Crystal plasticity finite element modelling of coarse-grained α-uranium

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ABSTRACT

The deformation behaviour of coarse-grained α-uranium is studied using crystal plasticity finite element simulations. The constitutive model includes 8 slip and 2 twin systems, based on dislocation densities as state variables. Polycrystal simulations are carried out to reproduce the manufacturing procedure: a quenching stage is followed by cutting out a sub volume to allow relaxation of the internal stresses. Room temperature tension and compression experiments are simulated for the textured samples that are generated by this process. Calibration of the model parameters is obtained by comparing simulated experiments against measured stress-strain curves and lattice strains from published in situ neutron diffraction studies. The comparison of the internal elastic strains allows the activity of slip and twin modes to be quantified, and to estimate their critical resolved shear stresses. The comparison between the present simulation results and previous models for fine-grained α-uranium provides information about the grain size dependence of the strength of slip and twin systems. The critical resolved shear stress of the most prominent twinning mode {130} is found to be similar to single crystal samples and much smaller for coarse-grained samples, showing the strong grain size dependence of this deformation mode.

1. Introduction

Understanding the deformation behaviour of α-uranium, which is the stable phase of uranium up to 670°C [1], is important for the development of safer manufacturing procedures and to predict fracture. α-uranium has a highly anisotropic crystal structure [2], elastic coefficients [3] and thermal expansion properties [4], which can give rise to significant thermal residual stresses [5]. The orthorhombic crystal structure of α-uranium can be thought of as a close-packed-hexagonal crystal structure distorted along the b axis [6].

Plastic deformation takes place by slip and twinning in α-uranium [7], depending on the temperature [8], loading conditions, hydrogen content [9], grain shape [10] and size [11]. The slip and twin systems were first studied by Cahn [12,7] using X-ray diffraction. 8 slip systems have been identified in α-uranium, which have very different critical resolved shear stresses (CRSS) [13]. 9 different twin types have been observed experimentally [14], but only the 2 variants of [130][310] are frequently observed and occupy a significant volume fraction of the crystal [15]. Some twin types appear only at high strain rate [16,17].

Polycrystalline samples show a high variability of the yield strength, with values between 250 and 400 MPa, and of the ultimate tensile stress [18]. The observed twin parting mechanism [7,19], in which crack surfaces form at the interface between the parent and twinned lattice [20], has led to different hypotheses: cracks may nucleate at the twin tips to accommodate strain [21] or they could be generated by the interaction between twins, dislocations and grain boundaries [20,22]. Therefore, modelling the plastic deformation in α-uranium and predicting the twin volume fraction in polycrystalline samples is required to understand the mechanisms leading to fracture.

The crystal plasticity finite element method (CPFEM) takes into account the set of discrete slip and twin systems [23] and can account for large strains, elastic anisotropy, texture evolution during deformation and the lattice reorientation given by twinning [24]. It can model the thermo-mechanical response of polycrysals using arbitrary boundary conditions and complex geometries. Therefore, CPFEM is ideally suited to interpret the lattice strain measured using neutron diffraction experiments, in which families of grains with different orientations with respect to the detector contribute to the measured signal [15]. This is important because the texture induced by deformation affects the recrystallization kinetics during heat treatment [25].

Low strain rate experiments on fine-grained α-uranium have previously been modelled using the elasto-plastic and visco-plastic self-consistent frameworks (EPSC and VPSC), with 8 slip systems and 6 twin systems [26,5]. These simulations are based on the approximation of grains as spherical inclusions embedded in a homogenised effective medium (HEM) [27], whose mechanical behaviour is given by the
volume weighted properties of the grains [28]. However, this approach does not take into account the interaction between neighbouring grains and cannot establish which grain combinations lead to the highest accumulation of plastic strain [29].

Most research on uranium has been focused on fine-grained α-uranium because of the higher availability of this material. Fine-grained α-uranium is normally obtained by several stages of heat treatment and rolling [30]. The grain size is typically in the range of 15–25 μm [30,31]. Cast α-uranium has a larger grain size [31] and is used in the first stage of the manufacturing process. The microstructure is characterised by grains with different sizes from centimetre to micrometre length scale [17]. The stress necessary to induce twinning is lower because of a Hall-Petch effect [11] and many twins are created during the cooling process. Because of the connection between twins and fracture [19], the coarse-grained material represents an ideal system to study plasticity and fracture mechanics in α-uranium. Moreover, large grains can form in the heat affected zone of welds in fine-grained α-uranium [19]. The CPFE method has not been applied to coarse-grained α-uranium, therefore no model parameters are available in the literature. Experiments on single crystals are, however, available [8], in which the CRSS of each slip system has been determined.

In this paper, CPFEM is used to model plastic slip and twinning in coarse-grained α-uranium, with an average grain size of 300 μm. The most important slip and twin systems identified by previous experiments are used. We show that neither the set of parameters identified for single crystals [8] nor the ones for the fine-grained material [26] are suitable for coarse-grained α-uranium. Quenching process simulations of polycrystals, followed by the cutting of samples from the quenched body and tension or compression on the resulting textured specimens, are carried out. The residual strains induced during manufacture are modelled, which have a significant effect on the mechanical properties. The residual strains depend on the characteristic temperature at which the CRSS of the slip systems decrease and this temperature dependence is included in the constitutive model.

Simulations are compared to in situ neutron diffraction experiments [32] carried out at the EPGN-X beamline of the ISIS Neutron Source, Rutherford Appleton Laboratory [33], and to tensile and compressive stress-strain curves obtained from the textured samples. This comparison required the simulated elastic lattice strain in each grain to be extracted. To achieve this a selection algorithm was developed to identify the set of grains which are suitably oriented to be detected by the diffractometer. The simulated twin volume fraction, predicted after sample cooling, is also compared to values found from electron backscatter diffraction (EBSD) images [32].

These comparisons allow validation of the CRSS values for the different slip and twin systems. The comparison between the CRSS values found in the present study and for fine-grained α-uranium shows that the grain-size dependence of the material parameters for this material is very different for slip and twinning. This can clarify the origin of the strong dependence of the ductility of α-uranium on the grain size [34]. The tension–compression asymmetry observed in neutron diffraction experiments is explained in terms of the relative activation of slip and twin modes.

The model developed is a first step to understand how fracture is affected by plastic deformation and texture in coarse-grained α-uranium.

2. Material model

A finite strain, crystal plasticity finite element framework is used [35]. The deformation gradient is decomposed into elastic and plastic parts:

\[ F = F_p F_e \]

where the plastic deformation gradient \( F_p \) transforms the crystal lattice into an intermediate (or relaxed) configuration [36]. The plastic deformation gradient \( F_p \) evolves according to [37]:

\[ \dot{\gamma}_p = \lambda_p \frac{\partial \tilde{\sigma}_p}{\partial \tilde{\varepsilon}_p} \]

where \( \dot{\gamma}_p \) is the shear rate on slip system \( \alpha \), \( \tilde{\sigma}_p \) is the temperature dependent shear stress and \( \tilde{\varepsilon}_p \) is the shear strain on the slip system. The tension–compression asymmetry observed in neutron diffraction experiments is explained in terms of the relative activation of slip and twin modes.

The model developed is a first step to understand how fracture is affected by plastic deformation and texture in coarse-grained α-uranium.

### Table 1

| Slip system | \( s_0^2 \) | \( n_0^2 \) |
|-------------|-------------|-------------|
| \( \alpha = 1 \) (wall) | [1, 0, 0] | [0, 1, 0] |
| \( \alpha = 2 \) (floor) | [1, 0, 0] | [0, 0, 1] |
| \( \alpha = 3 \) (chimney) | [0.437, -0.899, 0] | [0.899, 0.437, 0] |
| \( \alpha = 4 \) (chimney) | [0.437, 0.899, 0] | [0.899, -0.437, 0] |
| \( \alpha = 5 \) (roof) | [0.241, -0.495, 0.839] | [0.0, 0.860, 0.510] |
| \( \alpha = 6 \) (roof) | [0.241, -0.495, 0.839] | [0.0, 0.860, 0.510] |
| \( \alpha = 7 \) (roof) | [0.241, -0.495, -0.839] | [0.0, 0.860, -0.510] |
| \( \alpha = 8 \) (roof) | [0.241, -0.495, -0.839] | [0.0, 0.860, -0.510] |

### Twin system

| \( \beta \) | \( s_0^2 \) | \( n_0^2 \) |
|-------------|-------------|-------------|
| \( \beta = 1 \) | [0.825, -0.565, 0] | [0.565, 0.825, 0] |
| \( \beta = 2 \) | [-0.825, -0.565, 0] | [-0.565, 0.825, 0] |

where \( \gamma_p \) is the shear rate on slip system \( \alpha \), \( \tilde{\sigma}_p \) is the temperature dependent shear stress, \( \tilde{\varepsilon}_p \) is the shear strain on the slip system, and \( \lambda_p \) is the temperature dependent CRSS on slip system \( \beta \).

A power law slip rule is used for each slip system [26]:

\[ \dot{\gamma}_p = \left( \frac{\tilde{\sigma}_p}{\tilde{\varepsilon}_p} \right) \text{sign}(\tilde{\varepsilon}_p) \]

where \( \tilde{\sigma}_p \) and \( \tilde{\varepsilon}_p \) are the reference applied stress and strain rate sensitivity of the material. \( \lambda_p \) is the resolved shear stress and \( \tilde{\varepsilon}_p(T) \) is the temperature dependent CRSS on slip system \( \alpha \) [38]. A similar rate equation is used for the evolution of the twin volume fraction:

\[ \dot{\gamma}_{\text{twin}} = \dot{\gamma}_p \frac{\partial \tilde{\sigma}_\alpha}{\partial \tilde{\varepsilon}_\alpha} \]

where \( \gamma_{\text{twin}} \) and \( \gamma_p \) are the resolved shear stress and stress independent CRSS on twin system \( \beta \) respectively [39]. Twinning is active only if the resolved shear stress is positive [37].

A model based on dislocation densities, as developed by McCabe et al. [26], is used to calculate the evolution of the CRSS for each slip system:

\[ \tilde{\sigma}_p(T) = \exp \left( -\frac{T - \tilde{\theta}_p}{\tilde{\rho}_p} \right) \left( s_0^2 + 0.9\tilde{\mu}_p\tilde{\rho}_p^{\rho_{\text{sub}}} - 0.086\tilde{\mu}_p\tilde{\rho}_p^{\rho_{\text{sub}}}\log(\tilde{\rho}_p^{\rho_{\text{sub}}}) \right) \]

where \( \tilde{\rho}_p \) is the forest dislocation density on slip system \( \alpha \) and \( \rho_{\text{sub}} \) is the dislocation density in the substructures [40,41]. \( \rho_{\text{sub}} \) represents immobile dislocations that are debris left by dislocation annihilation, due to cross slip or climb. They do not multiply and, at the strain level used here, they do not recover, i.e. they remain sessile [26]. Their contribution to the CRSS is necessary to model stage IV hardening and
the last term in (5) is based on discrete dislocation dynamics studies [42].

\( b\) is the Burgers vector magnitude, \( c^\alpha \) is a constant friction stress, and \( \mu_a \) is the projected shear modulus of slip system \( \alpha \). This is found by assuming a deformation gradient of the form \( F = s_a \otimes n_a \) and a corresponding strain tensor \((F + F^T)/2\). This strain tensor is multiplied by the elasticity tensor \( C \) to find the Cauchy stress \( \sigma \). The projected shear modulus is defined as \( \mu_a = s_a \cdot n_a \). The CRSS is a constant friction stress, \( K \). In (5), \( L \) is a linear temperature dependence in the model.

The temperature dependence coefficient, reported by Daniel et al. [8] for the projected shear modulus on several combinations of planes and directions, is used in the present model. \( \Delta \sigma_{\text{xit}} \) is calculated using Eq. (2):  

\[
\Delta \sigma_{\text{xit}}(\sigma) = \frac{1}{2}(L_{\text{el}} + L_{\text{pl}}^T(\sigma))\Delta T.
\]  

A Newton-Raphson algorithm is used to find the zero of the entries of the \([3 \times 3]\) matrix \( \Psi(\Delta \sigma) \):  

\[
\theta = \Psi(\Delta \sigma) = C(\Delta \sigma - \alpha \Delta T - \Delta \sigma_{\text{rit}}(\sigma)) + (W_1 \sigma_1 - \sigma_1 W_1)\Delta T.
\]

The Cauchy stress increment \( \Delta \sigma \) at each time increment is calculated as follows [44]. The total velocity gradient \( L \) is given by:  

\[
L = FF^T - I.
\]

and it is used to calculate the small strain increment \( \Delta e \) in a time increment \( \Delta t \):  

\[
\Delta e = \frac{1}{2}(L + L^T)\Delta t.
\]  

The elastic continuum spin is given by [45]:  

\[
W_e = \frac{1}{2}(I_e - L_e^T)\Delta T.
\]  

and is used to calculate the Cauchy stress increment \( \Delta \sigma \) at every time increment [46]:  

\[
\Delta \sigma = C(\Delta e + (W_e \sigma_e - \sigma W_e))\Delta T.
\]

\[
= C(\Delta e - \alpha \Delta T - \Delta \sigma_{\text{rit}}(\sigma)) + (W_1 \sigma_1 - \sigma_1 W_1)\Delta T.
\]

where \( \sigma_a = \sigma - \Delta \sigma \) is the Cauchy stress at the start of the increment. \( \Delta \sigma_{\text{el}} \) and \( \Delta \sigma_{\text{rit}} \) are the elastic and plastic parts of the small strain increment. The fourth order elasticity tensor \( C \) has a linear temperature dependence [8]:  

\[
C = C(T_0)[1 - (9.35 \times 10^{-4} \text{ K}^{-1})(T - T_0)].
\]
Table 2
Model parameters.

| Twiss law parameters |          |
|----------------------|----------|
| CRSS of the twin system \( (c_{ij}) \) [8] | 25 MPa |
| Magnitude of shear due to twinning \( \gamma_{i}^{\text{min}} \) [7] | 0.299 |
| Initial twin volume fraction \( f_{t0} \) | 0 |

| Slip law parameters |          |
|---------------------|----------|
| Plastic strain rate coefficient \( (q_{p}) \) | 0.001 s^{-1} |
| Plastic strain rate exponent \( (n) \) [46] | 20 |

| Hardening law parameters |          |
|--------------------------|----------|
| Thermal activation parameter for slip \( (\theta_{a}) \) [24] | 140 K |
| Reference temperature \( (\theta_{0}) \) | 293 K |
| Constant friction stress (wall slip) \( (\Delta q_{w}) \) [5] | 7 MPa |
| Constant friction stress (floor slip) \( (\Delta q_{f}) \) [5] | 10 MPa |
| Constant friction stress (chimney slip) \( (\Delta q_{c}) \) [5] | 35 MPa |
| Constant friction stress (roof slip) \( (\Delta q_{r}) \) [5] | 235 MPa |
| Burgers vector (wall slip) \( (b_{w}) \) [49] | 0.285 nm |
| Burgers vector (floor slip) \( (b_{f}) \) [49] | 0.285 nm |
| Burgers vector (chimney slip) \( (b_{c}) \) [49] | 0.651 nm |
| Burgers vector (roof slip) \( (b_{r}) \) [49] | 1.185 nm |
| Projected shear modulus (wall slip) \( (\mu_{w}) \) [3] | 74.330 GPa |
| Projected shear modulus (floor slip) \( (\mu_{f}) \) [3] | 73.420 GPa |
| Projected shear modulus (chimney slip) \( (\mu_{c}) \) [3] | 92.255 GPa |
| Projected shear modulus (roof slip) \( (\mu_{r}) \) [3] | 115.670 GPa |

| Dislocation evolution law parameters |          |
|-------------------------------------|----------|
| Dislocation multiplication prefactor (wall slip) \( (\ell_{w}) \) [26] | 200.0 μm^{-1} |
| Dislocation multiplication prefactor (floor slip) \( (\ell_{f}) \) [26] | 500.0 μm^{-1} |
| Dislocation multiplication prefactor (chimney slip) \( (\ell_{c}) \) [26] | 150.0 μm^{-1} |
| Dislocation multiplication prefactor (roof slip) \( (\ell_{r}) \) [26] | 800.0 μm^{-1} |
| Dislocation annihilation length (wall slip) \( (d_{w}) \) [26] | 0.171 μm |
| Dislocation annihilation length (floor slip) \( (d_{f}) \) [26] | 0.256 μm |
| Dislocation annihilation length (chimney slip) \( (d_{c}) \) [26] | 0.117 μm |
| Dislocation annihilation length (roof slip) \( (d_{r}) \) [26] | 0.12 μm |
| Drag stress (wall slip) \( (D_{w}) \) [26] | 900 MPa |
| Drag stress (floor slip) \( (D_{f}) \) [26] | 6000 MPa |
| Drag stress (chimney slip) \( (D_{c}) \) [26] | 700 MPa |
| Drag stress (roof slip) \( (D_{r}) \) [26] | 1500 MPa |
| Reference strain rate \( (\dot{\varepsilon}) \) [26] | 10^{10} s^{-1} |
| Initial dislocation density \( \rho_{0} \) | 10^{10} m^{-2} |

Table 3
Elastic constants (GPa) at \( T = T_{0} \) for the orthorhombic structure of α-uranium [3,50] in Voigt notation.

| \( C_{11} \) | \( C_{12} \) | \( C_{13} \) | \( C_{22} \) | \( C_{23} \) | \( C_{33} \) | \( C_{44} \) | \( C_{55} \) | \( C_{66} \) |
|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 214.74 | 46.49 | 21.77 | 198.57 | 107.91 | 267.11 | 124.44 | 73.42 | 74.33 |

\( s_{a} = R e_{a} \) : \( R = \Delta \), (19)

\( n_{a} = R n_{a} \) : \( R = \Delta \), (20)

The rotation matrix \( R \) also transforms the thermal eigenstrain tensor \( \alpha \):

\( \alpha = R e_{a} \), (21)

where \( e_{a} \) is expressed in the lattice coordinate system and its diagonal entries are quadratic functions of the temperature \( T \) [51,4]:

\( e_{a}^{0} = 24.22 \times 10^{-8} - (9.83 \times 10^{-9} \text{ K}^{-1}) T + (46.02 \times 10^{-12} \text{ K}^{-2}) T^{2} \), (22)

\( e_{a}^{0} = 3.07 \times 10^{-8} + (3.47 \times 10^{-9} \text{ K}^{-1}) T - (38.45 \times 10^{-11} \text{ K}^{-2}) T^{2} \), (23)

\( e_{a}^{0} = 8.72 \times 10^{-6} + (37.04 \times 10^{-9} \text{ K}^{-1}) T + (9.08 \times 10^{-12} \text{ K}^{-2}) T^{2} \). (24)

At each time increment, the rotation matrix has to be updated based on the change of the elastic deformation gradient \( F_{e} \), since the plastic deformation, described by \( F_{p} \), does not induce lattice rotations. At each integration point, the continuum elastic spin is calculated as [52]:

\( R e_{a} = W_{e} \). (25)

and so the rotation matrix can be updated at the end of the increment:

\( R(t + \Delta t) = R(t) + R(t)\Delta t = (I + W_{e}\Delta t)R(t) \). (26)

The elastic velocity gradient \( L_{e} \) is calculated as:

\( L_{e} = L - E_{i}L_{e}F_{i}^{-1} \). (27)

The elastic lattice strain that is compared with neutron diffraction experiments is found by rotating the Green-LaGrange elastic strain tensor from the sample coordinate system to the lattice coordinate system:

\( E_{i}^{0} = \frac{1}{2} R^{T} F_{e}^{-1} F_{i} R \). (28)
a random angle $\psi$ around the x axis is performed to randomise the grain orientations. This is necessary because the experimental pole figures are available only along the load direction, therefore the experimental angle $\psi$ is unknown.

The orientation of the grains in the central part of the model (1000 grains in Fig. 3(b)) is assigned based on the experimental probability distribution functions [32]. These are repeated in Fig. 4(b) and (c) for the samples tested in tension and compression respectively. Note that the textures of these tested samples are different from each other, and this plays an important role in determining their material response, as demonstrated later. We designate these textures as T1, for the specimen tested in tension, and C2, for that tested in compression. A random texture is assigned to the grains that surround this central region, which are removed after the quenching stage. These cut grains are not included in subsequent stages of the simulations and do not contribute to the simulated neutron diffraction images.

5. Analysis of the neutron diffraction experiment

In order to compare the elastic lattice strains found using Eq. (28) and those measured using neutron diffraction [32], it is necessary to select the grains in which the lattice planes have an orientation such that the diffracted beam can be detected. A schematic view of the experimental setup used in [32] is shown in Fig. 5 (a). The sample load direction is along the x axis and the direction of the incoming beam, depicted in Fig. 5(b), is $\vec{q} = [1, 1, 0] / \sqrt{2}$. The detector is positioned at $90^\circ$ with respect to the incoming beam, therefore the segment connecting the region of the sample interacting with the neutron beam and the centre of the detector corresponds to the vector $\vec{d} = [1, 1, 0] / \sqrt{2}$, as shown in Fig. 5(a). Thus, the detector measures the spacing of lattice planes that have their plane normals approximately parallel to the load axis.

Specifically, if $\hat{n}$ is the lattice plane normal, the reflected beam $\vec{q}_r$ is given by:

$$\vec{q}_r = \vec{q} - 2(\vec{q} \cdot \hat{n})\hat{n},$$

as depicted in Fig. 5 (b). The factor of 2 in front of the second term on the right-hand side is due to the elastic scattering process, which reverses the sign of the component of the momentum that is parallel to $\hat{n}$.

Let $\vec{q}_r$ be the projection of $\vec{q}_r$ on the x-y plane and $\phi$, the angle between $\vec{q}_r$ and the x-y plane (vertical detector coverage). Let $\phi_0$ be the angle between the detector direction $\vec{q}_r$ and the projection $\vec{q}_r / ||\vec{q}_r||$ (horizontal detector coverage). The diffracted beam is detected only if $-14^\circ < \phi_0 < 14^\circ$ and $-21^\circ < \phi < 21^\circ$.

The simulated elastic lattice strain is found by averaging Eq. (28) over the integration points of the grains with $\phi_0$ and $\phi$ that satisfy this diffraction condition. Such grains will be called (DC) grains as they satisfy the diffraction condition for a specific plane $\hat{n}$. The planes $\hat{n}$ analysed are $(100)$, $(010)$ and $(001)$.

6. Simulation results

6.1. Stress-strain curves

Mechanical properties predicted by the model are found by
averaging the tensile or compressive stress on the x = 3000 μm surface, where the velocity boundary condition is applied in Fig. 3 (b). The resulting stress-strain curves are shown in Fig. 6 for tension and compression with the textures T1 and C1 of Fig. 3 respectively. The comparison with the experimental data shows that the model correctly predicts the material response for both the textures. The model is able to capture both the yield points and the hardening rate because of the calibration of the CRSS constants for slip and twinning (c_s and c_t) in addition to the dislocation multiplication pre-factors (k_s). The larger stress in the T1 sample is due to the presence of many grains with an orientation close to [001], as shown in Fig. 4 (b). These grains have fewer active slip and twin modes, therefore they are harder to deform.

6.2. Slip and twin activity

Fig. 7 shows the shear strain rate \( \chi \) on every slip and twin system during tension (T1 texture). The shear strain rate on the set of grains with an orientation such that the (100), (010), and (001) lattice planes are in the diffraction condition. Fig. 8 shows the same quantity during compression (C1 texture). The shear strain rate of deformation modes that include more than one slip or twin system, such as the chimney slip, roof slip and (130) twin, represents the sum of the shear strain rates of those systems. As expected from Schmid factor analysis and from Eq. (4), the twin systems in Table 1 are active only in tension for (100)-oriented grains and only in compression for (010)-oriented grains. For those grains, the twin systems have higher activity than the slip systems. The chimney slip system has a Schmid factor of 0.39 for (100) and (010) oriented grains; it is the most active slip system in tension for grains with the (010) plane in DC, as shown in Fig. 7 (b), and the most active in compression for grains with the (100) plane in DC, as shown in Fig. 8 (a). However, the chimney slip system is not active when the twin systems are active, as shown in Figs. 7(a) and 8(b). This is because they have similar slip directions and normals but the twin systems have lower CRSS. The roof slip system has a Schmid factor 0.43 in (001)-oriented grains, therefore it is the mostly active for grains with the (001) plane in DC, as shown in Figs. 7(c) and 8(c). The shear strain rate on most of the slip and twin modes increases or remains stable with increasing applied strain; a sensible decrease is predicted only for the chimney mode in the (010)-oriented grains in tension.

The simulated [130] twin volume fraction after the quenching stage in the central 1000 grains is shown in Fig. 9 (a) for the T1 texture. The distribution is highly heterogeneous; some grains have an orientation that favours twinning, given the thermal stress applied by neighbouring grains. The maximum value of the twin volume fraction is between 5% and 6%. A small number of grains with a [130] twin volume fraction up to 13% have been measured in an undeformed sample extracted from the same plate that the T1 sample was extracted [32], while annealed fine-grained \( \alpha \)-uranium is free of twins [26]. Therefore, the value chosen for the CRSS of the twin system (25 MPa) is reasonable. A higher value would lead to a smaller simulated [130] twin volume fraction, not compatible with the experiments on coarse-grained \( \alpha \)-uranium. The average of the [130] twin volume fraction as a function of temperature during cooling is shown in Fig. 9(b) for the T1 and C1 textures. Internal stresses are not strong enough to induce twinning during cooling from 400 °C to 200 °C. After that point, the [130] twin volume fraction increases linearly as temperature decreases. [172] twins were found to occupy up to 1% of the volume fraction in a small number of grains of an undeformed sample extracted from the same plate [32]. This justifies the assumption that only [130] twins contribute to the plastic deformation.
6.3. Elastic lattice strain

The simulated elastic lattice strain, averaged over grains with the (100), (010) and (001) planes in DC is shown in Figs. 10(a), (b) and 11 respectively. Experimental data correspond to single peak fits and the error bars are shown. The ordinate in Figs. 10 and 11 represents the macroscopic stress. The interpretation of these plots is the following. When plasticity is accommodated by a specific family of grains, the rate of increase of the elastic lattice strain in that grain family decreases. The macroscopic stress continues to increase and is accommodated by elastic deformation in harder grains. Therefore, an increase in the slope of a curve indicates that family of grains accommodates more plasticity.

For the tension sample, many grains have an orientation close to (10 0), as shown in Fig. 4(b), and 30 grains have the (10 0) plane in DC. For the compression sample, 16 grains are used for the average. The predicted elastic lattice strain agrees with the data for the tension sample, while it slightly overpredicts the elastic lattice strain for the compression one, as shown in Fig. 10(a). The asymmetry between the tension and compression results is due to the twinsystem activity in the (10 0)-oriented grains in tension only, as shown in Fig. 7(a), and to the higher macroscopic stress in the tensile sample, as shown in Fig. 6.

Texture T1 consists of two main grain families, as shown in Fig. 4(b): one family has an orientation close to (10 0) and the other family is close to (00 1). Because of twinning, (10 0)-oriented grains are softer in tension, while (00 1)-oriented grains are harder. Therefore, when plasticity initiates in the (100)-oriented grains, the rate of increase of the elastic lattice strain in those grains decreases, leading to the slope change observed in Fig. 10(a) for the tension sample. The macroscopic stress continues to increase because of the harder (00 1) grains.

The measured (010) elastic lattice strain in Fig. 10(b) has larger uncertainties, however, it does not show a clear slope change both for the compression and the tension samples. For the compression sample, many grains have an orientation close to (01 0), as shown in Fig. 4(c), and 56 grains have the (01 0) plane in DC. For the tension sample, only 4 grains are used for the average. The predicted (01 0) elastic lattice strain agrees with the data within the uncertainty interval both for the tension and compression samples. Even if twinning is present for the C1 texture in compression, as shown in Fig. 8(b), the slope change in tension and compression is not significant, in contrast to the (100) elastic lattice strain response. The present simulations indicate that this is due to the textures. In the T1 texture, plastic deformation is more relevant in (100)-oriented grains, while the (01 0)-oriented grains are harder. Therefore, none of them will accommodate much more plastic strain than the other. Therefore, the macroscopic stress is almost directly proportional to the lattice strain in those grain families.

Fig. 7. Simulated slip and twin activity during tension (T1 texture) in grains where the planes (a) (100), (b) (010) and (c) (001) are in diffraction condition respectively.

Fig. 8. Simulated slip and twin activity during compression (C1 texture) in grains where the planes (a) (100), (b) (010) and (c) (001) are in diffraction condition respectively.
The measured (001) elastic lattice strain in Fig. 11 does not show a strong slope change both for the compression and the tension samples. (001)-oriented grains have the lowest plastic deformation because only the roof slip system has a non-zero Schmid factor. Therefore, grains with the (001) plane in DC have the lowest slip activity, as shown in Figs. 7(c) and 8(c). Consequently, the simulated (001) elastic strain continues to increase, in qualitative agreement with the experimental data. The stress is higher for the tensile sample due to the harder texture, as shown by the stress-strain curve in Fig. 6. This trend is predicted by the present model.

7. Discussion

The CRSS for slip used in the present simulations are the same as those used for fine-grained α-uranium (25μm average grain size) by Calhoun et al. [5]. These values are smaller than the ones used by McCabe et al. for α-uranium with 12.5μm average grain size [26]. For instance, in that work, the constant friction stresses for wall and floor slip are 60MPa and 270MPa, while values of 7MPa and 10MPa are used in the present simulations.

A fitting procedure is performed by finding a value of the twin CRSS $c$ that is able to reproduce both the stress-strain curves and the asymmetry between tension and compression of the (100) elastic lattice strain (Figure 10(a)).

If the CRSS for slip is increased, the stress-strain curves are most affected, while there is little change in the elastic lattice strain-stress curves. Higher values of the CRSS for slip and twin cannot reproduce the experimental stress-strain curves, presented in Fig. 6. Indeed, McCabe et al. found stresses up to 600MPa at 1% strain during tension and compression tests [26]. This shows that the yield strength of the slip systems has a strong grain size dependence when the grain size is of
the order of 10 μm. The present simulations suggest that this grain size dependence is not strong in the interval between 25 μm and 300 μm.

On the other hand, the values found for the CRSS for a (130) twin in the present simulations is within the uncertainty interval determined for single crystals (25 MPa) [8], while Calhoun et al. [5] and McCabe et al. [26] use higher values: 80 MPa and 300 MPa for 25 μm and 12.5 μm average grain size respectively. If the CRSS for a (130) twin is increased, higher stresses are found, which are not comparable to the experimental stress-strain curves in Fig. 6. Moreover, if the CRSS for (130) twin is set much higher than the CRSS for slip, the twin activity, shown in Figs. 7 and 8, would be reduced. This would have two consequences: first, the asymmetry between the tension and compression (100) elastic strain in Fig. 10(a) would be reduced because the (100)-oriented grains would become harder in tension; second, the simulated (130) twin volume fraction, shown in Fig. 9(a), would be reduced. The maximum simulated value, between 5% and 6%, of the twin volume fraction depends on the initial temperature of the quenching simulation. However, a higher value of the CRSS for (130) twins would lead to a twin volume fraction that is too low compared with experimental observations, which are up to 13% in some grains.

Therefore, the present simulations suggest that the Hall-Petch dependence for (130) twinning is very strong in the grain size interval between 12.5 μm and 300 μm and the present coarse-grained material shows a twinning behaviour similar to single crystals.

The simulated twin volume fraction after quenching, between 5% and 6%, is normally found in fine-grained α-uranium after deformation. For instance, McCabe et al. [26] report a (130) twin volume fraction between 9% and 28% after 10% strain for 12.5 μm average grain size, depending on the texture and load condition. Brown et al. [15] report a (130) twin volume fraction between 8% and 10% after 5% strain for 25 μm average grain size.

The slip and twin activities found in the present simulations, shown in Figs. 7 and 8, are different from the fine-grained material. Calhoun et al. [5] show that wall slip is more active than the (130) twin mode for deformations between room temperature and 150 °C. Twin is the dominant deformation mechanism in the highly textured samples analysed by Knezevic et al. [53]. Their clock-rolled samples have a large fraction of (010)-oriented grains parallel to the rolling direction and (100)-oriented grains along the transverse direction. Twinning activity is higher than wall slip for compression along the rolling direction (IPC1 sample in [53]) and for tension along the transverse direction (IPT2 sample in [53]). Therefore, the slip and twin activity in the present coarse-grained cast α-uranium can be similar to highly textured fine-grained uranium, obtained by rolling followed by annealing.

As discussed in Section 6.3, the elastic lattice strain during deformation depends strongly on the texture. A slope change in the stress-elastic lattice strain curve is present only if different grain families have rather different yield strengths. This is the case for the T1 texture, as shown in Fig. 4, which has two different peaks near (100) and (001). The T1 texture under tension exhibits an evident slope change in the stress-elastic lattice strain curve, as shown in Fig. 10(a). The C1 texture does not show an evident slope change; however, plastic deformation is present, as shown by the twin activity in Fig. 8(b). This shows the need for CPFE simulations to understand the stress-elastic lattice strain curves obtained from neutron diffraction experiments: the absence of saturation of the elastic strain in a grain family can be due to the strong texture of the sample and not to the lack of plastic flow.

It is worth noting that the stress at which the slope change is present for the T1 sample in Fig. 10(a), which is about 115 MPa, does not necessarily correspond to the activation stress of a plastic deformation mode. At a macroscopic stress of 115 MPa, the resolved shear stress on the (130) twin system for a (100)-oriented grain is about 54 MPa. This value is higher than the CRSS used for twinning, which is 25 MPa. This is in part due to the orientation of the grain family detected by the diffractometer, which is not perfectly aligned to the [100] axis, but also to the presence of slip that partially accommodates plastic deformation. Therefore, a direct analysis of the experimental data, without using CPFE simulations, may lead to an overestimation of the twin CRSS.

One possible origin of the discrepancy between the experimental and simulated elastic lattice strain-stress curves is due to the fact that the neutron diffraction experiments analyse only the central part of the specimen. Strain concentrations may be present outside that region. Therefore, the measured strain may not coincide with the simulated one, which is the local strain in the region sampled by the neutron beam.

The thermal residual strains, included in the present simulations, give rise to the difference in the slope of the elastic lattice strain-stress curves of the T1 and C1 samples, in the elastic regime, as shown in Figs. 10 and 11. Such a difference, which is in qualitative agreement with the experimental results, is not present if the quenching stage is not simulated. The influence of thermal residual strains on the predictions of internal strains has already been noted by Calhoun et al. [13]. The thermal residual strains can also cause an apparent increase in hardness in some grain families.

8. Conclusions

A constitutive model to describe the plastic deformation of coarse-grained cast α-uranium is developed and implemented in ABAQUS. The model parameters are calibrated to fit stress-strain curves, internal strains measured using in situ neutron diffraction experiments and twin volume fractions measured by EBSD given by Earp et al. [32]. Simulations take into account thermal residual strains and relaxation after sample cutting, consistent with the sample preparation and testing method. Internal stresses change the slope of the elastic lattice stress-strain curves and the plastic activity.

Simulations include 8000 grains, oriented according to the experimental texture, in order to obtain statistically relevant results that can be compared directly with the neutron diffraction experiments, in which a similar number of grains is interrogated.

The model shows that the tension-compression asymmetry in the stress-strain curves and in the neutron diffraction data observed experimentally [32] is due to the activation of twinning and by the different textures of the tested samples. Specifically, the presence of grain families with different hardness is associated with the saturation of the elastic strain. The T1 texture, in which two families of grains with orientations close to (100) and (001) respectively are present, leads to harder samples.

Results are compared with previous studies on single crystal and fine-grained α-uranium. The calibration of the CRSS values for slip and twin reveals that coarse-grained α-uranium has a twin CRSS similar to single crystals, while the slip CRSS is similar to α-uranium with 25 μm average grain size as investigated by Calhoun et al. [5]. This indicates that the grain-size dependence for twinning is stronger than for slip.

The present work shows that CPFE simulations are necessary to extract the proper values of the CRSS for slip and twinning from neutron diffraction experiments. They allow the integral strains due to quenching to be studied and represent a step forward compared with the approximation of grains as spherical inclusions.

Data availability

The raw/processed data required to reproduce these findings cannot be shared at this time as the data also forms part of an ongoing study.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at https://doi.org/10.1016/j.commatsci.2019.109276.