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Task 1. Materials introduction (25 points, Lecture1)

Select one or more of the following modern items or devices and conduct an Internet search in order to determine what specific material(s) is (are) used and what specific properties this (these) material(s) possess(es) in order for the device/item to function properly. Finally, write a short essay in which you report your findings. (0.5-1 A4 Page)

- Cell phone/digital camera batteries
- Cell phone displays
- Solar cells
- Wind turbine blades
- Fuel cells
- Automobile engine blocks
- Automobile bodies
- Space telescope mirrors
- Military body armor
- Lightweight bicycle frames

Essay: I choose military body armor for materials analysis

- Military body armor: modern military body armour is usually divided into two material types: soft body armour which is easily moveable and not very rigid and hard body armour, which is usually integrated into a vest that covers vital parts (chest, back, torso, head, etc). [1].

In soft body armour, the commonly used materials are Kevlar, Dyneema and Polyethylene (PE). [2] The goal of soft body armour is to be flexible and allow wearers to use in combination with other tools and gears.

- Kevlar is a synthetic fiber invented by Stephanie Kwolek in the 1970s. Kevlar is known to be a strong and heat resistant material. In body armour, Kevlar mainly protects the body from medium to low velocity firearms but not against high ones => The more layers of Kevlar, the more protection the body armour gains. [2]
- Dyneema Composite Fabric (DCF) is an ultra-high-molecular-weight polyethylene (UHMWPE) that is known to be one of the world's current strongest fibers. Its form is a long molecule chain combined with strong intermolecular bonds. Its weight is 15 times less than steel, flexible and highly resistant, making it an ideal materials for soft body armour [3]
- Polyethylene (PE) or $(C_2H_4)_n$, is commonly used as PE armor plates that are usually worn together with carrier vests. PE armor plates are usually resistant on the same par with Dyneema (Dyneema is indeed laminated between two PE sheets) and much lighter than steel. However, it is expensive to produce and easily degraded in high temperatures [2]

In hard body armour, the commonly used materials are steel, ceramic or ceramic composites. Hard body armour is usually composed of multiple plates that are interlocked and covered by an armour shell, commonly known as a vest [1] Hard body armour is less flexible and heavier than its soft counterpart

- Steel: alloys of different metals that make it really resistant and hard. Steel is commonly used as ballistic plates that can reduce blunt trauma when they are hit with high velocity firearms, which Kevlar cannot withstand (although Kevlar being more resistant) [2] A drawback is that steel plates are heavy to carry around.
- Ceramic/ Ceramic composites: Ceramics are often covered in synthetic fibers that often considerably increase the protectiveness of the plates. Ceramic plates can also protect wearers from attacks of blunt or sharp objects. [1]

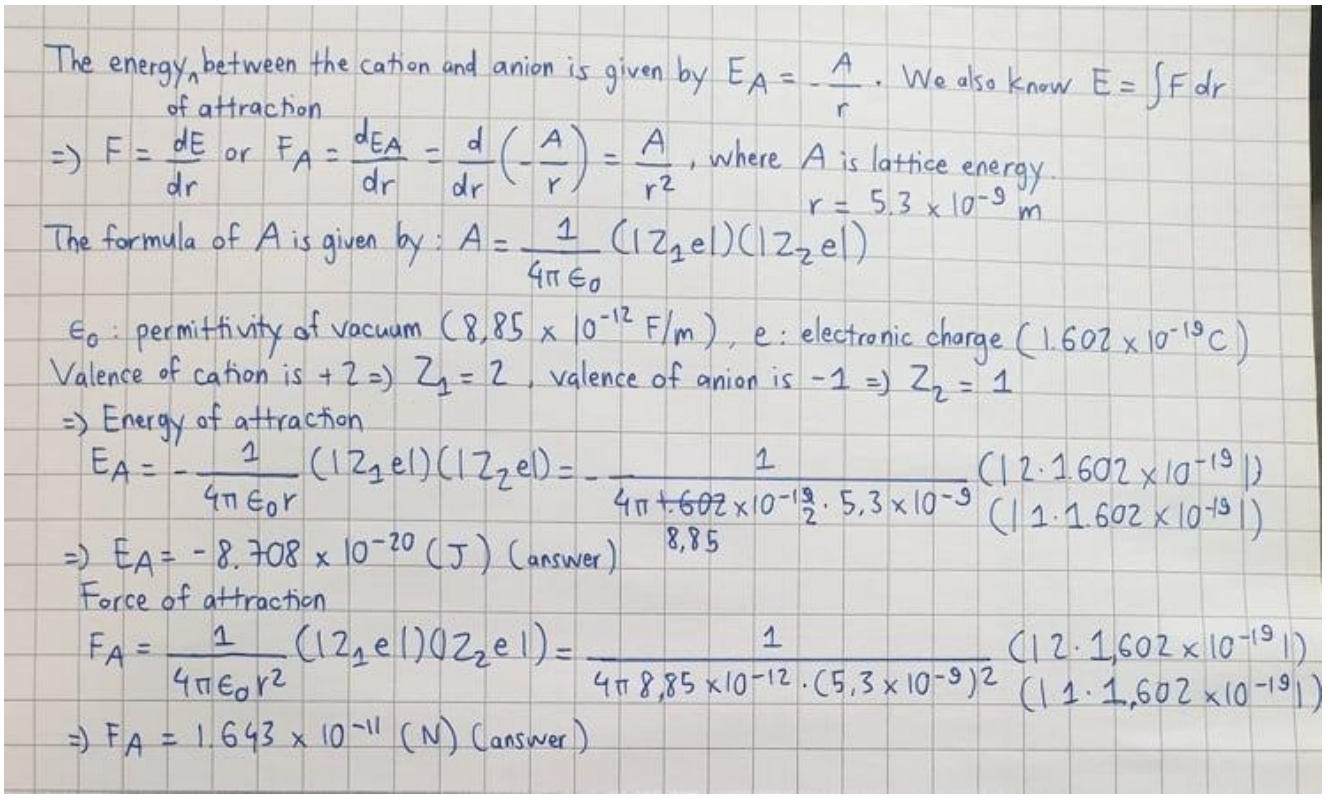
To obtain optimal protection, users should wear an armour that has both soft and hard body armour designs.

References:

1. Khalid, JANUARY 23, 2018. https://www.fortressarmour.com. [Online]
Available at: https://www.fortressarmour.com/difference-soft-hard-body-armour/
[Accessed 2 11 2021].
2. Anon., May 28, 2019. https://www.atomicdefense.com. [Online]
Available at: https://www.atomicdefense.com/blogs/news/materials-used-to-make-body-armor
[Accessed 2 11 2021].
3. Bowden, T., MAY 29, 2018. https://www.gearpatrol.com. [Online] Available at:
https://www.gearpatrol.com/outdoors/a462827/everything-you-need-to-know-about-dyneema/
[Accessed 2 11 2021].

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.)



The energy between the cation and anion is given by $E_A = -\frac{A}{r}$. We also know $E = \int F\,dr$

of attraction

$\Rightarrow F = \frac{dE}{dr}$ or $F_A = \frac{dE_A}{dr} = \frac{d}{dr}\left(-\frac{A}{r}\right) = \frac{A}{r^2}$, where A is lattice energy.

$r = 5.3 \times 10^{-9}$ m

The formula of A is given by: $A = \frac{1}{4\pi\epsilon_0}(|Z_1 e|)(|Z_2 e|)$

ϵ_0: permittivity of vacuum ($8{,}85 \times 10^{-12}$ F/m), e: electronic charge (1.602×10^{-19} C)

Valence of cation is $+2 \Rightarrow Z_1 = 2$, valence of anion is $-1 \Rightarrow Z_2 = 1$

$\Rightarrow$ Energy of attraction

$$E_A = -\frac{1}{4\pi\epsilon_0 r}(|Z_1 e|)(|Z_2 e|) = -\frac{1}{4\pi \frac{8{,}85}{1.602}\times 10^{-19} \cdot 5{,}3 \times 10^{-9}}(|2 \cdot 1.602 \times 10^{-19}|)(|1 \cdot 1.602 \times 10^{-19}|)$$

$\Rightarrow E_A = -8.708 \times 10^{-20}$ (J) (answer)

Force of attraction

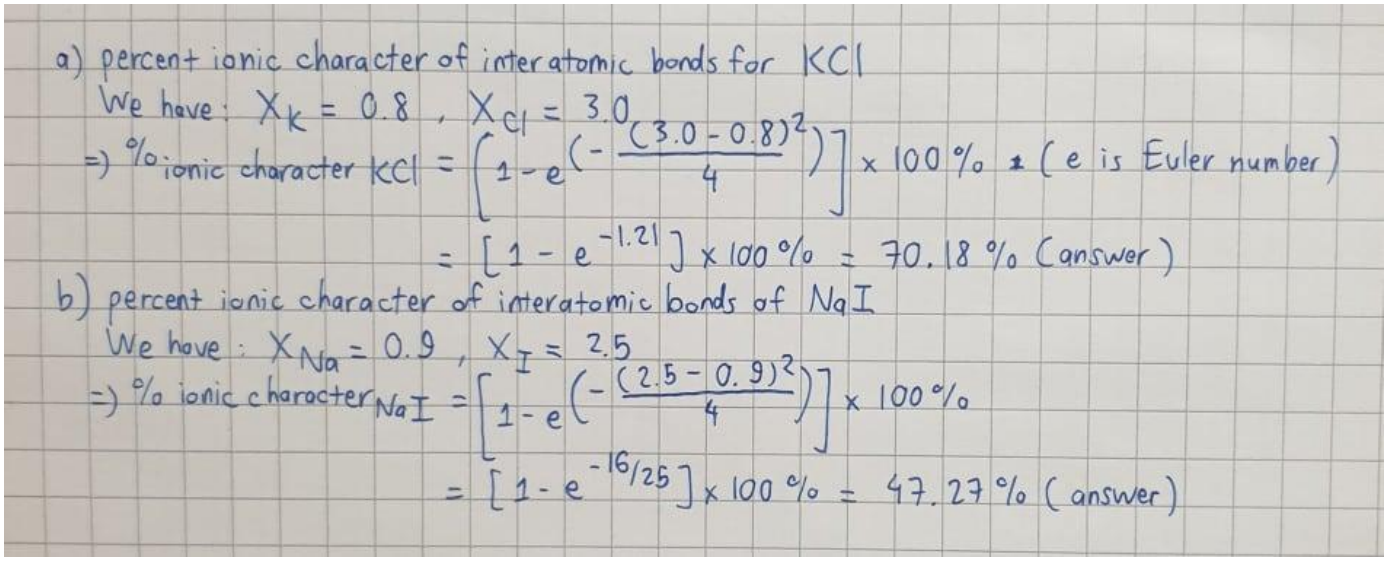
$$F_A = \frac{1}{4\pi\epsilon_0 r^2}(|Z_1 e|)(|Z_2 e|) = \frac{1}{4\pi\, 8{,}85 \times 10^{-12} \cdot (5{,}3 \times 10^{-9})^2}(|2 \cdot 1{,}602 \times 10^{-19}|)(|1 \cdot 1{,}602 \times 10^{-19}|)$$

$\Rightarrow F_A = 1.643 \times 10^{-11}$ (N) (answer)

2.2 Using the figure below, calculate the percent ionic character of the interatomic bonds for the following materials (Please give the detailed calculation process.):

(a) “KCl”; (b) “NaI”.

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															



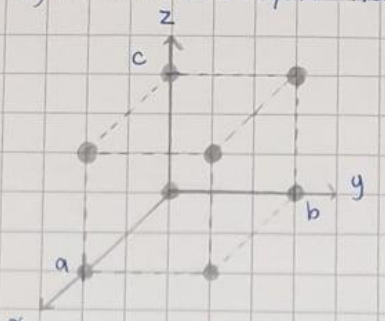
Task 3. Crystal structure (40 points, Lecture2)

3.1 Explain the lattice and unit cell of the crystal structure

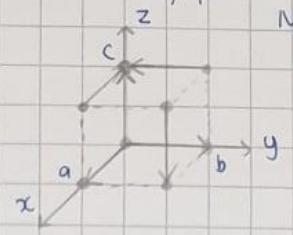
- Lattice of crystal structure: A lattice is an ordered network of lines of atoms forming a regular plane/layer that describes the atomic arrangement of the crystal.
- Unit cell of crystal structure: Unit cell is the smallest repeating pattern in a crystal => a regular crystal can be thought of as blocks of adjacent unit cells

3.2 For four types of crystal structure:
(a) Simple cubic (SC);
(b) Body-centered cubic (BCC);
(c) Face-centered cubic (FCC);
(d) 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)

a) Primitive cubic crystal structure



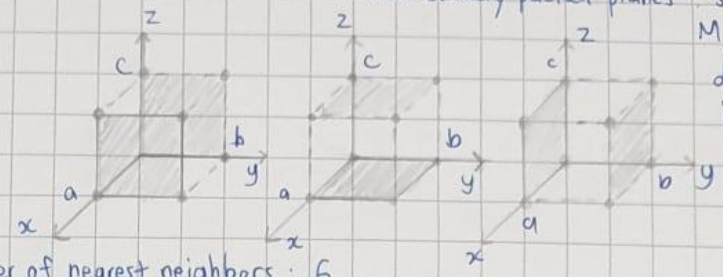
Most closely packed directions : along the cube edges



Miller indices of closely packed directions

$\langle 100 \rangle = [100], [010], [001]$
$[\bar{1}00], [0\bar{1}0], [00\bar{1}]$

Most closely packed planes : sides of the cube unit cell



Miller indices of closely packed directions

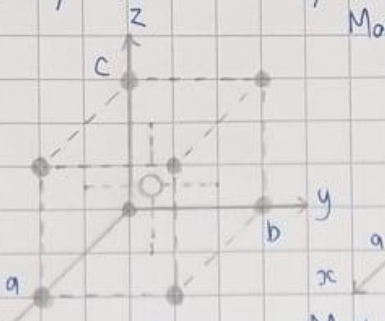
$\{100\} = (100), (010), (001)$
$(\bar{1}00), (0\bar{1}0), (00\bar{1})$

Number of nearest neighbors : 6

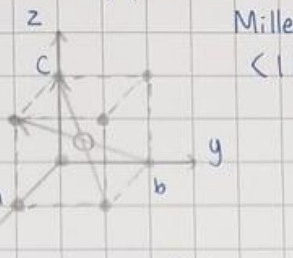
Atomic packing factor : unit cell has $8 \times 1/8 = 1$ atom / unitcell (uc)

$$\Rightarrow APF_{SC} = \frac{\text{atom/uc} \times V/\text{atom}}{V/uc} = \frac{1 \times 4/3\pi (0.5a)^3}{a^3} \approx 0.52$$

b) Body-centered cubic crystal structure



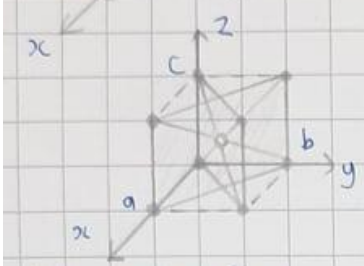
Most closely packed directions : along the unit cell diagonals



Miller indices of closely packed directions

$\langle 111 \rangle = [111], [\bar{1}11], [1\bar{1}\bar{1}]$
$[\bar{1}\bar{1}\bar{1}], [\bar{1}\bar{1}1], [11\bar{1}]$
$[1\bar{1}1], [\bar{1}1\bar{1}]$

Most closely packed planes : go through 4 diagonal 3 non-adjacent edges and the center cell



Miller indices of closely packed directions

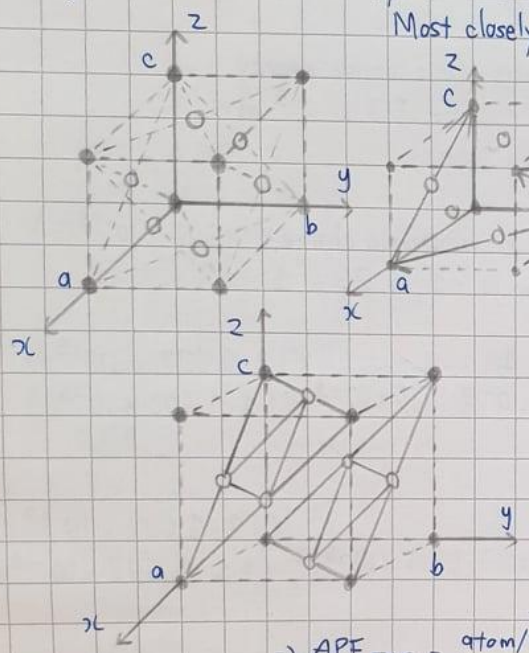
$\{110\} = (101), (110), (011)$
$(10\bar{1}), (1\bar{1}0), (01\bar{1})$

Number of nearest neighbors : 8

Atomic packing factor : unit cell has 1 center atom + 8 corners $\times$ 1/8 = 2 atoms / unit cell

$$\Rightarrow APF_{BCC} = \frac{\text{atom/uc} \times V/\text{atom}}{V/uc} = \frac{2 \times 4/3\pi (\sqrt{3}a/4)^3}{a^3} \approx 0.68$$

c) Face-centered cubic crystal structure



Most closely packed directions : along unit cell's face diagonals

Miller indices of closely packed directions

$\langle 110 \rangle = [110], [101], [011]$
$[\bar{1}10], [\bar{1}01], [0\bar{1}1]$

Most closely packed planes : go through 3 non-adjacent edges and 3 atoms in cell face

Miller indices of closely packed planes

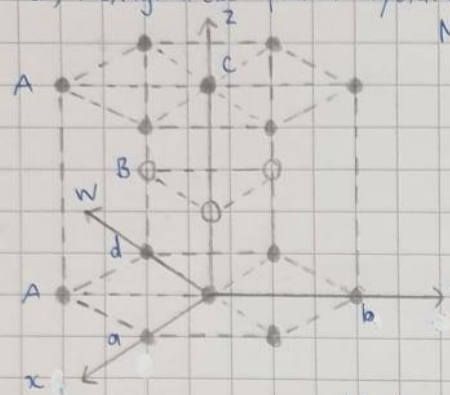
$\{111\} = (111), (1\bar{1}1), (11\bar{1})$
$(\bar{1}11)$

Number of nearest neighbors : 12

Atomic packing factor : unit cell has 6 face $\times$ 1/2 + 8 corners $\times$ 1/8 = 4 atoms / unit cell

$$\Rightarrow APF_{FCC} = \frac{\text{atom/uc} \times \text{V/atom}}{\text{V/uc}} = \frac{4 \times 4/3\,\pi(\sqrt{2}a/4)^3}{a^3} \approx 0.74$$

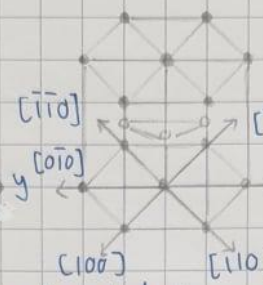
d) Hexagonal close-packed crystal structure



Most closely packed directions : along the hexagonal flat plane that separates the base

Miller indices of closely packed directions

$\langle 100 \rangle = [100], [010], [0\bar{1}0]$
$[\bar{1}00], [\bar{1}\bar{1}0], [110]$



Most closely packed planes : horizontal flat planes that go through the lattices

Miller indices of closely packed planes is the family of $\{001\}$ planes

Number of nearest neighbors : 12

Atomic packing factor : 3 midde atoms + 1/2 x 2 half center atoms + 1/6 x 12 corner atoms = 6 atoms / unit cell

$$\Rightarrow APF_{HCP} = \frac{\text{atom/uc} \times \text{V/atom}}{\text{V/uc}} = \frac{6 \times 4/3\,\pi r^3}{\frac{3\sqrt{3}}{2} b^2 c}$$ (r is radius of atom cell)

$$= \frac{8\pi r^3}{\frac{3\sqrt{3}}{2}(2r)^2 \frac{4\sqrt{6}}{3} r} = \frac{\sqrt{2}}{6}\pi \frac{r^3}{r^3} \approx 0.74$$

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

4.1 Answer these questions

(a) Describe briefly, what the dislocation is and the types of dislocations

In materials science, dislocations are one dimensional line defects within crystalline solids that make the solids structure irregular. Structured crystalline structures of atoms are misaligned along this dislocation line defect. The dislocations in crystalline solids strongly have strong influences on various properties of materials.

There are three types of dislocations: edge, screw and mixed dislocations

- Screw dislocations: the lattice plane on the two sides of the defect line shifts by a layer, which resembles a staircase
- Edge dislocations: there is an extra plane of atoms that ends abruptly halfway through the crystal lattice, making the layers converge into an edge.
- Mixed dislocations: dislocations that have both edge and screw dislocations

(b) Describe briefly, what the crystallographic orientation is.

Crystallographic orientation is defined by the Miller indices of the lattice plane of a crystal, that is, how a single crystal block (a grain) is oriented in 3d space

(c) Explain how the grain size distribution of polycrystals can be determined and represented.

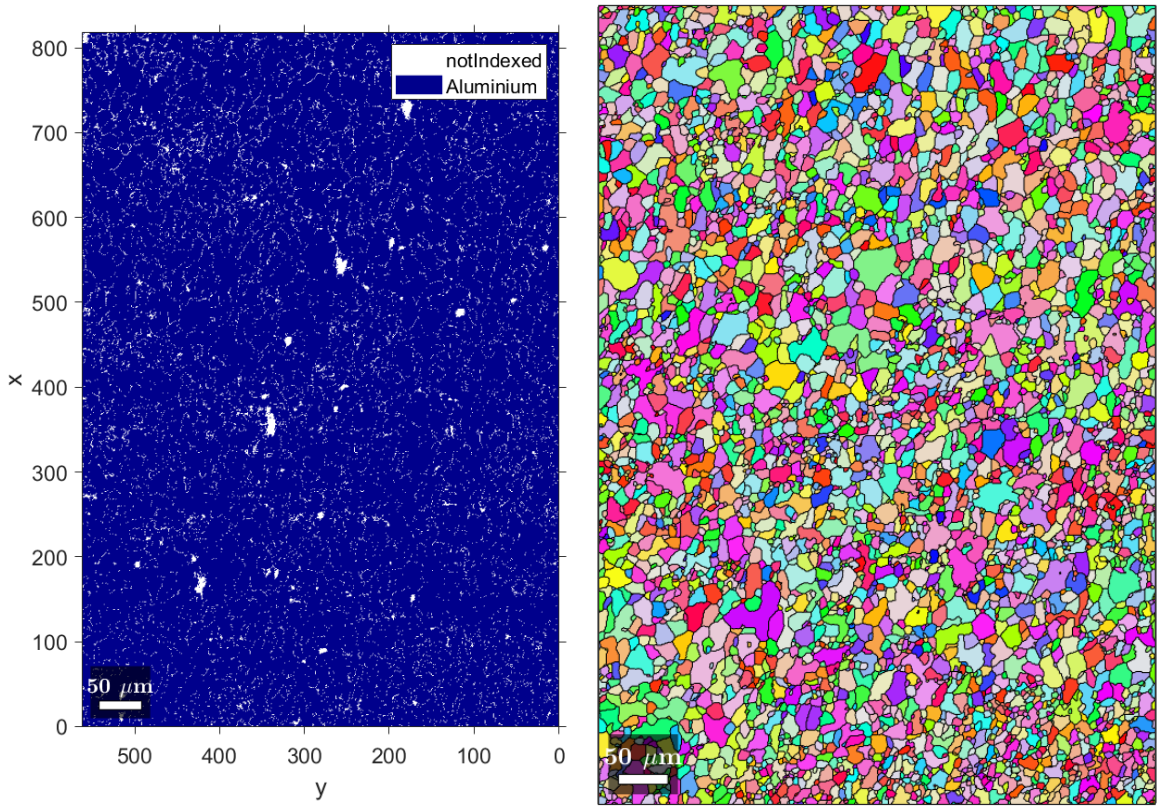
Grain size is the diameter of a circle whose area approximates the area of individual grain.

=> grain size distribution is how the diameters of the grains in a polycrystal are distributed.

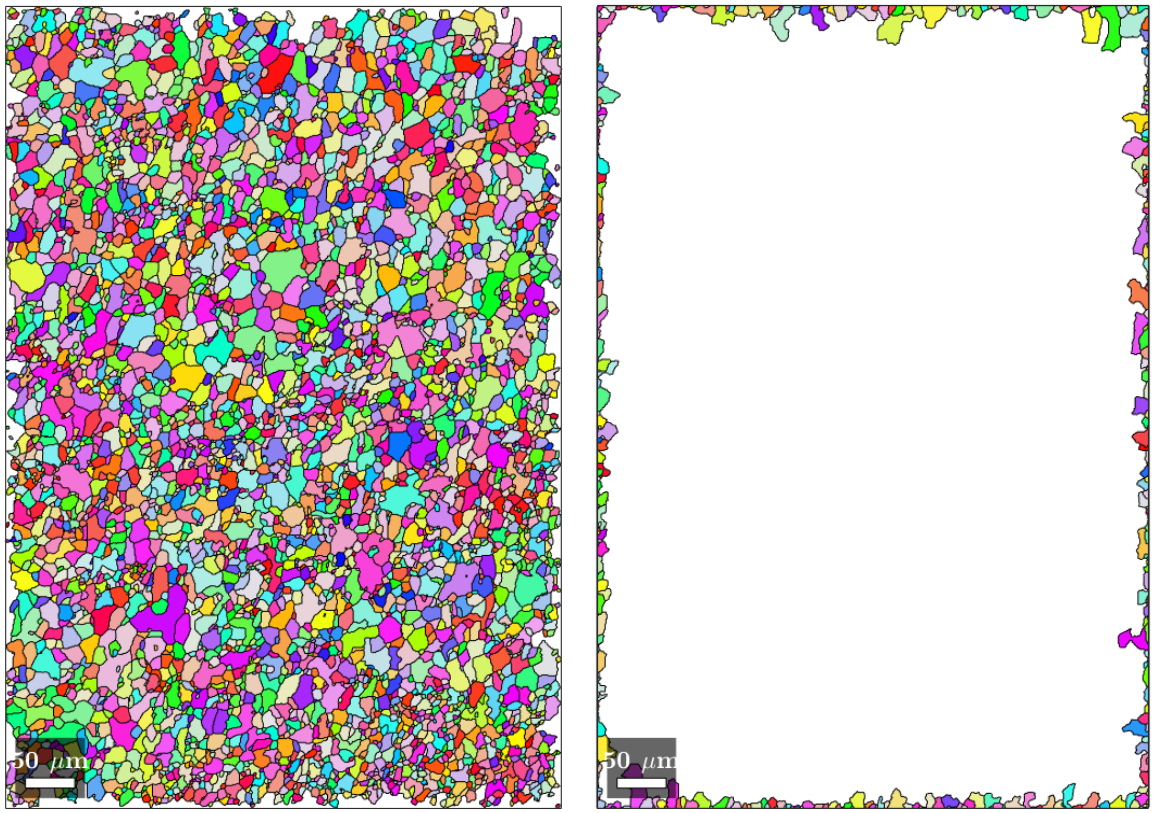
Grain size distribution can be determined by examining and collecting the data of the diameters of the grains based on experiments. Grain size distribution usually represented by lognormal distribution or gamma distribution

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)

Plot the EBSD phase map and colored grain map:



The inner and boundary grains map with their mean orientation:



The total grain number: 5323

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totalGrainNr =

        5323
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The inner grain number: 4977

```
innerGrainNr =

        4977
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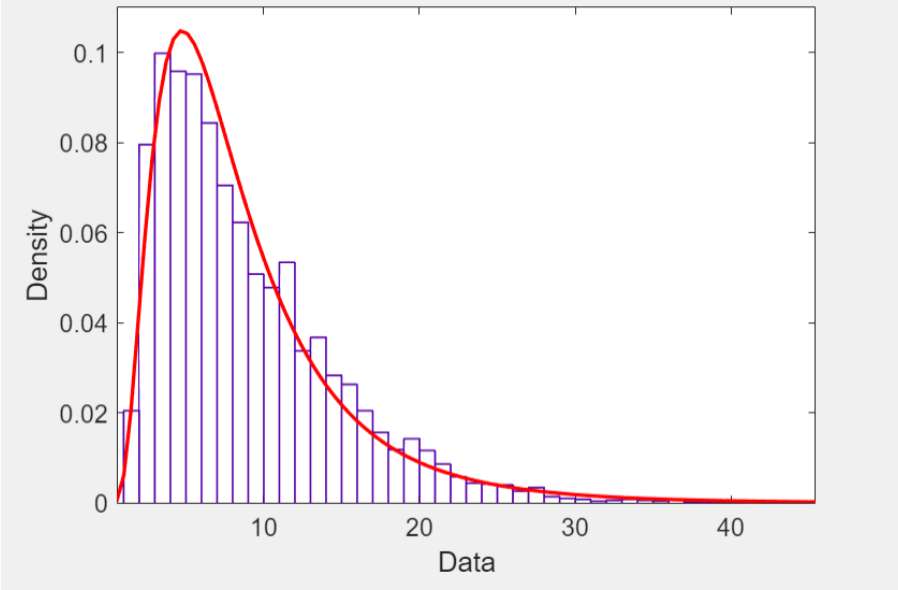
Lognormal distribution of the grain size data along with their characteristic parameters of the distribution, where
$\mu = 1.9787$, $\sigma = 0.649249$, mean(d) = 8.93043 μm



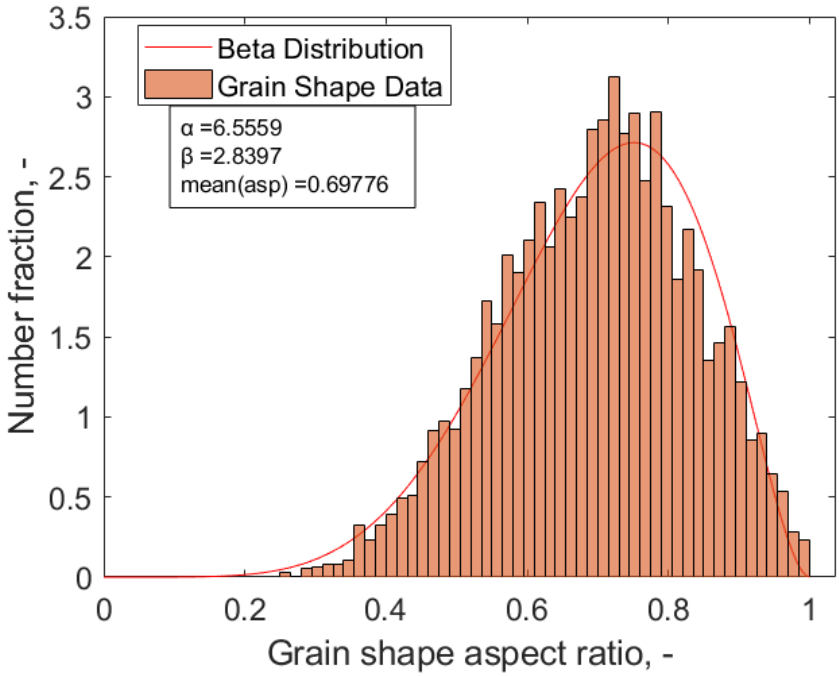
Results:

Distribution: Lognormal
Log likelihood: -14759.8
Domain: -Inf < y < Inf
Mean: 8.93043
Variance: 41.8128

Parameter	Estimate	Std. Err.
mu	1.9787	0.00920295
sigma	0.649249	0.00650845

Estimated covariance of parameter estimates:

	mu	sigma
mu	8.46943e-05	-6.82161e-20
sigma	-6.82161e-20	4.23599e-05



Beta distribution of the grain shapes along with their characteristic parameters of the distribution