N$$

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2.2 Using the figure below, calculate the percent ionic character of the interatomic bonds for the following materials:

      (a) "CsCl";

      (b) "CsBr".

(Please give the detailed calculation process.)

IA																		0
1 H 2.1	IIA											IIIA	IVA	VA	VIA	VIIA		2 He –
3 Li 1.0	4 Be 1.5											5 B 2.0	6 C 2.5	7 N 3.0	8 O 3.5	9 F 4.0		10 Ne –
11 Na 0.9	12 Mg 1.2	IIIB	IVB	VB	VIB	VIIB		VIII		IB	IIB	13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	17 Cl 3.0		18 Ar –
19 K 0.8	20 Ca 1.0	21 Sc 1.3	22 Ti 1.5	23 V 1.6	24 Cr 1.6	25 Mn 1.5	26 Fe 1.8	27 Co 1.8	28 Ni 1.8	29 Cu 1.9	30 Zn 1.6	31 Ga 1.6	32 Ge 1.8	33 As 2.0	34 Se 2.4	35 Br 2.8		36 Kr –
37 Rb 0.8	38 Sr 1.0	39 Y 1.2	40 Zr 1.4	41 Nb 1.6	42 Mo 1.8	43 Tc 1.9	44 Ru 2.2	45 Rh 2.2	46 Pd 2.2	47 Ag 1.9	48 Cd 1.7	49 In 1.7	50 Sn 1.8	51 Sb 1.9	52 Te 2.1	53 I 2.5		54 Xe –
55 Cs 0.7	56 Ba 0.9	57–71 La–Lu 1.1–1.2	72 Hf 1.3	73 Ta 1.5	74 W 1.7	75 Re 1.9	76 Os 2.2	77 Ir 2.2	78 Pt 2.2	79 Au 2.4	80 Hg 1.9	81 Tl 1.8	82 Pb 1.8	83 Bi 1.9	84 Po 2.0	85 At 2.2		86 Rn –
87 Fr 0.7	88 Ra 0.9	89–102 Ac–No 1.1–1.7																

Figure 1 The electronegativity values for the elements. [1]

Solution:

The percent ionic character is a function of the electronegativity of the ions χ_A and χ_B according to:

$$\%IC = \{1 - exp[-((\chi_A - \chi_B)/2)^2]\} \times 100\% \tag{Eq.5}$$

(a) For CsCl, $\chi_A = 0.7$ and $\chi_B = 3.0$, so

$$\%IC(CsCl) = \{1 - exp[-((0.7 - 3.0)/2)^2]\} \times 100\% = 73\%$$

(b) For CsBr, $\chi_A = 0.7$ and $\chi_B = 2.8$, so

$$\%IC(CsCl) = \{1 - exp[-((0.7 - 3.0)/2)^2]\} \times 100\% = 67\%$$

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Task 3. Crystal structure (25 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).
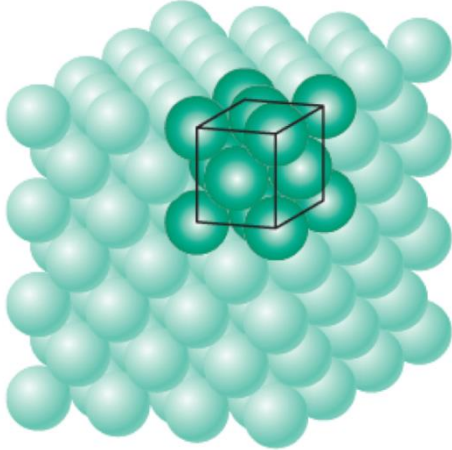
Solution:

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

(a) Lattice

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

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.

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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!);
- Mark the most closely packed planes and directions and list their Miller indices;
- Determine the number of nearest neighbors;
- Calculate the atomic packing factor (Please give the detailed calculation process.).

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:

(a)   (b)

(c)   (d)
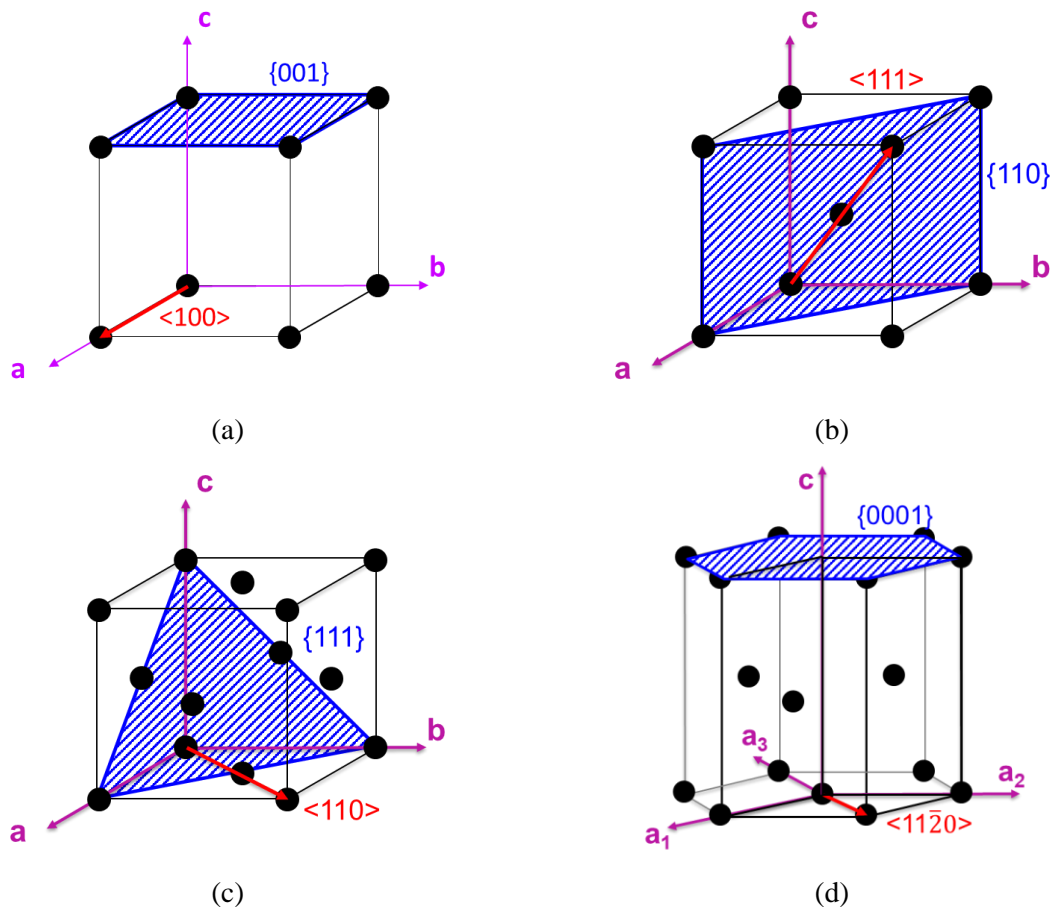
Figure 3 The schematic diagram of unit cells (cell with black solid lines) of (a) Primitive cubic, (b) BCC, (c) FCC, and (d) HCP crystal structure in the coordinate system. Their most closely packed planes are marked as the blue shaded areas and the most closely packed directions are marked with the 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	<100>	<111>	<110>	<11$\bar{2}$0>
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.
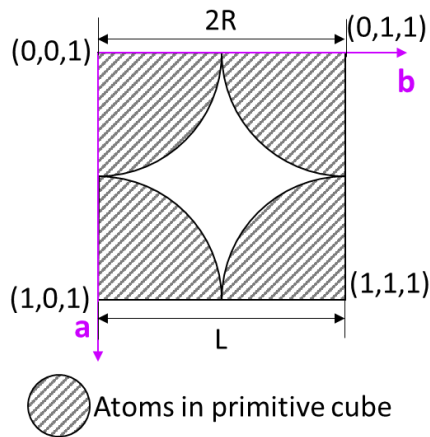
Atom radius: $R = \frac{L}{2}$,

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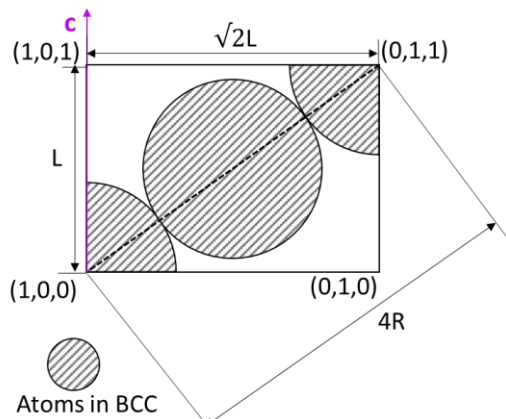
Atom radius: $R = \frac{\sqrt{3}L}{4}$,

Number of atoms in a unit cell:

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

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

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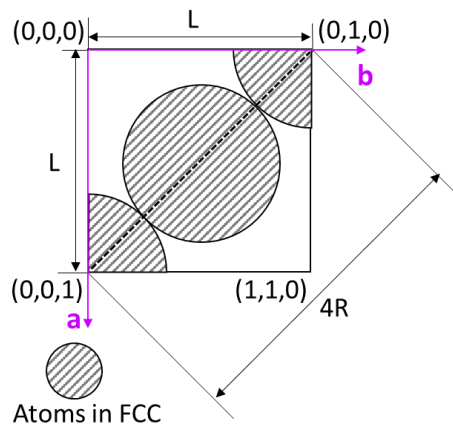
Atom radius: $R = \frac{\sqrt{2}L}{4}$,

Number of atoms in a unit cell:

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

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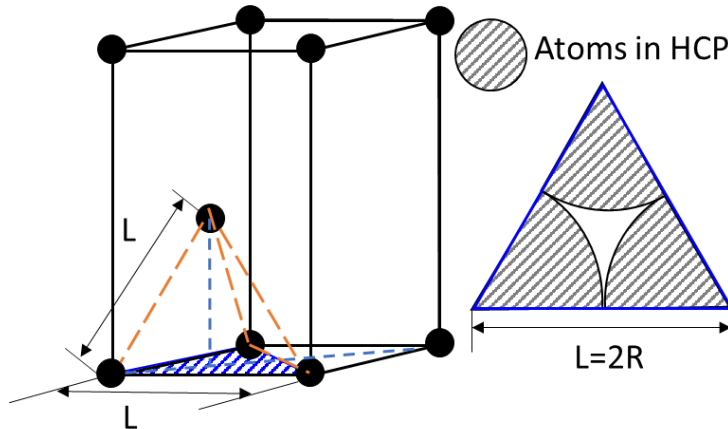
As the unit cell illustrated, the atoms touch one another across a pyramid line and the length of which is 2R, the pyramid structure is composed by three atoms in the bottom plane and one atom in the mid-plane. For ideal HCP ($L_c/L_a=1.6333$), the length of the pyramid is the HCP cell edge length L.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

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

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

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

Atomic packing factor:

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

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Task 4. Polycrystal structure (40 points, Lecture2&Exercise1)

4.1 (a) Describe briefly, what the crystallographic orientation is and how it can be measured and represented. (Hint: explain with examples of the technical relevance of crystallographic orientation investigations.) (b) Give the orientation matrix and Euler angle of the Brass orientation and plot the rotate cube of it. (Hint: Miller index of Brass orientation is $(011)[2\bar{1}1]$.)

Solution:

(a):

Definition of crystallographic orientation

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 **g**, which transforms the sample frame {**S**} into the crystal frame {**C**}: {**C**}=**g**·{**S**}.

Measurement of crystallographic orientation

The main measurement techniques for crystal orientation are the X-ray diffraction (XRD) method or electron backscatter diffraction (EBSD) method with the scanning electron microscopy (SEM).

(1) XRD:

According to Bragg's law:

$$2d\sin\theta = n\lambda \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\text{(Eq. 6)}$$

where the d is the distance between crystal planes, θ is the incident angle, and λ is the wavelength of incident X-ray. The reflection only happens when Bragg's law is fulfilled. Therefore, with the specific incident X-ray and angle θ, the reflection only occurs for the specific crystal planes family which have the plane distance of d. Or, with a pre-set incident angle θ for the X-ray source, only certain crystal planes show the peak intensity in the X-ray figures, as shown in Figure 4 (a). In this way, the crystal orientations can be indexed by XRD. XRD is normally used for macrotexture measurement with a large measurement area.
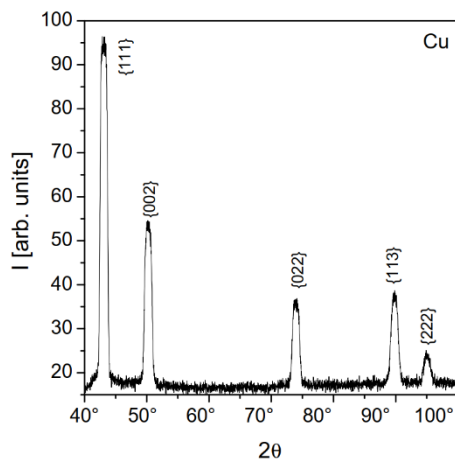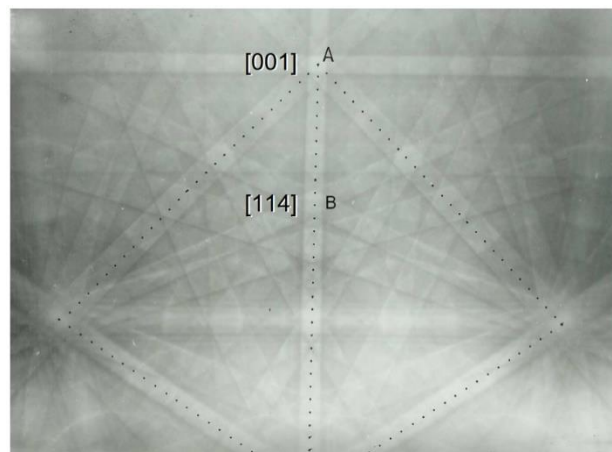
| (a) | (b) |

Figure 4 (a) An X-ray diffraction pattern of Cu. (b) A Kikuchi pattern of a [100]-oriented single crystal in EBSD.[2]

(2) EBSD

According to the diffraction law and crystal structure/orientation database, the Kikuchi pattern can be calibrated with reflection crystal planes in the EBSD method, as an example shown in Figure 4 (b). The corresponding crystal orientations can be calculated in the Euler angle method, and this progress is

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named as 'index'. With the point to point indexing, the orientation map can be obtained within a relatively small measurement area. Therefore, EBSD is preferred for local crystal orientation or microtexture measurements.

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 g is a 3×3 matrix, in terms of a rolled specimen with the cubic crystal symmetry,

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

As shown in Figure 5, 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.
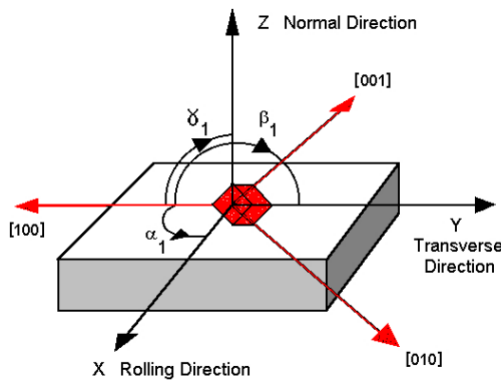

Figure 5 Relationship of the specimen and crystal coordinate system: the rotation matrix g. [2]

(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}<uvw>. 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 6, 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:

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

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

$$N_1 = \sqrt{u^2 + v^2 + w^2}$$
$$N_2 = \sqrt{q^2 + r^2 + s^2} \tag{Eq. 9}$$
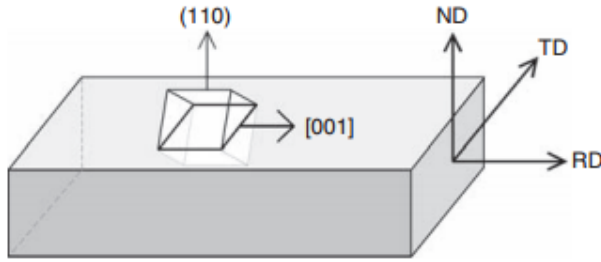$$N_3 = \sqrt{h^2 + k^2 + l^2}$$

Figure 6 Schematic illustration of the relationship between the crystal and specimen axes for the (110) [001] Goss orientation. [2]

(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 [3] is applied (Figure 7):

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;

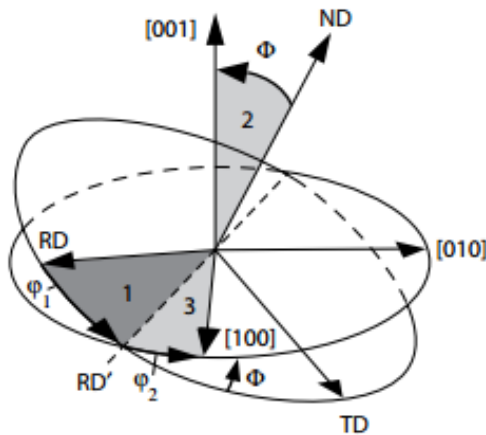3. rotation by φ_2 about ND" (in its new orientation, i.e. [001] direction).

Figure 7 Schematic presentation showing the Bunge definition of the Euler angles. [2]

Mathematically, these three rotations can be expressed as:

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

$$g_{\Phi} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\Phi & -\sin\Phi \\ 0 & -\sin\Phi & \cos\Phi \end{pmatrix}$$ (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:

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

(4) Rotation axis/angle parameters method and misorientation

The rotation axis/angle parameter [uvw]/θ 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 8. The rotation matrix g and rotation axis/angle parameter [uvw]/θ are related through:

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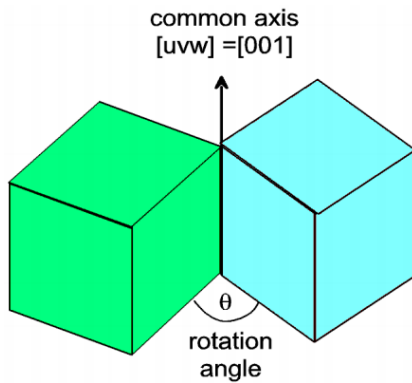
(Eq. 12)

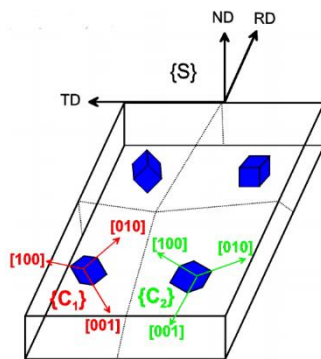Figure 8 The angle/axis of rotation between two cubes. [2]

Figure 9 Schematic diagram for grain misorientation definition. [2]

The rotation axis/angle method is useful in the misorientation description. The misorientation between two grains is the rotation matrix g^M to transform crystal frame {C_1} of grain 1 into the crystal frame {C_2} of grain 2: {C_2} = $g^M \cdot${C_1} or $g^M = g_I^{-1} \cdot g_2$ (Figure 9). The misorientation matrix g^M is analogous to the rotation matrix g, and it can be expressed in the rotation axis/angle parameter [uvw]/θ method. In general, only the misorientation angle θ is considered in misorientation distribution.

(b): Commands

```
%% Commands for Assignment1 Task4.1(a)
cs = crystalSymmetry('m-3m')
ss = specimenSymmetry('mmm')
oriBrass = orientation.byMiller([0 1 1],[2 -1 1],cs,ss)
GmatrixBrass = oriBrass.matrix'
cS = crystalShape.cube(cs)
figure
plot([0,0]+oriBrass * cS)
axis on
```

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Results:

```
oriBrass = orientation (show methods, plot)
  size: 1 x 1
  crystal symmetry : m-3m
  specimen symmetry: mmm

  Bunge Euler angles in degree
     phi1      Phi     phi2     Inv.
   35.2644       45       0        0


GmatrixBrass =

      0.8165     0.5774    -0.0000
     -0.4082     0.5774     0.7071
      0.4082    -0.5774     0.7071
```
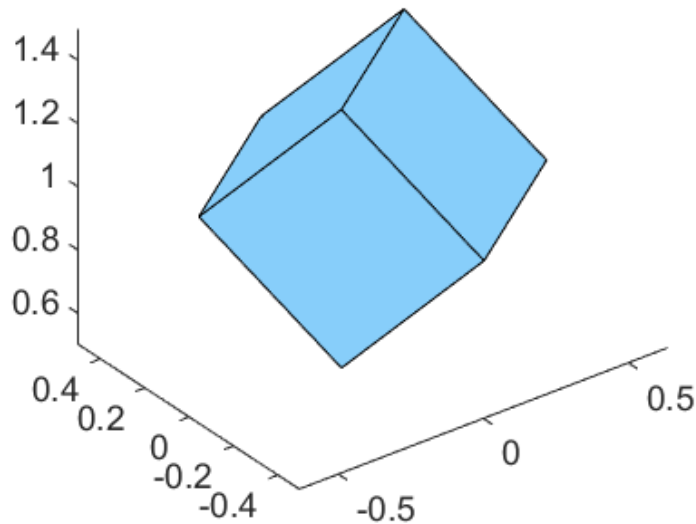

The Euler angle of the Brass orientation is (35.2644°, 45°, 0°) or (35°, 45°, 0°).

The orientation matrix is:

$$g = \begin{pmatrix} 0.8165 & 0.5774 & 0 \\ -0.4082 & 0.5774 & 0.7071 \\ 0.4082 & -0.5774 & 0.7071 \end{pmatrix} \ or \begin{pmatrix} 0.8192 & 0.5736 & 0 \\ -0.4056 & 0.5792 & 0.7071 \\ 0.4056 & -0.5792 & 0.7071 \end{pmatrix}$$

4.2 (a) Explain, how the grain size distribution of polycrystals can be determined and represented. (b) 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:

(a): 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.

(b): Commands: See the attached pages.

Results:
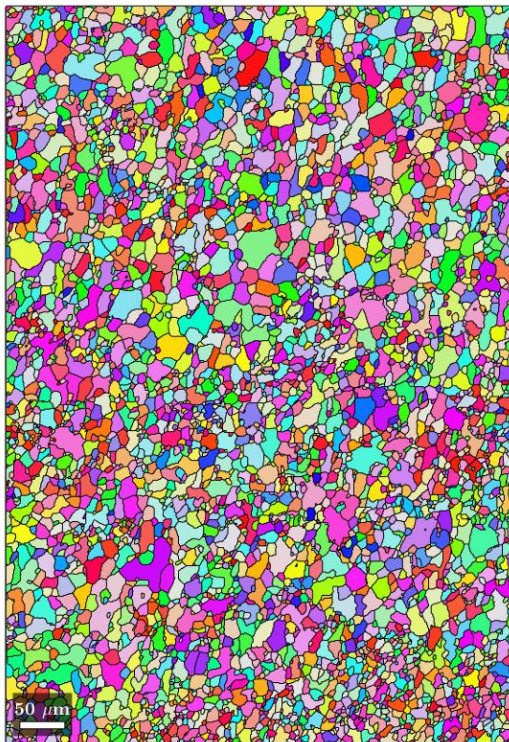
Figure 10 Grain mean orientation of the measured EBSD data.

After grain reconstruction with the misorientation as 15° for grain boundaries, the grain mean orientation map is shown in Figure 10. 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.

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The grain size and shape distribution are shown in Figure 11, and the fitted parameters are listed in Table 2. The average grain size is 8.9304 μm and the average grain shape aspect ratio is 0.6978.

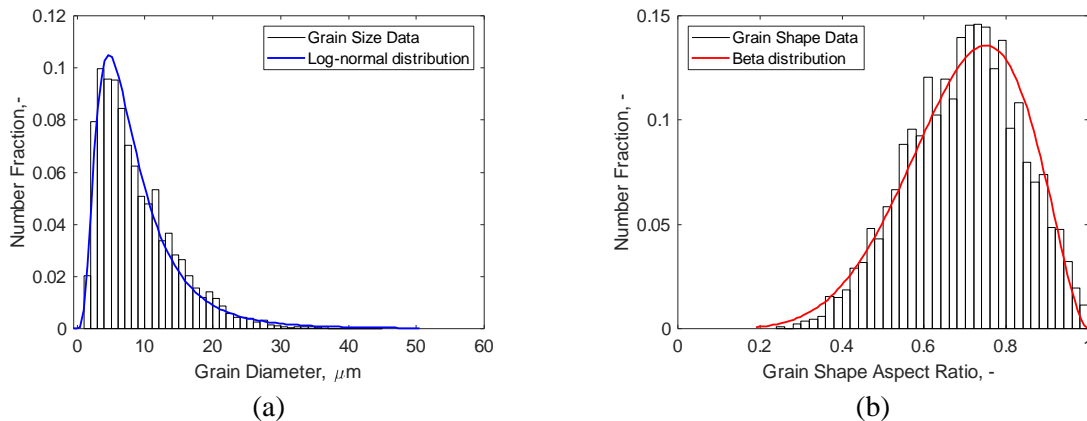(a)   (b)

Figure 11 (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

Reference:

[1] W. D. Callister and D. G. Rethwisch, *Materials Science and Engineering: An Introduction, 8th Edition*, Wiley, 2009.

[2] O. Engler and V. Randle, *Introduction to Texture Analysis: Macrotexture, Microtexture, and Orientation Mapping*, 2010.

[3] H.-J. Bunge, *Texture Analysis in Materials Science: Mathematical Methods*, Butterworth-Heinemann, London, 1982.

Due date: 23:00, 01.11.2020.
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```matlab
%% 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
%   ========        ==========       ================================
%  30-10-2020       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';
% Which files to be imported.
fname = [pname '\ebsd2.ctf'];
% Create an EBSD variable containing the data.
ebsd = EBSD.load(fname,CS,'interface','ctf',...
  'convertEuler2SpatialReferenceFrame');

%% Initial analyses - Phase, Orientation Map.
% Index/Phase analysis.
figure;plot(ebsd,'coordinates','on');
% Plot initial EBSD orientation map.
ipfKey = ipfColorKey(ebsd('Aluminium'));
ipfKey.inversePoleFigureDirection = vector3d.Z;
colors = ipfKey.orientation2color(ebsd('Aluminium').orientations);
figure;
plot(ebsd('Aluminium'),colors);
```

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```matlab
%% Grain reconstruction.
% Consider only indexed & corrected data.
ebsd_corrected = ebsd(ebsd.mad<1);
ebsdcorri=ebsd_corrected('indexed');
% Reconstruct the grain structure.
[grains,ebsdcorri.grainId,ebsdcorri.mis2mean] = calcGrains(ebsdcorri,'angle',15*degree);
initialGrainNr=length(grains);
% Delete the very small grains which might be caused by the measurement error.
ebsdcorri(grains(grains.grainSize<2)) = [];
% Redo grain segmentation.
[grains,ebsdcorri.grainId] = calcGrains(ebsdcorri,'angle',15*degree);
% Pick up the focused phase.
grainsAl=grains('Aluminium');
totalGrainNr=length(grainsAl);
% Plotting grain mean orientation maps.
figure;
plot(grainsAl,grainsAl.meanOrientation);

%% 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);
% Remove the boundary grains.
grainsAl(grain_id) = [];
innerGrainNr=length(grainsAl);
% Plot the inner grains with their mean orientations.
figure;plot(grainsAl,grainsAl.meanOrientation);
% Extract Grain Data.
Grainarea=grainsAl.area;
GraineqR=grainsAl.equivalentRadius;
GraineqD=GraineqR*2;
Grainasp=1./grainsAl.aspectRatio;
% Fit the equivalent ellipses of grains.
[GrainfitEangle,GrainfitElongA,GrainfitEshortb] = fitEllipse(grainsAl);
figure;
plot(grainsAl,grainsAl.meanOrientation,'linewidth',1);
hold on;
plotEllipse(grainsAl.centroid,GrainfitElongA,GrainfitEshortb,GrainfitEangle,'lineColor','r');
hold off;
```

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```matlab
%% 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;
```

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```matlab
%% 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);
BinHeight=BinHeight*0.05;
figure;
hLine = bar(BinCenter,BinHeight,'hist');
set(hLine,'DisplayName','Grain Shape Data','FaceColor','none','EdgeColor','k','LineStyle','-', 'LineWidth',1);
xlabel('Grain Shape Aspect Ratio, - ','fontsize',15);
ylabel('Number Fraction, -','fontsize',15)
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)*0.05;
hLine = plot(XGrid,YPlot,'Color','r','LineStyle','-', 'LineWidth',1.5,'DisplayName','Beta distribution');
legend('show','Location','northwest')
xlim([0 1]);
hold off;
```

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