crystallography IV



Useful concept for crystallography & diffraction

Think of sets of planes in lattice - each plane in set parallel to all others in set. All planes in set equidistant from one another

Infinite number of sets of planes in lattice



d interplanar spacing

Keep track of sets of planes by giving them names - Miller indices

(hkl)



Choose cell, cell origin, cell axes:



Choose cell, cell origin, cell axes Draw set of planes of interest:



Choose cell, cell origin, cell axes Draw set of planes of interest Choose plane nearest origin:



Choose cell, cell origin, cell axes Draw set of planes of interest Choose plane nearest origin Find intercepts on cell axes: origin

a

0

0

0

0

0

0

1,1,∞

Choose cell, cell origin, cell axes Draw set of planes of interest Choose plane nearest origin Find intercepts on cell axes

1,1,∞

Invert these to get (hkl) (110)









































Two things characterize a set of lattice planes:

interplanar spacing (d)

orientation (defined by normal)

Strange indices

For hexagonal lattices - sometimes see 4-index notation for planes (hkil) where i = - h - k



Zones

2 intersecting lattice planes form a zone



if $(h_1 k_1 l_1)$ and $(h_2 k_2 l_2)$ in same zone, then $(h_1+h_2 k_1+k_2 l_1+l_2)$ also in same zone

Zones

Example: zone axis for (111) & (100) - [011]

zone axis [uvw] is ui + vj + wk





(011) in same zone? hu + kv + lw = 0 0·0 + 1·1 − 1·1 = 0

if $(h_1 k_1 l_1)$ and $(h_2 k_2 l_2)$ in same zone, then $(h_1+h_2 k_1+k_2 l_1+l_2)$ also in same zone

Reciprocal lattice Real space lattice



Real space lattice - basis vectors



Real space lattice - choose set of planes



Real space lattice - interplanar spacing d



Real space lattice —> the (100) reciprocal lattice pt



Reciprocal lattice The (010) recip lattice pt



The (020) reciprocal lattice point



More reciprocal lattice points



The (110) reciprocal lattice point



Still more reciprocal lattice points



Reciprocal lattice notation











In general:

$$a^* = \frac{b \times c}{a \cdot b \times c}$$

 $b^* = \frac{c \times a}{a \cdot b \times c}$
 $c^* = \frac{a \times b}{a \cdot b \times c}$