Computation of Miller-Bravais indices to Miller indices conversion for hexagonal crystal

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1 Introduction

The Hexagonal Closed Packed (HCP) crystal systems are crystallographically better presented in Miller-Bravais (4-index) indices because of low symmetry and non-orthogonality of HCP crystals. With this 4-index notation, the planes and directions in HCP crystal systems are presented as $\{h\,k\,i\,l\}$ and $\langle u\,v\,t\,w\rangle$ respectively. These Miller-Bravais notation work perfectly in theoretical and even in visualization of planes and direction in HCP crystals. However, for computational analysis, a cartesian reference frame is preferred for easier computation. In cartesian space, the crystallographic planes and directions are represented as Miller indices i.e. 3-index notation. Therefore, it is very essential to convert Miller-Bravais indices to Miller indices correctly.

The conversion of Miller-Bravais (4-index) to Miller (3-index) can be found in numerous books [1, 2]. However, in most of the literature, this conversion does not account for the c/a ratio of HCP crystals which is very crucial in computational analysis. Furthermore, it is also very essential that the converted lattice must be orthonormal i.e. projected HCP unit should have $\alpha = \beta = \gamma = 90°$.

Therefore, in this article a procedure has been discussed to account for lattice-parameter of HCP crystal as well as lattice orthonormality while converting Miller-Bravais to Miller indices.

2 Procedure

The following steps are followed to convert the Miller-Bravais to Miller indices-

1. **Direct transformation**
2. Transforming **directions** in **direct (crystal) space** using transformation-matrix for directions
3. Projecting **planes** in **reciprocal space** using transformation-matrix for planes

Further, these Miller-Bravais to Miller conversion steps discussed in more detail.

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2.1 Direct transformation:

In this first step, one convert the 4-index to 3-index notations of planes and directions as per method explained in reference books [1, 3, 2]. These methods are as-
for planes: $(h\,k\,i\,l)$ plane in 4-index notation and $(h'\,k'\,l')$ are planes in 3-index notation.

$$(h\,k\,i\,l) = (h'\,k'\,l')$$

where, $h = h'$, $k = k'$ and $l = l'$
for directions: $[u\,v\,t\,w]$ direction in 4-index notation and $[u'\,v'\,w']$ are direction in 3-index notation.

$$[u\,v\,t\,w] = [u'\,v'\,w']$$

where, $u' = 2u + v$, $v' = 2v + u$ and $w' = w$

2.2 Transforming directions in direct (crystal) space using transformation-matrix (M) for directions:

This step is to construct the transformation matrix based on directions of the HCP'crystal coordinate. Since, for HCP crystal symmetry, the crystal coordinates are non-orthonormal, therefore an orthonormal coordinate system has to be associated with HCP'crystal axes [4, 3]. There are two ways to align the HCP'crystal axes to form the orthonormal crystal as shown in Fig. (1). Both approaches are correct, but here Fig.1(a) used i.e. a_1 axis of HCP lattice aligned with the x-axis of orthonormal axis.
Further, transformation-matrix (M) constructed for HCP crystal by transforming/aligning a_1, a_2 and c with x, y and z axis of orthonormal-axis respectively [4, 3].

$$M = \begin{bmatrix} a & -a/2 & 0 \\ 0 & a\sqrt{3}/2 & 0 \\ 0 & 0 & c \end{bmatrix} \tag{1}$$

The 'M' matrix can be constructed for any non-orthonormal crystal lattice as discussed in Appendix.

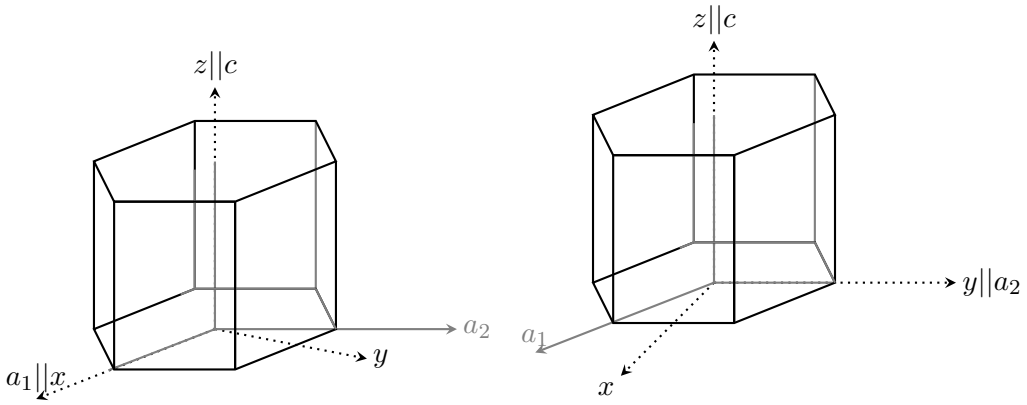

Figure 1: Orthonormal crystal coordinates system for a HCP lattice, when (a) a_1 align with x-axis and (b) a_2 align with y-axis

Further, a mapping can be done using M matrix to get the 3-index direction indices $[U\,V\,W]$ which accounted for orthonormality and lattice parameters from the direct transformed 3-index

direction indices $[u'\,v'\,w']$

$$\begin{bmatrix} U \\ V \\ W \end{bmatrix} = \begin{bmatrix} a & -a/2 & 0 \\ 0 & a\sqrt{3}/2 & 0 \\ 0 & 0 & c \end{bmatrix} \begin{bmatrix} u' \\ v' \\ w' \end{bmatrix}$$
$$\begin{bmatrix} U \\ V \\ W \end{bmatrix} = M \begin{bmatrix} u' \\ v' \\ w' \end{bmatrix} \tag{2}$$

2.3 Projecting planes in reciprocal space using transformation-matrix (M^P) for planes:

As it is know that crystallographic planes could be better understand using reciprocal lattice, which is lattice in Fourier space associated with crystal [5]. A reciprocal lattice for planes can be constructed using parameters b_1, b_2, b_3 from the lattice parameters in direct (crystal) space using parameters a_1, a_2, a_3 as following [5]-

$$b_1 = 2\pi \frac{a_2 \times a_3}{V}; b_2 = 2\pi \frac{a_3 \times a_1}{V}; b_3 = 2\pi \frac{a_1 \times a_2}{V}$$

where V is volume of the lattice in direct space. It can be seen from the above relationship that each reciprocal lattice's basis vector is orthonormal to two basis vectors of crystal lattice. With this establishment, the reciprocal crystal-lattice matrix for planes (M^P) could be constructed in reciprocal space as [5]-

$$M^P = 2\pi (M^{-1})^T \tag{3}$$

Here, it is worth to note a factor of 2π have been used, which ensures the periodicity of the reciprocal lattice in Fourier space. Further, using M^P the directly converted $[h'k'l']$ can be mapped to $[HKL]$ which accounted for c/a ratio, as-

$$\begin{bmatrix} H \\ K \\ L \end{bmatrix} = M^P \begin{bmatrix} h' \\ k' \\ l' \end{bmatrix} \tag{4}$$

3 Conclusion

To compute the crystal properties of HCP crystals, the crystallographic plane $\{HKL\}$ and direction $< UVW >$ should be used. Since, these corrected plane and direction account for both orthonormality of crystals and lattice parameters.

Appendix

For the general case i.e. for any kind of non-orthonormal crystal as shown in Fig. 2. The transformation matrix (M) can represented as for direction in direct space as - [4, 3].

$$M = \begin{bmatrix} a & bcos\gamma & cos\beta \\ o & bsin\gamma & \frac{c(cos\alpha - cos\beta cos\gamma)}{sin\gamma} \\ 0 & 0 & \frac{c\sqrt{(1+2cos\alpha cos\beta cos\gamma - (cos^2\alpha + cos^2\beta + cos^2\gamma))}}{sin\gamma} \end{bmatrix} \tag{5}$$

Further, from this M, M^P can be calculated for the planes for any general crystal system.

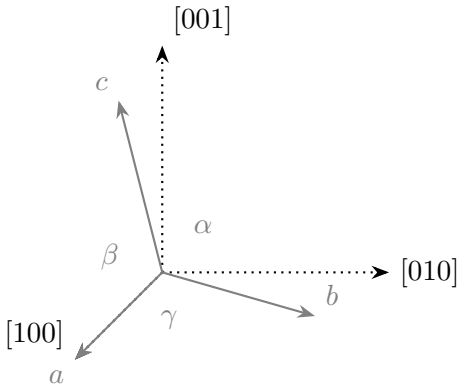

Figure 2: Orthonormalized crystal coordinates system for a general (triclinic) crystal system

References

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