## 6.3 Crystalline structure

### Bravais lattices

| | | | | |
|---|---|---|---|---|
| Volume of primitive cell | $V = (\boldsymbol{a}\times\boldsymbol{b})\cdot\boldsymbol{c}$ | (6.1) | $\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}$<br>$V$ | primitive base vectors<br>volume of primitive cell |
| Reciprocal primitive base vectors[a] | $\boldsymbol{a}^* = 2\pi\boldsymbol{b}\times\boldsymbol{c}/[(\boldsymbol{a}\times\boldsymbol{b})\cdot\boldsymbol{c}]$<br>$\boldsymbol{b}^* = 2\pi\boldsymbol{c}\times\boldsymbol{a}/[(\boldsymbol{a}\times\boldsymbol{b})\cdot\boldsymbol{c}]$<br>$\boldsymbol{c}^* = 2\pi\boldsymbol{a}\times\boldsymbol{b}/[(\boldsymbol{a}\times\boldsymbol{b})\cdot\boldsymbol{c}]$<br>$\boldsymbol{a}\cdot\boldsymbol{a}^* = \boldsymbol{b}\cdot\boldsymbol{b}^* = \boldsymbol{c}\cdot\boldsymbol{c}^* = 2\pi$<br>$\boldsymbol{a}\cdot\boldsymbol{b}^* = \boldsymbol{a}\cdot\boldsymbol{c}^* = 0$ (etc.) | (6.2)<br>(6.3)<br>(6.4)<br>(6.5)<br>(6.6) | $\boldsymbol{a}^*,\boldsymbol{b}^*,\boldsymbol{c}^*$ | reciprocal primitive base vectors |
| Lattice vector | $\boldsymbol{R}_{uvw} = u\boldsymbol{a} + v\boldsymbol{b} + w\boldsymbol{c}$ | (6.7) | $\boldsymbol{R}_{uvw}$<br>$u,v,w$ | lattice vector $[uvw]$<br>integers |
| Reciprocal lattice vector | $\boldsymbol{G}_{hkl} = h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$<br>$\exp(\mathbf{i}\boldsymbol{G}_{hkl}\cdot\boldsymbol{R}_{uvw}) = 1$ | (6.8)<br>(6.9) | $\boldsymbol{G}_{hkl}$<br>$\mathbf{i}$ | reciprocal lattice vector $[hkl]$<br>$\mathbf{i}^2 = -1$ |
| 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 $2\pi$ 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 $[UVTW]$ | $U = \dfrac{1}{3}(2u - v)$<br>$V = \dfrac{1}{3}(2v - u)$<br>$T = -\dfrac{1}{3}(u + v)$<br>$W = w$ | (6.13)<br>(6.14)<br>(6.15)<br>(6.16) | $U,V,T,W$<br>$u,v,w$<br>$[UVTW]$<br>$[uvw]$ | Weber indices<br>zone axis indices<br>Weber symbol<br>zone axis symbol |
| Converting $[UVTW]$ to $[uvw]$ | $u = (U - T)$<br>$v = (V - T)$<br>$w = W$ | (6.17)<br>(6.18)<br>(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] | $\boldsymbol{a}_1 = a\hat{\boldsymbol{x}}$<br>$\boldsymbol{a}_2 = a\hat{\boldsymbol{y}}$<br>$\boldsymbol{a}_3 = a\hat{\boldsymbol{z}}$ | $\boldsymbol{a}_1 = \frac{a}{2}(\hat{\boldsymbol{y}}+\hat{\boldsymbol{z}}-\hat{\boldsymbol{x}})$<br>$\boldsymbol{a}_2 = \frac{a}{2}(\hat{\boldsymbol{z}}+\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}})$<br>$\boldsymbol{a}_3 = \frac{a}{2}(\hat{\boldsymbol{x}}+\hat{\boldsymbol{y}}-\hat{\boldsymbol{z}})$ | $\boldsymbol{a}_1 = \frac{a}{2}(\hat{\boldsymbol{y}}+\hat{\boldsymbol{z}})$<br>$\boldsymbol{a}_2 = \frac{a}{2}(\hat{\boldsymbol{z}}+\hat{\boldsymbol{x}})$<br>$\boldsymbol{a}_3 = \frac{a}{2}(\hat{\boldsymbol{x}}+\hat{\boldsymbol{y}})$ |

[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]

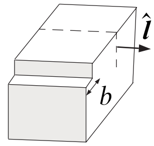
| *system* | *symmetry* | *unit cell*[b] | *lattices*[c] |
|---|---|---|---|
| triclinic | none | $a \neq b \neq c$;<br>$\alpha \neq \beta \neq \gamma \neq 90°$ | P |
| monoclinic | one diad $\parallel$ [010] | $a \neq b \neq c$;<br>$\alpha = \gamma = 90°,\ \beta \neq 90°$ | P, C |
| orthorhombic | three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

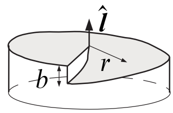
[a] The symbol "$\neq$" implies that equality is not required by the symmetry, but neither is it forbidden.
[b] The cell axes are $a$, $b$, and $c$ with $\alpha$, $\beta$, and $\gamma$ the angles between $b:c$, $c:a$, and $a:b$ respectively.
[c] The lattice types are primitive (P), body-centred (I),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

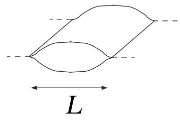
## Dislocations and cracks

| | | |
|---|---|---|
| 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 |
| $\mu$ | shear modulus |
| $R$ | outer cutoff for $r$ |
| $r_0$ | inner cutoff for $r$ |
| $L$ | critical crack length |
| $\alpha$ | surface energy per unit area |
| $E$ | Young modulus |
| $\sigma$ | 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 | $f(\boldsymbol{G})=\displaystyle\int_{\text{vol}}\mathrm{e}^{-\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{r}}\rho(\boldsymbol{r})\,\mathrm{d}^3r$ | (6.30) |
| Structure factor[b] | $S(\boldsymbol{G})=\displaystyle\sum_{j=1}^{n}f_j(\boldsymbol{G})\mathrm{e}^{-\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{d}_j}$ | (6.31) |
| Scattered intensity[c] | $I(\boldsymbol{K})\propto N^2\lvert S(\boldsymbol{K})\rvert^2$ | (6.32) |
| Debye–Waller factor[d] | $I_T=I_0\exp\left[-\dfrac{1}{3}\langle u^2\rangle\lvert\boldsymbol{G}\rvert^2\right]$ | (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) |
| $\lambda$ | 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 $j$th 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.