Simple tension within the framework of multiplicative crystal plasticity

The objective of the exercise is to investigate the influence of finite deformations on the computation of resolved shear stresses in a FCC single crystal in the case of pure tension. The slip systems are the usual slip systems of FCC crystals like pure copper. The tensile direction $\underline{e}_3$ is parallel to the [001] direction of the single crystal.

The multiplicative decomposition is used:

$$\underset{\sim}{\boldsymbol{F}} = \underset{\sim}{\boldsymbol{E}} \cdot \underset{\sim}{\boldsymbol{P}}, \quad J_e = \det \underset{\sim}{\boldsymbol{E}}, \quad J_p = \det \underset{\sim}{\boldsymbol{P}}, \quad J = J_e J_p = \det \underset{\sim}{\boldsymbol{F}} \tag{1}$$

where $\underset{\sim}{\boldsymbol{E}}$ and $\underset{\sim}{\boldsymbol{P}}$ respectively are the elastic and plastic deformation tensors. The elastic strain tensor is

$$\underset{\sim}{\boldsymbol{E}}^e = \frac{1}{2}(\underset{\sim}{\boldsymbol{E}}^T \cdot \underset{\sim}{\boldsymbol{E}} - \underset{\sim}{\boldsymbol{1}}) \tag{2}$$

where $\underset{\sim}{\boldsymbol{1}}$ is the identity matrix.

The Cauchy stress tensor is denoted by $\underset{\sim}{\boldsymbol{\sigma}}$. The following stress tensors are defined with respect to the intermediate configuration:

$$\underset{\sim}{\boldsymbol{\Pi}}^e = J_e \underset{\sim}{\boldsymbol{E}}^{-1} \cdot \underset{\sim}{\boldsymbol{\sigma}} \cdot \underset{\sim}{\boldsymbol{E}}^{-T}, \quad \underset{\sim}{\boldsymbol{\Pi}}^M = J_e \underset{\sim}{\boldsymbol{E}}^T \cdot \underset{\sim}{\boldsymbol{\sigma}} \cdot \underset{\sim}{\boldsymbol{E}}^{-T} \tag{3}$$

An isotropic elastic law is assumed:

$$\underset{\sim}{\boldsymbol{\Pi}}^e = \lambda(\operatorname{trace} \underset{\sim}{\boldsymbol{E}}^e)\underset{\sim}{\boldsymbol{1}} + 2\mu \underset{\sim}{\boldsymbol{E}}^e \tag{4}$$

where λ and μ are the Lamé elastic moduli. It is recalled that

$$\frac{\lambda}{\lambda + \mu} = 2\nu, \quad \frac{3\lambda + 2\mu}{\lambda + \mu} = 2(1 + \nu) \tag{5}$$

The Schmid law is adopted to predict the activation of slip system s. The slip system s is activated when the resolved shear stress τ^s reaches the critical value τ_c:

$$|\tau^s| = |\underset{\sim}{\boldsymbol{\Pi}}^M : (\underline{\boldsymbol{\ell}}^s \otimes \underline{\boldsymbol{n}}^s)| = \tau_c \tag{6}$$

where $\underline{\boldsymbol{\ell}}^s$ and $\underline{\boldsymbol{n}}^s$ respectively are the slip direction and the normal to the slip plane. In the whole problem, the Cauchy stress tensor takes the form

$$[\underset{\sim}{\boldsymbol{\sigma}}] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \sigma \end{bmatrix} \tag{7}$$

where σ is the tensile stress.

Stress and deformations are assumed to be homogeneous.

1 Determination of the yield stress

In this section, it is assumed that the material response is purely elastic so that $\underset{\sim}{\boldsymbol{P}} = \underset{\sim}{\mathbf{1}}$.
The deformation gradient takes the form:

$$[\underset{\sim}{\boldsymbol{F}}] = \begin{bmatrix} g & 0 & 0 \\ 0 & g & 0 \\ 0 & 0 & f \end{bmatrix} \tag{8}$$

where f is the applied axial deformation and g the transverse deformation component. It is recalled that $f = g = 1$ before straining.

1.1

Compute the matrix $\underset{\sim}{\boldsymbol{E}}^e$ as a function of f and g.
We find

$$[\underset{\sim}{\boldsymbol{E}}^e] = \frac{1}{2} \begin{bmatrix} g^2 - 1 & 0 & 0 \\ 0 & g^2 - 1 & 0 \\ 0 & 0 & f^2 - 1 \end{bmatrix} \tag{9}$$

1.2

Compute the matrix $\underset{\sim}{\boldsymbol{\Pi}}^e$ using the elasticity law Eq. (4). Its components are then expressed in terms of f, g, λ, μ.
We find

$$[\underset{\sim}{\boldsymbol{\Pi}}^e] = \begin{bmatrix} \frac{\lambda}{2}(f^2 + 2g^2 - 3) + \mu(g^2 - 1) & 0 & 0 \\ 0 & \frac{\lambda}{2}(f^2 + 2g^2 - 3) + \mu(g^2 - 1) & 0 \\ 0 & 0 & \frac{\lambda}{2}(f^2 + 2g^2 - 3) + \mu(f^2 - 1) \end{bmatrix} \tag{10}$$

1.3

Give then a second expression of $\underset{\sim}{\boldsymbol{\Pi}}^e$ starting from the Cauchy stress given by Eq. (7). This expression depends on σ, f and g.
We find

$$[\underset{\sim}{\boldsymbol{\Pi}}^e] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{g^2}{f}\sigma \end{bmatrix} \tag{11}$$

1.4

Compute in the same way as in Question 1.3 the matrix of $\underset{\sim}{\mathbf{\Pi}}^M$ depending on σ, f, g.
Check that this matrix is slightly different from that of $\underset{\sim}{\mathbf{\Pi}}^e$.
Show that these expressions coincide in the small deformation case.
We find

$$[\underset{\sim}{\mathbf{\Pi}}^M] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & fg^2\sigma \end{bmatrix} \tag{12}$$

In the small deformation case, $fg^2\sigma \simeq \sigma \simeq \frac{g^2}{f}\sigma$.

1.5

By combining the results of Questions 1.2 and 1.3, derive the expressions of g^2 and σ depending on f and the Lamé constants.
These results tell us that if we prescribe the axial strain f, we can then compute the transverse strain g and the axial stress σ according to isotropic elasticity.
Check that the usual formula are retrieved in the small strain case, that is when

$$f = 1 + \varepsilon_{33}, \quad g = 1 + \varepsilon_{11}, \quad |\varepsilon_{11}| \ll 1, \quad |\varepsilon_{33}| \ll 1$$

In the following, we do not replace g and σ by their expressions for the sake of brevity.
We find

$$2g^2(\lambda + \mu) + \lambda f^2 = 3\lambda + 2\mu \Longrightarrow 2g^2 = 2(1+\nu) - 2\nu f^2 \tag{13}$$

At small strain, $f^2 = 1 + 2\varepsilon_{33}$ and $\varepsilon_{11} = -\nu\varepsilon_{33}$, as expected.
We find also

$$\sigma = \frac{f}{2g^2}\left((\lambda + 2\mu)f^2 + 2\lambda g^2 - (3\lambda + 2\mu)\right) \tag{14}$$

At small strains, this gives $\sigma = (\lambda + 2\mu)\varepsilon_{33} + 2\lambda\varepsilon_{11}$, which gives $\sigma = E\varepsilon_{33}$ when $\varepsilon_{11} = -\nu\varepsilon_{33}$.

1.6

Give then the yield stress as a function of τ_c, f and g.
In fact, the expression of f as a function of σ found in Question 1.5 should be substituted in the previous expression so as to obtain an implicit equation for σ as a function of τ_c. We do not ask for the derivation of this equation.
How many slip systems are activated?
Check that the usual result is retrieved at small deformations.
We find

$$\tau = \frac{1}{\sqrt{6}} fg^2\sigma \Longrightarrow |\sigma| = \sqrt{6}\frac{\tau_c}{fg^2}$$

at yield. At small strains, $|\sigma| = \sqrt{6}\tau_c$, as usual. Eight slip systems are activated.

2 Deformation in the plastic regime

We assume now that the single crystal has deformed plastically:

$$[\underset{\sim}{\boldsymbol{P}}] = \begin{bmatrix} g^p & 0 & 0 \\ 0 & g^p & 0 \\ 0 & 0 & f^p \end{bmatrix} \tag{15}$$

where f^p and g^p are the axial and transverse plastic deformations.

The material element is still in simple tension described by Eq. (7) and the total deformation gradient is still given by Eq. (8).

2.1

Justify the form chosen for $\underset{\sim}{\boldsymbol{P}}$ in Eq. (15).
Express g^p as a function of f^p.
In tension along [001], the activation of eight symmetric slip systems results in isotropic transverse strains and no lattice rotation takes place for symmetry reasons so that the symmetry of the deformations remains the same.
Plastic slip is isochoric such that $J_p = 1$. It follows that $g^p = 1/\sqrt{f^p}$.

2.2

Explain why the elastic deformation is of the form

$$[\underset{\sim}{\boldsymbol{E}}] = \begin{bmatrix} g^e & 0 & 0 \\ 0 & g^e & 0 \\ 0 & 0 & f^e \end{bmatrix} \tag{16}$$

Give the relations between f, g, f^e, g^e, f^p, g^p.
Explain why the two relations between g^e, f^e, σ are the same as the ones derived in Question 1.5, after replacing f and g by f^e and g^e.
Similarly, the relation between σ and τ_c is the same as in Question 1.6 after replacing f by f^e.

2.3

The nominal stress, or first Piola–Kirchhoff stress tensor, $\underset{\sim}{\boldsymbol{S}}$, is associated with the ratio of current forces divided by initial surfaces:

$$\underset{\sim}{\boldsymbol{S}} = J\underset{\sim}{\boldsymbol{\sigma}} \cdot \underset{\sim}{\boldsymbol{F}}^{-T}$$

Prove that

$$S_{33} = \sqrt{6}\frac{\tau_c}{f} \tag{17}$$

Explain physically why it tends towards 0 for ever increasing f?
From the previous question we have

$$\tau_c = \frac{1}{\sqrt{6}} f^e g^{e2} \sigma$$

We get also $S_{33} = fg^2\sigma/f = f^e g^{e2}\sigma/f = \sqrt{6}\tau_c/f$.