Use of four-axes setting for trigonal and hexagonal crystals

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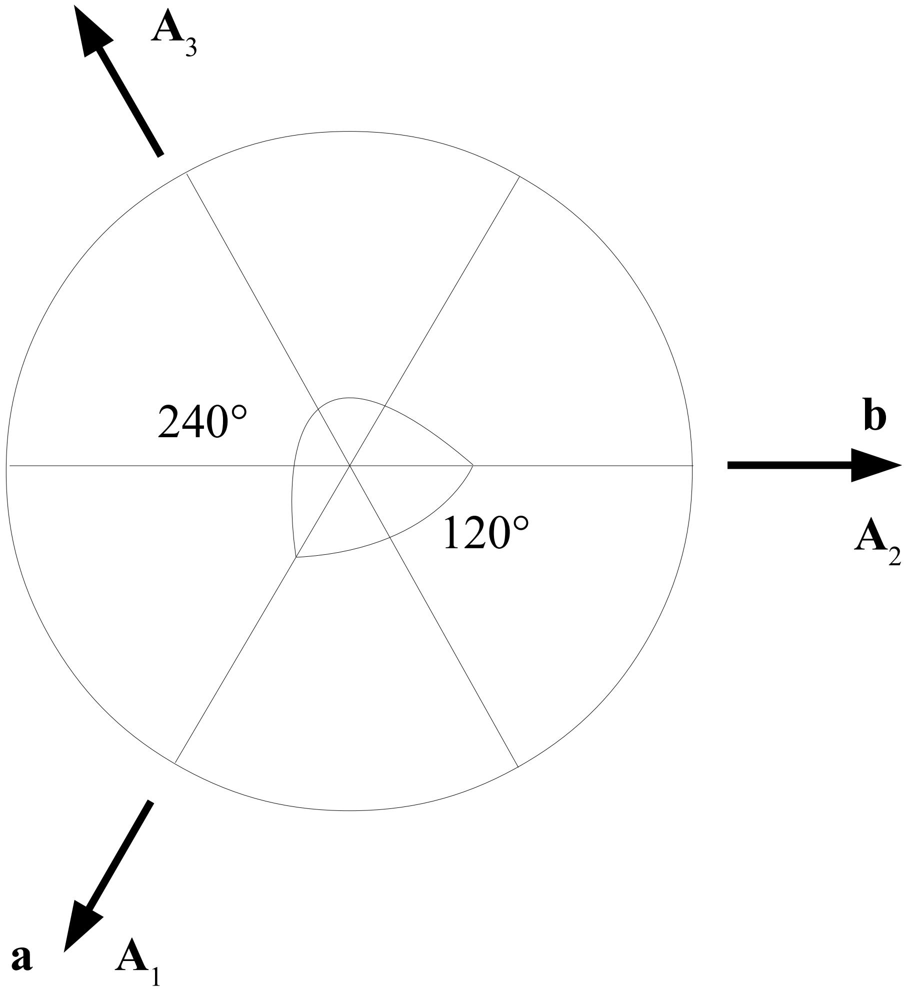
Bravais-Miller indices for hexagonal axes



$$\mathbf{abc} \rightarrow \mathbf{A}_1\mathbf{A}_2\mathbf{A}_3\mathbf{C}$$

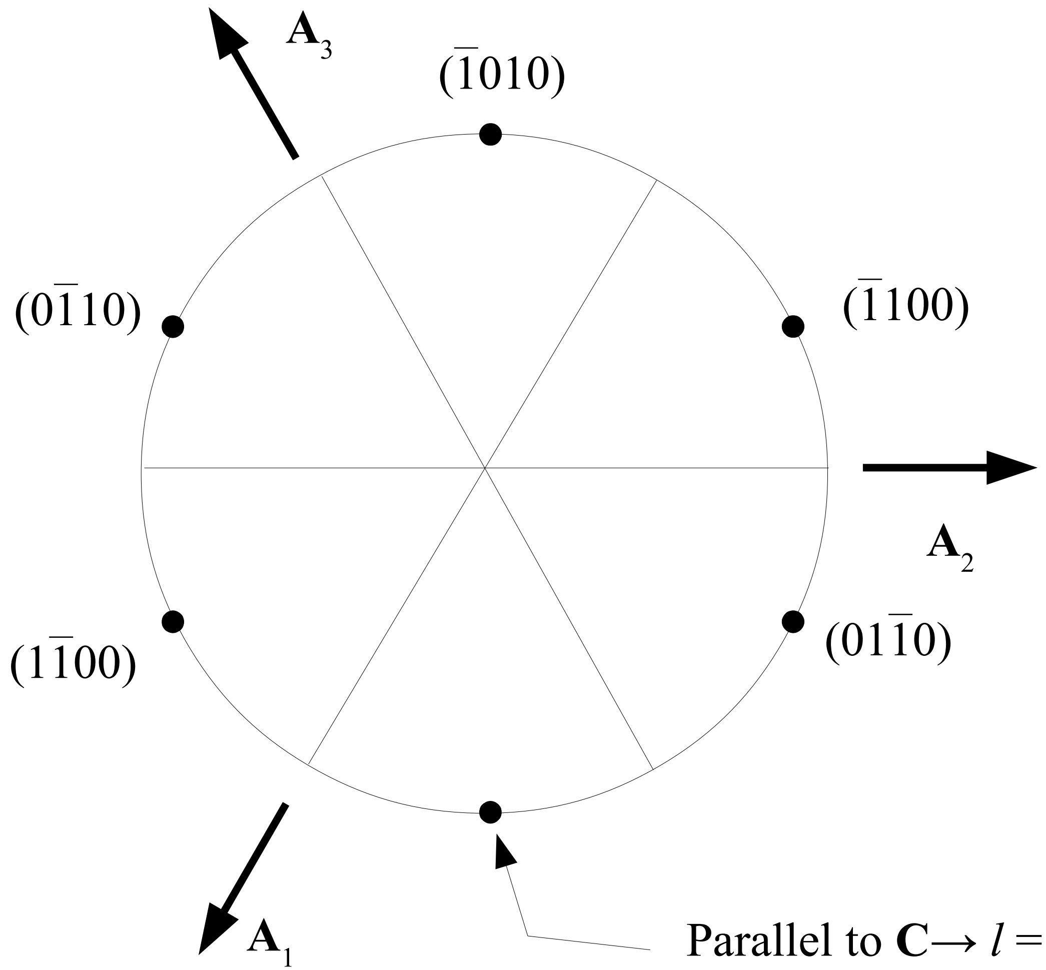
$$hkl \rightarrow hkil$$

Miller indices   Bravais-Miller indices

$$\mathbf{A}_3 = -\mathbf{A}_1-\mathbf{A}_2$$

$$i = -h-k$$

Example of Bravais-Miller indices



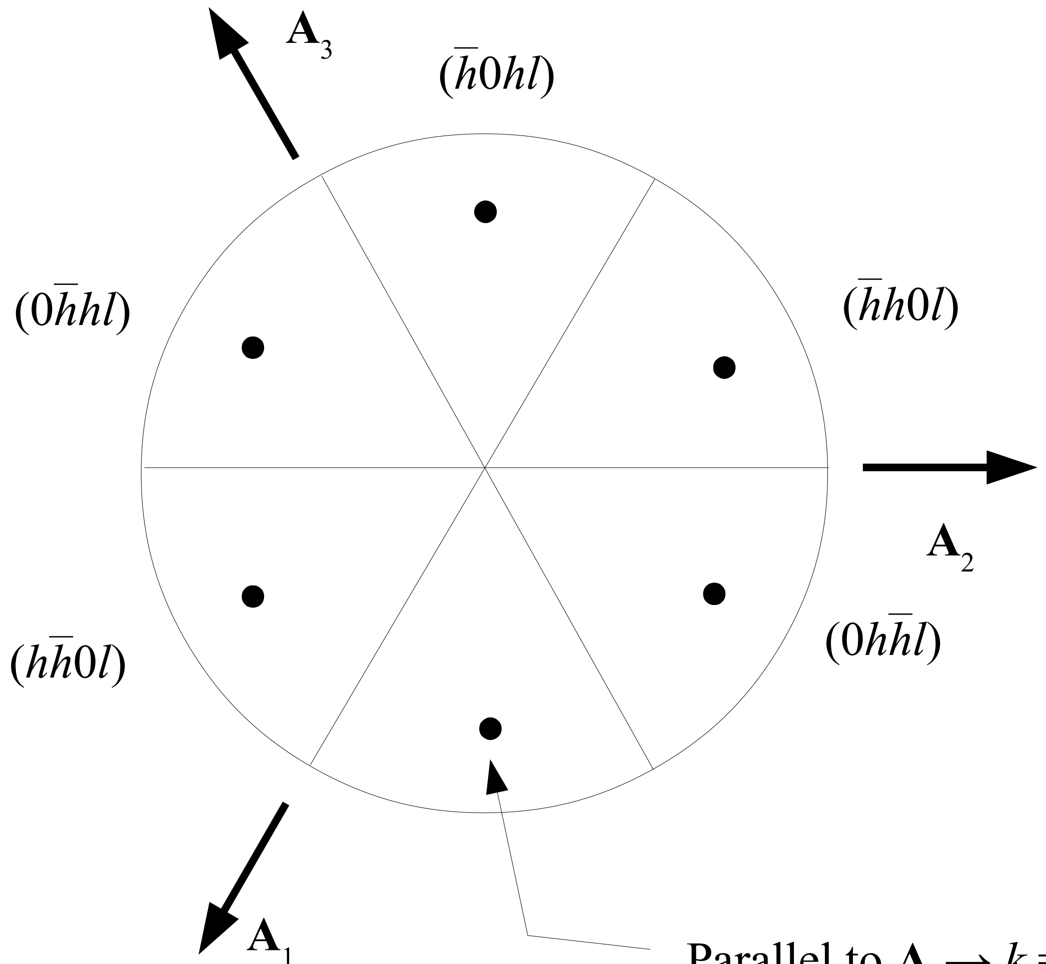
Symmetry is less evident with using Miller indices

(100)
(010)
$(\bar{1}10)$
$(\bar{1}00)$
$(0\bar{1}0)$
$(1\bar{1}0)$

Parallel to **C** $\rightarrow l = 0$
Parallel to $\mathbf{A}_2 \rightarrow k = 0$

$(hkil) \rightarrow (h0i0) \xrightarrow[i = -h-0]{} (h0\bar{h}0) \xrightarrow[\text{Remove common factor}]{} (10\bar{1}0)$

Example of Bravais-Miller indices



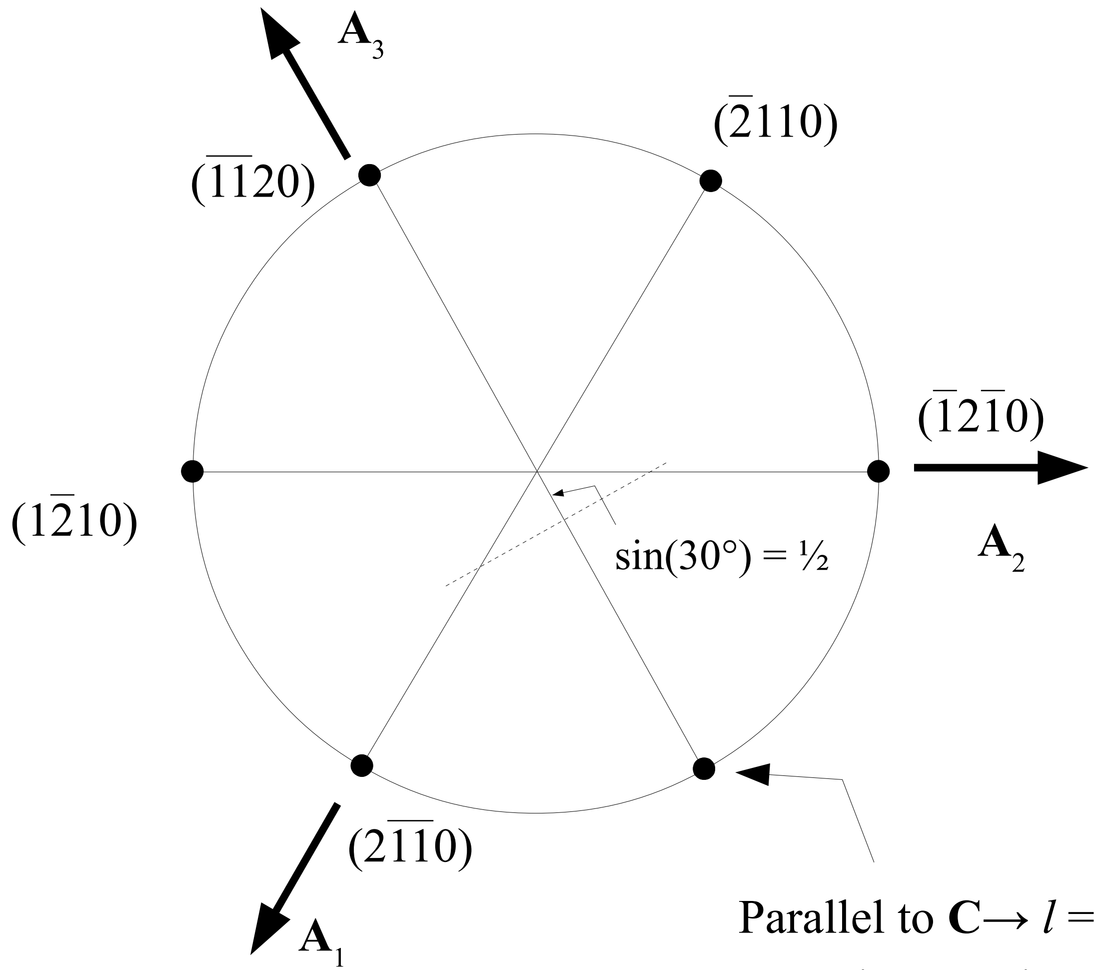
Parallel to $\mathbf{A}_2 \rightarrow k = 0$

Symmetry is less evident with using Miller indices

$(h0l)$
$(0hl)$
$(\bar{h}hl)$
$(\bar{h}0l)$
$(0\bar{h}l)$
$(h\bar{h}l)$

$$(hkil) \rightarrow (h0il) \xrightarrow[i = -h-0]{} (h0\bar{h}l)$$

Example of Bravais-Miller indices



Symmetry is less evident with using Miller indices

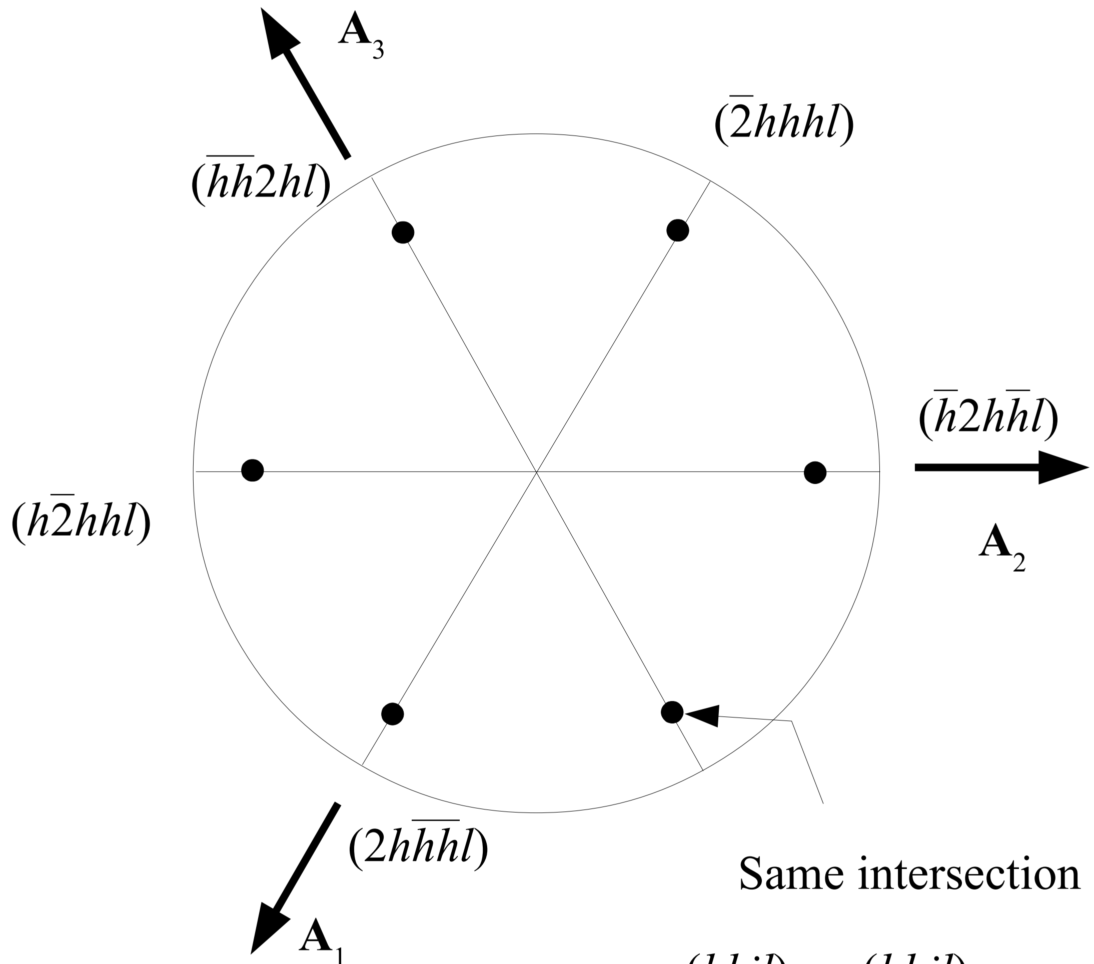
(110)
$(\bar{1}20)$
$(\bar{2}10)$
(110)
$(1\bar{2}0)$
$(2\bar{1}0)$

Parallel to **C** $\rightarrow l = 0$

Same intersection on $\mathbf{A}_1$ and $\mathbf{A}_2 \rightarrow k = h$

$$(hkil) \rightarrow (hhi0) \xrightarrow{i = -h-h} (hh\bar{2}h0) \xrightarrow{\text{Remove common factor}} (11\bar{2}0)$$

Example of Bravais-Miller indices



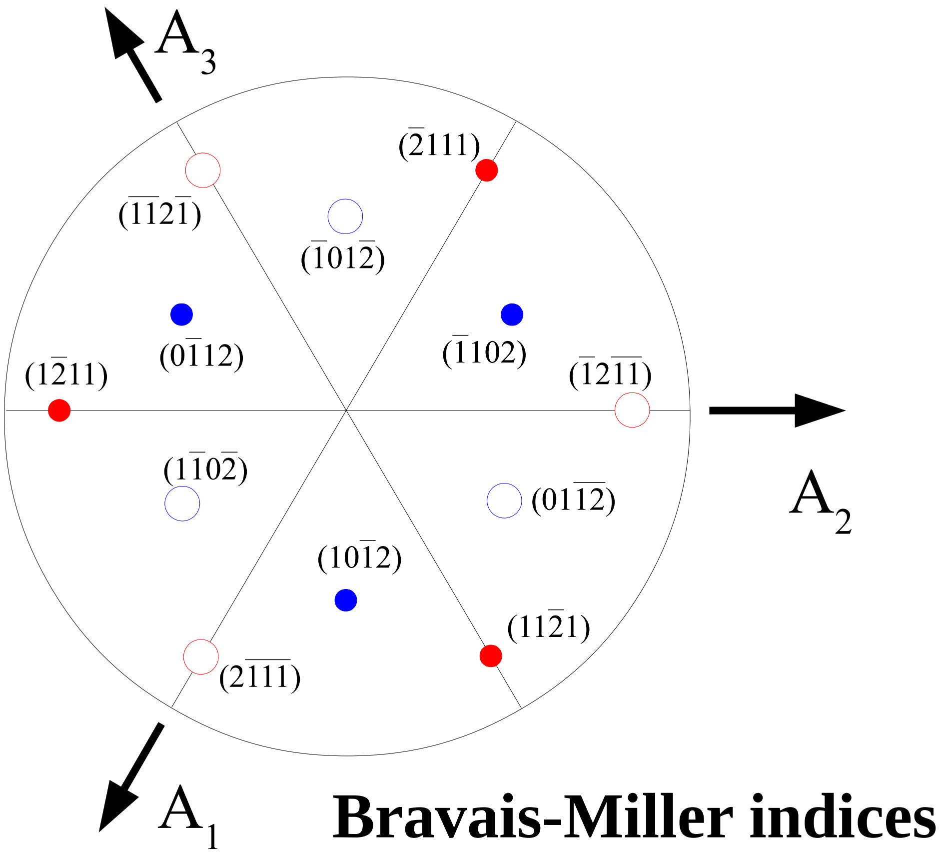
Symmetry is less evident with using Miller indices

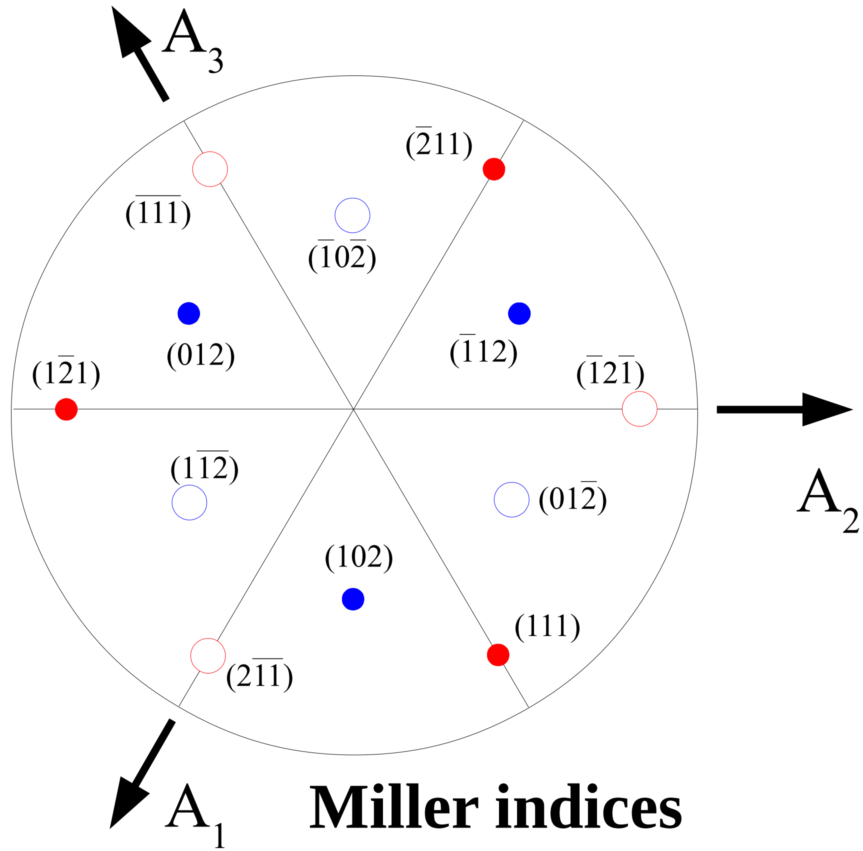
(hhl)
$(\bar{h}2hl)$
$(\bar{2}hhl)$
$(\bar{h}\bar{h}l)$
$(h\bar{2}hl)$
$(2h\bar{h}l)$

Same intersection on $\mathbf{A}_1$ and $\mathbf{A}_2 \rightarrow k = h$

$$(hkil) \rightarrow (hhil) \xrightarrow[i = -h-h]{} (hh\bar{2}hl)$$

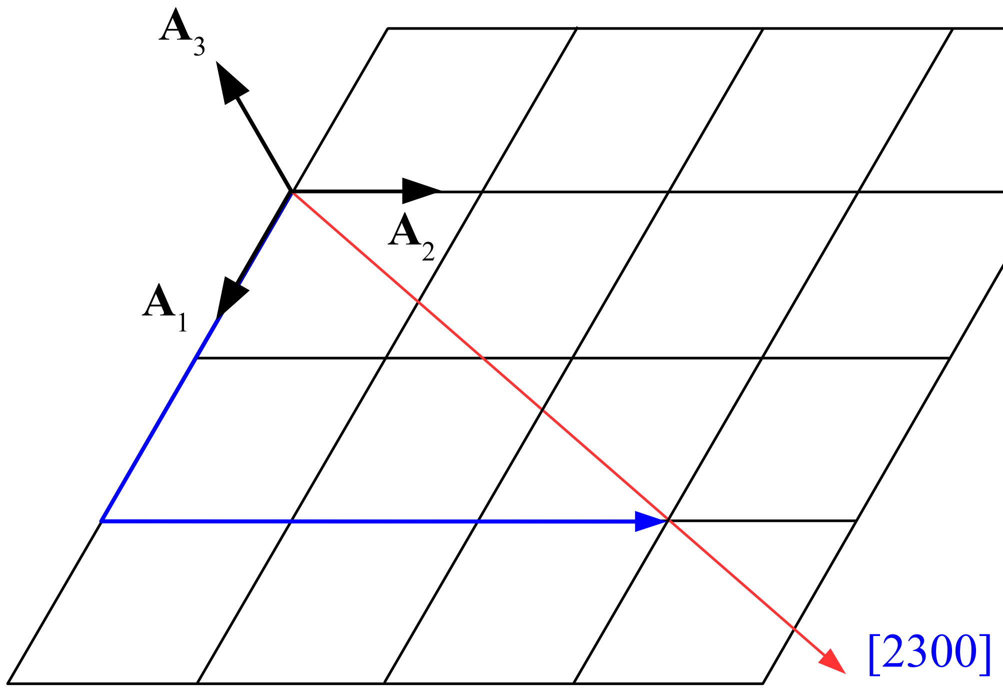
Comparison of Bravais-Miller and Miller indices



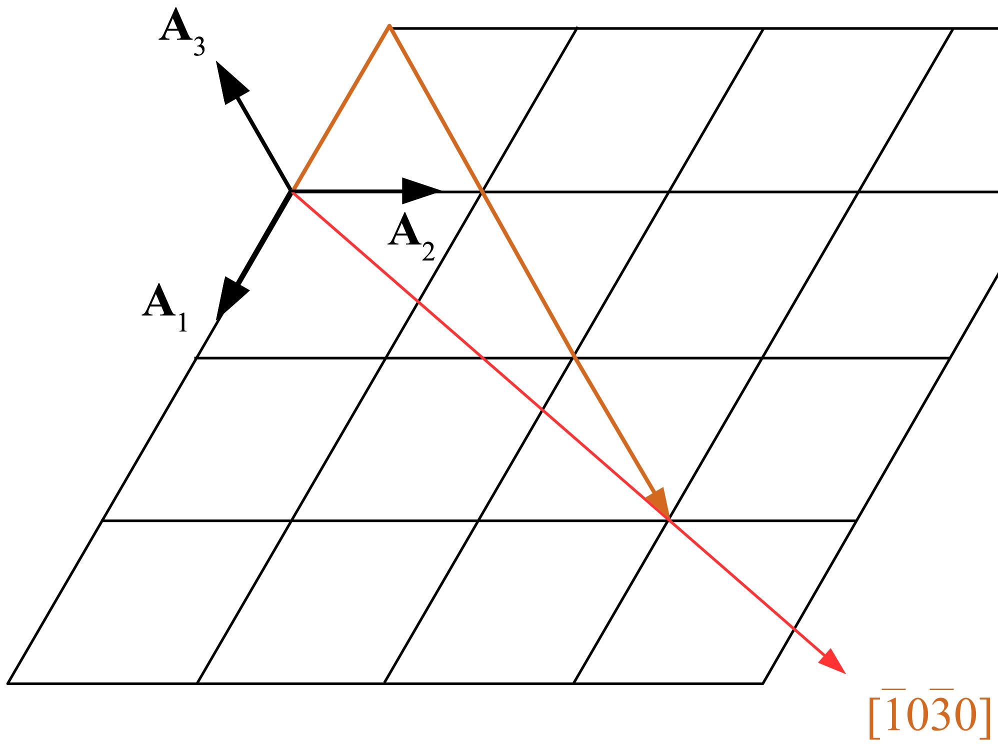


Whether we use Miller or Bravais-Miller indices, the indexing of the plane (face) is unique and unambiguous

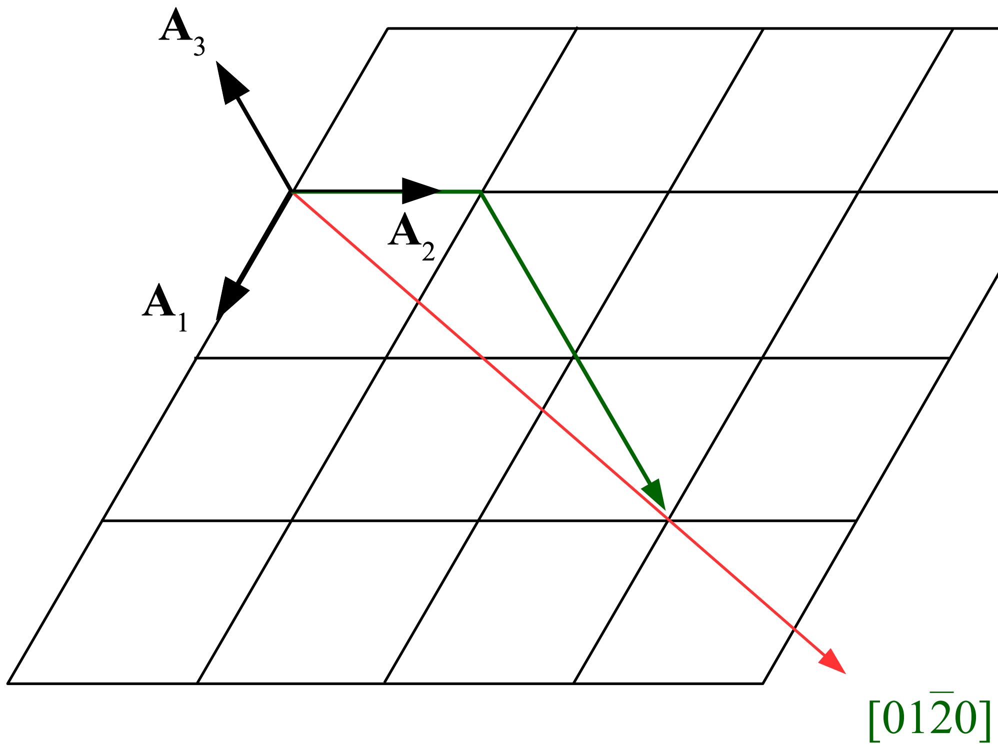
Direction indices with respect to four axes



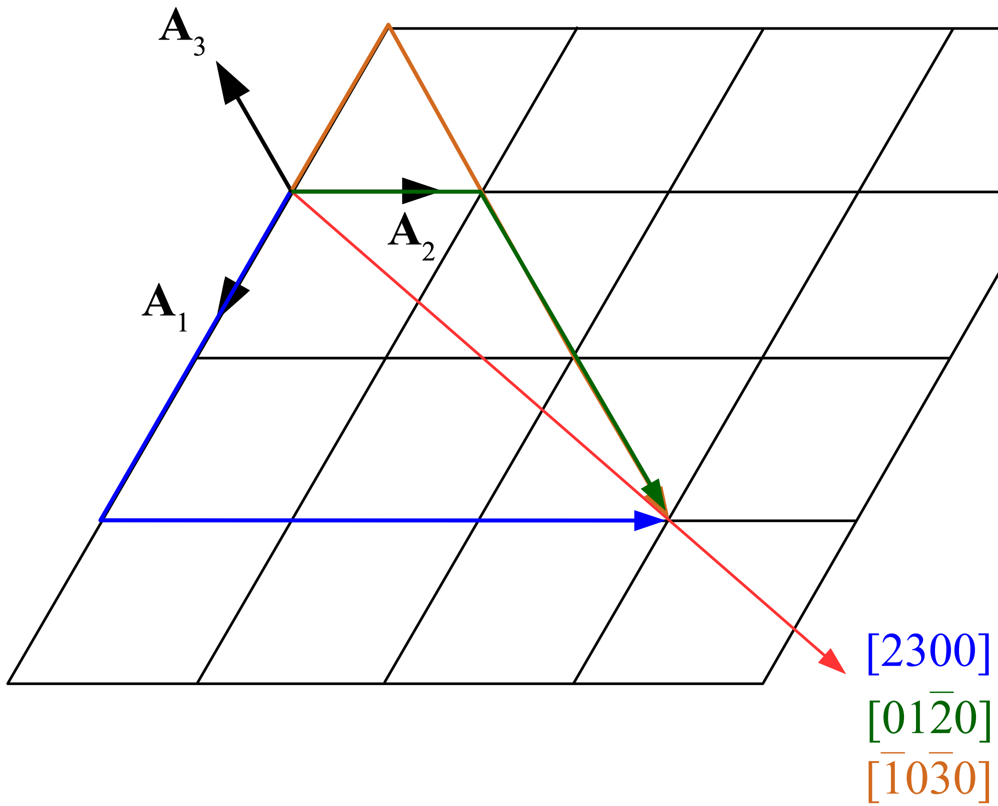
Direction indices with respect to four axes



Direction indices with respect to four axes

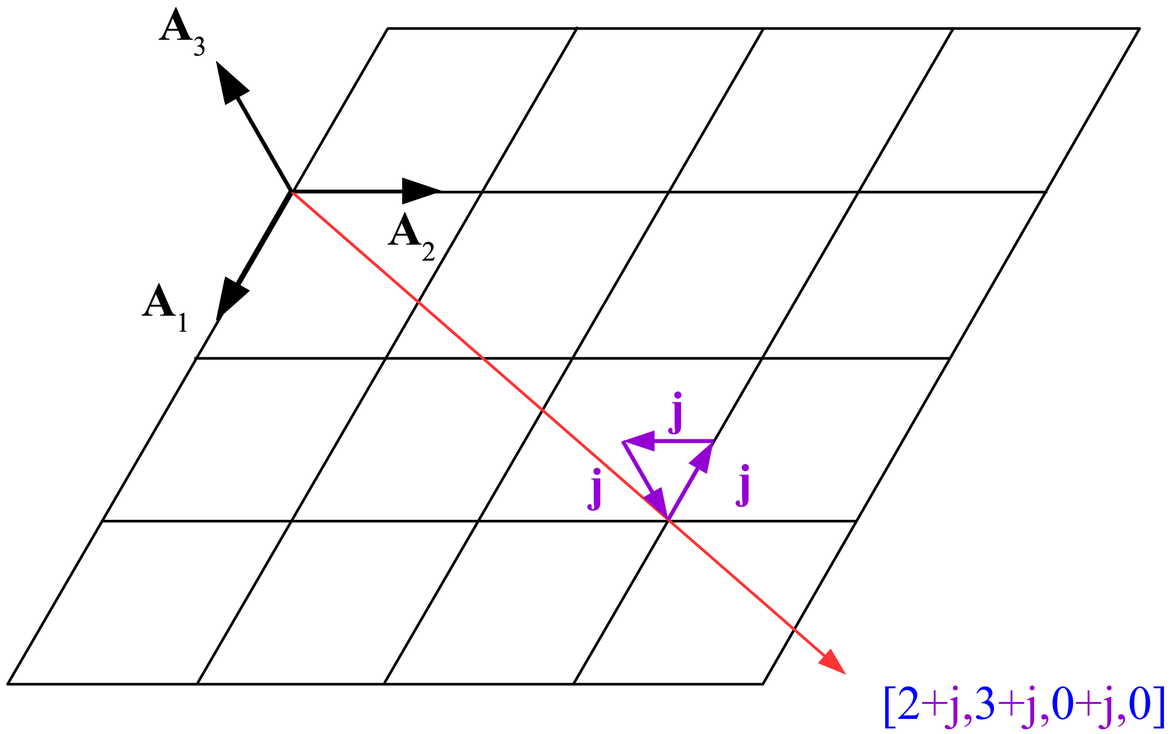


Direction indices with respect to four axes



The use of four axes makes the indexing of a direction no longer unique and unambiguous

Direction indices with respect to four axes



The use of four axes makes the indexing of a direction no longer unique and unambiguous

Weber indices: a bad idea to make indexing unique again

$$(u+j)+(v+j)+j = 0 \quad \rightarrow j = -(u+v)/3$$

$$[u-(u+v)/3, v-(u+v)/3, -(u+v)/3, w] = [(2u-v)/3, (2v-u)/3, -(u+v)/3, w]$$

$$U = (2u-v)/3$$
$$V = (2v-u)/3$$
$$T = -(u+v)/3$$
$$W = w$$

$$2U+V = (4u-2v)/3 + (2v-u)/3 = u$$

$$U+2V = (2u-v)/3 + (4v-2u)/3 = v$$

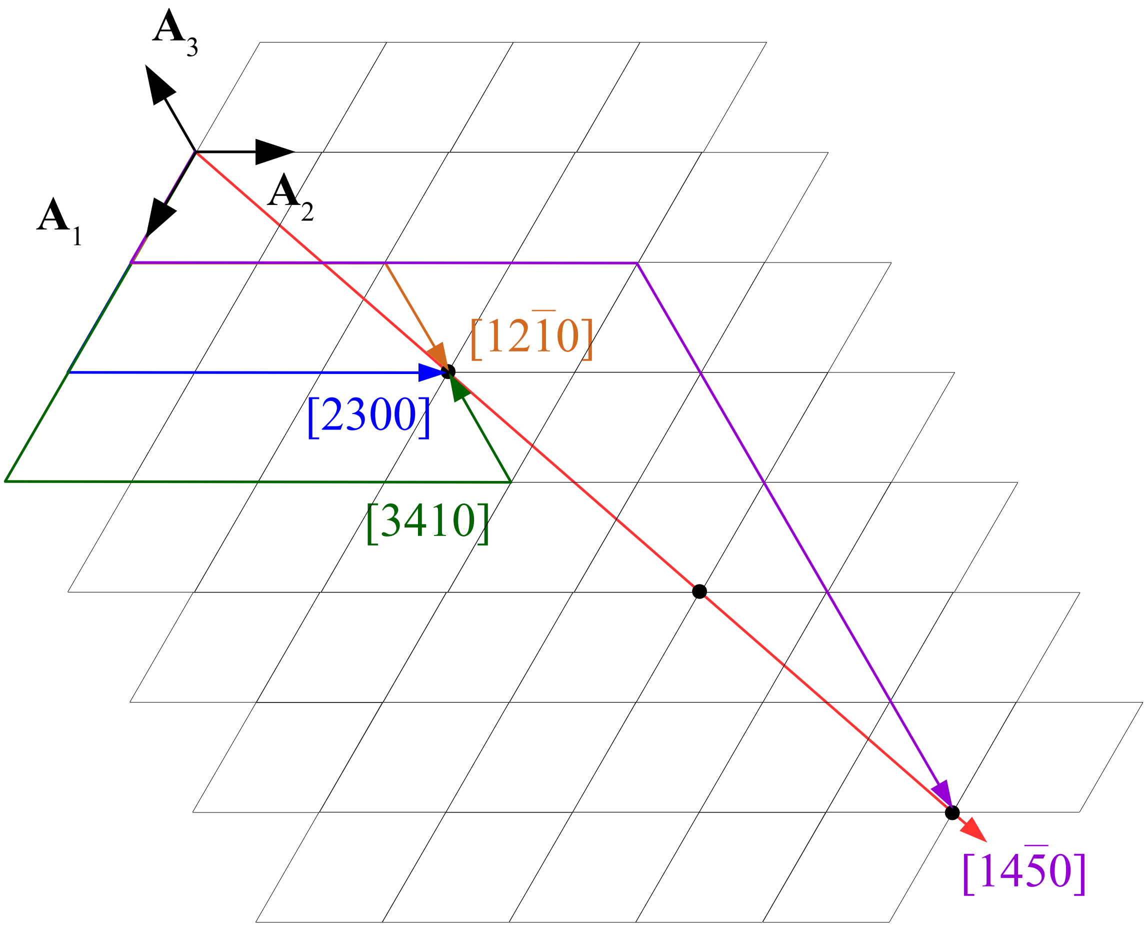
$$T = -(u+v)/3 = -(2U+V)/3-(U+2V)/3 = -(3U+3V)/3 = -U-V$$

Looks like $i = -h-k$!

Unfortunately, two problems are hidden in Weber indices

First problem: indices unduly made integer

[2300] → [3410], [$1 2 \bar{1} 0$], [$1/3, 4/3, \bar{5}/3, 0$], changed to [$1 4 \bar{5} 0$]



Second problem: mixed indexing in dual spaces

Expression of a reciprocal lattice direction in direct space and vice-versa

$$u\mathbf{a} + v\mathbf{b} + w\mathbf{c} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$$

$$(\mathbf{abc}|uvw) = (\mathbf{a}^*\mathbf{b}^*\mathbf{c}^*|hkl)$$

$$|\mathbf{abc})(\mathbf{abc}|uvw) = |\mathbf{abc})(\mathbf{a}^*\mathbf{b}^*\mathbf{c}^*|hkl)$$

$$(\mathbf{abc}| = \mathbf{B} = \begin{pmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{pmatrix}; \quad |\mathbf{abc}) = \tilde{\mathbf{B}} = \begin{pmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{pmatrix}$$

$$(\mathbf{a}^*\mathbf{b}^*\mathbf{c}^*| = \mathbf{B}^* = \begin{pmatrix} a_1^* & b_1^* & c_1^* \\ a_2^* & b_2^* & c_2^* \\ a_3^* & b_3^* & c_3^* \end{pmatrix}; \quad |\mathbf{a}^*\mathbf{b}^*\mathbf{c}^*) = \tilde{\mathbf{B}}^* = \begin{pmatrix} a_1^* & a_2^* & a_3^* \\ b_1^* & b_2^* & b_3^* \\ c_1^* & c_2^* & c_3^* \end{pmatrix}$$

$$|\mathbf{abc})(\mathbf{abc}| = \tilde{\mathbf{B}}\mathbf{B} = \mathbf{G}$$

$$|\mathbf{abc})(\mathbf{a}^*\mathbf{b}^*\mathbf{c}^*| = \tilde{\mathbf{B}}\mathbf{B}^* = \begin{pmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{pmatrix}\begin{pmatrix} a_1^* & b_1^* & c_1^* \\ a_2^* & b_2^* & c_2^* \\ a_3^* & b_3^* & c_3^* \end{pmatrix} =$$

$$= \begin{pmatrix} a_1 \cdot a_1^* + a_2 \cdot a_2^* + a_3 \cdot a_3^* & a_1 \cdot b_1^* + a_2 \cdot b_2^* + a_3 \cdot b_3^* & a_1 \cdot c_1^* + a_2 \cdot c_2^* + a_3 \cdot c_3^* \\ a_1 \cdot b_1^* + a_2 \cdot b_2^* + a_3 \cdot b_3^* & b_1 \cdot b_1^* + b_2 \cdot b_2^* + b_3 \cdot b_3^* & b_1 \cdot c_1^* + b_2 \cdot c_2^* + b_3 \cdot c_3^* \\ a_1 \cdot c_1^* + a_2 \cdot c_2^* + a_3 \cdot c_3^* & c_1 \cdot b_1^* + c_2 \cdot b_2^* + c_3 \cdot b_3^* & c_1 \cdot c_1^* + c_2 \cdot c_2^* + c_3 \cdot c_3^* \end{pmatrix} = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 3 \end{pmatrix} = 3\mathbf{I}$$

$$|uvw) = 3\mathbf{G}^*|hkl) \qquad |hkl) = \mathbf{G}|uvw)/3$$

Second problem: mixed indexing in dual spaces (2)

Expression of a reciprocal lattice direction in direct space and vice-versa with respect to hexagonal axes:

$a = b$, $\alpha = \beta = 90°$; $\gamma = 120°$;

$a^* = b^* = 2/3^{½}a$; $c^* = 1/c$; $\alpha^* = \beta^* = 90°$; $\gamma^* = 60°$

$$\mathbf{G} = \begin{pmatrix} a^2 & -a^2/2 & 0 \\ -a^2/2 & a^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}; \mathbf{G}^* = \begin{pmatrix} 4/3a^2 & 2/3a^2 & 0 \\ 2/3a^2 & 4/3a^2 & 0 \\ 0 & 0 & 1/c^2 \end{pmatrix}$$

$$|uvw) = 3\begin{pmatrix} 4/3a^2 & 2/3a^2 & 0 \\ 2/3a^2 & 4/3a^2 & 0 \\ 0 & 0 & 1/c^2 \end{pmatrix}|hkl) \rightarrow |uvw) = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 3a^2/2c^2 \end{pmatrix}|hkl)$$

$$|hkl) = \frac{1}{3}\begin{pmatrix} a^2 & -a^2/2 & 0 \\ -a^2/2 & a^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}|uvw) \rightarrow |hkl) = \frac{1}{3}\begin{pmatrix} 2 & \bar{1} & 0 \\ \bar{1} & 2 & 0 \\ 0 & 0 & 2c^2/a^2 \end{pmatrix}|uvw)$$

Second problem: mixed indexing in dual spaces (3)

$$|uvw) = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & {}^{3a^2}\!/\!_{2c^2} \end{pmatrix} |hkl) \quad \rightarrow u = 2h+k,\ v = h+2k,\ w = 3la^2/2c^2$$

$$|hkl) = \frac{1}{3}\begin{pmatrix} 2 & \bar{1} & 0 \\ \bar{1} & 2 & 0 \\ 0 & 0 & {}^{2c^2}\!/\!_{a^2} \end{pmatrix} |uvw) \quad \rightarrow h = (2u\text{-}v)/3 \text{ and } k = (-u+2v)/3,\ l = 2wc^2/3a^2$$

Cfr. $2U+V = (4u\text{-}2v)/3 + (2v\text{-}u)/3 = u;\ U+2V = (2u\text{-}v)/3 + (4v\text{-}2u)/3 = v$

$U = h$ and $V = k$ BUT $w \neq l$ (and thus $W \neq l$) unless $l = 0$ or $c = a(3/2)^{½}$

Weber indices: a bad idea to make indexing unique again

Miller indices	**Bravais-Miller indices**	**Perpendicular direction**		
		Direct space	Reciprocal space	Weber indices
(001)	(0001)	[001]	[001]*	[0001]
$(hk0)$	$(hki0)$	$[2h+k,h+2k,0]$	$[hk0]$*	$[hki0]$
Ex. (100)	$(10\bar{1}0)$	[210]	[100]*	$[10\bar{1}0]$
Ex. $(2\bar{1}0)$	$(2\bar{1}\bar{1}0)$	[100]	$[2\bar{1}0]$*	$[2\bar{1}\bar{1}0]$
(hkl)	$(hkil)$	---	$[hkl]$*	$[hkiw]$