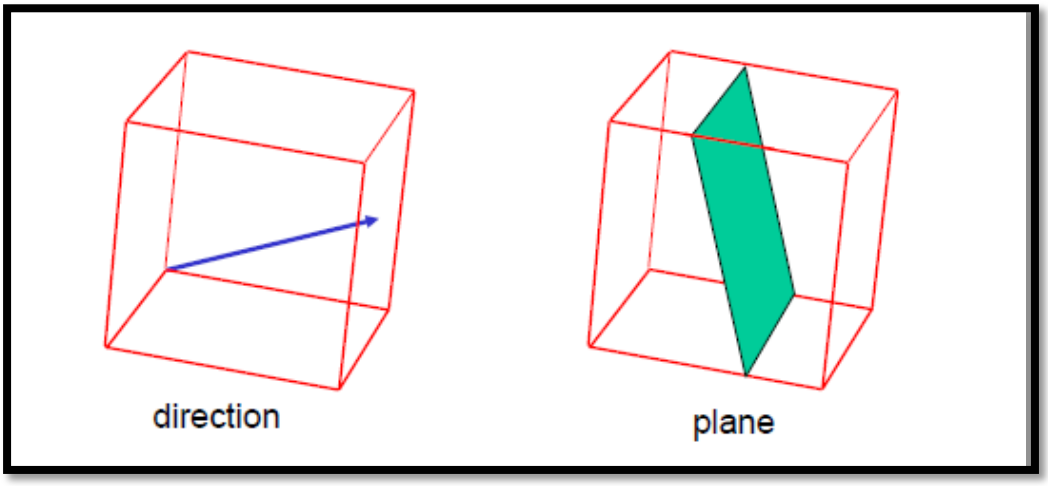
Crystallographic Directions, and Planes

we need a way to identify directions and planes of atoms. Why?

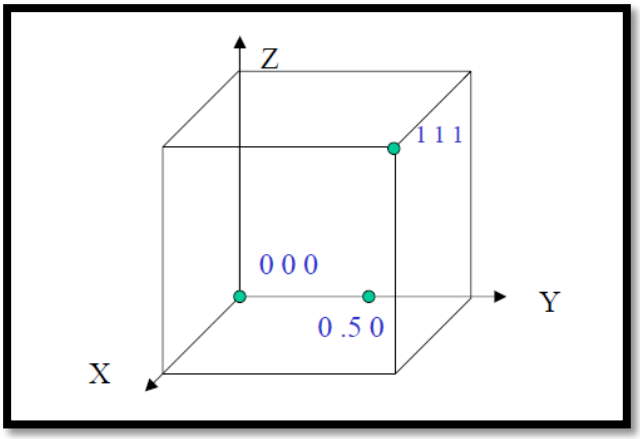
- Deformation under loading (*slip*) occurs on certain crystalline planes and in certain crystallographic directions.
- Before we can predict how materials fail, we need to know what modes of failure are more likely to occur.
- Other properties of materials (*electrical conductivity,thermal conductivity, elastic modulus*) can vary in a crystal with orientation.



- It is often necessary to be able to specify certain directions and planes in crystals.
- Many material properties and processes vary with direction in the crystal.
- Directions and planes are described using three integers -**Miller Indices**

Point coordinates

• Point position specified in terms of its coordinates as fractional multiples of the unit cell edge lengths



General Rules for Lattice Directions, Planes & Miller Indices

• Miller indices used to express lattice *planes* and *directions*

- x, y, z are the axes (on arbitrarily positioned origin)
- a, b, c are lattice parameters (*length of unit cell along a side*)
- h, k, l are the Miller indices for planes and directions - expressed as planes: (hkl) and directions: [hkl]
  - Negative values are expressed with a bar over the number

• *Example: -2 is expressed 2*

Crystallographic direction:

– [123]

– [100]

– … etc.

Miller Indices for Directions

Method

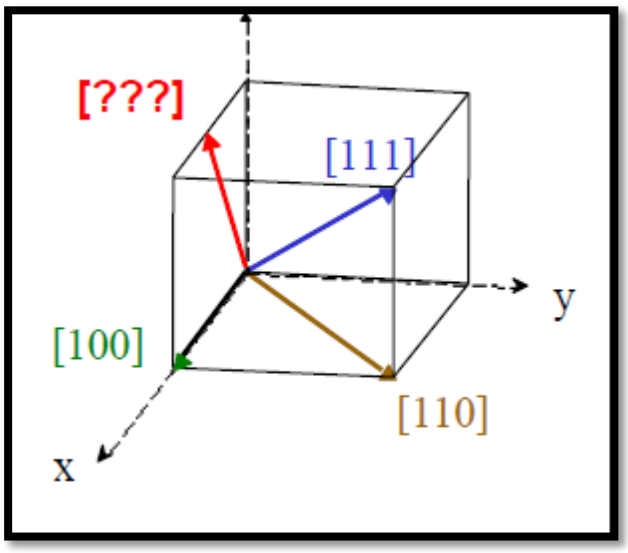
– Draw vector, and find the coordinates of the head, h_1,k_1,l_1 and the tail

h_2,k_2,l_2.

– subtract coordinates of tail from coordinates of head

– Remove fractions by multiplying by smallest possible factor

– Enclose in square brackets



Miller Indices for Planes

• (hkl) Crystallographic plane

• {hkl} Family of crystallographic planes

– e.g. (hkl), (lhk), (hlk) … etc.

In the cubic system planes having the same indices regardless of ***order*** *or* ***sign*** *are equivalent*

• Hexagonal crystals can be expressed in a four index system (u v t w)

– *Can be converted to a three index system using formulas*

Method

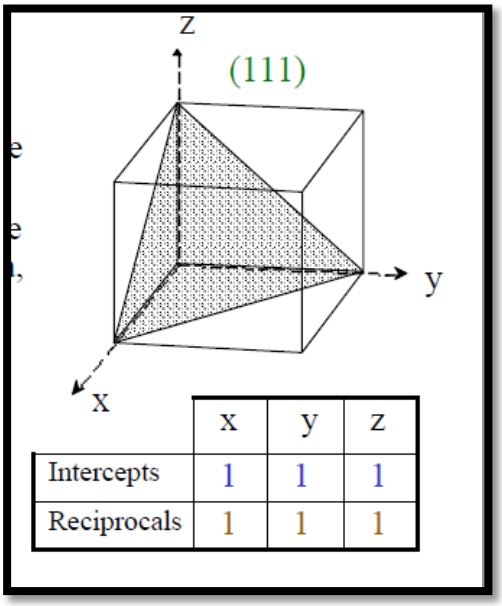
• If the plane passes through the origin, select an equivalent plane or move the origin.

• Determine the intersection of the plane with the axes in terms of a, b, and c

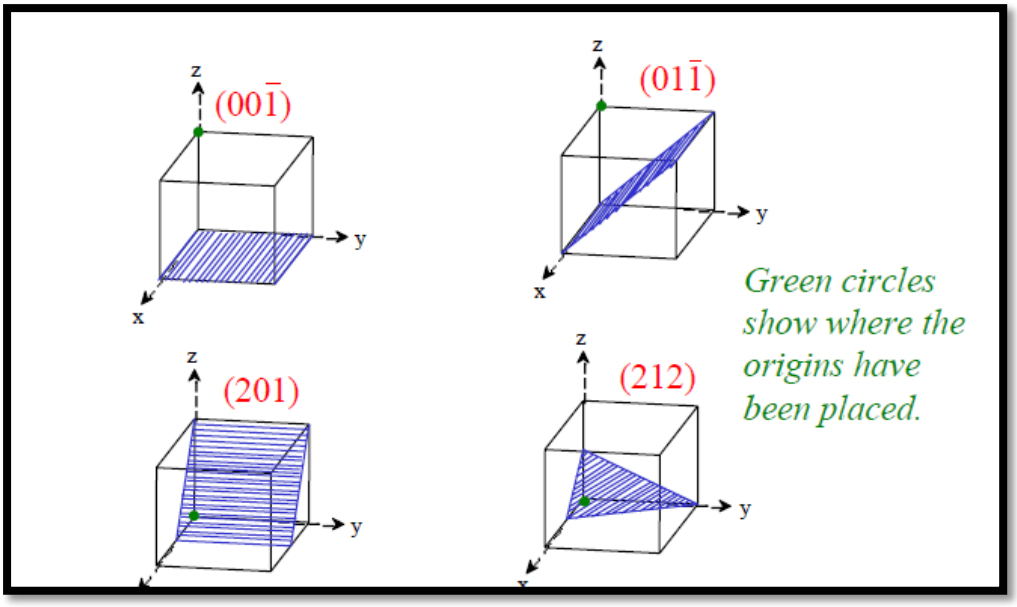
• Take the reciprocal *(1/∞ = 0)*

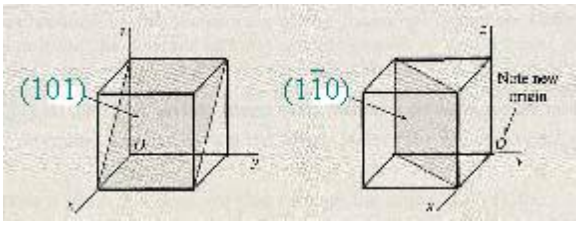
• Convert to smallest integers *(optional)*

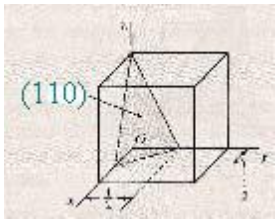
• Enclose by parentheses



	x	y	z
Intercepts	1	1	1
Reciprocals	1	1	1







(a) (101) **(b) (110)** **(c) (221)**

Linear and Planar density

Linear Density:

– Number of atoms per length whose centers lie on the direction vector for a specific crystallographic direction.

$$LD = \frac{\#\text{ of atoms centered on a direction vector}}{\text{length of direction vector}}$$

ex. calculate linear atomic density ρ_l in [110] direction in Cu crystal lattice in atoms/mm. (Cu is FCC and lattice constant a = 0.361 nm)

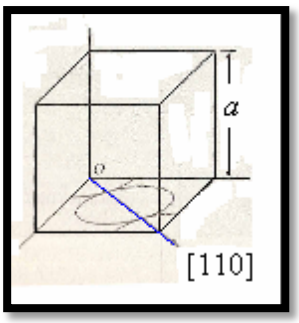
solution:

no. of atoms = ½ + 1 + ½ = 2 atoms

length = $\sqrt{2}\, a = \sqrt{2}\,(3.61 \times 10^{-7})$

$= 5.104 \times 10^{-7}$ mm

$$\rho_l = \frac{2 \text{ atoms}}{5.104 \times 10^{-7} \text{ mm}} = 3.92 \times 10^{6} \text{ atoms/mm}$$



Planar Density

– Number of atoms per unit area that are centered on a particular crystallographic plane.

$$PD = \frac{\#\text{ of atoms centered on a plane}}{\text{area of plane}}$$

ex. calculate planar atomic density ρ_p on (110) plane of the α-Fe in BCC lattice in atoms/mm^2. (lattice constant a = 0.287 nm)

solution:

1 atom (center) + ¼ atom (corner) × 4 = 2 atoms

area = $a \times \sqrt{2}\, a = \sqrt{2}\, a^2 = \sqrt{2}\, (2.87 \times 10^{-7})^2$

$= 1.164 \times 10^{-13}$ mm^2

$$\rho p = \frac{\text{2 atoms}}{1.164 \times 10^{-13}\ \text{mm}^2} = 1.72 \times 10^{13}\ \text{atoms/mm2}$$