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Supporting information for article:

Identifying the multiplicity of crystallographically equivalent variants generated by iterative phase transformations in Ti

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S1. Projection from a higher dimension

Before explaining how one can project a 4D object into 3D space, it would be helpful to describe the analogous procedure of projecting a 3D object onto a 2D space, i.e. a plane.

In figure SI-1a, a hexagon AEBFCD is shown. If an indexing scheme was required for it, the choice to index the direction **OA** as [1,0] and the direction **OB** as [0,1] would be an obvious one. Yet, it would not be a wise choice, because it does not reflect the symmetry of the hexagon. Direction **OE** would be indexed as [1,1], although it is physically indistinguishable from directions **OA** or **OB**.

Another option is to regard the hexagon as the 2D projection of a 3D cube viewed along its body diagonal OO'. Such a projection is shown in figure SI-1b. O', A', B' and C' are placed directly above O, A, B and C, respectively. Now, a use of a 3D Cartesian frame is possible for the cube. Naturally, **O'A'** is indexed as [100], **O'B'** as [010] and **O'C'** as [001]. Since the projection direction **O'O** is [111], the components of these primitive vectors resolved parallel to the plane of the projection can be easily proven to be **OA**=$\frac{1}{3}[2\bar{1}\bar{1}]$, **OB**=$\frac{1}{3}[\bar{1}2\bar{1}]$ and **OC**=$\frac{1}{3}[\bar{1}\bar{1}2]$. It can also be verified quite easily that the scalar product formed between any vectors in the 2D space and the projection direction [111] is zero. Because all three indices of the projection direction are the same (i.e. 1), this means that all vectors on the plane have indices that must add up to zero.

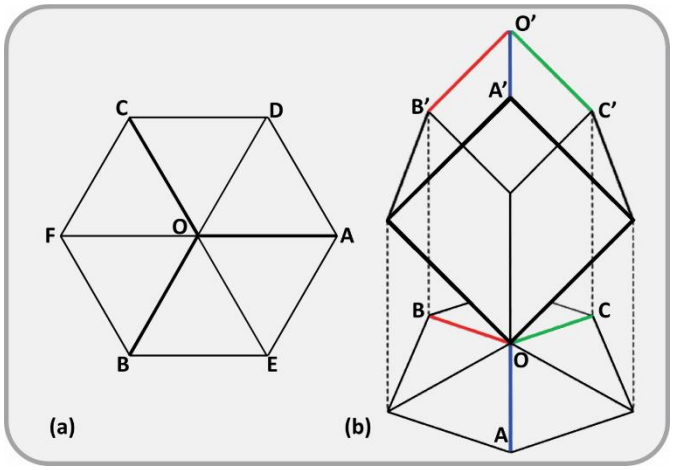

Figure SI-1: A hexagon in 2D space (a) can be regarded as the projection on the plane of a cube. The projection takes place along the body diagonal of the cube (b).

Thus, by exploiting the auxiliary dimension, a much more symmetrical algebraic representation was obtained. Using an analogous procedure, a 4D hypercube, with edges indexed as [1000], [0100], [0010] and [0001] can be projected along the direction [1110]. This results in three unit vectors indexed as $\frac{1}{3}[2\bar{1}\bar{1}0]$, $\frac{1}{3}[\bar{1}2\bar{1}0]$, $\frac{1}{3}[\bar{1}\bar{1}20]$ and another one, being perpendicular to the projection direction, indexed as [0001].

The system created by this procedure certainly resembles the Miller-Bravais system; three unit vectors describe all directions on a basal plane, whereas the fourth is perpendicular to this plane. Yet, for this system to describe a hexagonal unit cell, it is necessary to be rescaled in order for its dimensions to correspond to the lattice parameters, a and c, of a real hexagonal crystal.

If the unit 4-space vectors have magnitude e, it follows that the $\frac{1}{3}\langle 2\bar{1}\bar{1}0\rangle$ -type vectors will have a magnitude of $\sqrt{\frac{2}{3}}$e, while vector [0001] will still have magnitude e. This can be very easily verified by a single trigonometric study of the triangles that are created from 3D

and 4D unit vectors. Therefore, the ratio of the magnitude of [0001] to $\frac{1}{3}\langle 2\bar{1}\bar{1}0\rangle$ is $\sqrt{\frac{3}{2}}$. By increasing the length of 4-vector components parallel to [0001] by the appropriate factor, the 3D cell exhibits the $\frac{c}{a}$ ratio required for a particular problem. The required factor is simply equal to $\frac{c}{e} = \sqrt{\frac{2}{3}}\frac{c}{a}$. This was designated Λ by Frank [5].

In other words, a hexagonal unit cell is derived from the projection of a 4D cubic one only if the ratio of its basis vectors is a specific one: $\sqrt{\frac{3}{2}}$. This means that to be able to treat a hexagonal crystal as the projection of a cubic hyper-crystal, one has to rescale it using Λ, to obtain this specific ratio. Only then can the crystal be regarded as cubic and be manipulated by convenient linear algebra methods of orthogonal matrices.

S2. Transformation matrices for cubic-hexagonal Burgers OR

The Burgers OR states that closest packed planes and closest packed directions of two structures involved in a transformation are parallel. In the case studied here, the two structures involved are h.c.p. and b.c.c.; their relationship is schematically illustrated in figure SI-2. As indicated in the figure, when Ti is transformed from hcp to bcc, hexagonal directions $[0001]$, $[\bar{1}\bar{1}20]$ and $[\bar{1}100]$ transform into cubic directions $[0\bar{1}1]$, $[\bar{1}\bar{1}\bar{1}]$ and $[\bar{2}11]$, respectively.

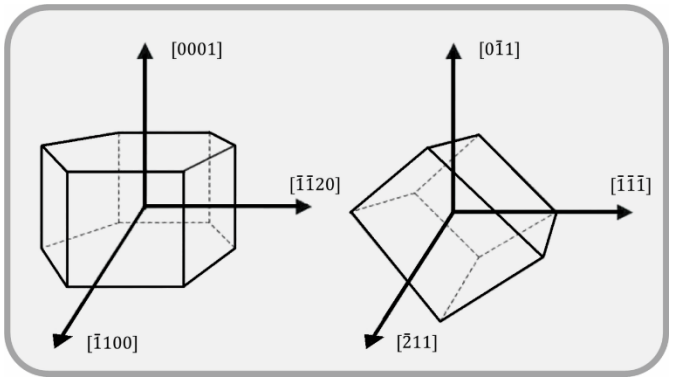

Figure SI-2: Hexagonal-cubic Burgers OR. Hexagonal directions [0001], [$\bar{1}\bar{1}$20] and [$\bar{1}$100] transform into cubic directions [0$\bar{1}$1], [$\bar{1}\bar{1}\bar{1}$] and [$\bar{2}$11], respectively.

P and **Q** are transformation matrices of coefficients. **P** is defined by (**a'**, **b'**, **c'**) = (**a**, **b**, **c**) **P**, where **a**, **b**, and **c** are the original basis vectors and **a'**, **b'**, and **c'** are the basis vectors after the transformation. Of course, since another, fourth, dimension was added for our study in Ti, another basis vector **d** (and **d'**, respectively) should be considered, as well. **Q** is the inverse of **P** [5].

The transformation described above is called a covariant transformation. Quantities that transform in the same way as the basis vectors are called covariant quantities. For a quantity to be transformed covariantly, it has to be post-multiplied by **P** or **Q**. Such quantities are indices of planes and coordinates of points in reciprocal space. Quantities that are transformed by a pre-multiplication by **P** or **Q** are called contra-variant quantities.

Since **P** transforms basis vectors of the one frame to basis vectors of the other, to determine its value, the information about the transformation given by the Burgers OR has to be manipulated so as to refer to basis vectors. To make things simple, the 3D cubic frame will be used first, since 3D directions were used in the Burgers OR (see figure SI-2). If the basis vectors of the cubic and the hexagonal system are $\mathbf{a}_1^{\boldsymbol{c}}$, $\mathbf{a}_2^{\boldsymbol{c}}$ and $\mathbf{a}_3^{\boldsymbol{c}}$ (where the superscript $\boldsymbol{c}$

stands for cubic) and $\mathbf{e_1}$, $\mathbf{e_2}$, $\mathbf{e_3}$ and $\mathbf{e_4}$, respectively, the covariant transformation described above, is:

$$(\mathbf{a}_1^c, \mathbf{a}_1^c, \mathbf{a}_1^c) = (\mathbf{e}_1, \mathbf{e}_1, \mathbf{e}_1, \mathbf{e}_1)\mathbf{P} = (\mathbf{e}_1, \mathbf{e}_1, \mathbf{e}_1, \mathbf{e}_1)\begin{bmatrix} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22} & p_{23} \\ p_{31} & p_{32} & p_{33} \\ p_{41} & p_{42} & p_{43} \end{bmatrix} \quad \text{SI.1}$$

Each column of matrix **P** is in fact the cubic ⟨100⟩-type vector, expressed in the hexagonal frame; this is the physical meaning of matrix **P**.

The ⟨100⟩-type directions can be decomposed with respect to the directions involved in the Burgers OR according to:

$$[100] = 0\left[0\bar{1}1\right] - \frac{1}{3}\left[\bar{1}\bar{1}\bar{1}\right] - \frac{1}{3}\left[\bar{2}11\right] \quad \text{SI.2}$$

$$[010] = -\frac{1}{2}\left[0\bar{1}1\right] - \frac{1}{3}\left[\bar{1}\bar{1}\bar{1}\right] + \frac{1}{6}\left[\bar{2}11\right] \quad \text{SI.3}$$

$$[001] = \frac{1}{2}\left[0\bar{1}1\right] - \frac{1}{3}\left[\bar{1}\bar{1}\bar{1}\right] + \frac{1}{6}\left[\bar{2}11\right] \quad \text{SI.4}$$

If magnitudes are taken into account by equating unit vectors, the three cubic directions and the three hexagonal directions involved in the Burgers OR can be related to each other. For example, the magnitude of $[\bar{2}11]$ has to equal that of $[\bar{1}100]$, leading to:

$$\frac{1}{\sqrt{6}\mathrm{a}_c}\left[\bar{2}11\right] = \frac{1}{\sqrt{2}\mathrm{e}}\left[\bar{1}100\right] \quad \text{SI.5}$$

If the value of Λ is taken into account, to transform e into a_h, equation SI.5 becomes:

$$\left[\bar{2}11\right] = \sqrt{2}\,\frac{\mathrm{a}_c}{\mathrm{a}_h}\left[\bar{1}100\right] \quad \text{SI.6}$$

For the other two directions, the expressions analogous to equation SI.6 are:

$$[111] = \frac{\mathrm{a}_c}{\sqrt{3}\mathrm{a}_h}\left[\bar{1}\bar{1}20\right] \quad \text{SI.7}$$

$$\left[0\bar{1}1\right] = \sqrt{2}\,\frac{a_c}{c_h}\left[0001\right] \qquad \text{SI.8}$$

Substituting SI.6, SI.7 and SI.8 in equations SI.2, SI.3 and SI.4, the 4 × 4 version of **P** can be obtained:

$$\mathbf{P} = \left(\frac{a_c}{3a_h}\right)\begin{bmatrix} \left(\frac{1}{\sqrt{3}}+\sqrt{2}\right) & \left(\frac{1}{\sqrt{3}}-\frac{\sqrt{2}}{2}\right) & \left(\frac{1}{\sqrt{3}}-\frac{\sqrt{2}}{2}\right) & -\sqrt{2} \\ \left(\frac{1}{\sqrt{3}}-\sqrt{2}\right) & \left(\frac{1}{\sqrt{3}}+\frac{\sqrt{2}}{2}\right) & \left(\frac{1}{\sqrt{3}}+\frac{\sqrt{2}}{2}\right) & -\sqrt{2} \\ \frac{-2}{\sqrt{3}} & \frac{-2}{\sqrt{3}} & \frac{-2}{\sqrt{3}} & -\sqrt{2} \\ 0 & \frac{-3}{\sqrt{3}} & \frac{3}{\sqrt{3}} & 0 \end{bmatrix} \qquad \text{SI.9}$$

where a_c and a_h for Ti are 0.332 and 0.295, respectively. **Q** being the inverse of **P** is given by:

$$\mathbf{Q}=\mathbf{P}^{-1} = \left(\frac{\sqrt{2}a_h}{12a_c}\right)\begin{bmatrix} \left(\sqrt{6}+6\right) & \left(\sqrt{6}-6\right) & -2\sqrt{6} & 0 \\ \left(\sqrt{6}-3\right) & \left(\sqrt{6}+3\right) & -2\sqrt{6} & -3\sqrt{6} \\ \left(\sqrt{6}-3\right) & \left(\sqrt{6}+3\right) & -2\sqrt{6} & 3\sqrt{6} \\ -6 & -6 & -6 & 0 \end{bmatrix} \qquad \text{SI.10}$$