# A simplified invariant line analysis for face-centred cubic/body-centred cubic precipitation systems

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#### Appendix

Let the unit rotation axis **u** as [$p_1$, $p_2$, $p_3$] and rotation angle as $\theta$, the rotation matrix ***R*** of an arbitrary axis **u** is

$$R=\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} = \begin{pmatrix} p_1^2(1-\cos\theta)+\cos\theta & p_1p_2(1-\cos\theta)-p_3\sin\theta & p_1p_3(1-\cos\theta)+p_2\sin\theta \\ p_2p_1(1-\cos\theta)+p_3\sin\theta & p_2^2(1-\cos\theta)+\cos\theta & p_2p_3(1-\cos\theta)-p_1\sin\theta \\ p_3p_1(1-\cos\theta)-p_2\sin\theta & p_3p_2(1-\cos\theta)+p_1\sin\theta & p_3^2(1-\cos\theta)+\cos\theta \end{pmatrix} \tag{A1}$$

The total strain matrix is

$$A=RB=\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}\begin{pmatrix} \eta_1 & 0 & 0 \\ 0 & \eta_2 & 0 \\ 0 & 0 & \eta_3 \end{pmatrix} \tag{A2}$$

Where $n_i$ ($i$ = 1,2,3) is the three main strains of Bain strain. The rigid-body rotation angle $\theta$ necessary to produce an invariant line can be obtained by setting the eigenvalues $\lambda$ equal to unity, so that

$$\cos\theta=\frac{\eta_1\eta_2\eta_3+p_1^2(\eta_1-\eta_2\eta_3)+p_2^2(\eta_2-\eta_3\eta_1)+p_3^2(\eta_3-\eta_1\eta_2)-1}{(1-p_1^2)(\eta_2\eta_3-\eta_1)+(1-p_2^2)(\eta_3\eta_1-\eta_2)+(1-p_3^2)(\eta_1\eta_2-\eta_3)} \tag{A3}$$

The eigenvalues are the roots of the equation

$$|A-\lambda I|=0 \tag{A4}$$

From which

$$|A-\lambda I|=|RB-\lambda I|=\lambda^3-S_1\lambda^2+S_2\lambda-S_3=0 \tag{A5}$$

Where, $S_1 = a_{11}n_1 + a_{22}n_2 + a_{33}n_3; S_2 = a_{11}n_2n_3 + a_{22}n_3n_1 + a_{33}n_1n_2; S_3 = n_1n_2n_3$

It is easy to prove that $S_2 - S_1 = S_3 - 1$.

The equation (A5) has a form of

$$\lambda^3 - S_1\lambda^2 + S_2\lambda - S_3 = (\lambda - 1)[\lambda^2 - (S_1 - 1)\lambda + S_3] = 0 \quad \text{(A6)}$$

The eigenvalues are then found to be

$$\lambda_1 = 1; \lambda_{2,3} = \frac{S_1 - 1 \pm \sqrt{(S_1 - 1)^2 - 4S_3}}{2} \quad \text{(A7)}$$

For the phase transformations, of which the range of $a_f/a_b$ meet the requirement, one can get three real eigenvalues $\lambda_i$ and three corresponding eigenvectors $V_i$ = [uvw], $i$ = 1, 2, 3

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} p_3p_1(1-a)(n_2+\lambda_i) + p_2b(\lambda_i - n_2) \\ p_3p_2(1-a)(n_1+\lambda_i) - p_1b(\lambda_i - n_1) \\ \dfrac{(n_1-\lambda_i)(n_2-\lambda_i) + (1-a)[(p_3^{\,2}-1)n_1n_2 + \lambda_i(1-p_1^{\,2})n_1 + \lambda_i(1-p_2^{\,2})n_2]}{n_3} \end{pmatrix} \quad \text{(A8)}$$

Here, a = cos $\theta$ and b = sin $\theta$.