Twinning in face centered cubic metals

We consider FCC (face centered cubic) single crystals. The lattice coordinate frame is defined by the Cartesian vectors:

$$\underline{\boldsymbol{d}}_1 = [100], \quad \underline{\boldsymbol{d}}_2 = [010], \quad \underline{\boldsymbol{d}}_3 = [001]$$

Vector components with respect to this coordinate system are denoted with the sign $\sharp$ in the form:

$$\underline{\boldsymbol{t}} = t_{\sharp i}\, \underline{\boldsymbol{d}}_i$$

where repeated indices are summed.
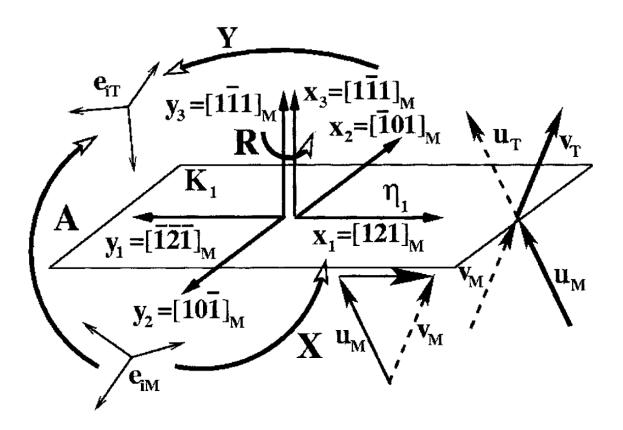
1 Elements of twinning in FCC metals and alloys

Figure 1: Characteristics of the twin boundary and orientations of crystals, after [1]. We call A the crystal below the plane and B the twin crystal above the plane. These names are not indicated on the drawing (the letter A here has a different meaning).

Twin crystals with FCC lattice possess specific orientations relationships represented in Fig. 1. We call A and B the two crystals separated a grain boundary called called twin boundary. The twin boundary is the $(1\bar{1}1)$ plane in crystals A and B. Let us define the vectors

$(\underline{\boldsymbol{X}}_1, \underline{\boldsymbol{X}}_2, \underline{\boldsymbol{X}}_3)$ where $\underline{\boldsymbol{X}}_3$ is parallel to the normal to the twin boundary, $\underline{\boldsymbol{X}}_1$ is parallel to the lattice direction [121] of the mother crystal A. In that case, according to figure 1, the vector $\underline{\boldsymbol{X}}_1$ coincides with the direction $[\bar{1}2\bar{1}]$ in the twinned crystal B. As a result:
In crystal A:

$$\underline{\boldsymbol{X}}_1 = [121]_A, \quad \underline{\boldsymbol{X}}_2 = [\bar{1}01]_A, \quad \underline{\boldsymbol{X}}_3 = [1\bar{1}1]_A$$

In crystal B:

$$\underline{\boldsymbol{X}}_1 = [\bar{1}2\bar{1}]_B, \quad \underline{\boldsymbol{X}}_2 = [10\bar{1}]_B, \quad \underline{\boldsymbol{X}}_3 = [1\bar{1}1]_B$$

Let us define the corresponding normalized vectors in crystal A:

$$\underline{\boldsymbol{e}}_1 = [121]/\sqrt{6}, \ \underline{\boldsymbol{e}}_2 = [\bar{1}01]/\sqrt{2}, \ \underline{\boldsymbol{e}}_3 = [1\bar{1}1]/\sqrt{3}$$

The transformation from mother orientation A to twin orientation B is the $180°$ rotation[1] with respect to axis $\underline{\boldsymbol{e}}_3$:

$$\underset{\sim}{\boldsymbol{S}}_1 = -\underline{\boldsymbol{e}}_1 \otimes \underline{\boldsymbol{e}}_1 - \underline{\boldsymbol{e}}_2 \otimes \underline{\boldsymbol{e}}_2 + \underline{\boldsymbol{e}}_3 \otimes \underline{\boldsymbol{e}}_3$$

Give the matrix form of this rotation using the components in the lattice coordinate system of crystal A.
Give the components of images of the basis vectors $\underline{\boldsymbol{e}}_1, \underline{\boldsymbol{e}}_2$ and $\underline{\boldsymbol{e}}_3$ in the lattice coordinate frame of crystal A.

The matrix form of the rotation in the lattice coordinate system $\sharp A$ is

$$\frac{1}{3}\begin{bmatrix} -1 & -2 & 2 \\ -2 & -1 & -2 \\ 2 & -2 & -1 \end{bmatrix}_{\sharp A}$$

This rotation transforms the frame $(\underline{\boldsymbol{e}}_1, \underline{\boldsymbol{e}}_2, \underline{\boldsymbol{e}}_3)$ into $(-\underline{\boldsymbol{e}}_1, -\underline{\boldsymbol{e}}_2, \underline{\boldsymbol{e}}_3)$.

$$\underline{\boldsymbol{e}}_1' = -\underline{\boldsymbol{e}}_1 = [\bar{1}\bar{2}\bar{1}]_A/\sqrt{6}, \ \underline{\boldsymbol{e}}_2' = -\underline{\boldsymbol{e}}_2 = [10\bar{1}]_A/\sqrt{2}, \ \underline{\boldsymbol{e}}_3' = \underline{\boldsymbol{e}}_3 = [1\bar{1}1]_A/\sqrt{3}$$

2 Anisotropic elasticity

In this section, the single crystals undergo only elastic deformation.

2.1 Fourth rank tensors for cubic elasticity

We introduce the fourth order tensors $\underset{\approx}{\boldsymbol{I}}, \underset{\approx}{\boldsymbol{J}}$ and $\underset{\approx}{\boldsymbol{K}}$ acting on symmetric second order tensors $\underset{\sim}{\boldsymbol{A}}$ in the following way:

$$\underset{\approx}{\boldsymbol{I}} : \underset{\sim}{\boldsymbol{A}} = \underset{\sim}{\boldsymbol{A}}, \quad \underset{\approx}{\boldsymbol{J}} : \underset{\sim}{\boldsymbol{A}} = \frac{1}{3}(\text{trace } \underset{\sim}{\boldsymbol{A}})\underset{\sim}{\boldsymbol{1}}, \quad \underset{\approx}{\boldsymbol{K}} : \underset{\sim}{\boldsymbol{A}} = \underset{\sim}{\boldsymbol{A}}^{\text{dev}} \tag{1}$$

where $\underset{\sim}{\boldsymbol{A}}^{\text{dev}}$ is the deviatoric part of $\underset{\sim}{\boldsymbol{A}}$. It is apparent that $\underset{\approx}{\boldsymbol{I}} = \underset{\approx}{\boldsymbol{J}} + \underset{\approx}{\boldsymbol{K}}$.
Isotropic fourth order tensors of elasticity take the form:

$$\underset{\approx}{\boldsymbol{C}} = 3\kappa\underset{\approx}{\boldsymbol{J}} + 2\mu\underset{\approx}{\boldsymbol{K}}, \quad \underset{\approx}{\boldsymbol{S}} = \frac{1}{3\kappa}\underset{\approx}{\boldsymbol{J}} + \frac{1}{2\mu}\underset{\approx}{\boldsymbol{K}}$$

---

[1]It is the composition of mirror symmetry with respect to $(1\bar{1}1)$ and a central symmetry to restore the orientation of the triad.

with κ, the bulk modulus, and μ, the shear modulus.

The fourth order tensor of elastic moduli is $\underset{\approx}{\boldsymbol{C}}$ and its inverse, $\underset{\approx}{\boldsymbol{S}}$, is the fourth rank tensor of elastic compliance.

For cubic tensors, we introduce

$$\underset{\approx}{\boldsymbol{D}} = \underline{\boldsymbol{d}}_1 \otimes \underline{\boldsymbol{d}}_1 \otimes \underline{\boldsymbol{d}}_1 \otimes \underline{\boldsymbol{d}}_1 + \underline{\boldsymbol{d}}_2 \otimes \underline{\boldsymbol{d}}_2 \otimes \underline{\boldsymbol{d}}_2 \otimes \underline{\boldsymbol{d}}_2 + \underline{\boldsymbol{d}}_3 \otimes \underline{\boldsymbol{d}}_3 \otimes \underline{\boldsymbol{d}}_3 \otimes \underline{\boldsymbol{d}}_3$$

where $\underline{\boldsymbol{d}}_i$ are the three cubic directions $< 100 >$ of the lattice, as earlier defined. The deviatoric projection tensor $\underset{\approx}{\boldsymbol{K}}$ is then decomposed into:

$$\underset{\approx}{\boldsymbol{K}} = \underset{\approx}{\boldsymbol{K}}_a + \underset{\approx}{\boldsymbol{K}}_b, \quad \text{with} \quad \underset{\approx}{\boldsymbol{K}}_a = \underset{\approx}{\boldsymbol{D}} - \underset{\approx}{\boldsymbol{J}}$$

. The action of $\underset{\approx}{\boldsymbol{K}}_a$ and $\underset{\approx}{\boldsymbol{K}}_b$ on symmetric second order tensors is as follows:

$$
\begin{bmatrix}
a_{\sharp 11} & a_{\sharp 12} & a_{\sharp 13} \\
a_{\sharp 12} & a_{\sharp 22} & a_{\sharp 23} \\
a_{\sharp 13} & a_{\sharp 23} & a_{\sharp 33}
\end{bmatrix}
\xrightarrow{\underset{\approx}{\boldsymbol{K}}_a}
\begin{bmatrix}
a_{\sharp 11} & 0 & 0 \\
0 & a_{\sharp 22} & 0 \\
0 & 0 & a_{\sharp 33}
\end{bmatrix}
- \frac{a_{\sharp 11} + a_{\sharp 22} + a_{\sharp 33}}{3}
\begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix}
$$

$$
\begin{bmatrix}
a_{\sharp 11} & a_{\sharp 12} & a_{\sharp 13} \\
a_{\sharp 12} & a_{\sharp 22} & a_{\sharp 23} \\
a_{\sharp 13} & a_{\sharp 23} & a_{\sharp 33}
\end{bmatrix}
\xrightarrow{\underset{\approx}{\boldsymbol{K}}_b}
\begin{bmatrix}
0 & a_{\sharp 12} & a_{\sharp 13} \\
a_{\sharp 12} & 0 & a_{\sharp 23} \\
a_{\sharp 13} & a_{\sharp 23} & 0
\end{bmatrix}
$$

in the cubic lattice coordinate frame.

The fourth tensor of elastic moduli takes the following form in the case of cubic elasticity [2, 3]:

$$\underset{\approx}{\boldsymbol{C}} = 3\kappa \underset{\approx}{\boldsymbol{J}} + 2\mu_a \underset{\approx}{\boldsymbol{K}}_a + 2\mu_b \underset{\approx}{\boldsymbol{K}}_b, \quad \underset{\approx}{\boldsymbol{S}} = \frac{1}{3\kappa} \underset{\approx}{\boldsymbol{J}} + \frac{1}{2\mu_a} \underset{\approx}{\boldsymbol{K}}_a + \frac{1}{2\mu_b} \underset{\approx}{\boldsymbol{K}}_b \tag{2}$$

The moduli κ, μ_a, μ_b are directly related to the three independent Voigt components:

$$3\kappa = C_{11} + 2C_{12}, \quad 2\mu_a = C_{11} - C_{12}, \quad 2\mu_b = 2C_{44}$$

The isotropic case is retrieved when the anisotropy coefficient

$$a = \frac{2C_{44}}{C_{11} - C_{12}} = 1$$

In the case of an austenitic steel 316L (used in particular for components in nuclear reactors) having the following elasticity moduli:

$$C_{11} = 199000\,\text{MPa}, \quad C_{12} = 136000\,\text{MPa}, \quad C_{44} = 105000\,\text{MPa}$$

compute the bulk and shear moduli κ, μ_a, μ_b and the anisotropy coefficient a. Comment the latter result.

We find

$$\kappa = 157000\,\text{MPa}, \quad \mu_a = 31500\,\text{MPa}, \quad \mu_b = 105000\,\text{MPa}, \quad a = 3.33$$

The anisotropy is strong and comparable to that of pure copper.

2.2 Single crystal in tension along an arbitrary direction

The tensile stress tensor is

$$\underset{\sim}{\boldsymbol{\sigma}} = \sigma\, \underline{\boldsymbol{t}} \otimes \underline{\boldsymbol{t}}$$

where the tensile direction $\underline{\boldsymbol{t}}$, taken as a unit vector, has the lattice components $t_{\sharp 1}, t_{\sharp 2}, t_{\sharp 3}$.

The strain tensor induced by tension is obtained from Hooke's law:

$$\underset{\sim}{\boldsymbol{\varepsilon}} = \sigma\, \underset{\approx}{\boldsymbol{S}} : (\underline{\boldsymbol{t}} \otimes \underline{\boldsymbol{t}})$$

Check that the application of Hooke's law (2) provides the following components of the strain in the lattice coordinate frame A:

$$
\begin{aligned}
\varepsilon_{\sharp 11} &= \sigma\left(\frac{1}{9\kappa} + \frac{1}{2\mu_a}(t_{\sharp 1}^2 - \frac{1}{3})\right)\\[4pt]
\varepsilon_{\sharp 22} &= \sigma\left(\frac{1}{9\kappa} + \frac{1}{2\mu_a}(t_{\sharp 2}^2 - \frac{1}{3})\right)\\[4pt]
\varepsilon_{\sharp 33} &= \sigma\left(\frac{1}{9\kappa} + \frac{1}{2\mu_a}(t_{\sharp 3}^2 - \frac{1}{3})\right)\\[4pt]
\varepsilon_{\sharp 12} &= \frac{\sigma}{2\mu_b}t_{\sharp 1}t_{\sharp 2}\\[4pt]
\varepsilon_{\sharp 23} &= \frac{\sigma}{2\mu_b}t_{\sharp 2}t_{\sharp 3}\\[4pt]
\varepsilon_{\sharp 31} &= \frac{\sigma}{2\mu_b}t_{\sharp 3}t_{\sharp 1}
\end{aligned}
$$

where $t_{\sharp 1}, t_{\sharp 2}$ and $t_{\sharp 3}$ are the components of the tensile direction in the lattice coordinate frame A.

2.3 Tension along [121]

Compute the elastic strain lattice components when the single crystal A is submitted to simple tension in the direction [121].
The components of this strain tensor with respect to the orthonormal basis $(\underline{\boldsymbol{e}}_1, \underline{\boldsymbol{e}}_2, \underline{\boldsymbol{e}}_3)$ can be computed as[2]:

$$[\underset{\sim}{\boldsymbol{\varepsilon}}]_{(\underline{\boldsymbol{e}}_1,\underline{\boldsymbol{e}}_2,\underline{\boldsymbol{e}}_3)} = \sigma \times 10^{-6}\begin{bmatrix} 2.867 & 0 & -1.309\\ 0 & -1.366 & 0\\ -1.309 & 0 & -0.4398 \end{bmatrix}_{(\underline{\boldsymbol{e}}_1,\underline{\boldsymbol{e}}_2,\underline{\boldsymbol{e}}_3)}$$

in the case of an austenitic steel single crystal. Give then the components with respect to the same coordinate frame $(\underline{\boldsymbol{e}}_1, \underline{\boldsymbol{e}}_2, \underline{\boldsymbol{e}}_3)$ of the strain tensor of single crystal B subjected to tension along the same direction $\underline{\boldsymbol{e}}_1$.
Justify then that the tensile deformation of the twin with periodic boundary conditions looks like the deformed finite element mesh of figure 2, when it is loaded along the direction $\underline{\boldsymbol{e}}_1$.

For $t_{\sharp 1} = 1/\sqrt{6}, t_{\sharp 2} = 2/\sqrt{6}, t_{\sharp 3} = 1/\sqrt{6}$, we find

$$\varepsilon_{\sharp 11} = \varepsilon_{\sharp 33} = \sigma\left(\frac{1}{9\kappa} - \frac{1}{6\mu_a}\right), \quad \varepsilon_{\sharp 22} = \sigma\left(\frac{1}{9\kappa} + \frac{1}{6\mu_a}\right)$$

---

[2]It is not requested to make the calculation.

$$\varepsilon_{\sharp 12} = \varepsilon_{\sharp 23} = \frac{\sigma}{6\mu_b}, \quad \varepsilon_{\sharp 31} = \frac{\sigma}{12\mu_b}$$

The basis $(\underline{e}_1, \underline{e}_2, \underline{e}_3)$ represents the definition basis for the finite element mesh of the twin laminate. The deformed crystal B is obtained by the 180°–rotation around $\underline{e}_3$. Therefore,

$$[\underline{\underline{\varepsilon}}]_{(\underline{e}_1, \underline{e}_2, \underline{e}_3)} = \sigma \times 10^{-6} \begin{bmatrix} 2.867 & 0 & 1.309 \\ 0 & -1.366 & 0 \\ 1.309 & 0 & -0.4398 \end{bmatrix}_{(\underline{e}_1, \underline{e}_2, \underline{e}_3)}$$

The shear component in the plane 1–3 is opposite. When both crystals are glued allowing for periodic boundary conditions, both deformations are compatible and the deformed shape is the arrow of figure 2.
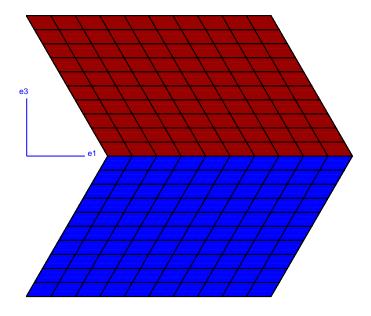

Figure 2: Tension of a twin laminate with periodicity conditions. The horizontal direction x is the tensile direction. The vertical direction z is the normal to the twin boundary. The red and blue colors denote the A and B crystals. Deformation is strongly magnified compared to reality.

3   Plastic slip activity in the twin boundary

The twin made of the crystals A and B is subjected to simple tension along the direction

$$\underline{t} = \cos\alpha\,\underline{e}_1 + \sin\alpha\,\underline{e}_3$$

where α denotes the angle between tensile direction and direction $\underline{e}_1$. It is assumed that the stress state in each crystal also simple tension along $\underline{t}$ with corresponding stress σ.

Compute the Schmid factors for the slip systems with slip plane parallel to the twin boundary. For which angle α does the resolved shear stress on these slip systems reach a maximum value?

The tensile direction can be written in the form:

$$\underline{t} = \frac{\cos\alpha}{\sqrt{6}}[121] + \frac{\sin\alpha}{\sqrt{3}}[1\bar{1}1]$$

The three candidate slip systems are $(1\bar{1}1)[\bar{1}01]$; $(1\bar{1}1)[110]$ and $(1\bar{1}1)[\bar{0}11]$. The first slip system cannot be activated since $[\bar{1}01]$ is orthogonal to both $\underline{e}_1$ and $\underline{e}_2$. We compute the following scalar products:

$$\underline{t} \cdot [1\bar{1}1]/\sqrt{3} = \sin \alpha$$

$$\underline{t} \cdot [110]/\sqrt{2} = \underline{t} \cdot [011]/\sqrt{2} = \frac{\sqrt{3}}{6} \cos \alpha$$

The two last slip systems therefore have the same Schmid factor equal to

$$M = \frac{\sqrt{3} \sin \alpha \cos \alpha}{6} = \frac{\sqrt{3}}{12} \sin 2\alpha$$

which takes the maximum value for $\alpha = \pm 45°$

References

[1] M Niewczas. *Dislocations in Solids, F.R.N. Nabarro and J.P. Hirth, editors, vol. 13*, chapter Dislocations and Twinning in Face Centered Cubic Crystals, pages 263–364. Elsevier, Berlin, 2007.

[2] M. Bornert, T. Bretheau, and P. Gilormini. *Homogénéisation en mécanique des matériaux.* Hermès, 2001.

[3] J. Qu and M. Cherkaoui. *Fundamentals of micromechanics of solids.* Wiley, Hoboken, New Jersey, USA, 2006.