a_i and b_i are augmented vectors representing the centroid of grain i in datasets A and B respectively:

$$[a_i]_{4x1} = \begin{bmatrix} a_i^x \\ a_i^y \\ a_i^z \\ 1 \end{bmatrix} \tag{1}$$

$$[b_i]_{4x1} = \begin{bmatrix} b_i^x \\ b_i^y \\ b_i^z \\ 1 \end{bmatrix} \tag{2}$$

$\boldsymbol{T}$ is a transformation mapping points from B to A:

$$\begin{aligned} [b_i']_{4x1} &= [\boldsymbol{T}]_{4x4}[b_i]_{4x1} \\ &= \begin{bmatrix} t_{11} & t_{12} & t_{13} & t_{14} \\ t_{11} & t_{12} & t_{13} & t_{14} \\ t_{11} & t_{12} & t_{13} & t_{14} \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} b_i^x \\ b_i^y \\ b_i^z \\ 1 \end{bmatrix} \\ &= \begin{bmatrix} b_i^x & b_i^y & b_i^z & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & b_i^x & b_i^y & b_i^z & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & b_i^x & b_i^y & b_i^z & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} t_{11} \\ t_{12} \\ t_{13} \\ t_{14} \\ t_{21} \\ t_{22} \\ t_{23} \\ t_{24} \\ t_{31} \\ t_{32} \\ t_{33} \\ t_{34} \\ 1 \end{bmatrix} \\ &= [\boldsymbol{B_i}]_{4x13}[t]_{13x1} \end{aligned} \tag{3}$$

The residual for a single centroid is the distance between its position in the two datasets after transforming dataset B with $\boldsymbol{T}$:

$$\begin{aligned} [r_i]_{1x1}^2 &= (a_i^x - b_i'^x)^2 + \left(a_i^y - b_i'^y\right)^2 + (a_i^z - b_i'^z)^2 \\ &= ([a_i]_{4x1} - [\boldsymbol{B_i}]_{4x13}[t]_{13x1})^T ([a_i]_{4x1} - [\boldsymbol{B_i}]_{4x13}[t]_{13x1}) \\ &= \left([a_i]_{1x4}^T - [t]_{1x13}^T[\boldsymbol{B_i}]_{13x4}^T\right) ([a_i]_{4x1} - [\boldsymbol{B_i}]_{4x13}[t]_{13x1}) \\ &= [a_i]_{1x4}^T[a_i]_{4x1} + [t]_{1x13}^T[\boldsymbol{B_i}]_{13x4}^T[\boldsymbol{B_i}]_{4x13}[t]_{13x1} \\ &\quad - [a_i]_{1x4}^T[\boldsymbol{B_i}]_{4x13}[t]_{13x1} - [t]_{1x13}^T[\boldsymbol{B_i}]_{13x4}^T[a_i]_{4x1} \\ &= [a_i]_{1x4}^T[a_i]_{4x1} + [t]_{1x13}^T[\boldsymbol{B_i}]_{13x4}^T[\boldsymbol{B_i}]_{4x13}[t]_{13x1} \\ &\quad - 2[a_i]_{1x4}^T[\boldsymbol{B_i}]_{4x13}[t]_{13x1} \end{aligned} \tag{4}$$

The total residual is the sum of residuals for each centroid pair:

$$\begin{aligned}[R]^2_{1x1} &= \sum_i [r_i]^2_{1x1} \\ &= \sum_i [a_i]^T_{1x4}[a_i]_{4x1} + \sum_i [t]^T_{1x13}[\boldsymbol{B_i}]^T_{13x4}[\boldsymbol{B_i}]_{4x13}[t]_{13x1} \\ &\quad - 2\sum_i [a_i]^T_{1x4}[\boldsymbol{B_i}]_{4x13}[t]_{13x1}\end{aligned} \tag{5}$$

R^2 is differentiated with respect to each component of $\boldsymbol{T}$ and equated with zero to find the least squares transformation:

$$\nabla_t [R]^2_{13x1} = 2\sum_i [\boldsymbol{B_i}]^T_{13x4}[\boldsymbol{B_i}]_{4x13}[t]_{13x1} - 2\sum_i [\boldsymbol{B_i}]^T_{13x4}[a_i]_{4x1} \tag{6}$$

$$\begin{aligned}[0]_{13x1} &= \nabla_t [R]^2_{13x1} \\ [t]_{13x1} &= \left(\sum_i [\boldsymbol{B_i}]^T_{13x4}[\boldsymbol{B_i}]_{4x13}\right)^{-1}\left(\sum_i [\boldsymbol{B_i}]^T_{13x4}[a_i]_{4x1}\right)\end{aligned} \tag{7}$$

This result can be simplified if the forms of each component are examined:

$$[\boldsymbol{B_i}]^T_{13x4}[\boldsymbol{B_i}]_{4x13} = \begin{bmatrix} & & & 0 \\ [b_i]_{4x1}[b_i]^T_{1x4} & [0]_{4x4} & [0]_{4x4} & \begin{matrix}0\\0\\0\end{matrix} \\ & & & \begin{matrix}0\\0\end{matrix} \\ [0]_{4x4} & [b_i]_{4x1}[b_i]^T_{1x4} & [0]_{4x4} & \begin{matrix}0\\0\\0\end{matrix} \\ & & & 0 \\ [0]_{4x4} & [0]_{4x4} & [b_i]_{4x1}[b_i]^T_{1x4} & \begin{matrix}0\\0\end{matrix} \\ 0\;0\;0\;0 & 0\;0\;0\;0 & 0\;0\;0\;0 & 1 \end{bmatrix} \tag{8}$$

$$\left([\boldsymbol{B_i}]_{13x4}^T[\boldsymbol{B_i}]_{4x13}\right)^{-1} = \begin{bmatrix} & & & 0 \\ & & & 0 \\ \left([b_i]_{4x1}[b_i]_{1x4}^T\right)^{-1} & [0]_{4x4} & [0]_{4x4} & 0 \\ & & & 0 \\ & & & 0 \\ & & & 0 \\ [0]_{4x4} & \left([b_i]_{4x1}[b_i]_{1x4}^T\right)^{-1} & [0]_{4x4} & 0 \\ & & & 0 \\ & & & 0 \\ & & & 0 \\ [0]_{4x4} & [0]_{4x4} & \left([b_i]_{4x1}[b_i]_{1x4}^T\right)^{-1} & 0 \\ & & & 0 \\ 0 \quad 0 \quad 0 \quad 0 & 0 \quad 0 \quad 0 \quad 0 & 0 \quad 0 \quad 0 \quad 0 & 1 \end{bmatrix} \tag{9}$$

$$[\boldsymbol{B_i}]_{13x4}^T[a_i]_{4x1} = \begin{bmatrix} b_i^x a_i^x \\ b_i^y a_i^x \\ b_i^z a_i^x \\ a_i^x \\ b_i^x a_i^y \\ b_i^y a_i^y \\ b_i^z a_i^y \\ a_i^y \\ b_i^x a_i^z \\ b_i^y a_i^z \\ b_i^z a_i^z \\ a_i^z \\ 1 \end{bmatrix} \tag{10}$$

Considering these forms, the transformation may expressed directly as a matrix (instead of as a vector of components):

$$
\begin{aligned}
[T]_{4x4} &= \begin{bmatrix} \left(\sum_i [b_i]_{4x1}[b_i]^T_{1x4}\right)^{-1} \sum_i \begin{bmatrix} b_i^x a_i^x & b_i^y a_i^x & b_i^z a_i^x & a_i^x \end{bmatrix}^T \\ \left(\sum_i [b_i]_{4x1}[b_i]^T_{1x4}\right)^{-1} \sum_i \begin{bmatrix} b_i^x a_i^y & b_i^y a_i^y & b_i^z a_i^y & a_i^y \end{bmatrix}^T \\ \left(\sum_i [b_i]_{4x1}[b_i]^T_{1x4}\right)^{-1} \sum_i \begin{bmatrix} b_i^x a_i^z & b_i^y a_i^z & b_i^z a_i^z & a_i^z \end{bmatrix}^T \\ 0 \quad 0 \quad 0 \quad 1 \end{bmatrix} \\
&= \begin{bmatrix} \left(\sum_i [b_i]_{4x1}[b_i]^T_{1x4}\right)^{-1} \sum_i \begin{bmatrix} b_i^x a_i^x & b_i^y a_i^x & b_i^z a_i^x & a_i^x \end{bmatrix}^T \\ \left(\sum_i [b_i]_{4x1}[b_i]^T_{1x4}\right)^{-1} \sum_i \begin{bmatrix} b_i^x a_i^y & b_i^y a_i^y & b_i^z a_i^y & a_i^y \end{bmatrix}^T \\ \left(\sum_i [b_i]_{4x1}[b_i]^T_{1x4}\right)^{-1} \sum_i \begin{bmatrix} b_i^x a_i^z & b_i^y a_i^z & b_i^z a_i^z & a_i^z \end{bmatrix}^T \\ \left(\sum_i [b_i]_{4x1}[b_i]^T_{1x4}\right)^{-1} \sum_i \begin{bmatrix} b_i^x & b_i^y & b_i^z & 1 \end{bmatrix}^T \end{bmatrix} \\
&= \left(\left(\sum_i [b_i]_{4x1}[b_i]^T_{1x4} \right)^{-1} \left(\sum_i \begin{bmatrix} b_i^x a_i^x & b_i^x a_i^y & b_i^x a_i^z & b_i^x \\ b_i^y a_i^x & b_i^y a_i^y & b_i^x a_i^z & b_i^y \\ b_i^z a_i^x & b_i^x a_i^y & b_i^z a_i^z & b_i^z \\ a_i^x & a_i^y & a_i^z & 1 \end{bmatrix} \right) \right)^T \\
&= \left(\left(\sum_i [b_i]_{4x1}[b_i]^T_{1x4} \right)^{-1} \left(\sum_i [b_i]_{4x1}[a_i]^T_{1x4} \right) \right)^T
\end{aligned}
\tag{11}
$$

This is equivalent to the familiar least squares regression solution:

$$\beta = \left(X^T X\right)^{-1} X^T Y \tag{12}$$

where:

$$
\begin{aligned}
\beta &= [\boldsymbol{T}]^T \\
X &= \begin{bmatrix} b_1^x & b_1^y & b_1^z & 1 \\ b_2^x & b_2^y & b_2^z & 1 \\ \vdots & \vdots & \vdots & \vdots \\ b_n^x & b_n^y & b_n^z & 1 \end{bmatrix} \\
Y &= \begin{bmatrix} a_1^x & a_1^y & a_1^z & 1 \\ a_2^x & a_2^y & a_2^z & 1 \\ \vdots & \vdots & \vdots & \vdots \\ a_n^x & a_n^y & a_n^z & 1 \end{bmatrix}
\end{aligned}
$$