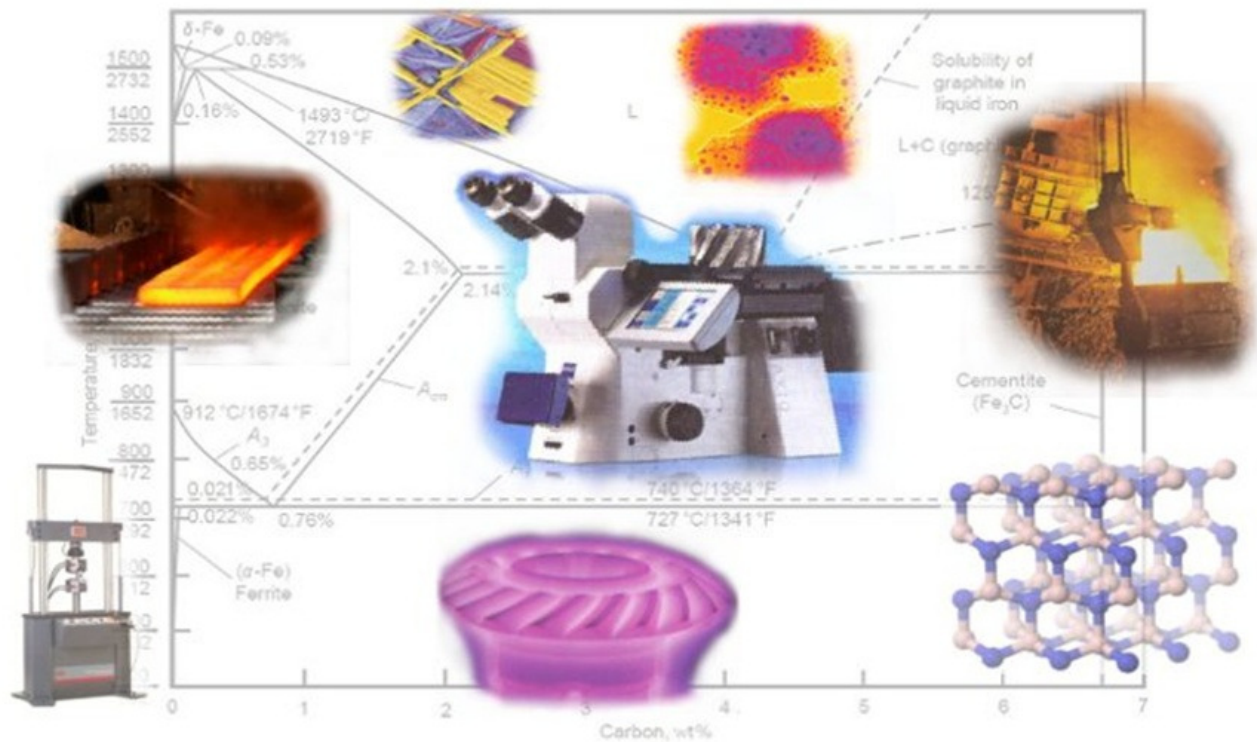


Mech 133 – Materials Technology



Assignment #2 *Crystallographic* *directions and planes*

Professor:
 Vladimir Neykov P.Eng.
 vneykov@okanagan.bc.ca
 (250) 762-5445 / 4758
 Office: C330B
 12:30 pm – 1:30 pm

1. Crystallographic directions and planes - glossary

The crystallographic directions - are fictitious lines linking nodes (atoms, ions or molecules) of a crystal.

The crystallographic planes - are fictitious planes linking nodes in the crystal.

Miller indices - are a notation system in crystallography for planes and directions in crystal (Bravais) lattices.

Use of terms crystal planes and crystal directions are related to the use of following terms:

Dislocations (plastic deformation) - in materials science, a dislocation is a crystallographic defect, or irregularity, within a crystal structure caused by a moving of the atoms on the specific crystallographic plane.

Cleavage - tendency of crystalline materials to split along definite crystallographic planes.

The ***pores*** and ***crystallites*** - tend to have straight grain boundaries following dense planes.

Optical properties - in condensed matter, the light "jumps" from one atom to the other with. The velocity of light thus varies according to the crystal directions.

The ***adsorption*** and the ***chemical reactions*** occur on atoms or molecules, these phenomena are thus sensitive to the density of nodes.

Surface tension - the condensation of a material means that the atoms, ions or molecules are more stable if they are surrounded by other similar species; the surface tension of an interface thus varies according to the density on the surface

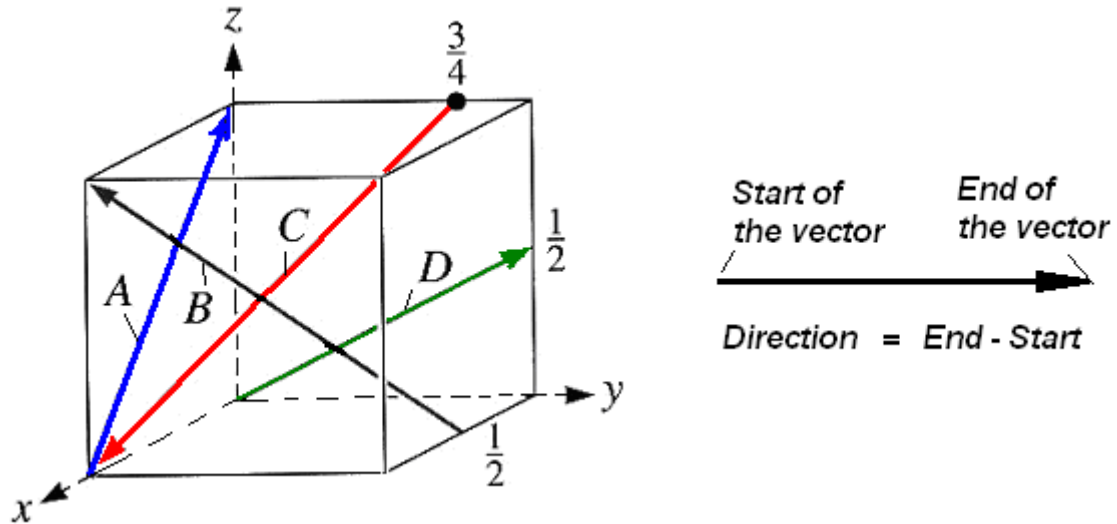
Wikipedia link:

http://en.wikipedia.org/wiki/Miller_index

2. Exercise

Example #1

Determine the indices for the directions in the cubic unit cell shown



Steps:

1. Subtract from end of the vector – start of the vector and write the result in x, y, z format;
2. Write result in fraction form;
3. Find common denominator and multiply numerator accordingly;
4. Remove denominator and put negative sign on top of the numerator;
5. Put result in square brackets.

Determine the indices for the directions in the cubic unit cell shown.

Solution:

A:

$$B: 1,0,1 - \frac{1}{2},1,0 = \frac{1}{2},-1,1 =$$

$$C: = [\overline{4}34]$$

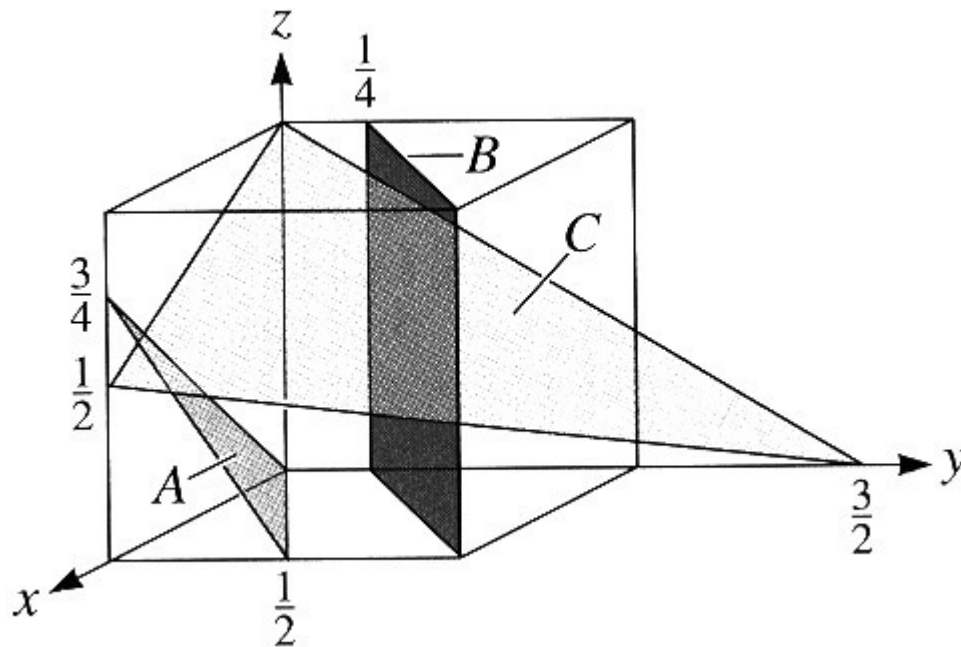
$$D: 0,1,\frac{1}{2} -$$

Example #2

Determine the indices for the planes in the cubic unit cell shown.

To determine coordinates x, y, z

1. Ask yourself where the plane cuts the Cartesian coordinate system? If one of the corners of the plane cuts through the origin \rightarrow origin must be relocated on the same plane to avoid getting infinite values in the next step;
2. Write x, y, z and take reciprocal values;
3. Find common denominator and multiply the numerator accordingly;
4. Remove denominator and put negative sign on top of the numerator;
5. Put result in parenthesis.



Determine the indices for the planes in the cubic unit cell shown.

Solutions:

$$\begin{array}{lll} \text{A: } x = -1 & 1/x = -1 \times 3 = -3 \\ y = 1/2 & 1/y = 2 \times 3 = 6 & (\bar{3}64) \text{ (origin at } 1,0,0) \\ z = 3/4 & 1/z = 4/3 \times 3 = 4 \\ \text{B: } x = & 1/x = & \\ y = & 1/y = & (3\bar{4}0) \text{ (origin at } 0,1,0) \\ z = & 1/z = & \\ \text{C: } x = & 1/x = & \\ y = & 1/y = & (346) \\ z = & 1/z = & \end{array}$$

3. Miller – Bravais indices for Hexagonal Crystals

Transfer formulas from 3 to 4 coordinates.

$$[u'v'w'] \rightarrow [u \ v \ t \ w]$$

$$u = \frac{1}{3}(2u' - v')$$

$$v = \frac{1}{3}(2v' - u')$$

$$t = -(u + v)$$

$$w = w'$$

To get $u'v'w'$ choose combination of axis that will give coordinates of the vector

Combinations could be: $a_1 \ a_2 \ c \rightarrow u' \ v' \ w'$

$a_2 \ a_3 \ c \rightarrow u' \ v' \ w'$

$a_1 \ a_3 \ c \rightarrow u' \ v' \ w'$

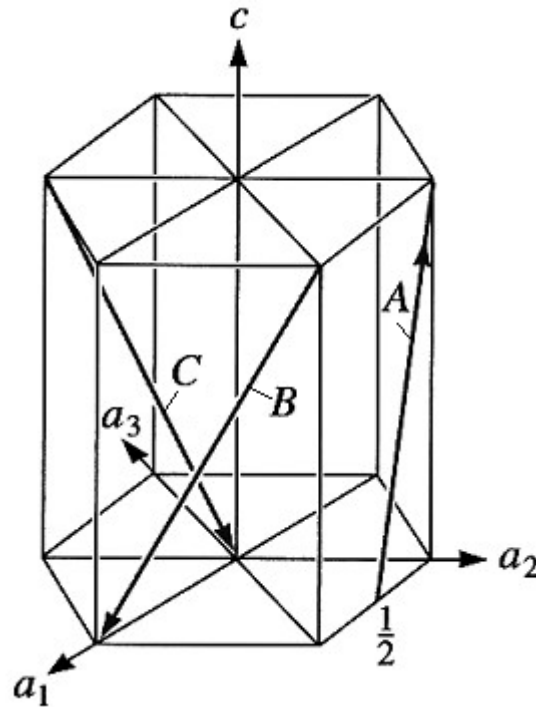
Note: Coordinate system can be anywhere so it can be always: $a_1 \ a_2 \ c \rightarrow u' \ v' \ w'$

Steps:

1. Calculate direction of the vector the way it is for single crystal: Subtract from end of the vector – start of the vector and write the result in $u'v'w'$ format;
2. Write result in fraction form;
3. Find common denominator and multiply numerator accordingly;
4. Remove denominator and put negative sign on top of the numerator;
5. Put result in square brackets.
6. Apply conversion formulas the way it is shown above;
7. For the converted result do again:
 - a. Find common denominator and multiply numerator accordingly;
 - b. Remove denominator and put negative sign on top of the numerator;
 - c. Put result in square brackets.

Example #3

Determine the indices for the directions in the hexagonal lattice shown.

**Solution:**

$$A: 0, 1, 1 - \frac{1}{2}, 1, 0 = -\frac{1}{2}, 0, 1 \rightarrow [\bar{1}02]$$

$$\begin{array}{ccc} a_1 & a_2 & c \\ \text{end} & \text{start} & \end{array} \quad \begin{array}{ccc} a_1 & a_2 & c \\ u' & v' & w' \end{array}$$

$$u = \frac{1}{3}(2(-1) - 0) = -\frac{2}{3}$$

$$v = \frac{1}{3}(2(0) - (-1)) = \frac{1}{3}$$

$$t = -\left(\left(-\frac{2}{3}\right) + \left(\frac{1}{3}\right)\right) = \frac{1}{3}$$

$$w = 2$$

Common denominator is 3. Multiplying every value by 3

$$-\frac{2}{3} \times 3 = -2; \quad \frac{1}{3} \times 3 = 1; \quad \frac{1}{3} \times 3 = 1; \quad 2 \times 3 = 6 \quad \rightarrow [\bar{2}116]$$

$$B: 1, 0, 0 - 1, 1, 1 = 0, -1, -1 \rightarrow [0\bar{1}\bar{1}]$$

$$\begin{array}{ccc} a_1 & a_2 & c \\ \text{end} & \text{start} & \end{array} \quad \begin{array}{ccc} a_1 & a_2 & c \\ u' & v' & w' \end{array}$$

$$u = \frac{1}{3}(2(0) - (-1)) =$$

$$v =$$

$$t = -\left(\left(\frac{1}{3}\right) + \left(-\frac{2}{3}\right)\right) = \frac{1}{3}$$

$$w = -1$$

$$\frac{1}{3} \times 3 = \quad ; \quad -\frac{2}{3} \times 3 = \quad ; \quad \frac{1}{3} \times 3 = \quad ; \quad -1 \times 3 = \quad \rightarrow [1\bar{2}1\bar{3}]$$

$$C: 0,0,0 - 1,1,1 =$$

$$a_1 \ a_3 \ c \quad a_1 \ a_3 \ c \quad u' \ v' \ w'$$

$$end \quad start$$

$$u =$$

$$v =$$

$$t =$$

$$w =$$

$$= \quad ; \quad = \quad ; \quad = \quad ; \quad = \quad \rightarrow [\bar{1}\bar{1}2\bar{3}]$$

For more information see pp.54 – 55, Materials science and engineering an introduction by W.D. Callister, WILEY

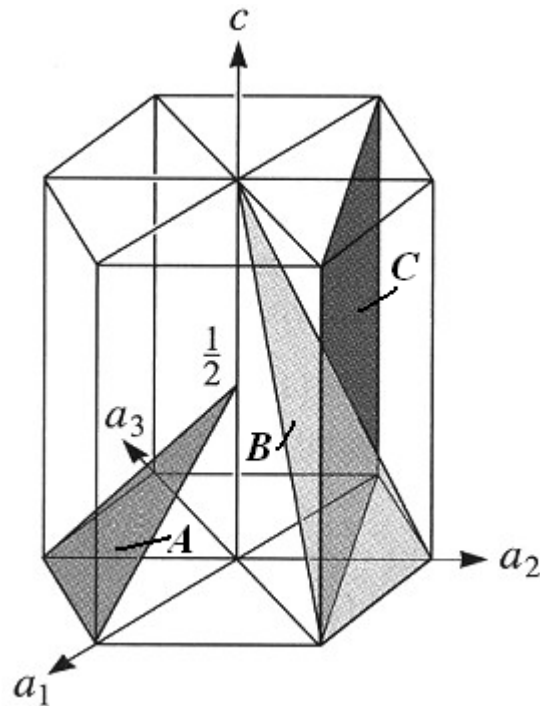
To determine crystalline planes for hexagonal crystal lattice:

Steps:

1. Find where plane cuts all four axis of the coordinate system. If the plane cuts through zero – change location of the origin in the same
2. Write them in format a_1, a_2, a_3, c
3. Calculate reciprocal values.
4. Find common denominator and multiply numerator accordingly;
5. Remove denominator and put negative sign on top of the numerator;
6. Put result in parentheses.

Example #4

Determine the indices for the planes in the hexagonal unit cell shown.



Determine the indices for the planes in hexagonal lattice shown:

Solution:

$A:$	$a_1 = 1$	$1/a_1 = 1$	
	$a_2 = -1$	$1/a_2 = -1$	$(1\bar{1}02)$
	$a_3 = \infty$	$1/a_3 = 0$	
	$c = 1/2$	$1/c = 2$	
$B:$	$a_1 =$	$1/a_1 =$	
	$a_2 =$	$1/a_2 =$	$(01\bar{1}1)$
	$a_3 =$	$1/a_3 =$	
	$c =$	$1/c =$	
$C:$	$a_1 =$	$1/a_1 =$	
	$a_2 =$	$1/a_2 =$	$(\bar{1}2\bar{1}0)$
	$a_3 =$	$1/a_3 =$	
	$c =$	$1/c =$	

4. Steps to determine standard ASTM grain size number and average grain size diameter.

Example 5: Given photo is of AISI 1018 annealed, magnification 500×, size of the photo 4in × 3in. Determine standard ASTM grain size number and average grain size diameter.

1. Count number of full size grains and half size grains. Mark them with different symbols:



Number of half size grains = 16 (squares), number of full size grains = 12 (triangles):

2. Calculate number of the grains:

$$\# \text{ full grains} + \frac{\# \text{ half grains}}{2} = \quad + \frac{\quad}{2} = \quad \text{grains}$$

3. Calculate area of the given photo. Size of the photo is 4in × 3in:

$$\text{width} \times \text{height} = 4 \times 3 = \quad \text{in}^2$$

4. Calculate number of the grains per square inch for magnification @500×

$$N_{500} = \frac{\# \text{ of grains}}{\text{area}} = \frac{\text{grains}}{\text{in}^2} = \quad \text{grains/in}^2$$

5. Re-calculate number of the grains per square inch for magnification 100×

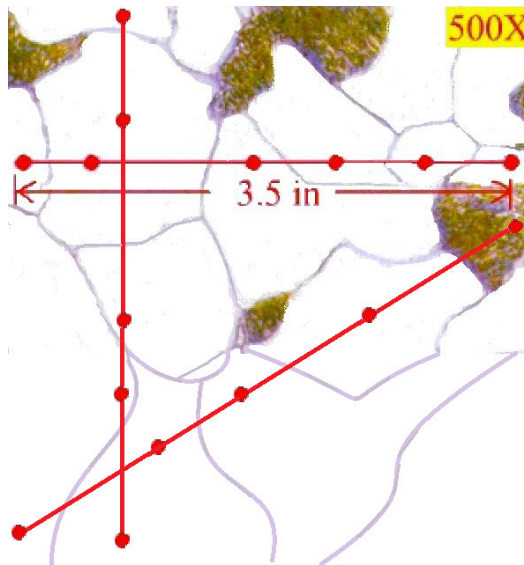
$$N_{100} = \left(\frac{\text{magnif. of the photo}}{\text{magnif. 100}\times} \right)^2 \times \text{grains/in}^2_{@500}$$

$$N_{100} = \left(\frac{500}{100} \right)^2 \times \quad = \quad \text{grains/in}^2$$

6. Calculate standard ASTM grain size number

$$n = \frac{\ln(N)}{\ln(2)} + 1 = \frac{\quad}{0.69315} + 1 = \quad \approx$$

7. To find average grain size diameter, draw two or three 3.5in long lines on the picture. Preferably in x, y direction and 45° angle.



8. Count the number of the intersected grains for each line. Divide length of each line by number of intercepted grains. Take average of all

$$N_{L1} = \frac{\# \text{ of grains}}{\text{length}} = \quad = \quad \text{grains/in}$$

$$N_{L2} =$$

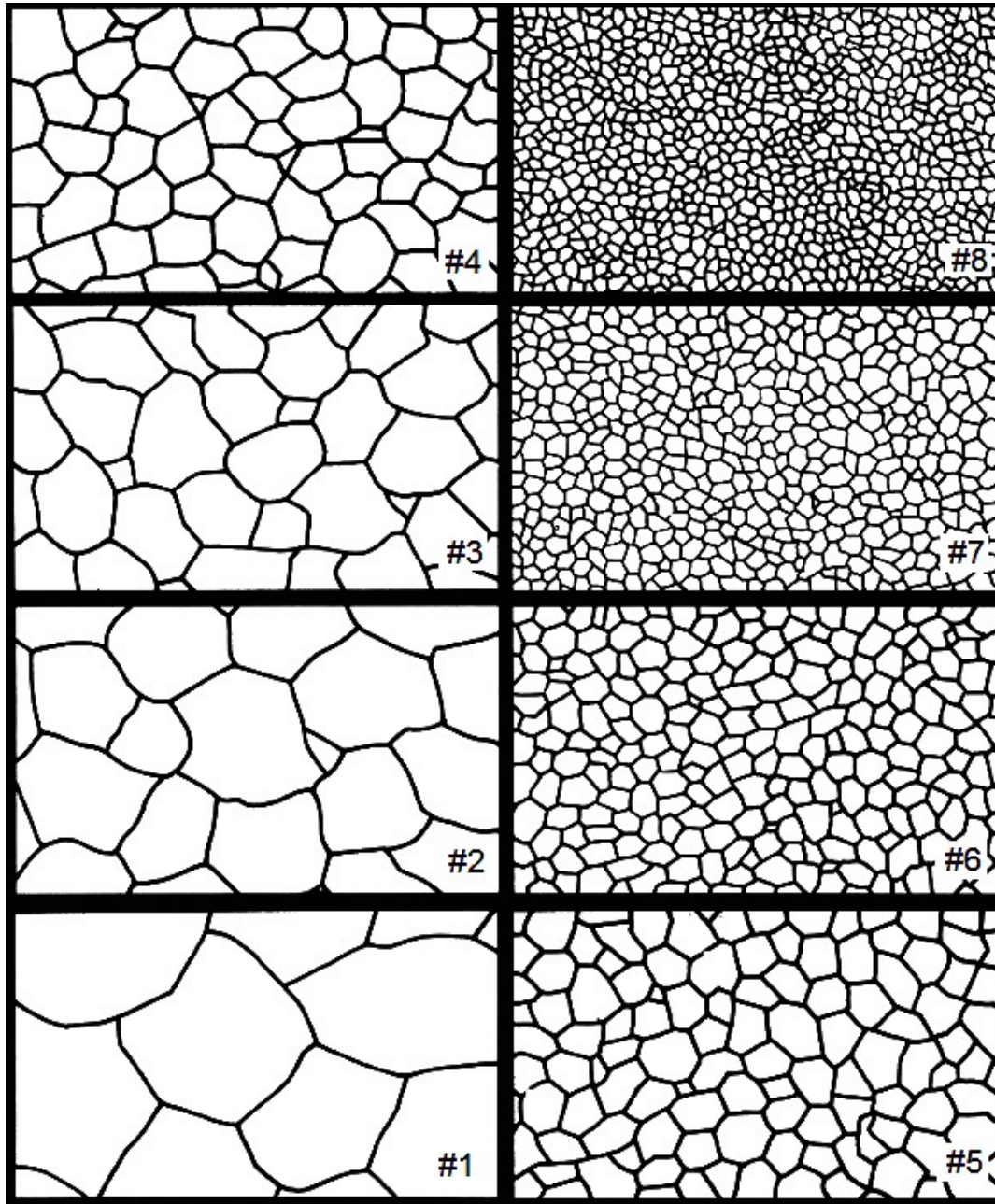
$$N_{L3} =$$

Average of the three results is

9. Calculate average grain size diameter

$$d = \frac{C}{N_L M} = \frac{1.5}{\times} = \quad in$$

Standard ASTM size of numbers



Standard grain size numbers. The grain size per square inch at a magnification of 100x

Example #6

Calculate density of the pure Gold Au atomic number 79. Find from table A2 in your work book p. 155 Atomic weight, crystal structure and atomic radius. After you find the answer compare it to the given density in table A2. Comment the result.

Table A2 - Physical properties of some elements

Element	Symbol	Atomic number	Atomic weight (amu)	Density (g/cm ³)	Crystal structure	Atomic radius (nm)
Aluminum	Al	13	26.98	2.71	FCC	0.143
Beryllium	Be	4	9.012	1.85	HCP	0.114
Boron	B	5	10.81	2.34	Rhomb.	-
Cadmium	Cd	48	112.41	8.65	HCP	0.149
Carbon	C	6	12.011	2.25	Hex.	0.071
Chromium	Cr	24	52.00	7.19	BCC	0.125
Cobalt	Co	27	58.93	8.9	HCP	0.125
Copper	Cu	29	63.55	8.94	FCC	0.128
Germanium	Ge	32	72.64	5.32	Dia. Cub.	0.122
Gold	Au	79	196.97	19.32	FCC	0.144
Hydrogen	H	1	1.008	-	-	-
Iron	Fe	26	55.85	7.87	BCC	0.124
Lead	Pb	82	207.2	11.35	FCC	0.175
Magnesium	Mg	12	24.31	1.74	HCP	0.160
Manganese	Mn	25	54.94	7.44	Cubic	0.112
Molybdenum	Mo	42	95.94	10.22	BCC	0.136
Nickel	Ni	28	58.69	8.90	FCC	0.125
Niobium	Nb	41	92.91	8.57	BCC	0.143
Silicon	Si	14	28.09	2.33	Dia. Cub.	0.118
Silver	Ag	47	107.87	10.49	FCC	0.144
Tin	Sn	50	118.71	7.27	Tetra.	0.151
Titanium	Ti	22	47.87	4.51	HCP	0.145
Tungsten	W	74	183.84	19.3	BCC	0.137
Vanadium	V	23	50.94	6.1	BCC	0.132
Zinc	Zn	30	65.41	7.13	HCP	0.133
Zirconium	Zr	40	91.22	6.51	HCP	0.159

<i>Crystal structure characteristics of some metals</i>		Atoms	Coordination	Packing	Examples
Structure	a_0 versus r	per Cell	Number	Factor	
Simple cubic (SC)	$a_0 = 2r$	1	6	0.52	Polonium (Po), α -Mn
Body-centered cubic (BCC)	$a_0 = 4r/\sqrt{3}$	2	8	0.68	Fe, Ti, W, Mo, Nb, Ta, K, Na, V, Zr, Cr
Face-centered cubic (FCC)	$a_0 = 4r/\sqrt{2}$	4	12	0.74	Fe, Cu, Au, Pt, Ag, Pb, Ni
Hexagonal close-packed (HCP)	$a_0 = 2r$ $c_0 \approx 1.633a_0$	2	12	0.74	Ti, Mg, Zn, Be, Co, Zr, Cd

Note:

1 nm = 1×10^{-7} cm

Avogadro number = 6.0221415×10^{23} atoms/mol

amu - stands for atomic mass, g/mol

Formulas:

$$\rho = \frac{\text{mass, g}}{\text{volume, cm}^3}$$

Formula 1:

$$\text{Density } \rho = \frac{\left(\frac{\# \text{ atoms}}{\text{cell}} \right) (\text{atomic mass, g/mol})}{(\text{volume of unit cell, cm}^3 / \text{cell}) (\text{Avogadro's } \# , \# \text{ atoms/mol})}, \text{ g/cm}^3$$

Formula 2 - volume of the unit cell: $V_0 = (a_0)^3 = \left(\frac{4r}{\sqrt{2}} \right)^3$ for FCC

Steps:

1. From table A2 – find atomic mass amu;
2. From table A2 – find atomic radius r ;
3. From the table above find # atoms per unit cell for gold;
4. Calculate formula 2;
5. Substitute parameters in formula 1;
6. Calculate density and compare it to the value given in table A2;
7. Comment on the result.

Solution:

amu =

r =

atoms per cell =

$V_0 =$

Density = _____ =

Answer:

$\rho =$