

Weekly Progress (Jan 30, 2026)

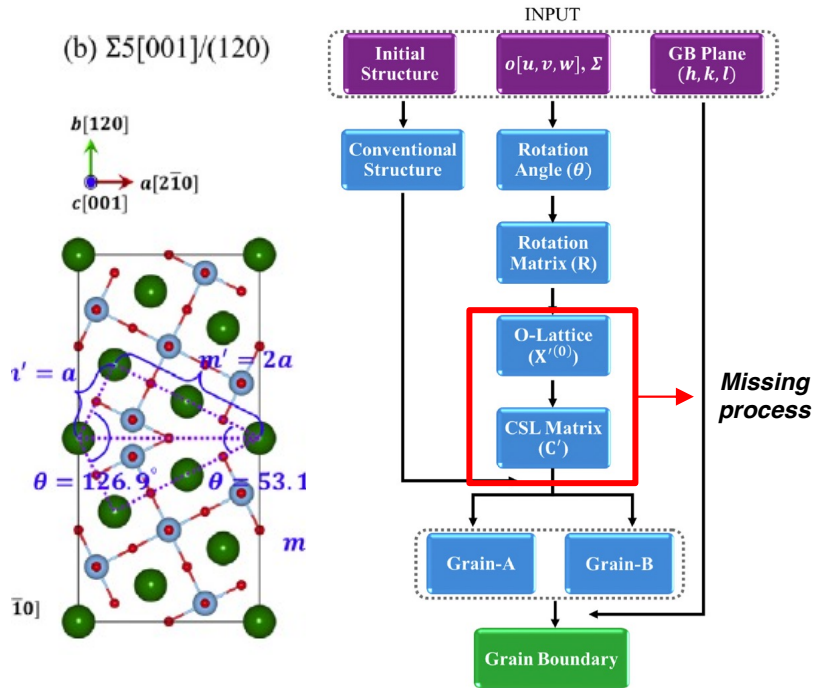


Fig. 5. The complete building procedure for generating atomic coordinates of periodic grain boundary models from the input Σ , rotation axis, grain boundary plane and initial crystal structure.

$$\alpha\Sigma = m^2 + (u^2 + v^2 + w^2)n^2 \quad (3)$$

and

$$\alpha = 1, 2, \text{ and } 4$$

$$\tan\left(\frac{\theta}{2}\right) = \frac{n}{m}(u^2 + v^2 + w^2)^{1/2} \quad (4)$$

$$\text{GCD}(u, v, w) = 1 \quad \text{and} \quad \text{GCD}(m, n) = 1 \quad (5)$$

$$K = \begin{bmatrix} 0 & -k_z & k_y \\ k_z & 0 & -k_x \\ -k_y & k_x & 0 \end{bmatrix} \quad (6)$$

$$R = I + (\sin\theta)K + (1-\cos\theta)K^2 \quad (7)$$

$$I - A'^{-1} = T' = I - US^{-1}R^{-1}S \quad (13)$$

$$\det(T') = \frac{n}{\Sigma} \quad (14)$$

$$X^{(0)} = T'^{-1} \quad (15)$$

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[illegible]

For the rotation axis $[001]$, we have the unit vector $\mathbf{k} = [0, 0, 1]$. Then using $\theta = 53.1^\circ$ and Eqs. (6) and (7), we are able to get a rotation matrix \mathbf{R} :

$$\mathbf{R} = \frac{1}{5} \begin{bmatrix} 3 & -4 & 0 \\ 4 & 3 & 0 \\ 0 & 0 & 5 \end{bmatrix} \quad (1)$$

Choose U:

$$\mathbf{U} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}$$

and plug it with \mathbf{R} into Eqs. (13) and (15), we can get:

$$\mathbf{T}' = \frac{1}{5} \begin{bmatrix} 2 & -4 & -5 \\ 4 & 2 & 0 \\ 4 & -3 & 0 \end{bmatrix} \quad (2)$$

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$\text{Kof}(\Pi') = \frac{1}{5} \begin{bmatrix} 0 & 0 & -20 \\ 15 & 20 & -10 \\ 10 & -20 & 20 \end{bmatrix} = \frac{1}{5} \begin{bmatrix} 0 & 0 & -20 \\ 15 & 20 & -10 \\ 10 & -20 & 20 \end{bmatrix} = \begin{bmatrix} 0 & 0 & -4 \\ 3 & 4 & -2 \\ 2 & -4 & 4 \end{bmatrix}$

$\text{adj}(\Pi') = \begin{bmatrix} 0 & 3 & 2 \\ 0 & 4 & -4 \\ -4 & -2 & 4 \end{bmatrix} = \begin{bmatrix} 0 & 3 & 1/2 \\ 0 & 4 & -1 \\ -1 & -1/2 & 1 \end{bmatrix}$

$X^{(0)} = \Pi'^{-1} = \text{adj}(\Pi') \cdot \text{factor det}(\Pi') \text{ neglected}$

$X^{(0)} = \begin{bmatrix} 0 & 3/4 & 1/2 \\ 0 & 1 & -1 \\ -1 & -1/2 & 1 \end{bmatrix}$ (3)

Hilangkan pecahan

$M = 4X^{(0)} = \begin{bmatrix} 0 & 3 & 2 \\ 0 & 4 & -4 \\ -4 & -2 & 4 \end{bmatrix}$

Sederhanakan tiap kolom

(1) $(0, 0, -4) = (0, 0, -1)$
 4

(2) $(3, 4, -2) \rightarrow \text{gcd} = 1$

(3) $(-4, -2, 4) = (-1, -1/2, 1)$
 4

$M_1 = \begin{bmatrix} 0 & 3 & 1 \\ 0 & 4 & -2 \\ -1 & -2 & 2 \end{bmatrix}$

$\det(M) = [0(8-4) - 3(0-2) + 1(0-(-4))]$
 $= 6 + 4 = 10 \rightarrow \text{mash belum minimal}$
 $2' = 10 \rightarrow \text{target } 5$

$v_1 = (0, 0, -1)$
 $v_2 = (3, 4, -2)$
 $v_3 = (1, -2, 2)$

$v_2 + v_3 = (4, 2, 0)$
 $(2, 1, 0)$

maka $v_2' = (2, 1, 0)$

$M_2 = \begin{bmatrix} 0 & 2 & 1 \\ 0 & 1 & -2 \\ -1 & 0 & 2 \end{bmatrix}$

$\det(M_2) = [0(2-0) - 2(0-2) + 1(0-(-1))]$
 $= 4 + 1 = 5$

(25)

and

$$X^{(0)} = \begin{bmatrix} 0 & 3/4 & 1/2 \\ 0 & 1 & -1 \\ -1 & -1/2 & 1 \end{bmatrix} \quad (3)$$

Still finding the step and transformation process

To obtain a CSL matrix, we make the matrix $X^{(0)}$ integral with each column vector having the shortest length, and meanwhile make its determinant equal to Σ , and get the following matrix C:

$$C = \begin{bmatrix} 0 & -1 & 2 \\ 0 & 2 & 1 \\ -1 & 0 & 0 \end{bmatrix}$$

We further reshape the matrix C by making its each column vector orthogonal and setting its third column vector same with the rotation axis \mathbf{o} , and get the CSL matrix:

$$C' = \begin{bmatrix} 2 & 1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

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$\begin{bmatrix} 2 \\ 8 \end{bmatrix} \begin{bmatrix} 110 \\ 110 \end{bmatrix}$
 $\begin{bmatrix} uvw \\ uvw \end{bmatrix} = \begin{bmatrix} 110 \\ 110 \end{bmatrix}$
 $d\vec{x} = m^2 + (u^2 + v^2 + w^2) n^2$
 $\alpha = 1, 2, 4$
 $d\vec{3} = m^2 + (1^2 + 1^2 + 0^2) n^2$
 $d\vec{3} = m^2 + 2n^2$
 $\alpha = 1 \rightarrow 3 = m^2 + 2n^2$ $(1, 1) \rightarrow \theta = 2(\tan^{-1}(\frac{1}{\sqrt{3}})) = 109.47^\circ$
 $\alpha = 2 \rightarrow 6 = m^2 + 2n^2$ $(2, 1) \rightarrow \theta = 2(\tan^{-1}(\frac{2}{\sqrt{3}})) = 70.53^\circ$
 $\alpha = 4 \rightarrow 12 = m^2 + 2n^2$ $(2, 2) \rightarrow \theta = 2(\tan^{-1}(\frac{2}{2})) = 109.47^\circ$
 \Rightarrow choose $\theta = 70.53^\circ$
 $\textcircled{2} k = [1, 1, 0]$
 $K = \begin{bmatrix} 0 & -k_3 & k_2 \\ k_3 & 0 & -k_1 \\ -k_2 & k_1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ -1 & 1 & 0 \end{bmatrix}$
 $R = I + (\sin \theta) K + (1 - \cos \theta) K^2$
 $K^2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ -1 & 1 & 0 \end{bmatrix}^2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ 1 & -1 & 0 \end{bmatrix} = \begin{bmatrix} -1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & -2 \end{bmatrix}$
 $R = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \sin 70.53^\circ \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ -1 & 1 & 0 \end{bmatrix} + (1 - \cos 70.53^\circ) \begin{bmatrix} -1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & -2 \end{bmatrix}$
 $= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \frac{9}{10} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ -1 & 1 & 0 \end{bmatrix} + \frac{1}{10} \begin{bmatrix} -1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & -2 \end{bmatrix}$
 $= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \frac{1}{10} \begin{bmatrix} 0 & 0 & 9 \\ 0 & 0 & -9 \\ -9 & 9 & 0 \end{bmatrix} + \begin{bmatrix} -1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & -14 \end{bmatrix}$
 $= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \frac{1}{10} \begin{bmatrix} -7 & 9 & 9 \\ 9 & -9 & -9 \\ -9 & 9 & -14 \end{bmatrix}$
 $10R = \begin{bmatrix} 10 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 10 \end{bmatrix} + \begin{bmatrix} -7 & 9 & 9 \\ 9 & -9 & -9 \\ -9 & 9 & -14 \end{bmatrix} = \begin{bmatrix} 3 & 9 & 9 \\ 9 & 1 & -9 \\ -9 & 9 & -4 \end{bmatrix}$
 $R = \frac{1}{10} \begin{bmatrix} 3 & 9 & 9 \\ 9 & 1 & -9 \\ -9 & 9 & -4 \end{bmatrix}$

$$T^{-1} = I - US^{-1}U^T S$$
$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 1 & 1 \\ -0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \frac{1}{1780} \begin{bmatrix} 69 & 109 & -90 \\ 109 & 69 & 90 \\ 90 & -90 & 40 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}$$
$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \frac{1}{1780} \begin{bmatrix} 69 & 109 & -90 \\ 109 & 69 & 90 \\ 90 & -90 & 40 \end{bmatrix}$$
$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \frac{1}{1780} \begin{bmatrix} 69 & 109 & -90 \\ 109 & 69 & 90 \\ 90 & -90 & 40 \end{bmatrix}$$
$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \frac{1}{1780} \begin{bmatrix} 159 & 19 & -50 \\ 109 & 69 & 90 \\ 189 & -21 & 130 \end{bmatrix}$$
$$\text{1860 } T^{-1} = \begin{bmatrix} 1860 & 0 & 0 \\ 0 & 1860 & 0 \\ 0 & 0 & 1860 \end{bmatrix} - \begin{bmatrix} 159 & 19 & -50 \\ 109 & 69 & 90 \\ 189 & -21 & 130 \end{bmatrix}$$
$$= \begin{bmatrix} 1621 & -19 & 50 \\ -109 & 1711 & -90 \\ -189 & 21 & 1650 \end{bmatrix}$$
$$T^{-1} = \frac{1}{1780} \begin{bmatrix} 1621 & -19 & 50 \\ -109 & 1711 & -90 \\ -189 & 21 & 1650 \end{bmatrix} = \begin{bmatrix} 91/100 & -1/100 & 3/100 \\ -6/100 & 96/100 & -5/100 \\ -9/100 & 1/100 & 93/100 \end{bmatrix}$$
$$X^{(10)} = T^{-1} \cdot \begin{bmatrix} 1 & -1 & 3 \\ -6 & 96 & -5 \\ -9 & 1 & 93 \end{bmatrix}$$
$$\det(T) = \frac{n}{\theta} = \frac{1}{3}$$
$$\text{For } T^{-1} = \frac{1}{100} \begin{bmatrix} (8928+5) & (-558-50) & (-6+960) \\ (-93-3) & (846+3+30) & (-91-10) \\ (5-288) & (-495+18) & (8736-6) \end{bmatrix}$$
$$= \frac{1}{100} \begin{bmatrix} 8933 & 608 & 954 \\ 96 & 8493 & -81 \\ -283 & 421 & 8730 \end{bmatrix}$$
$$\text{adj}(T^{-1}) = \frac{1}{100} \begin{bmatrix} 8933 & 96 & -81 \\ 608 & 8493 & -94 \\ 954 & 421 & 8730 \end{bmatrix}, T^{-1} = \frac{3}{100} \begin{bmatrix} 8933 & 96 & 954 \\ 608 & 8493 & -81 \\ 954 & 421 & 8730 \end{bmatrix}$$

$$x(0)' = \frac{3}{100} \begin{bmatrix} 8933 & 96 & 954 \\ 608 & 8493 & -81 \\ 954 & 437 & 8730 \end{bmatrix}$$

???

$$C = \begin{bmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 2 & 0 \end{bmatrix}$$