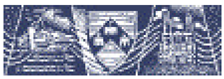
Mathematics Refresher

Peter Main

1123581321 ...

$ax^2+bx+c=0$

$1 + 1 = 2$

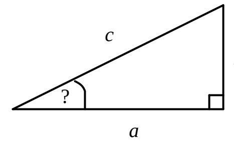


$\tan(?) = \dfrac{\sin(?)}{\cos(?)}$

Trigonometry

$$\sin(?) = \frac{b}{c} \qquad \cos(?) = \frac{a}{c}$$

$$\tan(?) = \frac{\sin(?)}{\cos(?)} = \frac{b}{a}$$



Pythagoras' theorem: $a^2 + b^2 = c^2$

$\cos^2(?) + \sin^2(?) = 1$

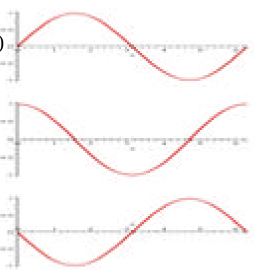
Differentiation

$$\frac{d}{d?}(\sin(?)) = \cos(?) \qquad \frac{d}{d?}(\cos(?)) = -\sin(?)$$

sin(?)

cos(?)

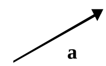
-sin(?)



Vectors

A vector has a magnitude and a direction.

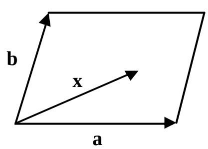
It is drawn as an arrow and written in bold as **a**.



Examples:	velocity	magnitude gives speed
		direction is direction of travel
	displacement	position of atom in cell

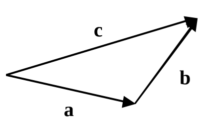
$\mathbf{x} = x\,\mathbf{a} + y\,\mathbf{b} + z\,\mathbf{c}$

$\mathbf{h} = h\,\mathbf{a}^* + k\,\mathbf{b}^* + l\,\mathbf{c}^*$

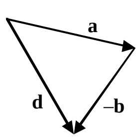


Vector addition and subtraction

Addition: $\mathbf{a} + \mathbf{b} = \mathbf{c}$



Subtraction: $\mathbf{a} - \mathbf{b} = \mathbf{d}$



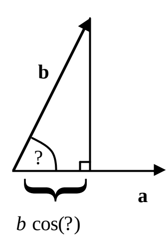
Scalar product

- also called a dot product

$\mathbf{a}.\mathbf{b} = a\,b\cos(?)$

$\mathbf{a}.\mathbf{b} = 0$ when vectors are orthogonal

$\mathbf{a}.\mathbf{a} = a^2$



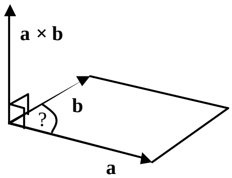
Vector product

- also called a cross product

$\mathrm{a} \times \mathbf{b} = a\, b \sin(?)\, \mathbf{n}$

$\mathbf{n}$ is perpendicular to $\mathbf{a}$ and $\mathbf{b}$

$\mathbf{a}, \mathbf{b}, \mathbf{n}$ form a right-handed set



$\mathbf{a} \times \mathbf{b} = 0$ when $\mathbf{a}$ is parallel to $\mathbf{b}$

$\mathbf{a} \times \mathbf{b} = -\mathbf{b} \times \mathbf{a}$

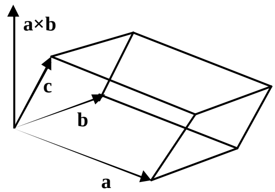
$|\mathbf{a} \times \mathbf{b}|$ = area of parallelogram defined by $\mathbf{a}$ and $\mathbf{b}$

Volume of a unit cell

If you need convincing that vectors are useful, consider the expression for the volume of a unit cell.

$V = \underbrace{\mathbf{a}\times\mathbf{b}}.\mathbf{c} = \mathbf{a}.\mathbf{b}\times\mathbf{c}$

area of base × vertical height



Without vectors, the volume is:

$$V = a\,b\,c\left(1 - \cos^2 a - \cos^2 b - \cos^2 g + 2\cos a \cos b \cos g\right)^{1/2}$$

Reciprocal lattice

The reciprocal lattice is defined by three vectors **a*, b*** and **c***.

They are defined in terms of the direct lattice vectors as:

$$\mathbf{a}^* = \frac{\mathbf{b}\times\mathbf{c}}{V} \qquad \mathbf{a}\,.\,\mathbf{a}^* = \frac{\mathbf{a}\,.\mathbf{b}\times\mathbf{c}}{V} = 1$$

$$\mathbf{b}^* = \frac{\mathbf{c}\times\mathbf{a}}{V} \qquad \mathbf{b}\,.\,\mathbf{a}^* = \frac{\mathbf{b}\,.\mathbf{b}\times\mathbf{c}}{V} = 0$$

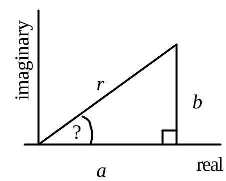
$$\mathbf{c}^* = \frac{\mathbf{a}\times\mathbf{b}}{V} \qquad \mathbf{c}\,.\,\mathbf{a}^* = \frac{\mathbf{c}\,.\mathbf{b}\times\mathbf{c}}{V} = 0$$

$$\begin{aligned}\mathbf{h.x} &= (h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*)\,.\,(x\mathbf{a} + y\mathbf{b} + z\mathbf{c}) \\ &= hx\mathbf{a}^*.\mathbf{a} + hy\mathbf{a}^*.\mathbf{b} + hz\mathbf{a}^*.\mathbf{c} + kx\mathbf{b}^*.\mathbf{a} + ky\mathbf{b}^*.\mathbf{b} + \ldots \\ &= hx + ky + lz\end{aligned}$$

Complex numbers

A complex number consists of two components called the real and imaginary parts.

It can be plotted on an Argand diagram and written as $a + i\,b$ where $i^2 = -1$



$$\begin{aligned}a + i\,b &= r\cos(?) + i\,r\sin(?) \\ &= r\,(\cos(?) + i\sin(?)) \\ &= r\,e^{i?} = r\exp(i?)\end{aligned}$$

Complex conjugate

complex conjugate: $(a + i\,b)^* = a - i\,b$

note that: $(a + i\,b)\,(a - i\,b) = a^2 + iab - iab - i^2b^2$

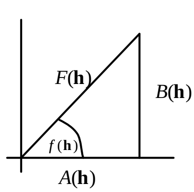
$= a^2 + b^2$

$= r^2$

Structure factors are conveniently represented as complex numbers:

$F(\mathbf{h}) = A(\mathbf{h}) + i\,B(\mathbf{h})$

$= |F(\mathbf{h})| \exp(if\,(\mathbf{h}))$



Friedel's law

Friedel's law is a direct result of real electron density:

Electron density equation $r\,(\mathbf{x}) = \frac{1}{V}\sum_h F(\mathbf{h})\exp(-2p\;i\,\mathbf{h.x})$

Take the pair of terms $F(\mathbf{h})\exp(-2p\;i\,\mathbf{h.x}) + F(\bar{\mathbf{h}})\exp(2p\;i\,\mathbf{h.x})$

The imaginary parts must cancel to obtain a real result:

$(a + i\,b) + (a - i\,b) = 2\,a$

It follows that $F^*(\mathbf{h}) = F(\bar{\mathbf{h}})$

i.e. $|F(\mathbf{h})| = |F(\bar{\mathbf{h}})|$ and $f(\mathbf{h}) = -f(\bar{\mathbf{h}})$

Centrosymmetric structure

For a centrosymmetric structure $?(\mathbf{x}) = ?(-\mathbf{x})$

$$\therefore \sum_{\mathbf{h}} F(\mathbf{h}) \exp(-2p\, i\mathbf{h.x}) = \sum_{\mathbf{h}} F(\mathbf{h}) \exp(2p\, i\mathbf{h.x})$$

Equate equivalent terms:

$$F(\mathbf{h}) \exp(-2p\, i\mathbf{h.x}) = F(\bar{\mathbf{h}}) \exp(-2p\, i\mathbf{h.x})$$

$$\therefore \; F(\mathbf{h}) = F(\bar{\mathbf{h}})$$

This means the structure factors must be real, so the phases can only be 0 or p.

Since $\exp(i\,0) = 1$ and $\exp(i\,\mathrm{p}) = -1$, the structure factor may be written as $|F(\mathbf{h})|$ or $-|F(\mathbf{h})|$.