University of Anbar/ Faculty of Engineering

Department of Mechanical Engineering

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Subject: Engineering of Metallurgy

Course Code: ME2304

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Lecturer. Osama Ibrahim

Lecture # 6

CHAPTER THREE/ THE STRUCTURE OF CRYSTALLINE SOLIDS

THEORETICAL DENSITY COMPUTATIONS

A knowledge of the crystal structure of a metallic solid permits computation of its theoretical density through the relationship

$$\rho = \frac{nA}{V_C N_A}$$

where;

n = number of atoms associated with each unit cell

A = atomic weight

V_C = volume of the unit cell

N_A= Avogadro's number 6.022×10^{23} atoms/mol

Examples: ***Copper*** *has an atomic radius of 0.128 nm, an* ***FCC*** *crystal structure, and an atomic weight of 63.5 g/mol. Compute its theoretical density and compare the answer with its measured density?*

Solution:

Because the crystal structure is FCC,
n, the number of atoms per unit cell, is 4.
atomic weight (A_{Cu}) = 63.5 g/mol.
The unit cell volume V_C for FCC was determined in Example above as where *R*, the atomic radius, is 0.128 nm.

$$V_c = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2}$$

Substitution for the various parameters into Equation below:

$$\rho = \frac{nA}{V_C N_A} = \frac{nA_{cu}}{(16R^3\sqrt{2}) \times N_A}$$

$$\rho = \frac{(4\ atoms/u\ nitcell) \times (63.5\ \text{g/mol})}{[16\sqrt{2}(1.28 \times 10^{-8} cm)^3/u\ nitcell] \times (6.022 \times 10^{23}\ \text{atoms/mol})}$$

$$\rho = 8.89\ \text{g/cm}^3$$

The literature value for the density of copper is 8.94 g/cm^3, which is in very close agreement with the previous result.

Table 2. presents the atomic radii for a number of metals. Three relatively simple crystal structures are found for most of the common metals: face centered cubic, body centered cubic, and hexagonal close-packed.

Table 2. Atomic Radii and Crystal Structures for 16 Metals

Metal	Crystal Structure[a]	Atomic Radius[b] (nm)	Metal	Crystal Structure	Atomic Radius (nm)
Aluminum	FCC	0.1431	Molybdenum	BCC	0.1363
Cadmium	HCP	0.1490	Nickel	FCC	0.1246
Chromium	BCC	0.1249	Platinum	FCC	0.1387
Cobalt	HCP	0.1253	Silver	FCC	0.1445
Copper	FCC	0.1278	Tantalum	BCC	0.1430
Gold	FCC	0.1442	Titanium (α)	HCP	0.1445
Iron (α)	BCC	0.1241	Tungsten	BCC	0.1371
Lead	FCC	0.1750	Zinc	HCP	0.1332

[a]FCC = face-centered cubic; HCP = hexagonal close-packed; BCC = body-centered cubic.

[b]A nanometer (nm) equals 10^{-9} m; to convert from nanometers to angstrom units (Å), multiply the nanometer value by 10.

H.W. (4) Calculate the radius of a vanadium atom, given that V has a BCC crystal structure, a density of 5.96 g/cm^3, and an atomic weight of 50.9 g/mol?

H.W. (5) Rhodium has an atomic radius of 0.1345 nm and a density of 12.41 g/cm^3. Determine whether it has an FCC or BCC crystal structure?

CHARACTERISTICS OF SELECTED ELEMENTS

element	symbol	Z	at. wt.	ρ (g/cm^3)	structure	r_{atomic}	r_{ionic}	valence	M.P (°C)
Aluminum	Al	13	26.98	2.71	FCC	0.143	0.053	3+	660.4
Argon	Ar	18	39.95	—	—	—	—	—	-189.2
Barium	Ba	56	137.33	3.5	BCC	0.217	0.136	2+	725
Beryllium	Be	4	9.012	1.85	HCP	0.149	0.095	3+	1278
Boron	B	5	10.81	2.34	rhomb.	—	0.023	3+	2300
Bromine	Br	35	79.90	—	—	—	0.196	1-	-7.2
Cadmium	Cd	48	112.41	8.65	HCP	0.149	0.095	2+	321
Calcium	Ca	20	40.08	1.55	FCC	0.197	0.100	2+	839
Carbon	C	6	12.011	2.25	hexag.	0.071	~0.016	4+	—
Cesium	Cs	55	132.91	1.87	BCC	0.265	0.170	1+	28.4
Chlorine	Cl	17	35.45	—	—	—	0.181	1-	-101
Chromium	Cr	24	52.00	7.19	BCC	0.125	0.063	3+	1875
Cobalt	Co	27	58.93	8.9	HCP	0.125	0.072	2+	1495
Copper	Cu	29	63.55	8.94	FCC	0.128	0.096	1+	1084
Fluorine	F	9	19.00	—	—	—	0.133	1-	-220
Gold	Au	79	196.97	19.32	FCC	0.144	0.137	1+	1064
Hydrogen	H	1	1.008	—	—	—	—	1+	-259
Iodine	I	53	126.91	4.93	ortho.	0.136	0.220	1-	114
Iron	Fe	26	55.85	7.87	BCC	0.124	0.077	2+	1538
Lead	Pb	82	207.2	11.35	FCC	0.175	0.120	2+	327
Lithium	Li	3	6.94	0.534	BCC	0.152	0.068	1+	181
Magnesium	Mg	12	24.31	1.74	HCP	0.160	0.072	2+	649
Manganese	Mn	25	54.94	7.44	cubic	0.112	0.067	2+	1244
Mercury	Hg	80	200.59	—	—	—	0.110	2+	-38.8
Molybdenum	Mo	42	95.94	10.22	BCC	0.136	0.070	4+	2617
Neon	Ne	10	20.18	—	—	—	—	—	-248.7
Nickel	Ni	28	58.69	8.90	FCC	0.125	0.069	2+	1453
Nitrogen	N	7	14.007	—	—	—	0.01-0.02	5+	-209.9
Oxygen	O	8	16.00	—	—	—	0.140	2-	-218.4
Platinum	Pt	78	195.08	21.45	FCC	0.139	0.080	2+	1772
Potassium	K	19	39.10	0.862	BCC	0.231	0.138	1+	63
Silicon	Si	14	28.09	2.33	diamond	0.118	0.040	4+	1410
Silver	Ag	47	107.87	10.49	FCC	0.144	0.126	1+	962
Sodium	Na	11	22.99	0.971	BCC	0.186	0.102	1+	98
Sulfur	S	16	32.06	2.07	ortho.	0.106	0.184	2-	113
Tin	Sn	50	118.69	7.3	tetra.	0.151	0.071	4+	232
Titanium	Ti	22	47.88	4.51	HCP	0.145	0.068	4+	1668
Tungsten	W	74	183.85	19.3	BCC	0.137	0.070	4+	3410
Vanadium	V	23	50.94	6.1	BCC	0.132	0.059	5+	1890
Zinc	Zn	30	65.39	7.13	HCP	0.133	0.074	2+	420
Zirconium	Zr	40	91.22	6.51	HCP	0.159	0.079	4+	1852

CRYSTALLOGRAPHIC DIRECTIONS AND PLANES

Crystallographic Directions

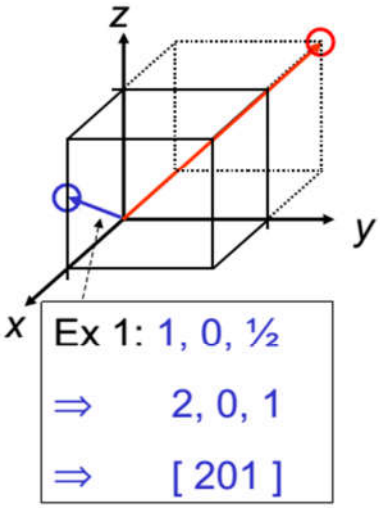
- Vectors or lines between two points described by indices.
- Direction [hkl]
- Families of directions <hkl>
- The following steps are used to determine the three directional indices:

1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions a, b, and c.
3. Adjust to smallest integer values (multiply by a factor).
4. Enclose in square brackets, no commas **[hkl]**

(note: If the value is –ve put the – sign over the number)

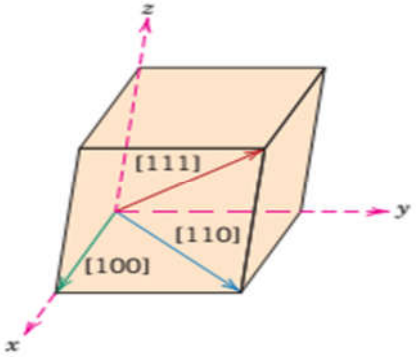
Instead of 1 and 2: you can;

1. Determine coordinates of head (H) and tail (T)
2. Subtract: head – tail
3. Then as before (steps 3 and 4)



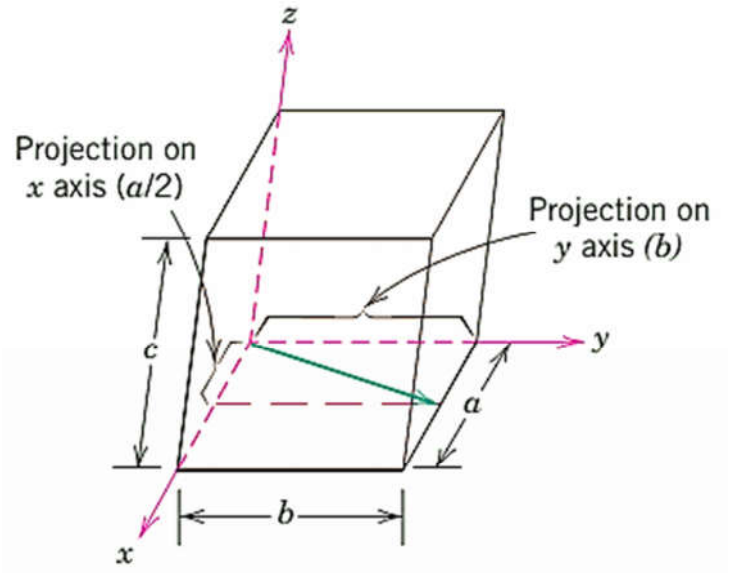
Ex 2: -1, 1, 1 ==== [$\bar{1}$11] (overbar represents a negative index)

The [100], [110], and [111] directions are common ones; they are drawn in the unit cell shown in Figure below;



Determination of Directional Indices

Example*: Determine the indices for the direction shown in the accompanying figure.*



Solution:

1. The vector, as drawn, passes through the origin of the coordinate system, and therefore no translation is necessary.
2. Projections of this vector onto the x, y, and z axes are, respectively, a/2, b, and 0c, which become 1/2, 1, and 0 in terms of the unit cell parameters (i.e., when the a, b, and c are dropped).
3. Reduction of these numbers to the lowest set of integers is accompanied by multiplication of each by the factor 2. This yields the integers 1, 2, and 0, which are then
4. enclosed in brackets as [120].

This procedure may be summarized as follows:

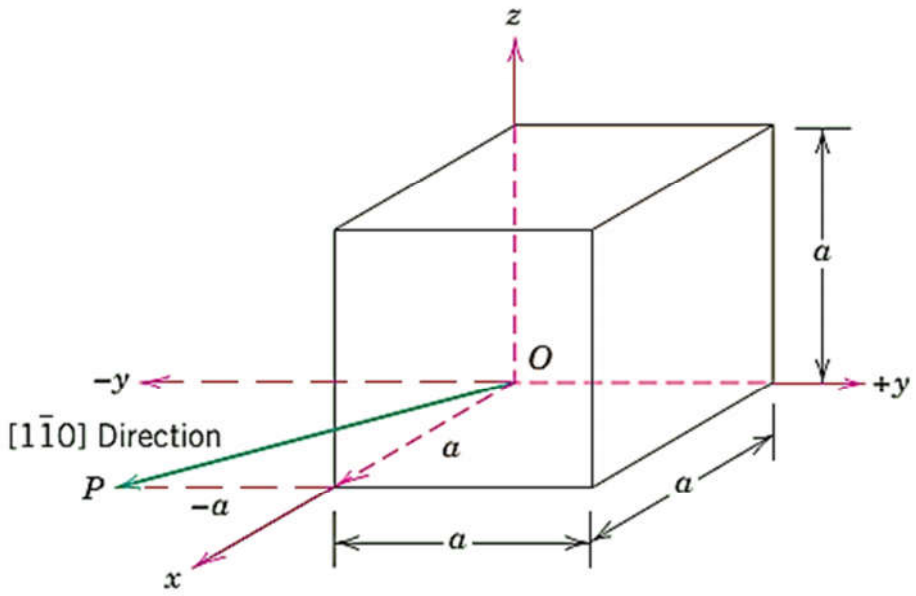
	x	*y*	*z*
Projections	*a*/2	*b*	0*c*
Projections (in terms of *a*, *b*, and *c*)	$\frac{1}{2}$	1	0
Reduction	1	2	0
Enclosure		[120]	

Construction of Specified Crystallographic Direction

Example*: Draw a [1$\bar{1}$0] direction within a cubic unit cell.*

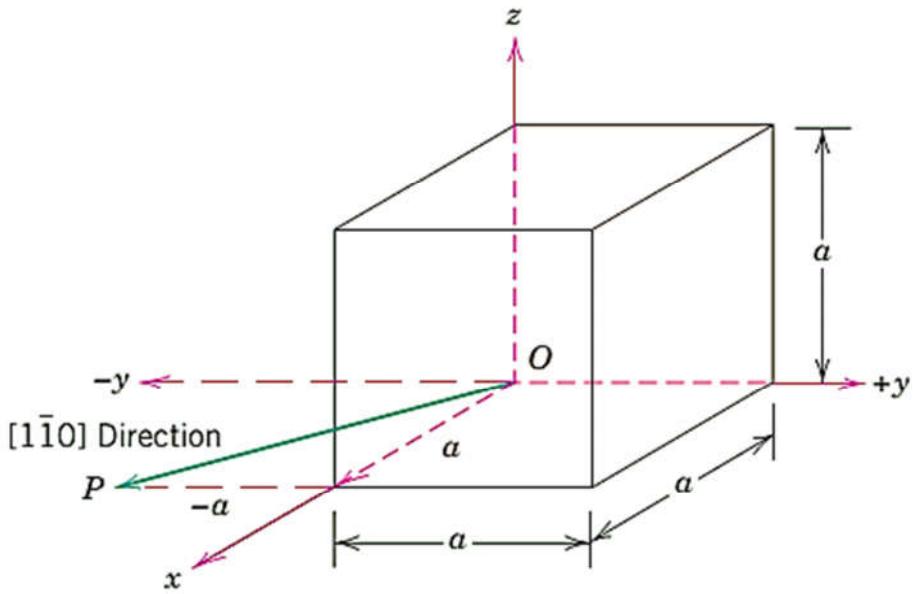
Solution

First construct an appropriate unit cell and coordinate axes system. In the accompanying figure the unit cell is cubic, and the origin of the coordinate system, point O, is located at one of the cube corners.



This problem is solved by reversing the procedure of the preceding example. For this [1$\bar{1}$0] direction, the projections along the *x*, *y*, and *z* axes are *a*, - *a*, and 0*a*, respectively. This direction is defined by a vector passing from the origin to point *P*, which is located by first moving along the *x* axis *a* units, and from this position, parallel to the *y* axis *a* units, as indicated in the figure. There is no *z* component to the vector, because the *z* projection is zero.

Example: *What are the indices for the direction indicated by the vector in the following sketch?*

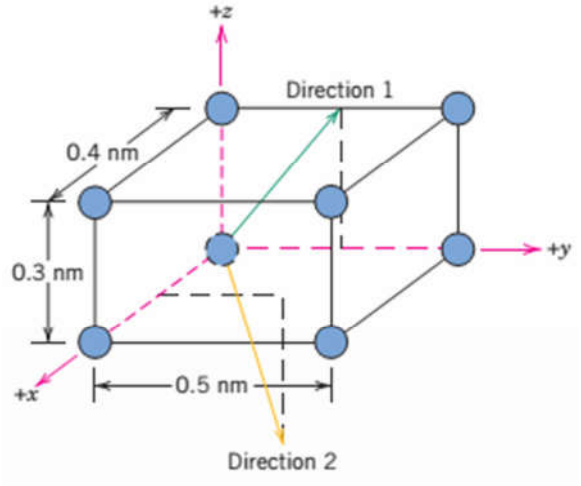


Solution:

For Vector OP;

Vector OP	**x**	**y**	**z**
Coordination of point P	1	-1	0
Coordination of point O	0	0	0
Vector OP = P-O	1	-1	0
Direction		[1$\bar{1}$0]	

H.W. (6): *What are the indices for the direction indicated by the vector in the following sketch?*



H.W. (7): *Within a cubic unit cell, sketch the following directions:*

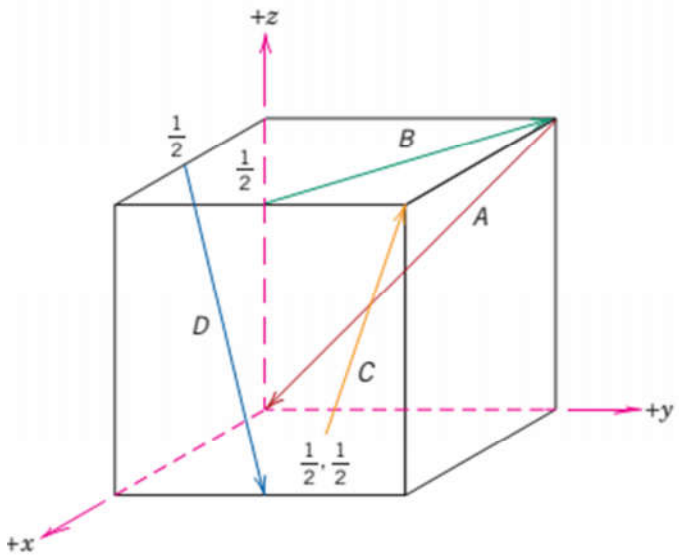
(a) $[\bar{1}10]$ **(e)** $[\bar{1}\bar{1}1]$

(b) $[\bar{1}\bar{2}1]$ **(f)** $[\bar{1}22]$

(c) $[0\bar{1}2]$ **(g)** $[1\bar{2}\bar{3}]$

(d) $[1\bar{3}3]$ **(h)** $[\bar{1}03]$

H.W. (8): *Determine the indices for the directions shown in the following cubic unit cell:*



Crystallographic Planes

- Crystallographic planes are specified by three Miller indices as (hkl).
- Miller indices: a set of integers that determine the crystallographic planes, as determined from reciprocal of fractional axis intercept.
- Family of Planes {hkl}

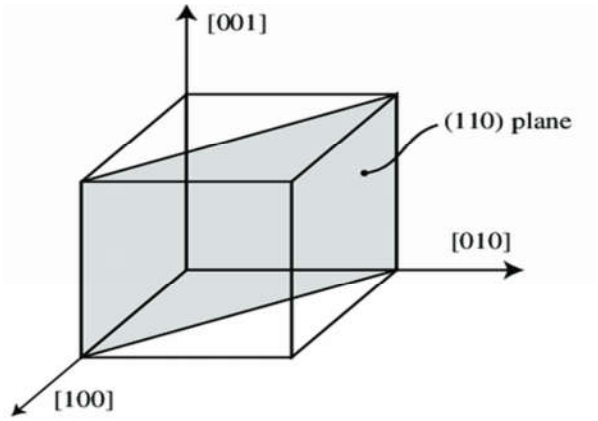
Algorithm (for obtaining Miller Indices):

Note: if the plane passes through the origin, choose another origin

1. Read off **intercepts** of plane with axes (in terms of *a*, *b*, *c)*
2. Take **reciprocals** of intercepts
3. Reduce to smallest **integer** values
4. Enclose in **parentheses ( )**, no commas i.e., **(hkl)**

Note: *if the plane is parallel to one axis then the intercept is (∞) and the indices is (0).*

Example: *Determine the Miller indices for the plane shown in the accompanying sketch:*



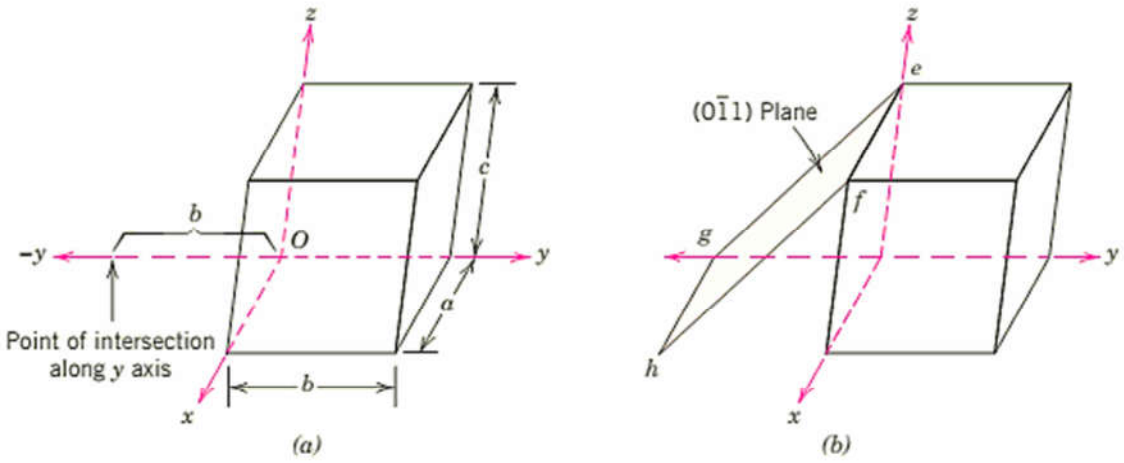
	x	y	z
Intercepts	a	b	∞c
Intercepts (in terms of lattice parameters)	1	1	∞
Reciprocals	1/1	1/1	$1/\infty$
Reductions (integer)	1	1	0
Enclosure (hkl)		**(110)**	

Example: *Construct a $(0\bar{1}\bar{1})$ plane within a cubic unit cell.*

Solution:

To solve this problem, carry out the procedure used in the preceding example in reverse order. To begin,

1. The indices are removed from the parentheses
2. reciprocals are taken, which yields ∞, -1, and 1. This means that the particular plane parallels the *x* axis while intersecting the *y* and *z* axes at *b* and *c*, respectively, as indicated in the accompanying sketch (*a*).
3. This plane has been drawn in sketch (*b*).
4. A plane is indicated by lines representing its intersections with the planes that constitute the faces of the unit cell or their extensions.



Angle between two planes, directions is given by:

$$\cos\theta = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\sqrt{h_2^2 + k_2^2 + l_2^2}}$$

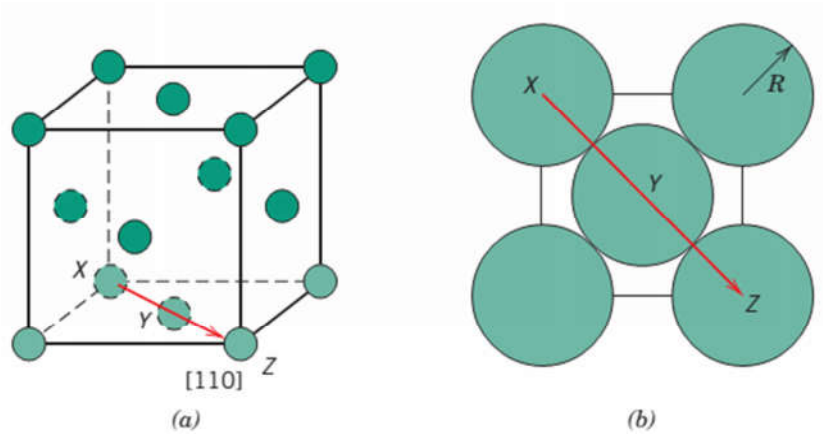
Ex: Calculate the angle between the (111) and (200) planes? (ans. $\Theta = 54.75°$)

LINEAR AND PLANAR DENSITIES

- Linear Density of Atoms calculated by eq.:

$$\text{LD} = \frac{\text{number of atoms centered on direction vector}}{\text{length of direction vector}} \quad nm^{-1} \; or \; m^{-1}$$

For **example**, let us determine the linear density of the [110] direction for the FCC crystal structure shown below:



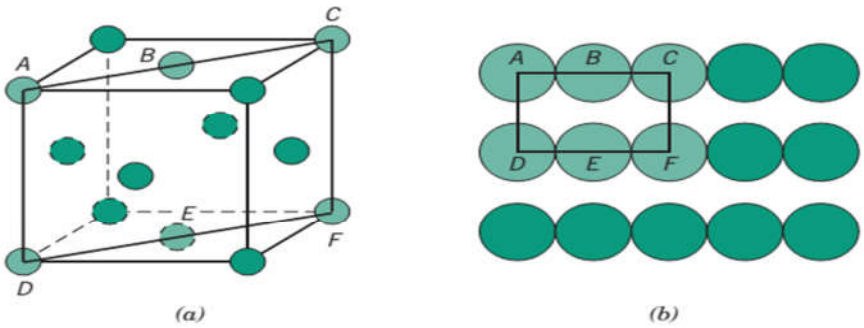
$$\text{LD}_{110} = \frac{2 \text{ atoms}}{4R} = \frac{1}{2R}$$

H.W. (8) *Find linear density of Aluminum in [110] direction, lattice constant is 0.405 nm?*

- planar density (PD) is taken as the number of atoms per unit area that are centered on a particular crystallographic plane, or

$$\text{PD} = \frac{\text{number of atoms centered on a plane}}{\text{area of plane}} \quad nm^{-2} \; or \; m^{-2}$$

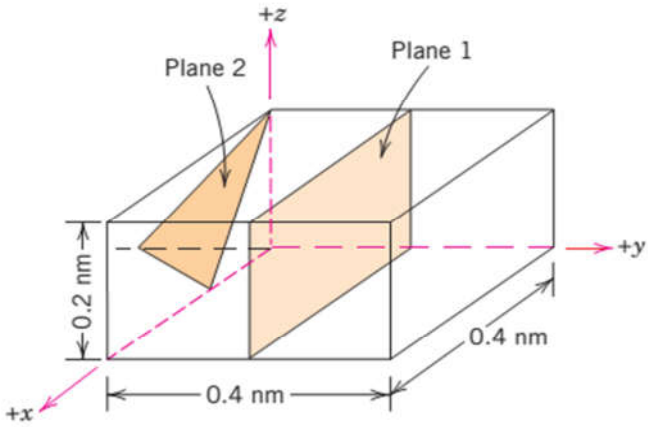
For example, consider the section of a (110) plane within an FCC unit cell as represented in Figure below:



$$\mathrm{PD}_{110} = \frac{2 \text{ atoms}}{4\mathrm{R} \times 2\mathrm{R}\sqrt{2}} = \frac{2 \text{ atoms}}{8\mathrm{R}^2\sqrt{2}} \quad nm^{-2} \text{ or } m^{-2}$$

H.W. (9) *Derive linear density expressions for FCC [100] and [111] directions in terms of the atomic radius R.*

H.W. (10) *What are the indices for the two planes drawn in the following sketch:*



H.W. (10) *Determine the Miller indices for the planes shown in the following unit cell:*