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New method for determining hexagonal direction indices and their relationship to crystallographic directions

D. C. Hofmann and V. A. Lubarda*

Department of Mechanical and Aerospace Engineering, University of California, San Diego, La Jolla, CA 92093-0411,USA. Correspondence e-mail: vlubarda@ucsd.edu

A new method for determining the hexagonal direction indices is introduced, which is more practical than other commonly used methods. The relationship between the crystallographic directions and hexagonal direction indices for face-centered cubic crystals is derived. Different sets of hexagonal indices for equivalent crystallographic directions are discussed.

1. Introduction

The hexagonal direction indices are well known and routinely applied to designate the crystallographic directions in hexagonal close packed (h.c.p.) crystals. They can also be used to designate the crystallographic directions in face-centered cubic (f.c.c.) crystals, although these are commonly, and more conveniently, labeled by using the standard crystallographic direction indices (*e.g.* Askeland, 1994; Smith, 1999). In this paper, we describe a new method to determine the hexagonal indices in f.c.c. and h.c.p. crystals, which is more practical and easier to apply than other commonly used methods. We then elaborate on the relationship between the hexagonal direction indices and the crystallographic directions for f.c.c. crystals, and derive two different but related four-index notations for equivalent crystallographic directions. The results may be of interest in the geometric analysis of the faults in stacking sequences, diffraction patterns, and related problems in the theory of crystalline lattices and their defects (Barrett & Massalski, 1980; McKie & McKie, 1986; Kelly *et al.*, 2000).

2. Geometric preliminaries

Consider a unit cell of an f.c.c. crystal with the lattice parameter a. The stacking sequence $ABC\ldots$ of the close-packed (111) planes of interplanar spacing $a/(3^{1/2})$ is shown in Fig. 1. The unit vectors along the edges of the cubic cell are $\mathbf{i}_1$, $\mathbf{i}_2$ and $\mathbf{i}_3$. The crystallographic direction indices for a lattice direction parallel to the vector $\mathbf{x} = x_1\mathbf{i}_1 + x_2\mathbf{i}_2 + x_3\mathbf{i}_3$ are the set of integers $[m_1\, m_2\, m_3]$, where

$$x_1 = m_1 a\,, \quad x_2 = m_2 a\,, \quad x_3 = m_3 a\,. \tag{1}$$

The hexagonal atomic packing within the (111) plane through the origin at one of the atoms, A, is shown in Fig. 2. The directions along the cell edges project in the (111) plane along the unit directions $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$. These vectors are at the angle $2\pi/3$, so that

$$\mathbf{e}_i \cdot \mathbf{e}_j = \begin{cases} 1 & \text{if } i = j, \\ -1/2 & \text{if } i \neq j. \end{cases} \tag{2}$$

The projected axes ξ_1, ξ_2 and ξ_3 do not pass through the first-nearest neighbors to A, but through the second-nearest neighbors. Denoting the unit vector normal to the octahedral (111) plane by $\mathbf{n} = (\mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3)/(3^{1/2})$, the direction vector $\mathbf{x}$ can be decomposed into the component $\boldsymbol{\xi}$ within the (111) plane, and the orthogonal component $(\mathbf{x} \cdot \mathbf{n})\,\mathbf{n}$, such that

$$\mathbf{x} = \boldsymbol{\xi} + \frac{1}{3^{1/2}}(x_1 + x_2 + x_3)\mathbf{n}. \tag{3}$$

If a_1, a_2 and a_3 are the components of $\boldsymbol{\xi}$ along the edges of the cubic cell,

$$\boldsymbol{\xi} = a_1\mathbf{i}_1 + a_2\mathbf{i}_2 + a_3\mathbf{i}_3, \tag{4}$$

it readily follows that

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \frac{1}{3}\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}, \tag{5}$$

and

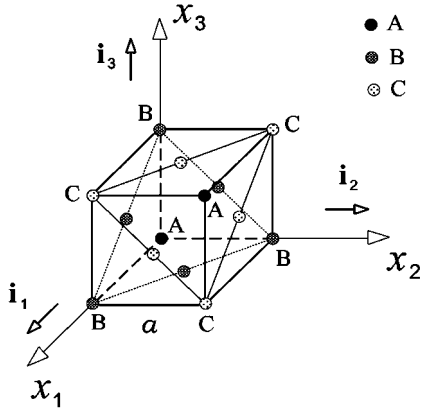

Figure 1
A unit cell of an f.c.c. crystal with the lattice parameter a. The $ABC\ldots$ stacking sequence of close-packed (111) planes is indicated.

$$\begin{bmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \end{bmatrix} = \frac{1}{6^{1/2}} \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} \cdot \begin{bmatrix} \mathbf{i}_1 \\ \mathbf{i}_2 \\ \mathbf{i}_3 \end{bmatrix}. \tag{6}$$

The constraint conditions are

$$a_1 + a_2 + a_3 = 0, \quad \mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3 = 0. \tag{7}$$

Note that the coefficient $1/(6^{1/2})$ in equation (6) appears in crystalline plasticity as the Schmid factor in f.c.c. crystals for uniaxial loading along the [001] direction. Indeed, the product $(\mathbf{n} \cdot \mathbf{i}_3)(\mathbf{m} \cdot \mathbf{i}_3)$, where $\mathbf{m}$ is the vector in the close-packed direction $[0\bar{1}1]$, is equal to this value.

3. New method for determining the hexagonal direction indices

The in-plane hexagonal decomposition of the vector $\boldsymbol{\xi}$ along the three axes $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$,

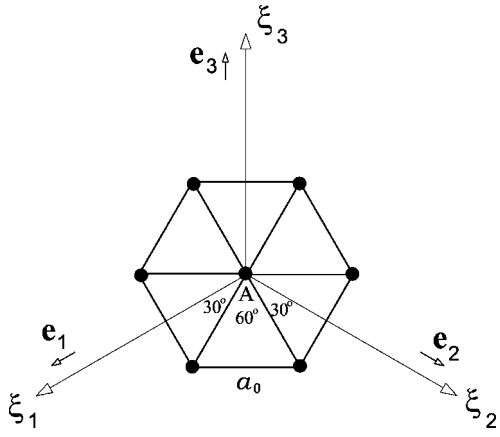

Figure 2
The hexagonal atomic arrangement within a (111) plane. The directions along the cubic cell edges project in this plane along the directions $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$. The interatomic spacing is $a_0 = a/(2^{1/2})$.

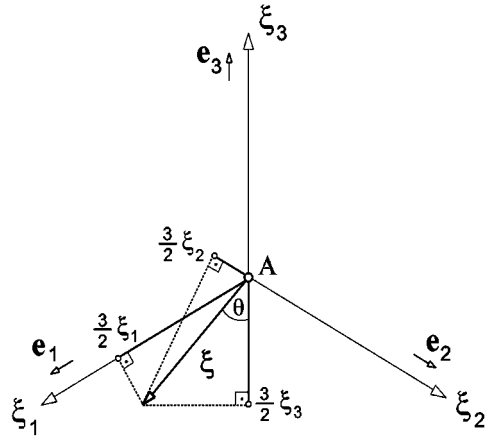

Figure 3
Geometric interpretation of the vector decomposition $\boldsymbol{\xi} = \xi_1\mathbf{e}_1 + \xi_2\mathbf{e}_2 + \xi_3\mathbf{e}_3$, subject to the constraint $\xi_1 + \xi_2 + \xi_3 = 0$. The components ξ_1, ξ_2, ξ_3 are defined by the orthogonal projections on the axes $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$, with the appropriate sign and the scaling factor of 2/3.

$$\boldsymbol{\xi} = \xi_1\mathbf{e}_1 + \xi_2\mathbf{e}_2 + \xi_3\mathbf{e}_3, \tag{8}$$

is defined such that ξ_1 is the projection of the vector component $a_1\mathbf{i}_1$ onto $\mathbf{e}_1$, and similarly for ξ_2 and ξ_3, *i.e.*

$$\xi_1 = a_1(\mathbf{i}_1 \cdot \mathbf{e}_1), \quad \xi_2 = a_2(\mathbf{i}_2 \cdot \mathbf{e}_2), \quad \xi_3 = a_3(\mathbf{i}_3 \cdot \mathbf{e}_3). \tag{9}$$

Since $\mathbf{i}_1 \cdot \mathbf{e}_1 = \mathbf{i}_2 \cdot \mathbf{e}_2 = \mathbf{i}_3 \cdot \mathbf{e}_3 = (2/3)^{1/2}$, it follows that

$$\begin{aligned} \begin{bmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{bmatrix} &= \left(\frac{2}{3}\right)^{1/2} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} \\ &= \left(\frac{2}{3}\right)^{1/2} \frac{1}{3} \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}, \end{aligned} \tag{10}$$

with the redundancy condition

$$\xi_1 + \xi_2 + \xi_3 = 0. \tag{11}$$

The following equalities are observed

$$\xi_1 = \frac{2}{3}(\boldsymbol{\xi} \cdot \mathbf{e}_1), \quad \xi_2 = \frac{2}{3}(\boldsymbol{\xi} \cdot \mathbf{e}_2), \quad \xi_3 = \frac{2}{3}(\boldsymbol{\xi} \cdot \mathbf{e}_3). \tag{12}$$

To prove the first, for example, it is enough to observe that

$$\boldsymbol{\xi} \cdot \mathbf{e}_1 = \xi_1 - \frac{1}{2}\xi_2 - \frac{1}{2}\xi_3 = \frac{3}{2}\xi_1, \tag{13}$$

because $\xi_1 + \xi_2 + \xi_3 = 0$, and similarly for $\boldsymbol{\xi} \cdot \mathbf{e}_2$ and $\boldsymbol{\xi} \cdot \mathbf{e}_3$. The formulae (12) have simple but convenient geometric interpretations, shown in Fig. 3. The orthogonal projections of the vector $\boldsymbol{\xi}$ onto the axes $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$, scaled by the factor of 2/3, define the hexagonal components ξ_1, ξ_2 and ξ_3. The simple recipe (12) is probably the most convenient method to determine the hexagonal in-plane indices, although it is surprisingly not mentioned in any of the standard texts on the subject (*e.g.* Askeland, 1994; Smith, 1999). There, instead, the vector $\boldsymbol{\xi}$ is first decomposed into the directions $\mathbf{e}_1$ and $\mathbf{e}_2$ as

$$\boldsymbol{\xi} = \hat{\xi}_1\mathbf{e}_1 + \hat{\xi}_2\mathbf{e}_2, \tag{14}$$

so that comparison with equation (8) establishes the connections

$$\hat{\xi}_1 = \xi_1 - \xi_3 = 2\xi_1 + \xi_2, \quad \hat{\xi}_2 = \xi_2 - \xi_3 = 2\xi_2 + \xi_1, \tag{15}$$

with the inverse relationships

$$\xi_1 = \frac{1}{3}\left(2\hat{\xi}_1 - \hat{\xi}_2\right), \quad \xi_2 = \frac{1}{3}\left(2\hat{\xi}_2 - \hat{\xi}_1\right). \tag{16}$$

These formulae are clearly not needed if the simple recipe (12) is used.

As an illustration, consider a unit direction ($|\boldsymbol{\xi}| = 1$) at an angle of 30° to the ξ_1 axis. From Fig. 4 it immediately follows that $(3/2)\xi_1 = \cos 30° = 3^{1/2}/2$ and $\xi_2 = 0$ (because $\boldsymbol{\xi}$ is orthogonal to ξ_2). Thus, the hexagonal indices are $[10\bar{1}0]$. On the other hand, if the classical method is used, we first need to calculate the components $\hat{\xi}_1 = 2/(3^{1/2})$ and $\hat{\xi}_2 = 1/(3^{1/2})$, then apply equations (16) to obtain $\xi_1 = 1/(3^{1/2})$ and $\xi_2 = 0$, which finally yields $[10\bar{1}0]$. The advantage of the former method is clear.

3.1. Trigonometric relations

Several useful trigonometric expressions are derived as follows. From Fig. 3 it is recognized that

$$\boldsymbol{\xi}\cdot\mathbf{e}_1=\xi\cos\Big(\frac{\pi}{3}-\theta\Big),\ \ \boldsymbol{\xi}\cdot\mathbf{e}_2=\xi\cos\Big(\frac{\pi}{3}+\theta\Big),\ \ \boldsymbol{\xi}\cdot\mathbf{e}_3=-\xi\cos\theta, \tag{17}$$

where $\xi = |\boldsymbol{\xi}|$ is the length of the vector $\boldsymbol{\xi}$. Consequently, the following relationships hold:

$$\cos\theta=-\frac{3}{2}\frac{\xi_3}{\xi},\quad \cos\Big(\frac{\pi}{3}-\theta\Big)=\frac{3}{2}\frac{\xi_1}{\xi},\quad \cos\Big(\frac{\pi}{3}+\theta\Big)=\frac{3}{2}\frac{\xi_2}{\xi}. \tag{18}$$

Similarly,

$$\sin\theta=\frac{3^{1/2}}{2}\frac{\xi_1-\xi_2}{\xi} \tag{19}$$

and

$$\sin\Big(\frac{\pi}{3}-\theta\Big)=\frac{3^{1/2}}{2}\frac{\xi_2-\xi_3}{\xi},\quad \sin\Big(\frac{\pi}{3}+\theta\Big)=\frac{3^{1/2}}{2}\frac{\xi_1-\xi_3}{\xi}. \tag{20}$$

Since $\cos 3\theta = 4\cos^3\theta - 3\cos\theta$, and $\sin 3\theta = 3\sin\theta - 4\sin^3\theta$, we also have

$$\cos 3\theta=-\frac{27}{2}\frac{\xi_1\xi_2\xi_3}{\xi^3},$$

$$\sin 3\theta=-\frac{3(3^{1/2})}{2}\frac{(\xi_1-\xi_2)(\xi_2-\xi_3)(\xi_3-\xi_1)}{\xi^3}. \tag{21}$$

The length of the vector $\boldsymbol{\xi}$ can be calculated from

$$\xi^2=\frac{3}{2}\big(\xi_1^2+\xi_2^2+\xi_3^2\big)=\frac{1}{2}\big[(\xi_1-\xi_2)^2+(\xi_2-\xi_3)^2+(\xi_3-\xi_1)^2\big]. \tag{22}$$

The identity

$$x_1-x_2=a_1-a_2=\left(\frac{3}{2}\right)^{1/2}(\xi_1-\xi_2), \tag{23}$$

with similar identities for $\xi_2 - \xi_3$ and $\xi_3 - \xi_1$ are noted, in addition to

$$\xi_1^2+\xi_2^2+\xi_3^2=-2(\xi_1\xi_2+\xi_2\xi_3+\xi_3\xi_1). \tag{24}$$

Analogous expressions in terms of the principal deviatoric stress components are well known from the theory of plasticity and geometric representation of the yield locus in the deviatoric π plane (*e.g.* Kachanov, 1971; Lubarda, 2002).

4. Transformation rules under rotation within the (111) plane

For the derivation of the relationship between the crystallographic directions and hexagonal direction indices for an f.c.c. crystal, it is useful first to derive the general formulae for the transformation of coordinates (ξ_1, ξ_2, ξ_3) under the rotation of the coordinate system within the (111) plane. If φ is the angle of counterclockwise rotation (Fig. 5), it can be readily verified that

$$\xi_1=\frac{2}{3}\xi\cos\Big(\frac{\pi}{3}-\theta\Big),\quad \xi_2=\frac{2}{3}\xi\cos\Big(\frac{\pi}{3}+\theta\Big),$$

$$\xi_3=-\frac{2}{3}\xi\cos\theta, \tag{25}$$

and

$$\xi_1^*=\frac{2}{3}\xi\cos\Big(\frac{\pi}{3}-\theta^*\Big),\quad \xi_2^*=\frac{2}{3}\xi\cos\Big(\frac{\pi}{3}+\theta^*\Big),$$

$$\xi_3^*=-\frac{2}{3}\xi\cos\theta^*. \tag{26}$$

where $\theta^* = \theta + \varphi$. By expanding the right-hand sides of equation (26) and by using equations (18), (19) and (20), it follows that

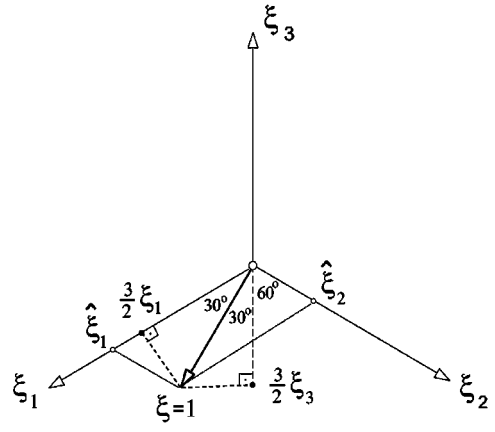

Figure 4
The unit direction at an angle of 30° relative to the ξ_1 axis. Two types of projections on the coordinate directions are shown, both of which can be used to determine the corresponding hexagonal indices.

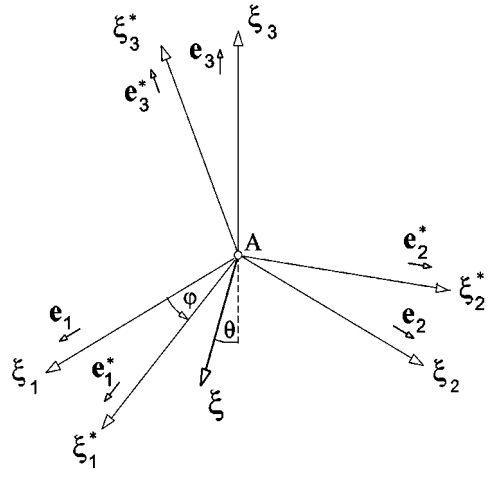

Figure 5
The coordinate system $(\xi_1^*, \xi_2^*, \xi_3^*)$ is obtained from the coordinate system (ξ_1, ξ_2, ξ_3) through a counterclockwise rotation by an angle φ. The vector $\boldsymbol{\xi}$ makes an angle θ with the negative ξ_3 axis.

$$\begin{bmatrix} \xi_1^* \\ \xi_2^* \\ \xi_3^* \end{bmatrix} = \frac{2}{3^{1/2}} \begin{pmatrix} \sin\left(\frac{\pi}{3}-\varphi\right) & 0 & -\sin\varphi \\ -\sin\varphi & \sin\left(\frac{\pi}{3}-\varphi\right) & 0 \\ 0 & -\sin\varphi & \sin\left(\frac{\pi}{3}-\varphi\right) \end{pmatrix} \cdot \begin{bmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{bmatrix}. \quad (27)$$

The same transformation relates the unit direction vectors $\mathbf{e}_1^*$, $\mathbf{e}_2^*$, $\mathbf{e}_3^*$ and $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$. A text by Sands (1982) can be consulted for further analysis of the transformation rules for vectors and tensors in crystallography.

5. Relationship between crystallographic and hexagonal direction indices

If the angle of rotation discussed in the previous section is $\varphi = \pi/6$, we obtain the hexagonal coordinates ξ_1^o, ξ_2^o, ξ_3^o within the (111) plane, which are shown in Fig. 6. The transformation rules for the unit vectors in this case reduce to

$$\begin{bmatrix} \mathbf{e}_1^o \\ \mathbf{e}_2^o \\ \mathbf{e}_3^o \end{bmatrix} = \frac{1}{3^{1/2}} \begin{pmatrix} 1 & 0 & -1 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix} \cdot \begin{bmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \end{bmatrix} = \frac{1}{2^{1/2}} \begin{pmatrix} 1 & 0 & -1 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix} \cdot \begin{bmatrix} \mathbf{i}_1 \\ \mathbf{i}_2 \\ \mathbf{i}_3 \end{bmatrix}, \quad (28)$$

and similarly for the two sets of coordinates ξ_1^0, ξ_2^0, ξ_3^0 and ξ_1, ξ_2, ξ_3. By using the expressions (10) for the components ξ_1, ξ_2, ξ_3 in terms of the rectangular components $x_1 = m_1 a$, $x_2 = m_2 a$, $x_3 = m_3 a$, it follows that

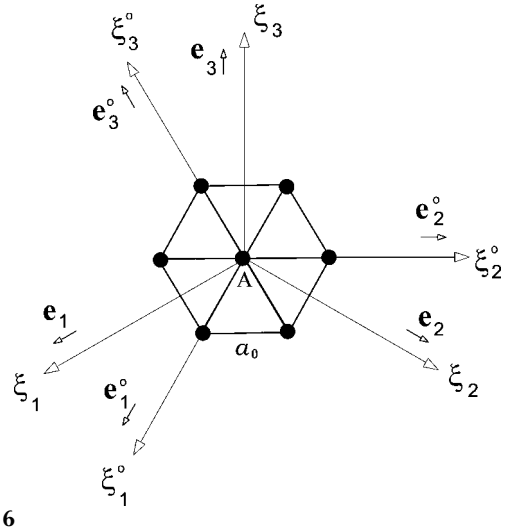

Figure 6
The coordinate system $(\xi_1^o, \xi_2^o, \xi_3^o)$ is obtained from the coordinate system (ξ_1, ξ_2, ξ_3) through a counterclockwise rotation by an angle $\pi/6$. The new axes ξ_1^o, ξ_2^o, and ξ_3^o are aligned along the close-packed atomic directions of interatomic spacing a_0.

$$\begin{bmatrix} \xi_1^o \\ \xi_2^o \\ \xi_3^o \end{bmatrix} = \frac{2a_0}{3} \begin{pmatrix} 1 & 0 & -1 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix} \cdot \begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix}, \quad (29)$$

where $a_0 = a/(2^{1/2})$ is the atomic distance between the first neighbors in the close-packed (111) plane. Thus, the projected vector $\boldsymbol{\xi}$ can be written as

$$\boldsymbol{\xi} = \frac{2}{3} a_0 \left[(m_1 - m_3)\mathbf{e}_1^o + (m_2 - m_1)\mathbf{e}_2^o + (m_3 - m_2)\mathbf{e}_3^o\right]. \quad (30)$$

On the other hand, the component of the vector $\mathbf{x}$ orthogonal to $\boldsymbol{\xi}$ is

$$\frac{1}{3^{1/2}}(x_1 + x_2 + x_3)\mathbf{n} = \frac{1}{3}(m_1 + m_2 + m_3)c_0\mathbf{n}, \quad (31)$$

where $c_0 = 3^{1/2}a = 6^{1/2}a_0$ represents the interplanar spacing between the A-type planes. This scale in the $\mathbf{n}$ direction is chosen so that the spacing between the A, B and C planes is equal to $c_0/3$. Therefore, the direction vector $\mathbf{x}$ can be decomposed as

$$\mathbf{x} = \frac{2}{3} a_0 [(m_1 - m_3)\mathbf{e}_1^o + (m_2 - m_1)\mathbf{e}_2^o + (m_3 - m_2)\mathbf{e}_3^o] + \frac{1}{3}(m_1 + m_2 + m_3)c_0\mathbf{n}. \quad (32)$$

This representation defines the hexagonal indices $[h_o\, k_o\, i_o\, l_o]$ for the considered direction, which are

$$\begin{aligned} h_o &= 2(m_1 - m_3), \quad & k_o &= 2(m_2 - m_1), \\ i_o &= 2(m_3 - m_2), \quad & l_o &= m_1 + m_2 + m_3; \end{aligned} \quad (33)$$

then

$$3\mathbf{x} = a_0(h_o\mathbf{e}_1^o + k_o\mathbf{e}_2^o + i_o\mathbf{e}_3^o) + l_o c_0\mathbf{n}. \quad (34)$$

The reduction to lowest integers usually needs to be made in equation (33). In the matrix notation, the transformation between the two sets of indices is

$$\begin{bmatrix} h_o \\ k_o \\ i_o \\ l_o \end{bmatrix} = \begin{pmatrix} 2 & 0 & -2 \\ -2 & 2 & 0 \\ 0 & -2 & 2 \\ 1 & 1 & 1 \end{pmatrix} \cdot \begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix}. \quad (35)$$

The inverse relations are

$$m_1 = h_o - k_o + 2l_o, \; m_2 = k_o - i_o + 2l_o, \; m_3 = i_o - h_o + 2l_o \quad (36)$$

with the matrix counterpart

$$\begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix} = \begin{pmatrix} 1 & -1 & 0 & 2 \\ 0 & 1 & -1 & 2 \\ -1 & 0 & 1 & 2 \end{pmatrix} \cdot \begin{bmatrix} h_o \\ k_o \\ i_o \\ l_o \end{bmatrix}. \quad (37)$$

The clearing of fractions was used in the above derivation, so that in this case $m_1 + m_2 + m_3 = 6l_o$. In general, an additional reduction to lowest integers is needed.

As an example which illustrates the use of the transformation formulae (35) and (37), consider the direction $[12\bar{1}]$ in the crystallographic direction notation. From equation (35) it follows that $h_o = 4$, $k_o = 2$, $i_o = -6$ and $l_o = 2$, so that upon the

reduction to lowest integers the hexagonal indices become $[21\bar{3}1]$. On the other hand, for the direction with the hexagonal indices $[2\bar{2}01]$, equation (37) gives $m_1 = 6$, $m_2 = m_3 = 0$, which yield the crystallographic direction indices [100].

5.1. Transformation to three-axis hexagonal indices

Returning to equation (32), the substitution of $\mathbf{e}_3^o = -(\mathbf{e}_1^o + \mathbf{e}_2^o)$ yields

$$3\mathbf{x} = 2a_0[(m_1 + m_2 - 2m_3)\mathbf{e}_1^o + (-m_1 + 2m_2 - m_3)\mathbf{e}_2^o] + (m_1 + m_2 + m_3)c_0\mathbf{n}. \quad (38)$$

Thus, the transformation rule between the crystallographic direction indices $[m_1\, m_2\, m_3]$ and the three-axis hexagonal direction indices $[h'_o\, k'_o\, l'_o]$ is

$$\begin{bmatrix} h'_o \\ k'_o \\ l'_o \end{bmatrix} = \begin{pmatrix} 2 & 2 & -4 \\ -2 & 4 & -2 \\ 1 & 1 & 1 \end{pmatrix} \cdot \begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix}. \quad (39)$$

The inverse transformation (after clearing the fractions) is

$$\begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix} = \begin{pmatrix} 1 & -1 & 2 \\ 0 & 1 & 2 \\ -1 & 0 & 2 \end{pmatrix} \cdot \begin{bmatrix} h'_o \\ k'_o \\ l'_o \end{bmatrix}. \quad (40)$$

The well known connections between the two sets of indices $[h'_o\, k'_o\, l'_o]$ and $[h_o\, k_o\, i_o\, l_o]$ are

$$h'_o = 2h_o + k_o, \quad k'_o = h_o + 2k_o, \quad (41)$$

$$h_o = \frac{1}{3}(2h'_o - k'_o), \quad k_o = \frac{1}{3}(2k'_o - h'_o), \quad (42)$$

$$i_o = -(h_o + k_o) = -\frac{1}{3}(h'_o + k'_o), \quad l_o = l'_o. \quad (43)$$

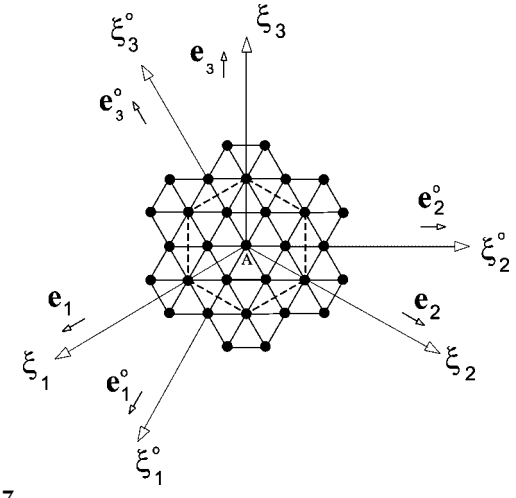

Figure 7
The coordinate axes ξ_1^o, ξ_2^o, ξ_3^o are aligned along directions of the first-nearest atoms to the atom at the origin A. The coordinate axes ξ_1, ξ_2, ξ_3 are along directions of the second-nearest atoms to the origin at A. The corresponding six atoms form the hexagon (indicated by dashed lines) of interatomic spacing $\hat{a}_0 = 3^{1/2}a_0$, where a_0 is the interatomic distance between the first-nearest neighbors.

6. An alternative set of hexagonal indices

The hexagonal direction indices $[h_o\, k_o\, i_o\, l_o]$ were derived in the previous section by using the coordinate axes ξ_1^o, ξ_2^o, ξ_3^o that pass through the first-nearest neighbors relative to an atom A at the origin. Another set of four hexagonal indices $[h\, k\, i\, l]$ for the same crystallographic direction can be obtained by using the coordinate axes ξ_1, ξ_2, ξ_3 that pass through the second-nearest neighbors (Fig. 7). The direction ξ_2 is a reciprocal direction to ξ_1^0, in the sense that $\mathbf{e}_2 \cdot \mathbf{e}_1^0 = 0$. The distance between the second-nearest neighbors is $\hat{a}_0 = 3^{1/2}a_0 = (3/2)^{1/2}a$. Thus, considering a direction $\mathbf{x}$ with the crystallographic direction indices $[m_1\, m_2\, m_3]$, such that $\mathbf{x} = m_1a\mathbf{i}_1 + m_2a\mathbf{i}_2 + m_3a\mathbf{i}_3$, from equation (10) it follows that

$$\begin{bmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{bmatrix} = \left(\frac{2}{3}\right)^{1/2}\frac{a}{3}\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} \cdot \begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix} \quad (44)$$

and

$$\mathbf{x} = \frac{2}{9}\hat{a}_0[(2m_1 - m_2 - m_3)\mathbf{e}_1 + (-m_1 + 2m_2 - m_3)\mathbf{e}_2 + (-m_1 - m_2 + 2m_3)\mathbf{e}_3] + \frac{1}{3}(m_1 + m_2 + m_3)c_0\mathbf{n}. \quad (45)$$

This defines the four indices

$$h = 2(2m_1 - m_2 - m_3), \quad k = 2(-m_1 + 2m_2 - m_3), \quad i = 2(-m_1 - m_2 + 2m_3), \quad l = 3(m_1 + m_2 + m_3), \quad (46)$$

i.e.

$$\begin{bmatrix} h \\ k \\ i \\ l \end{bmatrix} = \begin{pmatrix} 4 & -2 & -2 \\ -2 & 4 & -2 \\ -2 & -2 & 4 \\ 3 & 3 & 3 \end{pmatrix} \cdot \begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix}, \quad (47)$$

such that

$$9\mathbf{x} = \hat{a}_0(h\mathbf{e}_1 + k\mathbf{e}_2 + i\mathbf{e}_3) + lc_0\mathbf{n}. \quad (48)$$

On the other hand, if the direction indices $[h\, k\, i\, l]$ are known, the corresponding crystallographic direction indices are determined from

$$m_1 = 3h + 2l, \quad m_2 = 3k + 2l, \quad m_3 = 3i + 2l, \quad (49)$$

with the matrix counterpart

$$\begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix} = \begin{pmatrix} 3 & 0 & 0 & 2 \\ 0 & 3 & 0 & 2 \\ 0 & 0 & 3 & 2 \end{pmatrix} \cdot \begin{bmatrix} h \\ k \\ i \\ l \end{bmatrix}. \quad (50)$$

For example, for the previously considered direction $[12\bar{1}]$ in the crystallographic direction notation, from equation (47) we have $h = 2$, $k = 8$, $i = -10$, $l = 6$, so that upon reducing to lowest integers the set of four indices becomes $[14\bar{5}3]$. Similarly, for the direction with the indices $[h\, k\, i\, l] \simeq [2\bar{2}01]$, from equation (50) we have $m_1 = 8$, $m_2 = -4$, $m_3 = 2$, which is equivalent to the $[4\bar{2}1]$ crystallographic direction. It can also be easily veri-

fied that the crystallographic direction [100] corresponds to $[h\,k\,i\,l] \simeq [4\bar{2}\bar{2}3]$.

7. Discussion

It is of interest to establish a transformation rule between the two sets of indices $[h\,k\,i\,l]$ and $[h_o\,k_o\,i_o\,l_o]$. This can be accomplished by equating the expressions for **x** from equations (34) and (48), *i.e.*

$$\frac{a_0}{3}(h_o\mathbf{e}_1^o + k_o\mathbf{e}_2^o + i_o\mathbf{e}_3^o) + \frac{c_0}{3}l_o\mathbf{n} = \frac{\hat{a}_0}{9}(h\mathbf{e}_1 + k\mathbf{e}_2 + i\mathbf{e}_3) + \frac{c_0}{9}l\mathbf{n}. \tag{51}$$

In view of $\hat{a}_0 = 3^{1/2}a_0$ and the relationship (28) between the two sets of unit vectors, it follows that

$$\begin{bmatrix} h \\ k \\ i \\ l \end{bmatrix} = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix} \cdot \begin{bmatrix} h_o \\ k_o \\ i_o \\ l_o \end{bmatrix}. \tag{52}$$

The inverse relations are

$$\begin{bmatrix} h_o \\ k_o \\ i_o \\ l_o \end{bmatrix} = \frac{1}{3}\begin{pmatrix} 1 & 0 & -1 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \cdot \begin{bmatrix} h \\ k \\ i \\ l \end{bmatrix}. \tag{53}$$

For instance, the direction $[h_o\,k_o\,i_o\,l_o] \simeq [21\bar{3}1]$ is equivalent to $[h\,k\,i\,l] \simeq [14\bar{5}3]$, while $[h_o\,k_o\,i_o\,l_o] \simeq [2\bar{2}01]$ is equivalent to $[h\,k\,i\,l] \simeq [4\bar{2}\bar{2}3]$, in agreement with earlier calculations. The fact that the equivalent directions have different indices is a natural consequence of different hexagonal axes used for two sets of indices. It is well known that innumerable different sets of axes can be chosen for any crystal, with the corresponding direction indices related by appropriate transformation matrices [*e.g.* rhombohedral *versus* hexagonal axes for hexagonal crystals (see Barrett & Massalski, 1980; Hahn, 1995; Kelly *et al.*, 2000)].

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