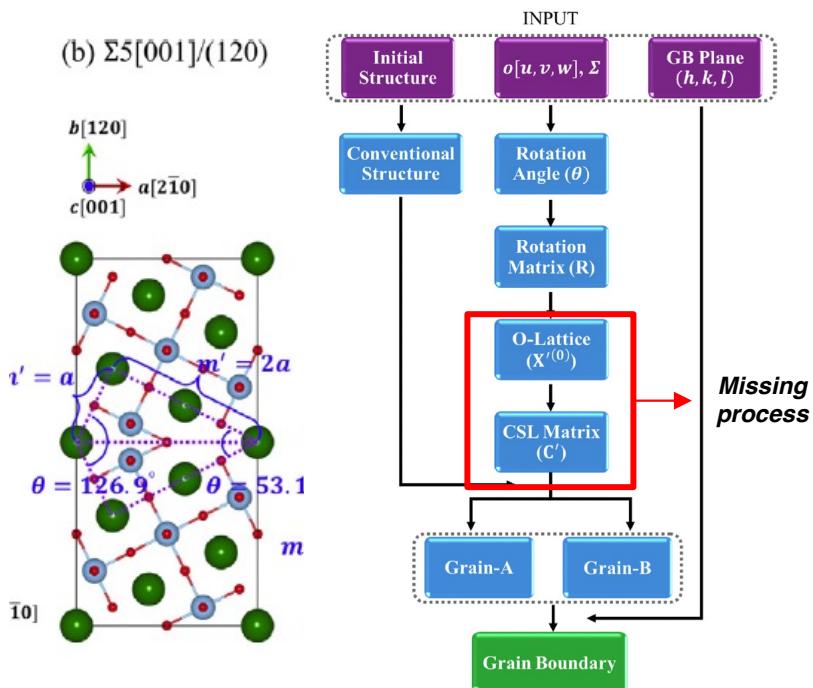


## Weekly Progress (Jan 30, 2026)



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

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

and

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

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

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

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

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

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

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

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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  $\mathbf{R}$ :

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

Inverse matrix

$$A^{-1} = \frac{1}{\det(A)} \cdot \text{adj}(A) \quad \text{kof}(A) = \begin{bmatrix} - & + & - \\ - & + & - \\ + & - & + \end{bmatrix}$$

$$A = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \quad \text{adj}(A) = \begin{pmatrix} + | e f | & - | b c | & + | b c | \\ - | h f | & + | a c | & - | a c | \\ + | g f | & - | a b | & + | a b | \end{pmatrix}$$

$$\text{adj } A = (\text{kof}(A))^T$$

$$\text{kof}(A) = \begin{pmatrix} |ef| & - |df| & |de| \\ - |bf| & |ac| & |gh| \\ - |bc| & - |ac| & |ab| \end{pmatrix}$$

$$\text{kof}(A)^T = \begin{pmatrix} |ef| & - |bc| & |eg| \\ - |hi| & |ac| & |bc| \\ - |df| & - |gi| & |ad| \\ |de| & - |gb| & |de| \end{pmatrix}$$


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$$S^{-1} = \frac{1}{\det(S)} \text{adj}(S)^T \quad S = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\det(S) = 1(1 \cdot 0) - 0(0 \cdot 0) + 0(0 \cdot 0) = 1$$

$$\text{kof}(S) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{kof}(S)^T = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \text{adj}(S)$$

$$S^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$


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$$R = \begin{bmatrix} 3 & -4 & 0 \\ 4 & 3 & 0 \\ 5 & 0 & 5 \end{bmatrix}, \quad \det(R) = \frac{1}{5} (3(15-0) + 20-0) + 0(0-0) = \frac{1}{5} (45+80) = \frac{1}{5} 125 = 25$$

## 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:

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

$$\text{adj}(R) = \begin{bmatrix} 15 & 20 & 0 \\ 0 & 0 & 25 \\ -20 & 15 & 0 \end{bmatrix}^T = \begin{bmatrix} 15 & 20 & 0 \\ -20 & 15 & 0 \\ 0 & 0 & 25 \end{bmatrix}$$

$$R^{-1} = \frac{1}{25} \begin{bmatrix} 15 & 20 & 0 \\ -20 & 15 & 0 \\ 0 & 0 & 25 \end{bmatrix} \cdot 25 R^{-1} = \begin{bmatrix} 15 & 20 & 0 \\ -20 & 15 & 0 \\ 0 & 0 & 25 \end{bmatrix}$$

$$= \frac{1}{5} \begin{bmatrix} 3 & 4 & 0 \\ -4 & 3 & 0 \\ 0 & 0 & 5 \end{bmatrix}$$

$$T' = I - US^{-1}R^{-1}S$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \frac{1}{5} \begin{bmatrix} 3 & 4 & 0 \\ -4 & 3 & 0 \\ 0 & 0 & 5 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \frac{1}{5} \begin{bmatrix} 3 & 4 & 0 \\ -4 & 3 & 0 \\ 0 & 0 & 5 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \frac{1}{5} \begin{bmatrix} 3 & 4 & 0 \\ -4 & 3 & 0 \\ 0 & 0 & 5 \end{bmatrix}$$

$$= \begin{bmatrix} 5 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 5 \end{bmatrix} - \begin{bmatrix} 3 & 4 & 5 \\ -4 & 3 & 0 \\ -4 & 3 & 5 \end{bmatrix}$$

$$= \begin{bmatrix} 2 & -4 & -5 \\ 4 & 2 & 0 \\ 4 & -3 & 0 \end{bmatrix}$$

$$T' = \begin{bmatrix} 2 & -4 & -5 \\ 4 & 2 & 0 \\ 4 & -3 & 0 \end{bmatrix}$$

$$\text{adj}(T') = \begin{bmatrix} 0 & 0 & 1 \\ -15 & 20 & -20 \\ 10 & -20 & 20 \end{bmatrix} = \begin{bmatrix} 0 & 0 & \frac{4}{5} \\ -3 & 4 & -4 \\ 2 & -4 & 4 \end{bmatrix}, \text{adj}(T') = \begin{bmatrix} 0 & -3 & 2 \\ 0 & 4 & -4 \\ 4 & -4 & 1 \end{bmatrix}$$

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$$\begin{aligned}
 \text{ko}_f(\Pi') &= \frac{1}{5} \begin{bmatrix} 0 & -0 & -20 \\ -15 & 20 & -10 \\ 10 & -20 & 20 \end{bmatrix} = \frac{1}{5} \begin{bmatrix} 0 & 0 & -20 \\ 15 & 20 & -10 \\ 10 & -20 & 20 \end{bmatrix} = \begin{bmatrix} 0 & 0 & -4 \\ 3 & 4 & -2 \\ 2 & -4 & 4 \end{bmatrix} \\
 \text{adj}(\Pi') &= \begin{bmatrix} 0 & 3 & 2 \\ 0 & 4 & -4 \\ -4 & -2 & 4 \end{bmatrix} = \begin{bmatrix} 0 & 3/4 & 1/2 \\ 0 & 1 & -1 \\ -1 & -1/2 & 1 \end{bmatrix} \\
 X'^{(0)} &= \Pi'^{-1} \quad \text{factor } \det(\Pi') \text{ neglected} \\
 &= \text{adj}(\Pi') \\
 &= \begin{bmatrix} 0 & 3/4 & 1/2 \\ 0 & 1 & -1 \\ -1 & -1/2 & 1 \end{bmatrix} \quad \boxed{3} \\
 \text{Hilangkan pecahan} \\
 M &= 4X'^{(0)} = \begin{bmatrix} 0 & 3 & 2 \\ 0 & 4 & -4 \\ -4 & -2 & 4 \end{bmatrix} \\
 \text{Sederhanakan tiap kolom} \\
 (1) \quad \underline{(0, 0, -4)} &= (0, 0, -1) \\
 &\quad 4 \\
 (2) \quad (3, 4, -2) &\rightarrow \text{gcd} = 1 \\
 (2) \quad \underline{(2, -4, 4)} &= (1, -2, 2) \\
 &\quad 2 \\
 M_1 &= \begin{bmatrix} 0 & 3 & 1 \\ 0 & 4 & -2 \\ -1 & -2 & 2 \end{bmatrix} \quad \det(M) = [0(8-4) - 3(0-2) + 1(0-(-4))] \\
 &= 6 + 4 = 10 \rightarrow \text{masih belum minimal} \\
 v_1 &= (0, 0, -1) \\
 v_2 &= (3, 4, -2) \\
 v_3 &= (1, -2, 2) \quad v_2 + v_3 = (4, 2, 0) \\
 &\quad (2, 1, 0) \\
 \text{maka } v_2' &= (2, 1, 0) \\
 M_2 &= \begin{bmatrix} 0 & 3 & 1 \\ 0 & 1 & -2 \\ -1 & 0 & 2 \end{bmatrix} \quad \det(M_2) = [0(2-0) - 2(0-2) + 1(0-(-1))] \\
 &= 4 + 1 = 5
 \end{aligned}$$

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and

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

**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  $\Sigma$ , 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  $o$ , and get the CSL matrix:

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

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$\text{① } \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$   
 $\begin{bmatrix} uvw \\ uvw \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$   
 $\alpha_1 = m^2 + (u^2 + v^2 + w^2) n^2$   
 $\alpha_2 = 1, 2, 4$   
 $\alpha_3 = m^2 + (1^2 + 1^2 + 0^2) n^2$   
 $\alpha_4 = m^2 + 2n^2$   
 $\alpha_5 = 1 \rightarrow 3 = m^2 + 2n^2$   
 $\alpha_6 = 2 \rightarrow 6 = m^2 + 2n^2$   
 $\alpha_7 = 4 \rightarrow 12 = m^2 + 2n^2$   
 $m, n$   
 $\tan\left(\frac{\theta}{2}\right) = \frac{n}{m} \sqrt{u^2 + v^2 + w^2}$   
 $= \frac{n}{m} \sqrt{1^2 + 1^2 + 0^2}$   
 $\theta = \tan^{-1}\left(\frac{n}{m}\sqrt{2}\right)$   
 $\theta = \tan^{-1}\left(\frac{1}{1}\sqrt{2}\right) = 45^\circ$   
 $\theta = 2 \tan^{-1}\left(\frac{1}{2}\sqrt{2}\right) = 70.53^\circ$   
 $\theta = 2 \tan^{-1}\left(1\sqrt{2}\right) = 109.47^\circ$   
 $\therefore \text{Choose } \theta = 70.53^\circ$   
 $\text{② } K = [1, 1, 0]$   
 $K = \begin{bmatrix} 0 & -k_3 & k_2 \\ k_2 & 0 & -k_1 \\ -k_3 & k_1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ 1 & 1 & 0 \end{bmatrix}$   
 $RK = I + (\sin\theta)K + (1 - \cos\theta)K^2$   
 $RK^2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ -1 & 1 & 0 \end{bmatrix}^2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ -1 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ -1 & 1 & 0 \end{bmatrix} = \begin{bmatrix} -1 & 1 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & -2 \end{bmatrix}$   
 $RK = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \sin 70.53^\circ \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ -1 & 1 & 0 \end{bmatrix} + (1 - \cos 70.53^\circ) \begin{bmatrix} -1 & 1 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & -2 \end{bmatrix}$   
 $= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \frac{9}{10} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ -1 & 1 & 0 \end{bmatrix} + \frac{3}{10} \begin{bmatrix} -1 & 1 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & -2 \end{bmatrix}$   
 $= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \frac{1}{10} \begin{bmatrix} 0 & 0 & 9 \\ 0 & 0 & -9 \\ -9 & 9 & 0 \end{bmatrix} + \begin{bmatrix} -3 & 7 & 0 \\ 3 & -7 & 0 \\ 0 & 0 & -14 \end{bmatrix}$   
 $= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \frac{1}{10} \begin{bmatrix} -9 & 7 & 9 \\ 7 & -9 & -9 \\ -9 & 9 & -14 \end{bmatrix} = \begin{bmatrix} 3 & 7 & 9 \\ 7 & -9 & -9 \\ 9 & 9 & -4 \end{bmatrix}$   
 $10RK = \begin{bmatrix} 10 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 10 \end{bmatrix} + \begin{bmatrix} -9 & 7 & 9 \\ 7 & -9 & -9 \\ -9 & 9 & -14 \end{bmatrix} = \begin{bmatrix} 3 & 7 & 9 \\ 7 & -9 & -9 \\ 9 & 9 & -4 \end{bmatrix}$   
 $R = \frac{1}{10} \begin{bmatrix} 3 & 7 & 9 \\ 7 & -9 & -9 \\ 9 & 9 & -4 \end{bmatrix}$

$$\begin{aligned}
 \textcircled{B} \quad V &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
 \text{II}' &= \text{II} - U S^{-1} R^{-1} S \\
 S &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad S^{-1} = \frac{1}{\det(S)} \text{adj}(S) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
 \text{det}(S) &= 1(1-0) - 0(0-0) + 0(0-0) \\
 &= 1 \\
 \text{ref}(S) &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \text{adj}(S) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
 R &= \frac{1}{10} \begin{bmatrix} 3 & 7 & 9 \\ 3 & 3 & -9 \\ -9 & 9 & 9 \end{bmatrix} \\
 \text{det}(R) &= \frac{1}{10} (3(-12 - (-81)) - 7(-28 - 81) + 9(63 - (-27))) \\
 &= \frac{1}{10} (3(69) - 7(-109) + 9(90)) \\
 &= \frac{1}{10} (207 + 763 + 810) = \frac{1}{10} (1780) = 178 \\
 \text{ref}(R) &= \frac{1}{10} \begin{bmatrix} -12+81 & -(-28-81) & (63+27) \\ (-28-81) & -12+81 & -(27+63) \\ (-63-27) & -(-27-63) & (9-48) \end{bmatrix} = \frac{1}{10} \begin{bmatrix} 69 & -(-109) & 90 \\ -109 & 69 & -90 \\ -90 & -90 & -48 \end{bmatrix} \\
 &= \frac{1}{10} \begin{bmatrix} 69 & 109 & 90 \\ 109 & 69 & -90 \\ -90 & -90 & -48 \end{bmatrix} = \begin{bmatrix} 69/10 & 109/10 & 90 \\ 109/10 & 69/10 & -90 \\ -9 & 9 & -4 \end{bmatrix} \\
 \text{adj}(R) &= \begin{bmatrix} 69/10 & 109/10 & -9 \\ 109/10 & 69/10 & 9 \\ 9 & -9 & -4 \end{bmatrix} \\
 R^{-1} &= \frac{1}{1780} \cdot \frac{1}{10} \begin{bmatrix} 69 & 109 & -90 \\ 109 & 69 & 90 \\ 90 & -90 & -40 \end{bmatrix} = \frac{1}{1780} \begin{bmatrix} 69 & 109 & -90 \\ 109 & 69 & 90 \\ 90 & -90 & -40 \end{bmatrix}
 \end{aligned}$$

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

???

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