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The Simplicity of Miller–Bravais Indexing

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The most important crystallographic formulae for hexagonal crystals are tabulated for both orthohexagonal and Miller–Bravais indexing. It is shown that the Miller–Bravais formulae can be expressed as simply as those of the orthohexagonal system while still retaining the virtues of symmetry and a primitive unit cell.

This note sets out to link two recent papers dealing with the indexing of hexagonal crystals (Otte & Crocker, 1965; Frank, 1965) and to give a table of important crystallographic formulae in various systems of indexing.

Otte & Crocker (1965) describe in detail the indexing of hexagonal crystals according to the orthohexagonal, the three-axis hexagonal, and the four-axis hexagonal (using Miller–Bravais indices) systems. They list some important crystallographic formulae for each system and conclude that the simplicity of the formulae, as given, warrants widespread use of the orthohexagonal system. However, the argument overlooks one complication of the orthohexagonal system and some significant simplifications which can be made to the four-axis formulae. With these changes incorporated, the four-axis formulae are comparable in simplicity with those of the orthohexagonal system.

The following definitions are needed:

$d^0 = d/Q$ = identity distance along a direction **d**,
$n^0 = n/Q^*$ = interplanar spacing between planes with normal **n***,
ϱ = angle between directions $\mathbf{d}_1$, $\mathbf{d}_2$,
φ = angle between plane normals $\mathbf{n}^*_1$, $\mathbf{n}^*_2$,
η = angle between direction **d** and normal **n***,
$\gamma = c/a$ = axial ratio of hexagonal lattice.

These symbols have been chosen to agree, where possible, with those used by Otte & Crocker, but new symbols d^0 and n^0 have been introduced for identity distances and interplanar spacings. This is necessary since the orthohexagonal system is based on a non-primitive unit cell and the simple formulae quoted by Otte & Crocker for d and n do not always correspond to true identity distances or spacings in *this* system. The present definitions allow both d and d^0, and n and n^0, to be determined by specifying that:
for orthohexagonal indexing,

$$Q = \begin{cases} 2, \text{ if } p+q \text{ and } r \text{ are both even,} \\ 1, \text{ otherwise,} \end{cases}$$
$$Q^* = \begin{cases} 2, \text{ if } e+f \text{ is odd,} \\ 1, \text{ otherwise; and} \end{cases}$$

for the other systems,

$$Q = Q^* = 1 \text{ throughout.}$$

For the Miller–Bravais system, algebraic manipulation, based largely on the result that, if

$$x+y+z=0\,,$$

then

$$xy \equiv \tfrac{1}{2}(x+y)^2 - \tfrac{1}{2}x^2 - \tfrac{1}{2}y^2 = \tfrac{1}{2}(z^2 - x^2 - y^2)\,,$$

allows the formulae in Otte & Crocker's Table 2† to be simplified to those in the top part of Table 1 here. For the sake of completeness, the formulae for the three-axis hexagonal system are also included in Table 1.

As Frank (1965) has shown, Miller–Bravais indices are proportional to the components of certain four-dimensional cartesian vectors. The simple formulae can therefore be derived as a series of scalar products of such vectors and the tensorial formulae quoted by Otte & Crocker for d, n, *etc.* hold true with the metrics

$$a_{ij} = (3a^2/2) \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \lambda^2 \end{pmatrix}$$

and

$$a^{ij} = (2a^{-2}/3) \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \lambda^{-2} \end{pmatrix},$$

where $\lambda = \sqrt{\frac{2}{3}}\gamma$ is the scaling factor introduced by Frank.

The lower rows of Table 1 list some other formulae of crystallographic interest. The particularly simple forms for transforming between planes and directions in the Miller–Bravais system are worthy of note. Further, in deriving the Miller–Bravais forms for directions common to planes *etc*, where essentially the problem is to calculate a vector product, both Frank (1965) and Weber (1922) advise calculation *via* one of

† It should be noted that, in Table 2, the formula for $\cos\varrho$ in the three-index form of the four-axis system needs a factor of $\frac{1}{3}$ before $\gamma^2 w_1 w_2$, while among the four-index formulae, that for $\cos\varphi$ needs a factor of $\frac{3}{4}$ before $\gamma^{-2} l_1 l_2$ and that for $\cos\eta$ a factor of $\frac{3}{2}$ before lw.

Table 1. *Crystallographic formulae for hexagonal lattices*

	Orthohexagonal indexing $\gamma=c/a$	Miller–Bravais indexing $\lambda=\sqrt{(\frac{2}{3})}c/a$	Three-axis hexagonal indexing $\gamma=c/a$
Direction, **d**	$[pqr]$	$[uvtw]$	$[UVW]$
$(d/a)^2=(Qd^0/a)^2$	$p^2+3q^2+\gamma^2r^2$	$(\frac{3}{2})(u^2+v^2+t^2+\lambda^2w^2)$	$U^2+V^2-UV+\gamma^2W^2$
$Q=2$ when	$p+q$ and r, both even	never	never
$(d_1d_2/a^2)\cos\varrho$	$p_1p_2+3q_1q_2+\gamma^2r_1r_2$	$(\frac{3}{2})(u_1u_2+v_1v_2+t_1t_2+\lambda^2w_1w_2)$	$U_1U_2+V_1V_2-\frac{1}{2}(U_1V_2+U_2V_1)+\gamma^2W_1W_2$
Plane normal, **n***	(efg)	$(hkil)$	(HKL)
$(a/n)^2=(a/Q^*n^0)^2$	$e^2+f^2/3+g^2/\gamma^2$	$(\frac{3}{4})(h^2+k^2+i^2+l^2/\lambda^2)$	$(\frac{4}{3})(H^2+HK+K^2)+L^2/\gamma^2$
$Q^*=2$ when	$e+f$ is odd	never	never
$(a^2/n_1n_2)\cos\varphi$	$e_1e_2+f_1f_2/3+g_1g_2/\gamma^2$	$(\frac{4}{3})(h_1h_2+k_1k_2+i_1i_2+l_1l_2/\lambda^2)$	$(\frac{4}{3})(H_1H_2+K_1K_2)+\frac{2}{3}(H_1K_2+H_2K_1)+L_1L_2/\gamma^2$
$(d/n)\cos\eta$	$ep+fq+gr$	$hu+kv+it+lw$	$HU+KV+LW$
Direction of normal **n***	$[e\ f/3\ g/\gamma^2]$	$[h\ k\ i\ l/\lambda^2]$	$[2H+K\ H+2K\ 3L/2\gamma^2]$
Plane with normal **d**	$(p\ 3q\ \gamma^2r)$	$(u\ v\ t\ \lambda^2w)$	$(2U-V\ -U+2V\ 2\gamma^2W)$
Direction common to planes with normals **n***$_1$, **n***$_2$	$[f_1g_2-f_2g_1\ g_1e_2-g_2e_1\ e_1f_2-e_2f_1]$	$[l_1(k_2-i_2)-l_2(k_1-i_1)\ l_1(i_2-h_2)-l_2(i_1-h_1)\ l_1(h_2-k_2)-l_2(h_1-k_1)\ -3(h_1k_2-h_2k_1))]$	$[K_1L_2-K_2L_1\ L_1H_2-L_2H_1\ H_1K_2-H_2K_1]$
Plane containing directions **d**$_1$, **d**$_2$	$(q_1r_2-q_2r_1\ r_1p_2-r_2p_1\ p_1q_2-p_2q_1)$	$(w_1(v_2-t_2)-w_2(v_1-t_1)\ w_1(t_2-u_2)-w_2(t_1-u_1)\ w_1(u_2-v_2)-w_2(u_1-v_1)\ -3(u_1v_2-u_2v_1))$	$(V_1W_2-V_2W_1\ W_1U_2-W_2U_1\ U_1V_2-U_2V_1)$
Direction perpendicular to **d**, and in plane with normal **n***	$[\gamma^2fr-3gq\ gp-\gamma^2er\ 3eq-fp]$	$[l(v-t)-\lambda^2w(k-i)\ l(t-u)-\lambda^2w(i-h)\ l(u-v)-\lambda^2w(h-k)\ -3(hv-ku)]$	$[L(U-2V)+2\gamma^2KW\ L(2U-V)-2\gamma^2HW\ (-U+2V)H-(2U-V)K]$
Plane with normal perpendicular to **n***, and containing **d**	$(\gamma^2fr-3gq\ 3(gp-\gamma^2er)\ \gamma^2(3eq-fp))$	$(l(v-t)-\lambda^2w(k-i)\ l(t-u)-\lambda^2w(i-h)\ l(u-v)-\lambda^2w(h-k)\ -3\lambda^2(hv-ku))$	$((H+2K)W-3LV/2\gamma^2\ -(2H+K)W+3LU/2\gamma^2\ (2H+K)V-(H+2K)U)$

the three-axis systems, but this seems an unnecessary complication since it involves transformation of indices. The problem can be tackled directly. For example, in order to find the direction $[UVTW]$ in the plane $(hkil)$ and perpendicular to $[uvtw]$, all that is necessary is to solve, for $U:V:T:W$, the three linear equations

$$hU+kV+iT+lW=0$$
$$uU+vV+tT+\lambda^2wW=0$$
$$U+V+T=0\,.$$

The result is easily shown to be as given in Table 1 and is, of course, identical with that found by working through a three-axis system.

While any assessment of the relative merits of different systems must be subjective and must depend on the particular application being considered, I believe it is fair to say that Table 1 shows that there is little to commend the three-axis hexagonal system and that, for the other systems,

(1) for distances and spacings, the Miller–Bravais system is simpler in that there is no confusion over Q and Q^*,

(2) for ϱ, φ, and η, there is little to choose between the formulae,

(3) for the remaining results, the essential difference is that one requires the calculation of three terms and the other four, but the Miller–Bravais system contains a simple inbuilt symmetry check.

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