Silicate Ceramics

Some Si – O bonding patterns

Kaolinite
Carbon polymorphs
Identification of planes and directions in crystals
Finding Crystallographic Directions

- When vector passes through the origin, project onto x y z axes
- Measure in terms of lattice constants a, b, c
- Clear fractions
- Multiply or divide to get smallest integers
- Enclose in [ ]

Point method:
Head – tail (in terms of lattice constants)
Clear fractions
Get smallest integers
Enclose in [ ]
Finding Crystallographic Directions

- When vector passes through the origin, project onto x y z axes
- Measure in terms of lattice constants a, b, c
- Clear fractions
- Multiply or divide to get smallest integers
- Enclose in [ ]

This method holds for all crystal systems regardless of angles.

Tetragonal cell, two lattice constants a and c

1. 1a, 0a, 0c = [1,0,0]
2. 1/2a, 0a, 1c = [1,0,2]
• **Directions only** – not vectors – magnitude not important!
• Lattice points have equivalent surroundings, so can choose origin
• Many directions crystallographically equivalent (family of directions) $<100>$
• Different directions have different atomic spacing (linear packing density - Fraction of unit cell length occupied by atom)
• **Direction + crystal structure** needed to know atom location
  
  for **Simple cubic:**
  Linear packing density
  
  $[100] \quad 1/a \text{ nm}^{-1}$
  $[110] \quad 1/(a \sqrt{2}) \text{ nm}^{-1}$
Crystallographic Planes – packing density

Atom positions for simple cubic planes

1 atom in each square

Po: \( a = 0.33 \text{nm} \)

Planar packing density

\[
\frac{1}{(0.33)^2} \text{nm}^{-2}
\]

\[
\frac{1}{(0.33)^2 \sqrt{2}} \text{nm}^{-2}
\]

Within a crystal structure:
Family of planes have equivalent area packing density
Crystallographic Planes – packing density

The same index may have different atomic packing for different crystal structures. Example: (011) on SC vs BCC

Planar packing density

\[
\frac{2}{(a)^2 \sqrt{2}} \text{ nm}^{-2}
\]
SINGLE VS POLYCRYSTALS

• Single Crystals
  - Properties vary with direction: **anisotropic**.
  - Example: the modulus of elasticity (E) in BCC iron:
    
    \[
    E \text{ (diagonal) } = 273 \text{ GPa} \\
    E \text{ (edge) } = 125 \text{ GPa}
    \]

• Polycrystals
  - Properties may/may not vary with direction.
  - If grains are randomly oriented: **isotropic**.
    
    \(E_{\text{poly iron}} = 210 \text{ GPa}\)
  - If grains are **textured**, anisotropic.

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(a) | (b) | (c) | (d)
Crystallographic planes - repeating

Crystals have repeating unit cells so planes repeat

Distance between planes, measured perpendicular to the plane: “d-spacing”

In cubic system

\[ d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \]
X-RAYS TO CONFIRM CRYSTAL STRUCTURE

• Incoming X-rays **diffract** from crystal planes.

- Critical angles, $\theta_c$, for X-rays provide atomic spacing, $d$.  

\[ d = n\lambda / 2\sin\theta_c \]

- Measurements include:
  - Critical angles, $\theta_c$, for X-rays provide atomic spacing, $d$.  
  - X-ray intensity (from detector)

Adapted from Fig. 3.2W, *Callister 6e*. 

Incoming X-rays diffract from crystal planes. Reflections must be in phase to detect signal.