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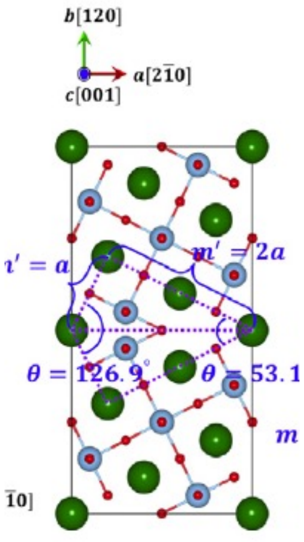
(b) Σ5[001]/(120)



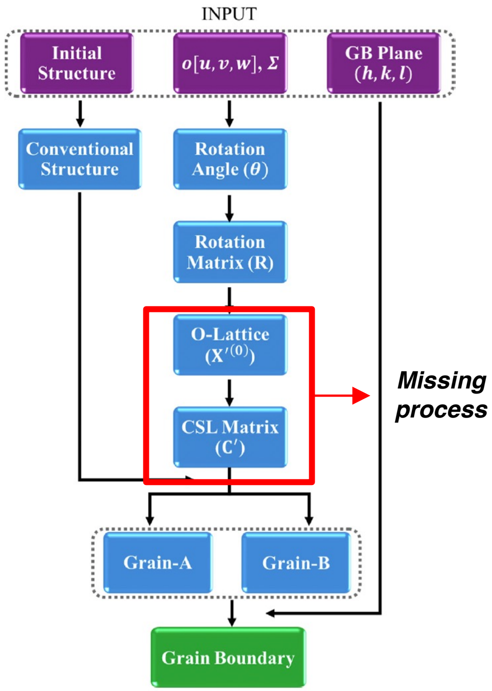


Fig. 5. The complete building procedure for generating atomic coordinates of periodic grain boundary models from the input Σ, rotation axis, grain boundary plane and initial crystal structure.

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

and $\alpha = 1, 2, and\ 4$

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

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

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

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

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

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

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

Jianli Cheng, Jian Luo, Kesong Yang, Aimsgb: An algorithm and open-source python library to generate periodic grain boundary structures, Computational Materials Science, Volume155, 2018, Pages 92-103, ISSN 0927-0256, https://doi.org/10.1016/j.commatsci.2018.08.029.

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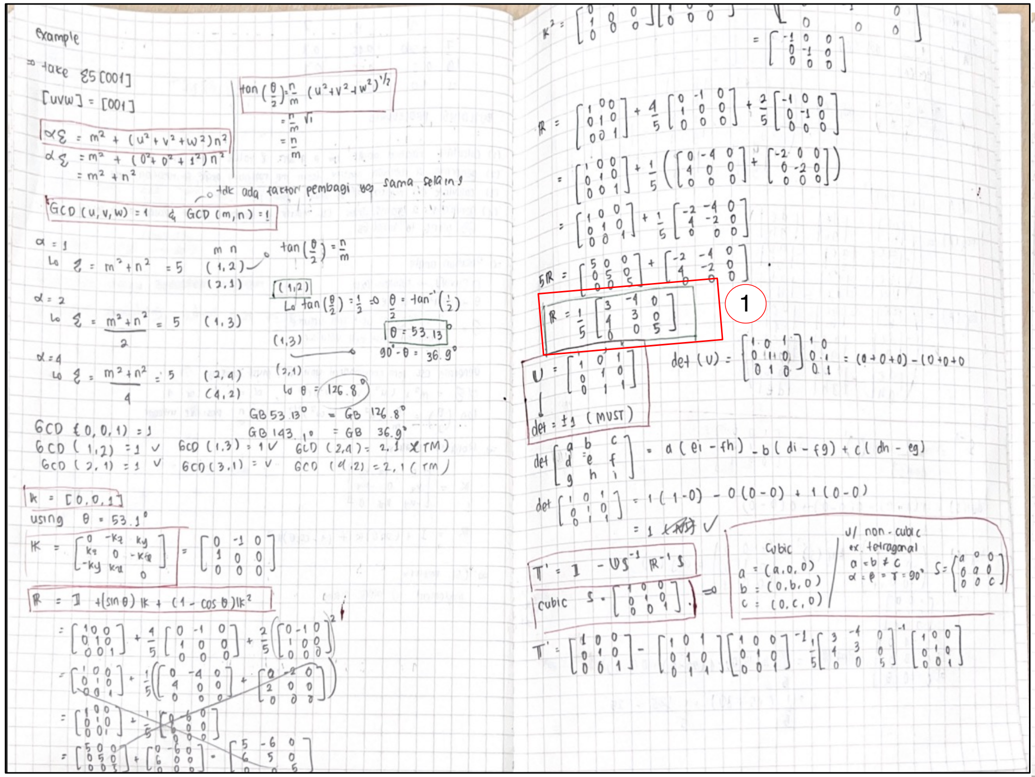

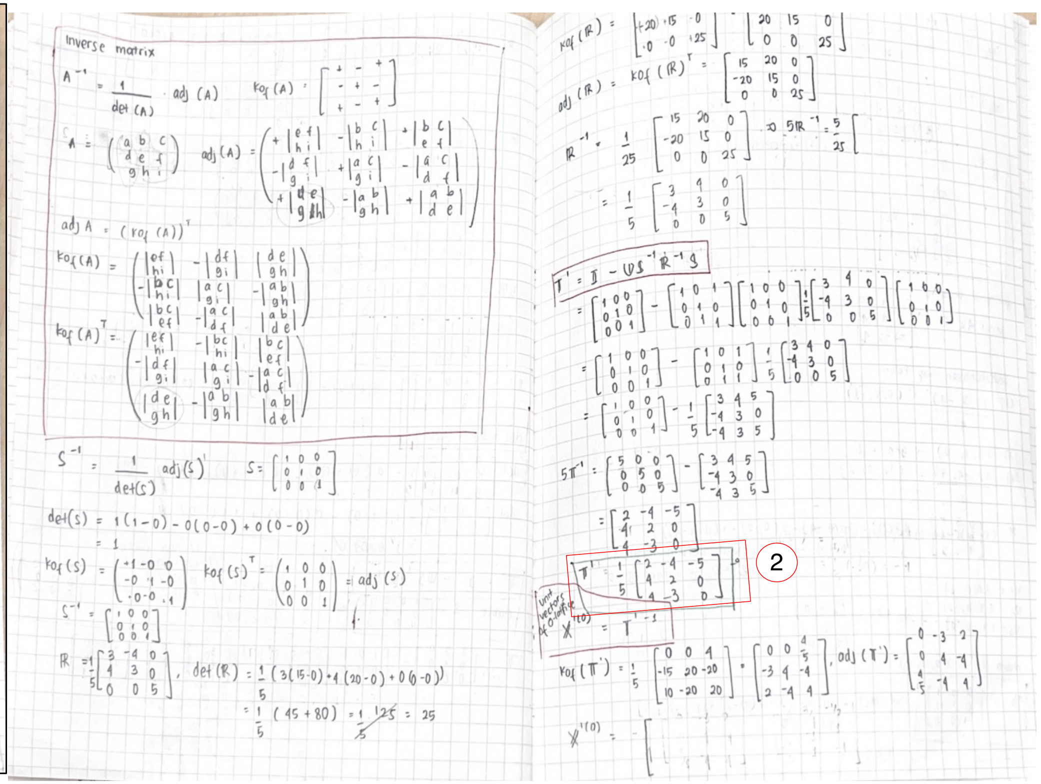

For the rotation axis [001], we have the unit vector $\boldsymbol{k} = [0,0,1]$. Then using $\theta = 53.1^\circ$ and Eqs. (6) and (7), we are able to get a rotation matrix $\mathbf{R}$:

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

Choose $\mathbf{U}$:

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

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

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

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

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

$$X'^{(0)} = \pi'^{-1} \quad \text{faktor det}(\pi') \text{ neglected}$$
$$= \text{adj}(\pi')$$
$$= \begin{bmatrix} 0 & 3/4 & 1/2 \\ 0 & 1 & -1 \\ -1 & -1/2 & 1 \end{bmatrix}$$

3

Hilangkan pecahan

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

Sederhanakan tiap kolom

(1) $\frac{(0, 0, -4)}{4} = (0, 0, -1)$

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

(3) $\frac{(2, -4, 4)}{2} = (1, -2, 2)$

$$M_1 = \begin{bmatrix} 0 & 3 & 1 \\ 0 & 4 & -2 \\ -1 & -2 & 2 \end{bmatrix} \quad \det(M) = [0(8-4) - 3(0-2) + 1(0-(-4))]$$
$$= 6 + 4 = 10 \rightarrow \text{masih belum minimal}$$
$$\Sigma = 10 \rightarrow \text{target } \Sigma = 5$$

$v_1 = (0, 0, -1)$

$v_2 = (3, 4, -2)$

$v_3 = (1, -2, 2)$

$\left.\begin{matrix} v_2 \\ v_3 \end{matrix}\right\} v_2 + v_3 = (4, 2, 0) \rightarrow (2, 1, 0)$

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

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

$$\boxed{M_2 = \begin{bmatrix} 0 & 2 & 1 \\ 0 & 1 & -2 \\ -1 & 0 & 2 \end{bmatrix}} \quad \det(M_2) = [0(2-0) - 2(0-2) + 1(0-(-1))]$$
$$= 4 + 1 = 5$$

Σ5

and

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

Still finding the step and transformation process

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

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

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

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

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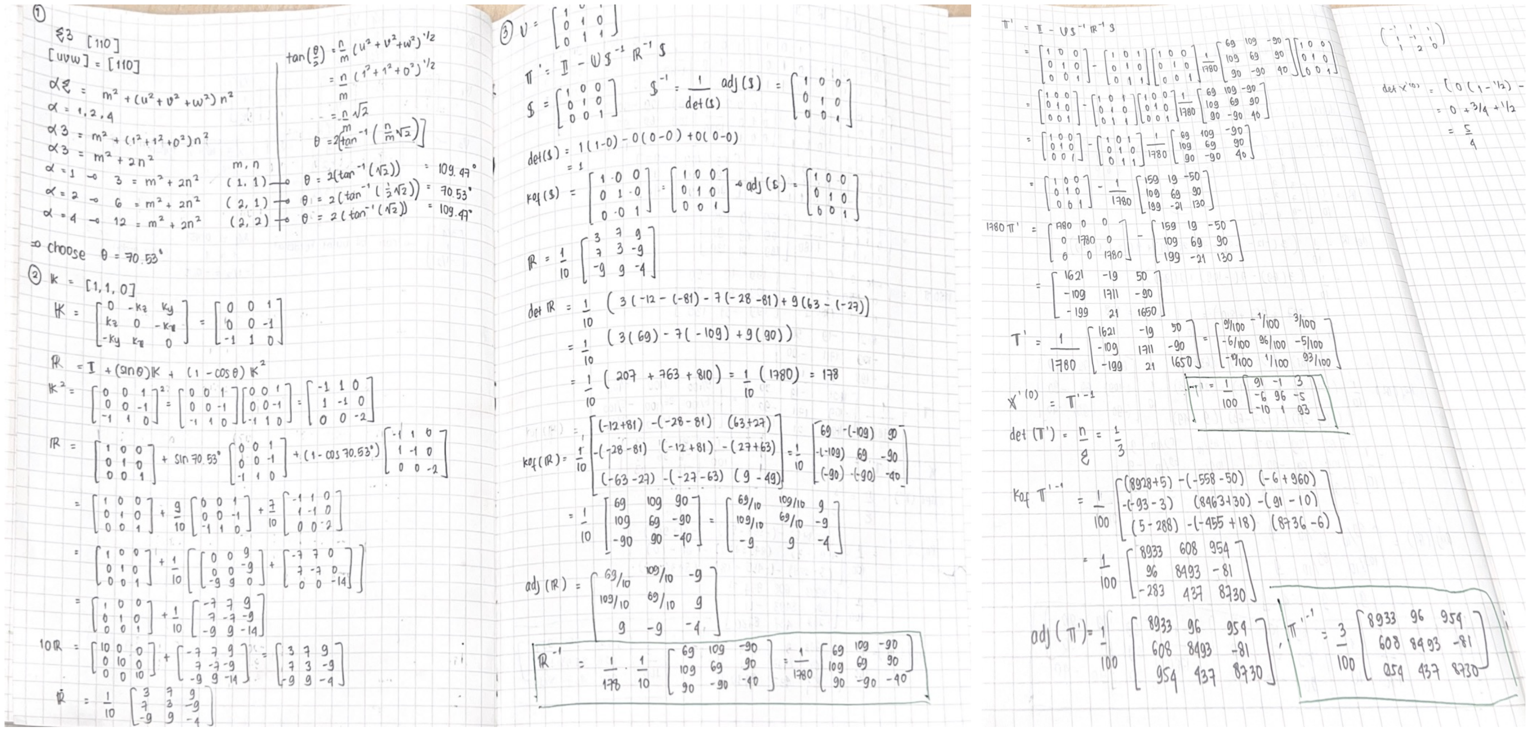

$$x(0)' = \frac{3}{100}\begin{bmatrix} 8933 & 96 & 954 \\ 608 & 8493 & -81 \\ 954 & 437 & 8730 \end{bmatrix}$$

???

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