

Crystallographic Notation

position: x,y,z, coordinates, sep^d by commas, no enclosure

O: 0,0,0 **A:** 0,1,1 **B:** 1,0, 1/2

direction: move coordinate axes so that line passes through origin

- define vector from **O** to point on the line
- choose smallest set of integers
- no commas, enclose in brackets, clear fractions

\xrightarrow{OB} 1 0 1/2 clear fractions ☞ [201]

\xrightarrow{AO} [0 $\bar{1}\bar{1}$] minus denoted by macron

can denote entire family of directions by carats < >

e.g., all body diagonals: <111> = [111], [$\bar{1}\bar{1}\bar{1}$], [$\bar{1}\bar{1}1$], [$1\bar{1}\bar{1}$], etc.

all cube edges: <001>

all face diagonals: <011>

all body diagonals: <111>

plane: Miller¹ indices – recall equation of a plane in space

$$\frac{x}{a} + \frac{y}{b} + \frac{z}{c} = 1, \text{ where } a, b, c \text{ are intercepts of the plane with the } x, y, z \text{ axes, respectively}$$

- let $h = \frac{1}{a}$, $k = \frac{1}{b}$, and $l = \frac{1}{c}$, so that $hx + ky + lz = 1$

- no commas², enclose in parentheses (hkl)

- can denote entire family of planes by braces $\{ \}$

e.g., all faces of unit cell: $\{001\} = (001), (00\bar{1}), (\bar{1}00), (0\bar{1}0), \text{ etc.}$

- cool property: $(hkl) \perp [hkl]$

¹ William Hallows Miller, British mineralogist, 1839

² plane must not include the origin