

6.3 Crystalline structure

Bravais lattices

Volume of primitive cell	$V = (\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c}$	(6.1)	$\mathbf{a}, \mathbf{b}, \mathbf{c}$ V	primitive base vectors volume of primitive cell
Reciprocal primitive base vectors ^a	$\mathbf{a}^* = 2\pi \mathbf{b} \times \mathbf{c} / [(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c}]$	(6.2)	$\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$	reciprocal primitive base vectors
	$\mathbf{b}^* = 2\pi \mathbf{c} \times \mathbf{a} / [(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c}]$	(6.3)		
	$\mathbf{c}^* = 2\pi \mathbf{a} \times \mathbf{b} / [(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c}]$	(6.4)		
	$\mathbf{a} \cdot \mathbf{a}^* = \mathbf{b} \cdot \mathbf{b}^* = \mathbf{c} \cdot \mathbf{c}^* = 2\pi$	(6.5)		
	$\mathbf{a} \cdot \mathbf{b}^* = \mathbf{a} \cdot \mathbf{c}^* = 0$ (etc.)	(6.6)		
Lattice vector	$\mathbf{R}_{uvw} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$	(6.7)	$\mathbf{R}_{uvw}$ u, v, w	lattice vector $[uvw]$ integers
Reciprocal lattice vector	$\mathbf{G}_{hkl} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$	(6.8)	$\mathbf{G}_{hkl}$	reciprocal lattice vector $[hkl]$
	$\exp(i\mathbf{G}_{hkl} \cdot \mathbf{R}_{uvw}) = 1$	(6.9)	$\mathbf{i}$	
Weiss zone equation ^b	$hu + kv + lw = 0$	(6.10)	(hkl)	Miller indices of plane ^c
Interplanar spacing (general)	$d_{hkl} = \frac{2\pi}{G_{hkl}}$	(6.11)	d_{hkl}	distance between (hkl) planes
Interplanar spacing (orthogonal basis)	$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$	(6.12)		

^aNote that this is 2π times the usual definition of a “reciprocal vector” (see page 20).

^bCondition for lattice vector $[uvw]$ to be parallel to lattice plane (hkl) in an arbitrary Bravais lattice.

^cMiller indices are defined so that $\mathbf{G}_{hkl}$ is the shortest reciprocal lattice vector normal to the (hkl) planes.

Weber symbols

Converting $[uvw]$ to $[UVTW]$	$U = \frac{1}{3}(2u - v)$	(6.13)	U, V, T, W u, v, w $[UVTW]$ $[uvw]$	Weber indices zone axis indices Weber symbol zone axis symbol
	$V = \frac{1}{3}(2v - u)$	(6.14)		
	$T = -\frac{1}{3}(u + v)$	(6.15)		
	$W = w$	(6.16)		
Converting $[UVTW]$ to $[uvw]$	$u = (U - T)$	(6.17)		
	$v = (V - T)$	(6.18)		
	$w = W$	(6.19)		
Zone law ^a	$hU + kV + iT + lW = 0$	(6.20)	$(hkil)$	Miller–Bravais indices

^aFor trigonal and hexagonal systems.

Cubic lattices

lattice	primitive (P)	body-centred (I)	face-centred (F)
lattice parameter	a	a	a
volume of conventional cell	a^3	a^3	a^3
lattice points per cell	1	2	4
1st nearest neighbours ^a	6	8	12
1st n.n. distance	a	$a\sqrt{3}/2$	$a/\sqrt{2}$
2nd nearest neighbours	12	6	6
2nd n.n. distance	$a\sqrt{2}$	a	a
packing fraction ^b	$\pi/6$	$\sqrt{3}\pi/8$	$\sqrt{2}\pi/6$
reciprocal lattice ^c	P	F	I
primitive base vectors ^d	$\mathbf{a}_1 = a\hat{\mathbf{x}}$	$\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}})$	$\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}})$
	$\mathbf{a}_2 = a\hat{\mathbf{y}}$	$\mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}} - \hat{\mathbf{y}})$	$\mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}})$
	$\mathbf{a}_3 = a\hat{\mathbf{z}}$	$\mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}})$	$\mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}})$

^aOr “coordination number.”

^bFor close-packed spheres. The maximum possible packing fraction for spheres is $\sqrt{2}\pi/6$.

^cThe lattice parameters for the reciprocal lattices of P, I, and F are $2\pi/a$, $4\pi/a$, and $4\pi/a$ respectively.

^d $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ are unit vectors.

Crystal systems^a

system	symmetry	unit cell ^b	lattices ^c
triclinic	none	$a \neq b \neq c$; $\alpha \neq \beta \neq \gamma \neq 90^\circ$	P
monoclinic	one diad $\parallel [010]$	$a \neq b \neq c$; $\alpha = \gamma = 90^\circ$, $\beta \neq 90^\circ$	P, C
orthorhombic	three orthogonal diads	$a \neq b \neq c$; $\alpha = \beta = \gamma = 90^\circ$	P, C, I, F
tetragonal	one tetrad $\parallel [001]$	$a = b \neq c$; $\alpha = \beta = \gamma = 90^\circ$	P, I
trigonal ^d	one triad $\parallel [111]$	$a = b = c$; $\alpha = \beta = \gamma < 120^\circ \neq 90^\circ$	P, R
hexagonal	one hexad $\parallel [001]$	$a = b \neq c$; $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$	P
cubic	four triads $\parallel \langle 111 \rangle$	$a = b = c$; $\alpha = \beta = \gamma = 90^\circ$	P, F, I

^aThe symbol “ $\neq$ ” implies that equality is not required by the symmetry, but neither is it forbidden.

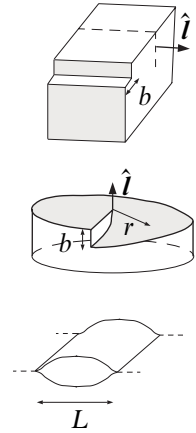
^bThe cell axes are a , b , and c with α , β , and γ the angles between $b:c$, $c:a$, and $a:b$ respectively.

^cThe lattice types are primitive (P), body-centred (I), all face-centred (F), side-centred (C), and rhombohedral primitive (R).

^dA primitive hexagonal unit cell, with a triad $\parallel [001]$, is generally preferred over this rhombohedral unit cell.

Dislocations and cracks

Edge dislocation	$\hat{l} \cdot \mathbf{b} = 0$	(6.21)	$\hat{l}$ unit vector $\parallel$ line of dislocation
Screw dislocation	$\hat{l} \cdot \mathbf{b} = b$	(6.22)	$\mathbf{b}, b$ Burgers vector ^a
Screw dislocation energy per unit length ^b	$U = \frac{\mu b^2}{4\pi} \ln \frac{R}{r_0}$	(6.23)	U dislocation energy per unit length
	$\sim \mu b^2$	(6.24)	μ shear modulus
Critical crack length ^c	$L = \frac{4\alpha E}{\pi(1-\sigma^2)p_0^2}$	(6.25)	R outer cutoff for r
			r_0 inner cutoff for r
			L critical crack length
			α surface energy per unit area
			E Young modulus
			σ Poisson ratio
			p_0 applied widening stress



^aThe Burgers vector is a Bravais lattice vector characterising the total relative slip were the dislocation to travel throughout the crystal.

^bOr “tension.” The energy per unit length of an edge dislocation is also $\sim \mu b^2$.

^cFor a crack cavity (long $\perp L$) within an isotropic medium. Under uniform stress p_0 , cracks $\geq L$ will grow and smaller cracks will shrink.

Crystal diffraction

Laue equations	$a(\cos \alpha_1 - \cos \alpha_2) = h\lambda$	(6.26)	a, b, c lattice parameters
	$b(\cos \beta_1 - \cos \beta_2) = k\lambda$	(6.27)	$\alpha_1, \beta_1, \gamma_1$ angles between lattice base vectors and input wavevector
	$c(\cos \gamma_1 - \cos \gamma_2) = l\lambda$	(6.28)	$\alpha_2, \beta_2, \gamma_2$ angles between lattice base vectors and output wavevector
			h, k, l integers (Laue indices)
Bragg's law ^a	$2\mathbf{k}_{\text{in}} \cdot \mathbf{G} + \mathbf{G} ^2 = 0$	(6.29)	λ wavelength
			$\mathbf{k}_{\text{in}}$ input wavevector
			$\mathbf{G}$ reciprocal lattice vector
Atomic form factor	$f(\mathbf{G}) = \int_{\text{vol}} e^{-i\mathbf{G} \cdot \mathbf{r}} \rho(\mathbf{r}) d^3r$	(6.30)	$f(\mathbf{G})$ atomic form factor
			$\mathbf{r}$ position vector
			$\rho(\mathbf{r})$ atomic electron density
Structure factor ^b	$S(\mathbf{G}) = \sum_{j=1}^n f_j(\mathbf{G}) e^{-i\mathbf{G} \cdot \mathbf{d}_j}$	(6.31)	$S(\mathbf{G})$ structure factor
			n number of atoms in basis
			$\mathbf{d}_j$ position of j th atom within basis
Scattered intensity ^c	$I(\mathbf{K}) \propto N^2 S(\mathbf{K}) ^2$	(6.32)	$\mathbf{K}$ change in wavevector ($= \mathbf{k}_{\text{out}} - \mathbf{k}_{\text{in}}$)
			$I(\mathbf{K})$ scattered intensity
			N number of lattice points illuminated
Debye–Waller factor ^d	$I_T = I_0 \exp \left[-\frac{1}{3} \langle u^2 \rangle \mathbf{G} ^2 \right]$	(6.33)	I_T intensity at temperature T
			I_0 intensity from a lattice with no motion
			$\langle u^2 \rangle$ mean-squared thermal displacement of atoms

^aAlternatively, see Equation (8.32).

^bThe summation is over the atoms in the basis, i.e., the atomic motif repeating with the Bravais lattice.

^cThe Bragg condition makes $\mathbf{K}$ a reciprocal lattice vector, with $|\mathbf{k}_{\text{in}}| = |\mathbf{k}_{\text{out}}|$.

^dEffect of thermal vibrations.