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

Hongwei Liu\textsuperscript{a}, Eric R Waclawik\textsuperscript{b} and Chengping Luo\textsuperscript{c}

\textsuperscript{a} School of Materials Science and Engineering, Guangxi University, Nanning, 530004, People’s Republic of China, \textsuperscript{b} Discipline of Chemistry, School of Science and Technology, Queensland University of Technology, Brisbane 4001 QLD, Australia, and \textsuperscript{c} School of Materials Science and Engineering, South China University of Technology, Guangzhou 510640, People’s Republic of China. *Correspondence author, E-mail: hwliu@gxu.edu.cn

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

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

(A1)

The total strain matrix is

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

(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

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

(A3)

The eigenvalues are the roots of the equation

$$|A - \lambda I| = 0$$

(A4)

From which

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

(A5)
Where, 

\[ S_1 = a_{11}n_1 + a_{22}n_2 + a_{33}n_3; S_2 = a_{11}n_2n_3 + a_{22}n_1n_3 + a_{33}n_1n_2; S_3 = n_1n_2n_3 \]

It is easy to prove that \( S_2 - S_1 = S_3 - 1 \).

The equation (A5) has a form of

\[ \lambda^3 - S_1\lambda^2 + S_2\lambda - S_3 = (\lambda - 1)[\lambda^2 - (S_1 - 1)\lambda + S_3] = 0 \]

The eigenvalues are then found to be

\[ \lambda_1 = 1; \lambda_{2,3} = \frac{S_1 - 1 \pm \sqrt{(S_1 - 1)^2 - 4S_3}}{2} \]

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

\[
\begin{bmatrix}
  u \\
  v \\
  w
\end{bmatrix} = \begin{bmatrix}
  \frac{p_3p_1(1-a)(n_2 + \lambda_i) + p_2b(\lambda_i - n_2)}{p_3p_1p_2(1-a)(n_1 + \lambda_i) - p_1b(\lambda_i - n_1)} \\
  \frac{(n_1 - \lambda_i)(n_2 - \lambda_i) + (1-a)((p_3^2 - 1)n_1n_2 + \lambda_i(1-p_1^2)n_1 + \lambda_i(1-p_2^2)n_2)}{n_3}
\end{bmatrix}
\]

Here, \( a = \cos \theta \) and \( b = \sin \theta \).