

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 [1]:

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

2. Reuss [2]:

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

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

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

4. Lekhnitskii [4] and Salvati *et al.* [5]:

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

5. Dunne *et al.* [6] (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. [7] within $\pm 4\%$.

Please note the difference in the shear components definition as here it follows ϵ_{xy} , ϵ_{xz} , and ϵ_{yz} and Ref. [7] uses a different order of ϵ_{yz} , ϵ_{xz} , and ϵ_{xy} instead. We also like to note that Ref. [5] uses Bunge rotation (X Z' X'') where Bunge-Euler rotation (Z X' Z'') is conventionally used for EBSD [8]. From these comparisons, we do not think a recalculation of the results is warranted, however, this discussion on this is now included to the Section B of the Supplementary Information. The amended text now reads:

“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 Bunge-Euler rotation (Z X' Z'') is conventionally used for EBSD [8]. For stiffness rotation, there are differences in the notation for ordering of the shear components [18],[20]. A comparison between rotations in the example of silicon (111), using different methods and notations: Voigt [21], Reuss [22], Hill [23], Lekhnitskii [24] and Salvati *et al.* [25], Dunne *et al.* [18] methods can be found here¹.”

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

References

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