Density Calculations

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

n = number of atoms associated with each unit cell
A = atomic weight
V_C = volume of the unit cell
N_A = Avogadro's number (6.023×10^{23} atoms/mol)

Example Calculate the radius of a tantalum atom, given that Ta has a BCC crystal structure, a density of 16.6 g/cm^3, and an atomic weight of 180.9 g/mol.

$$16.6 = \frac{2 * 180.9}{V_C * 6.022 * 10^{23}}$$

$$R = 8.23 * 10^{-9}\ cm$$

Crystallographic Directions, and Planes

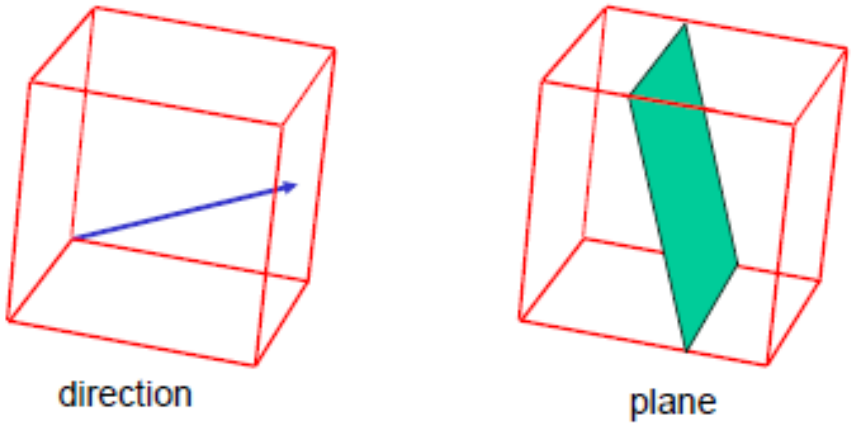
Now that we know how atoms arrange themselves to form crystals, *we need a way to identify directions and planes of atoms.*

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.

Crystallographic Directions, and Planes

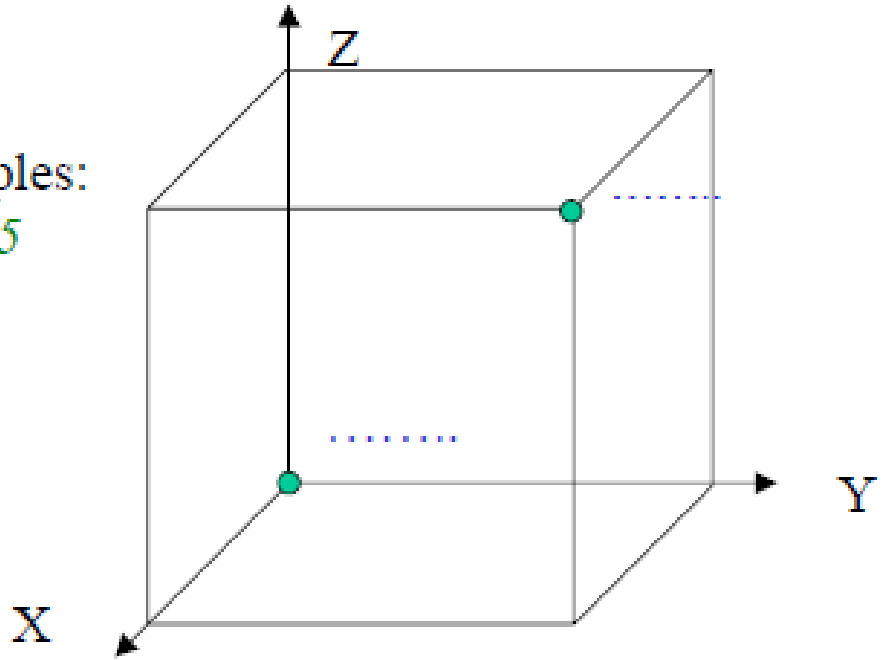


- It is often necessary to be able to specify certain directions and planes in crystals.
- Many material properties and processes vary with direction in the crystal.

Point coordinates

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

See examples:
3.4 and 3.5



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)
  - *in some crystal systems these are not mutually ⊥*
- 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]

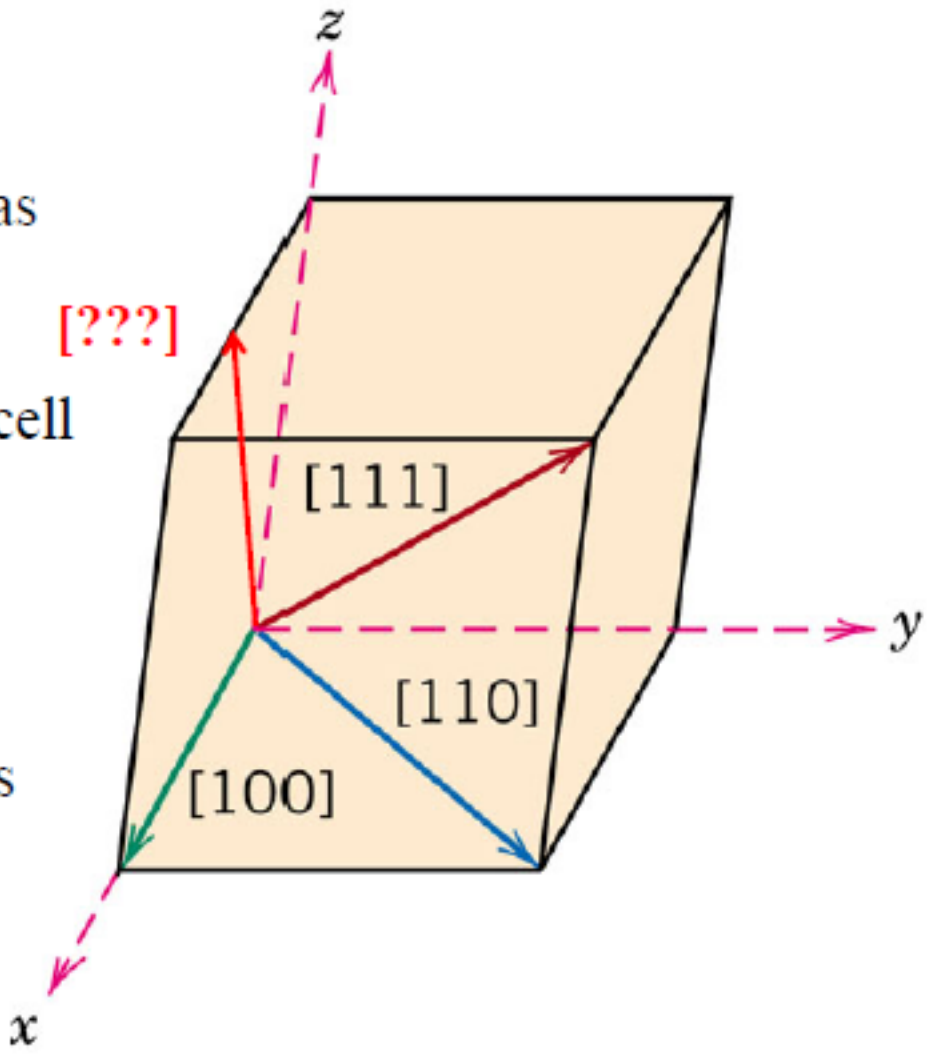
- Conventions for naming
  - There are NO COMMAS between numbers
  - Negative values are expressed with a bar over the number
    - *Example: -2 is expressed* $\bar{2}$

- Crystallographic direction:
  - [123]
  - [100]
  - … etc.

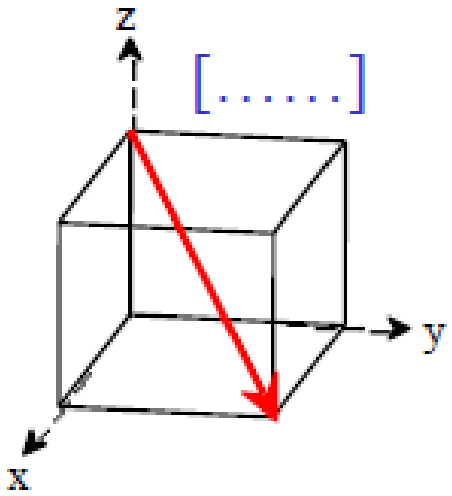
Miller Indices for Directions

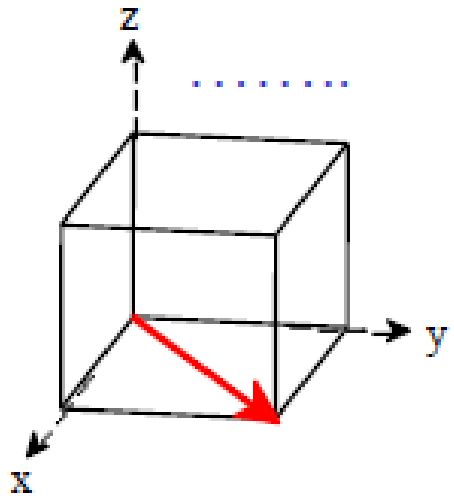
Method

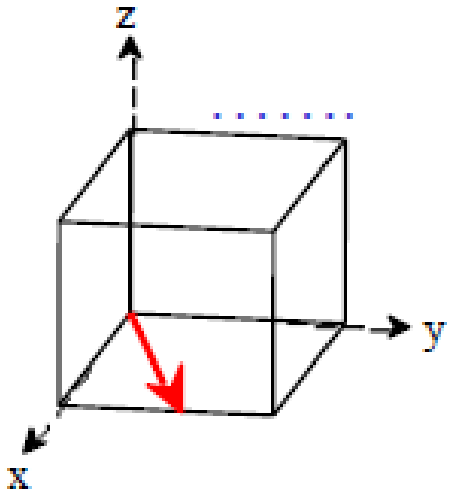
- Draw vector, define tail as origin.
- Determine length of the vector projection in unit cell dimensions, a, b, and c
- Remove fractions by multiplying by smallest possible factor
- Enclose in square brackets

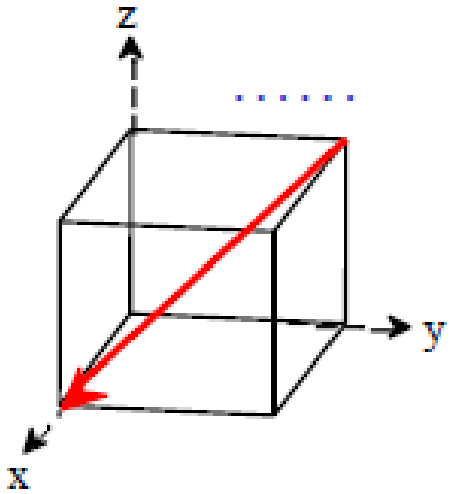


Example - Naming Directions



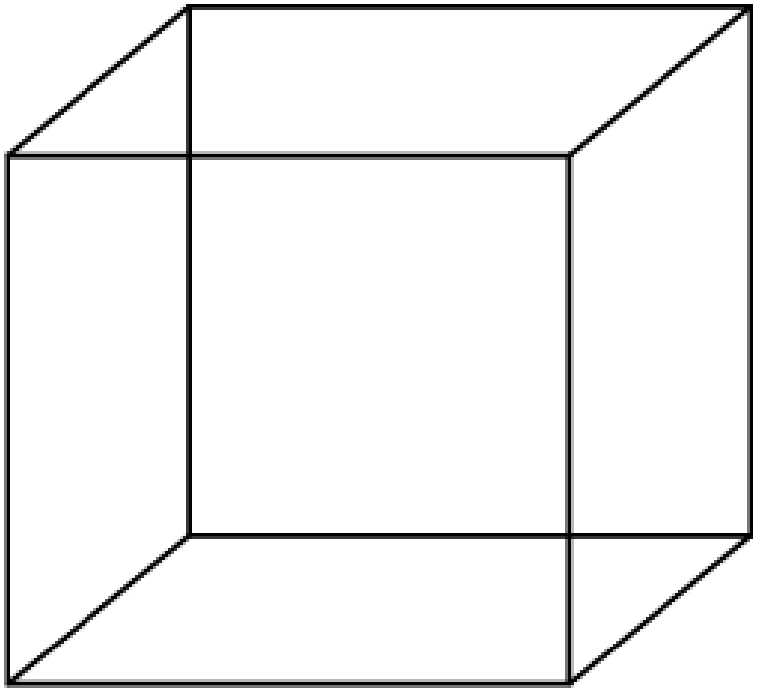


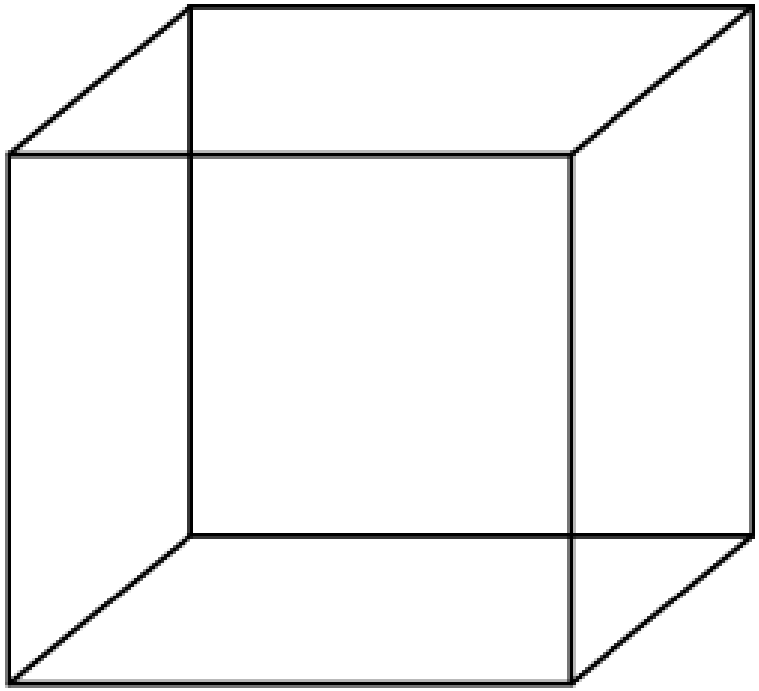




Example - Drawing Directions

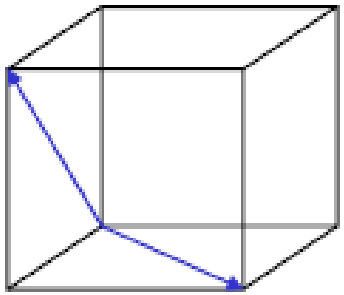
Draw $[11\bar{2}]$ and $[\bar{1}\bar{1}\bar{1}]$





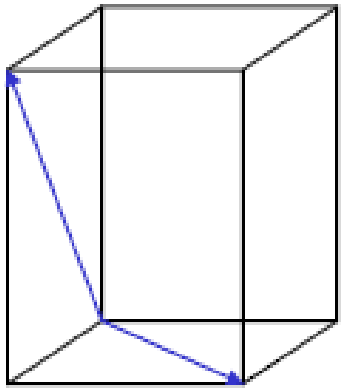
Families of Directions

- Equivalence of directions



[101] = [110]

cubic



[101] ≠ [110]

tetragonal

- <123> Family of directions
  - [123], [213], [312], [132], [231], [321]
    - *– only in a cubic crystal*

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

Miller Indices for Planes

- (hkl) Crystallographic plane
- {hkl} Family of crystallographic planes
  - e.g. (hkl), (lhk), (hlk) … etc.

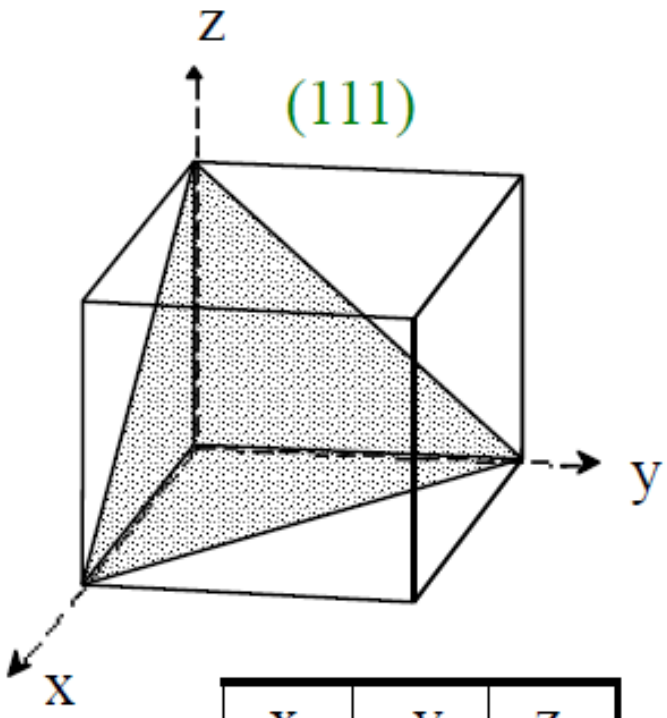
*In the cubic system planes having the same indices regardless of **order** or **sign** are equivalent*

- Hexagonal crystals can be expressed in a four index system (u v t w)
  - *Can be converted to a three index system using formulas*

Miller Indices for planes

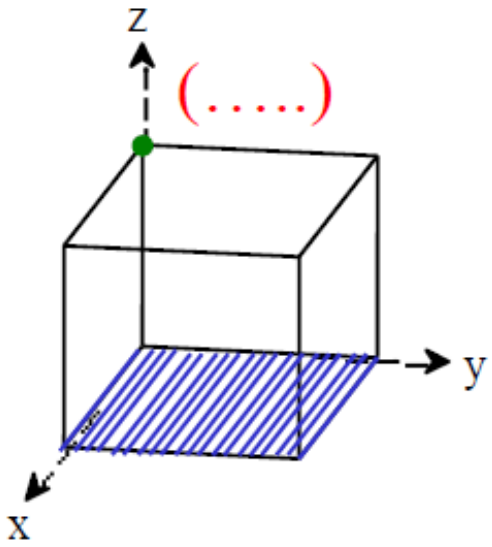
Method

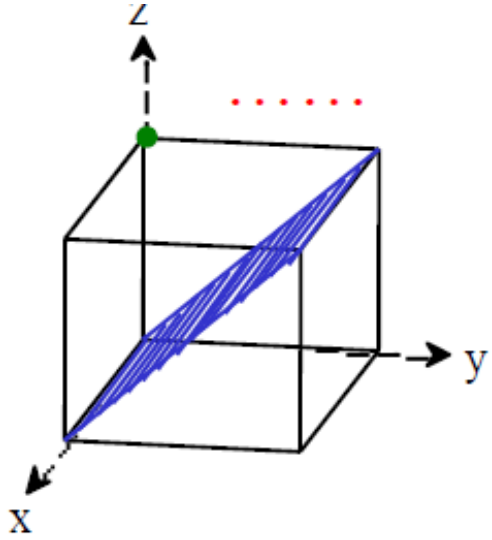
- If the plane passes through the origin, select an equivalent plane or move the origin
- Determine the intersection of the plane with the axes in terms of a, b, and c
- Take the reciprocal *(1/∞ = 0)*
- Convert to smallest integers *(optional)*
- Enclose by parentheses

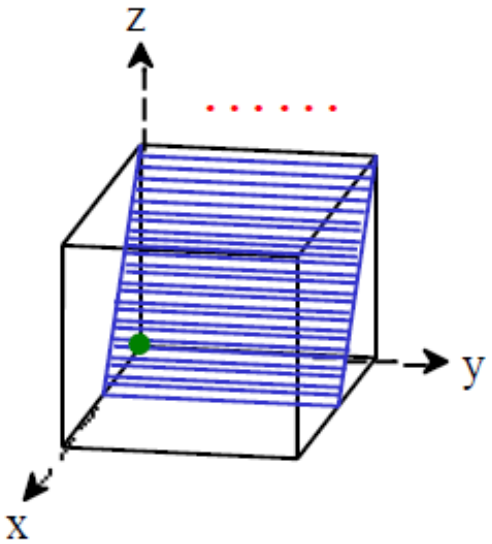


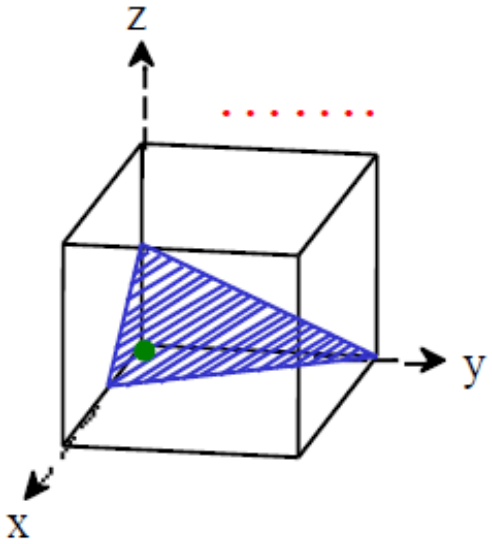
	x	y	z
Intercepts	1	1	1
Reciprocals	1	1	1

see example 3.8


z
(.....)
y
x


z
.....
y
x


z
.....
y
x


z
.....
y
x