Anisotropic Elastic Stiffness Matrix Rotation

A rotation matrix ($R_{\varphi_1,\Phi,\varphi_2}$) was constructed from the Euler angles ($\varphi_1, \Phi, \varphi_2$) of the reference pattern ($EBSP_0$) as in equation (1) [1].

$$R_{\varphi_1,\Phi,\varphi_2} =$$

$$\begin{bmatrix} \cos\varphi_1 \cos\varphi_2 - \cos\Phi \sin\varphi_1 \sin\varphi_2 & \cos\Phi \cos\varphi_1 \sin\varphi_2 + \sin\varphi_1 \cos\varphi_2 & \sin\Phi \sin\varphi_2 \\ -\cos\varphi_1 \sin\varphi_2 - \cos\Phi \sin\varphi_1 \cos\varphi_2 & \cos\Phi \cos\varphi_1 \cos\varphi_2 - \sin\varphi_1 \sin\varphi_2 & \sin\Phi \cos\varphi_2 \\ \sin\Phi \sin\varphi_1 & -\sin\Phi \cos\varphi_1 & \cos\Phi \end{bmatrix} \quad (1)$$

The local crystal anisotropic elastic stiffness matrix, C, is defined as [2]:

$$C = \begin{bmatrix} 230 & 135 & 135 & 0 & 0 & 0 \\ & 230 & 135 & 0 & 0 & 0 \\ & & 230 & 0 & 0 & 0 \\ & & & 117 & 0 & 0 \\ & & Sym. & & 117 & 0 \\ & & & & & 117 \end{bmatrix} GPa \quad (2)$$

Then by using the rotation matrix, the anisotropic elastic stiffness matrix, C_{EBSP_0}, can be mapped from the reference crystal coordinate system to the local coordinate system as below [3]:

$$C_{EBSP_0} = T_\sigma^{-1}\, C\, T_\varepsilon \quad (3)$$

Where:

$$T_\sigma =$$

$$\begin{bmatrix} R_{11}^2 & R_{21}^2 & R_{31}^2 & 2R_{11}R_{21} & 2R_{21}R_{31} & 2R_{31}R_{11} \\ R_{12}^2 & R_{22}^2 & R_{32}^2 & 2R_{12}R_{22} & 2R_{22}R_{32} & 2R_{32}R_{12} \\ R_{13}^2 & R_{23}^2 & R_{33}^2 & 2R_{13}R_{23} & 2R_{23}R_{33} & 2R_{33}R_{13} \\ R_{11}R_{12} & R_{21}R_{22} & R_{31}R_{32} & R_{11}R_{22} + R_{12}R_{21} & R_{21}R_{32} + R_{31}R_{22} & R_{31}R_{12} + R_{32}R_{11} \\ R_{12}R_{13} & R_{22}R_{23} & R_{33}R_{32} & R_{23}R_{12} + R_{13}R_{22} & R_{22}R_{33} + R_{32}R_{23} & R_{32}R_{13} + R_{12}R_{33} \\ R_{11}R_{13} & R_{23}R_{21} & R_{33}R_{31} & R_{13}R_{21} + R_{11}R_{23} & R_{23}R_{31} + R_{21}R_{33} & R_{33}R_{11} + R_{31}R_{13} \end{bmatrix} \quad (4)$$

$$T_\varepsilon =$$

$$\begin{bmatrix} R_{11}^2 & R_{21}^2 & R_{31}^2 & R_{11}R_{21} & R_{21}R_{31} & R_{31}R_{11} \\ R_{12}^2 & R_{22}^2 & R_{32}^2 & R_{12}R_{22} & R_{22}R_{32} & R_{32}R_{12} \\ R_{13}^2 & R_{23}^2 & R_{33}^2 & R_{13}R_{23} & R_{23}R_{33} & R_{33}R_{13} \\ 2R_{11}R_{12} & 2R_{21}R_{22} & 2R_{31}R_{32} & R_{11}R_{22}+R_{12}R_{21} & R_{21}R_{32}+R_{31}R_{22} & R_{31}R_{12}+R_{32}R_{11} \\ 2R_{12}R_{13} & 2R_{22}R_{23} & 2R_{33}R_{32} & R_{23}R_{12}+R_{13}R_{22} & R_{22}R_{33}+R_{32}R_{23} & R_{32}R_{13}+R_{12}R_{33} \\ 2R_{11}R_{13} & 2R_{23}R_{21} & 2R_{33}R_{31} & R_{13}R_{21}+R_{11}R_{23} & R_{23}R_{31}+R_{21}R_{33} & R_{33}R_{11}+R_{31}R_{13} \end{bmatrix} \quad (5)$$

Descriptions and notations for rotation, and T_σ, T_ε and T matrices are different across literature. The transformation (Q) matrix is used for rotation of the coordinate system, and this differs from the rotation (R) matrix to rotate tensors (counterclockwise) in a fixed coordinate system. Also, the Bunge rotation (X Z' X'') where Bunger-Euler rotation (Z X' Z'') is conventionally used for EBSD [4]. For stiffness rotation, there are differences in the notation for ordering of the shear components [3,5]. A comparison between rotations in the example of silicon (111), using different methods and notations: Voigt [6], Reuss [7], Hill [8], Lekhnitskii [9] and Salvati *et al.* [10], Dunne *et al.* [3] methods can be found here [1].

To confirm the validity of our rotations, we show below values for the (001) Silicon stiffness tensor – in Voigt matrix representation – rotated to (111) using various methods:

1. Voigt [6]:

$$\begin{bmatrix} 193.35 & 57.65 & 42.5 & -8.61 & -0.38 & 0.85 \\ 57.65 & 183.94 & 51.91 & 12.84 & 1.21 & -0.98 \\ 42.5 & 51.91 & 199.09 & -4.24 & -0.83 & 0.13 \\ -8.61 & 12.84 & -4.24 & 67.61 & 0.13 & 1.21 \\ -0.38 & 1.21 & -0.83 & 0.13 & 58.2 & -8.61 \\ 0.85 & -0.98 & 0.13 & 1.21 & -8.61 & 73.35 \end{bmatrix}$$

2. Reuss [7]:

$$\begin{bmatrix} 191.86 & 58.39 & 43.25 & -8.61 & -0.38 & 0.85 \\ 58.39 & 182.45 & 52.66 & 12.84 & 1.21 & -0.98 \\ 43.25 & 52.66 & 197.6 & -4.24 & -0.83 & 0.13 \\ -8.61 & 12.84 & -4.24 & 66.49 & 0.13 & 1.21 \\ -0.38 & 1.21 & -0.83 & 0.13 & 57.08 & -8.61 \\ 0.85 & -0.98 & 0.13 & 1.21 & -8.61 & 72.23 \end{bmatrix}$$

[1] See https://bit.ly/3hrmZlo for code and Silicon (111) dataset for verification.

3. Hill [8] (which in principle is Voight and Reuss methods average):

$$\begin{bmatrix} 192.61 & 58.02 & 42.87 & -8.61 & -0.38 & 0.85 \\ 58.02 & 183.19 & 52.28 & 12.84 & 1.21 & -0.98 \\ 42.87 & 52.28 & 198.34 & -4.24 & -0.83 & 0.13 \\ -8.61 & 12.84 & -4.24 & 67.05 & 0.13 & 1.21 \\ -0.38 & 1.21 & -0.83 & 0.13 & 57.64 & -8.61 \\ 0.85 & -0.98 & 0.13 & 1.21 & -8.61 & 72.79 \end{bmatrix}$$

1. Lekhnitskii [9] and Salvati *et al.* [10]:

$$\begin{bmatrix} 194.49 & 58.93 & 40.08 & -10.70 & -0.48 & 1.05 \\ 58.93 & 182.78 & 51.80 & 15.97 & 1.50 & -1.21 \\ 40.08 & 51.80 & 201.62 & -5.27 & -1.02 & 0.17 \\ -10.70 & 15.97 & -5.27 & 67.50 & 0.17 & 1.50 \\ -0.48 & 1.50 & -1.02 & 0.165 & 55.78 & -10.70 \\ 1.05 & -1.21 & 0.17 & 1.50 & -10.70 & 74.63 \end{bmatrix}$$

2. Dunne *et al.* [3] (used in the current paper):

$$\begin{bmatrix} 194.49 & 58.92 & 40.08 & 3.76 & -10.70 & -0.48 \\ 58.93 & 182.78 & 51.80 & -6.03 & 15.97 & 1.50 \\ 40.08 & 51.80 & 201.62 & 2.27 & -5.27 & -1.02 \\ 1.05 & -1.21 & 0.17 & 84.78 & 1.50 & -10.70 \\ -10.70 & 15.97 & -5.27 & 67.50 & 67.50 & 0.17 \\ -0.48 & 1.50 & -1.02 & 12.57 & 0.17 & 55.78 \end{bmatrix}$$

These values are consistent with Ref. [5] within ±4% with Lekhnitskii [9] and Salvati *et al.* [10] being the most accurate.

Please note the difference in the shear components definition as here it follows ϵ_{xy}, ϵ_{xz}, and ϵ_{yz} and Ref. [5] uses a different order of ϵ_{yz}, ϵ_{xz}, and ϵ_{xy} instead. We also like to note that Ref. [10] uses Bunge rotation (X Z' X'') where Bunger-Euler rotation (Z X' Z'') is conventionally used for EBSD [4].

References

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