6.3 Crystalline structure

Bravais lattices

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

[a] Note that this is 2π times the usual definition of a "reciprocal vector" (see page 20).
[b] Condition for lattice vector $[uvw]$ to be parallel to lattice plane (hkl) in an arbitrary Bravais lattice.
[c] Miller indices are defined so that G_{hkl} is the shortest reciprocal lattice vector normal to the (hkl) planes.

Weber symbols

Converting $[uvw]$ to $[UVTW]$	$U = \dfrac{1}{3}(2u - v)$	(6.13)	U,V,T,W u,v,w $[UVTW]$ $[uvw]$	Weber indices zone axis indices Weber symbol zone axis symbol
	$V = \dfrac{1}{3}(2v - u)$	(6.14)		
	$T = -\dfrac{1}{3}(u + v)$	(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

[a] For 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]	$\boldsymbol{a}_1 = a\hat{\boldsymbol{x}}$ $\boldsymbol{a}_2 = a\hat{\boldsymbol{y}}$ $\boldsymbol{a}_3 = a\hat{\boldsymbol{z}}$	$\boldsymbol{a}_1 = \frac{a}{2}(\hat{\boldsymbol{y}}+\hat{\boldsymbol{z}}-\hat{\boldsymbol{x}})$ $\boldsymbol{a}_2 = \frac{a}{2}(\hat{\boldsymbol{z}}+\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}})$ $\boldsymbol{a}_3 = \frac{a}{2}(\hat{\boldsymbol{x}}+\hat{\boldsymbol{y}}-\hat{\boldsymbol{z}})$	$\boldsymbol{a}_1 = \frac{a}{2}(\hat{\boldsymbol{y}}+\hat{\boldsymbol{z}})$ $\boldsymbol{a}_2 = \frac{a}{2}(\hat{\boldsymbol{z}}+\hat{\boldsymbol{x}})$ $\boldsymbol{a}_3 = \frac{a}{2}(\hat{\boldsymbol{x}}+\hat{\boldsymbol{y}})$

[a] Or "coordination number."
[b] For close-packed spheres. The maximum possible packing fraction for spheres is $\sqrt{2}\pi/6$.
[c] The lattice parameters for the reciprocal lattices of P, I, and F are $2\pi/a$, $4\pi/a$, and $4\pi/a$ respectively.
[d] $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$ are unit vectors.

Crystal systems[a]

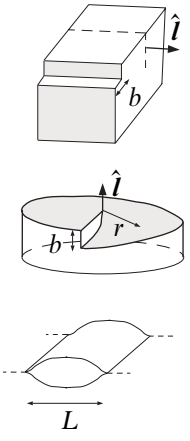
system	*symmetry*	*unit cell*[b]	*lattices*[c]
triclinic	none	$a \neq b \neq c$; $\alpha \neq \beta \neq \gamma \neq 90°$	P
monoclinic	one diad ∥ [010]	$a \neq b \neq c$; $\alpha = \gamma = 90°$, $\beta \neq 90°$	P, C
orthorhombic	three orthogonal diads	$a \neq b \neq c$; $\alpha = \beta = \gamma = 90°$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

[a] The symbol "≠" implies that equality is not required by the symmetry, but neither is it forbidden.
[b] The cell axes are a, b, and c with α, β, and γ the angles between $b:c$, $c:a$, and $a:b$ respectively.
[c] The lattice types are primitive (P), body-centred (I), all face-centred (F), side-centred (C), and rhombohedral primitive (R).
[d] A primitive hexagonal unit cell, with a triad ∥ [001], is generally preferred over this rhombohedral unit cell.

Dislocations and cracks

Edge dislocation	$\hat{\boldsymbol{l}}\cdot\boldsymbol{b}=0$	(6.21)
Screw dislocation	$\hat{\boldsymbol{l}}\cdot\boldsymbol{b}=b$	(6.22)
Screw dislocation energy per unit length[b]	$U=\dfrac{\mu b^2}{4\pi}\ln\dfrac{R}{r_0}$	(6.23)
	$\sim\mu b^2$	(6.24)
Critical crack length[c]	$L=\dfrac{4\alpha E}{\pi(1-\sigma^2)p_0^2}$	(6.25)

$\hat{\boldsymbol{l}}$	unit vector ∥ line of dislocation
$\boldsymbol{b}$,b	Burgers vector[a]
U	dislocation energy per unit length
μ	shear modulus
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



[a]The Burgers vector is a Bravais lattice vector characterising the total relative slip were the dislocation to travel throughout the crystal.
[b]Or "tension." The energy per unit length of an edge dislocation is also $\sim\mu b^2$.
[c]For 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)
	$b(\cos\beta_1-\cos\beta_2)=k\lambda$	(6.27)
	$c(\cos\gamma_1-\cos\gamma_2)=l\lambda$	(6.28)
Bragg's law[a]	$2\boldsymbol{k}_{\text{in}}.\boldsymbol{G}+\lvert\boldsymbol{G}\rvert^2=0$	(6.29)
Atomic form factor	$f(\boldsymbol{G})=\int_{\text{vol}}\mathrm{e}^{-\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{r}}\rho(\boldsymbol{r})\,\mathrm{d}^3r$	(6.30)
Structure factor[b]	$S(\boldsymbol{G})=\sum_{j=1}^{n}f_j(\boldsymbol{G})\mathrm{e}^{-\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{d}_j}$	(6.31)
Scattered intensity[c]	$I(\boldsymbol{K})\propto N^2\lvert S(\boldsymbol{K})\rvert^2$	(6.32)
Debye–Waller factor[d]	$I_T=I_0\exp\left[-\frac{1}{3}\langle u^2\rangle\lvert\boldsymbol{G}\rvert^2\right]$	(6.33)

a,b,c	lattice parameters
$\alpha_1,\beta_1,\gamma_1$	angles between lattice base vectors and input wavevector
$\alpha_2,\beta_2,\gamma_2$	angles between lattice base vectors and output wavevector
h,k,l	integers (Laue indices)
λ	wavelength
$\boldsymbol{k}_{\text{in}}$	input wavevector
$\boldsymbol{G}$	reciprocal lattice vector
$f(\boldsymbol{G})$	atomic form factor
$\boldsymbol{r}$	position vector
$\rho(\boldsymbol{r})$	atomic electron density
$S(\boldsymbol{G})$	structure factor
n	number of atoms in basis
$\boldsymbol{d}_j$	position of jth atom within basis
$\boldsymbol{K}$	change in wavevector ($=\boldsymbol{k}_{\text{out}}-\boldsymbol{k}_{\text{in}}$)
$I(\boldsymbol{K})$	scattered intensity
N	number of lattice points illuminated
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

[a]Alternatively, see Equation (8.32).
[b]The summation is over the atoms in the basis, i.e., the atomic motif repeating with the Bravais lattice.
[c]The Bragg condition makes $\boldsymbol{K}$ a reciprocal lattice vector, with $\lvert k_{\text{in}}\rvert=\lvert k_{\text{out}}\rvert$.
[d]Effect of thermal vibrations.