



Texture formation in orthorhombic alpha-uranium under simple compression and rolling to high strains



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HIGHLIGHTS

- A multi-scale finite element model is built to simulate behavior of α -U to large plastic strains.
- Development of texture gradients during rolling in α -U is captured by the model.
- Role of deformation mechanisms in texture formation of α -U is discussed.
- Twinning is profuse during rolling but not active during through-thickness compression.
- Floor slip is responsible for the formation of two pronounced {001} texture peaks in rolling.

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ABSTRACT

We study the mechanical response and texture evolution of alpha-uranium during simple compression and rolling at 573 K. In order to determine the underlying mechanisms governing plasticity and texture formation, we perform detailed characterizations using electron backscattered diffraction and constitutive modeling using a dislocation-density based hardening law within a visco-plastic self-consistent homogenization. We show that the model achieves good agreement with experimental measurements in terms of texture and stress–strain response. From detailed comparison of experimental and modeling results, we infer that in both through-thickness compression (TTC) and rolling at 573K, the active slip modes are floor slip (001)[100] and chimney slip $1/2\{110\}\langle 1\bar{1}0\rangle$ with slightly different ratios. However, $\{130\}\langle 3\bar{1}0\rangle$ twinning is not active in TTC compression but profuse during rolling. Further analysis indicates that during rolling, floor slip (001)[100] results in the formation of two pronounced (001) texture peaks tilted 10–15° away from the normal toward the rolling direction.

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1. Introduction

Polycrystalline uranium (U) is a metal that is desired for its nuclear properties and high density. The manufacturing of U components involves complex sequences of thermo-mechanical processes, such as forging, rolling, swaging, extrusion, and recrystallization. As the metal undergoes these processes, its microstructure, including grain sizes and shapes, crystal orientations, and defect densities, continuously evolves. The final microstructure, which significantly depends on the processing path taken,

determines its mechanical properties and performance in service. For understanding the structural properties of U, it is essential to understand its microstructural evolution as a function of processing path and the responsible underlying deformation mechanisms leading to microstructure formation. Such understanding would facilitate designing the processing path for prescribed material properties.

Microstructural evolution is linked to the predominant deformation mechanisms, which for U are much more diverse and complex than cubic materials, such as Al, Ni, and steels. Pure U, over the pressures and temperatures tested here, has an orthorhombic crystal structure and is referred to as α -uranium (α -U) with lattice parameters $a = 0.2852$ nm, $b = 0.5865$ nm, and $c = 0.4945$ nm [1]. To deform plastically, α -U exhibits multiple slip and twinning modes. The geometry of the predominant slip/twin systems has

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been depicted in Refs. [2,3]. Like most metals, possessing a low-symmetry crystal structure [4–6], activation barriers of these modes are not equivalent. It is known that the easiest slip mode is (010)[100] [7,8] possessing only one slip system. The (001)[100] slip mode operates at room and becomes the primary slip mode at elevated temperatures [7,8], and is also comprised of only a single slip system. The next easiest slip mode is the $1/2\{110\}\langle\bar{1}\bar{0}\rangle$ slip mode, which has two slip systems. Finally, the $1/2\{1\bar{1}2\}\langle 021\rangle$ slip mode is necessary to accommodate plastic strain in the [001] direction and, thus, to accommodate an arbitrary plastic strain. However, its activation requires a larger driving force than the other slip modes. The most commonly observed twinning modes are $\{130\}\langle\bar{3}\bar{1}0\rangle$, $\{172\}\langle\bar{3}\bar{1}2\rangle$ and $\{112\}\langle\bar{3}\bar{7}2\rangle$ [1,8,9], with the former being the easiest to activate. The twin shear S of the $\{130\}\langle\bar{3}\bar{1}0\rangle$ twin is 0.299 and it reorients the lattice by 69.3° about [001]. For the $\{172\}\langle\bar{3}\bar{1}2\rangle$ twin, $S = 0.227$, and it reorients the lattice by 92.6° about $\langle\bar{1}070\rangle$.

Making the link between these mechanisms and the deformation response of α -U is usually accomplished by crystal plasticity based constitutive models [1,2,8–15]. It is generally found that the multiple slip and twinning modes are active within individual crystals of α -U and such complex combinations are needed to explain its strong plastic anisotropy in macroscopic behavior [2,16,17]. Further, the slip modes differ in their sensitivity to temperature and strain rate leading to interesting and substantial changes in the constitutive response as temperature or strain rate changes [18]. This sensitivity can lead to significant thermal residual stresses upon cooling from the processing temperature to room temperature [14,19].

It has been shown that the deformation modes have very different activation stresses, and the active modes are significantly affected by the initial texture [16]. Such studies on texture effects have involved mechanical tests involving monotonic deformation. In forming operations like rolling, the deformation state is not as homogeneous as in uniaxial tests. In particular, the deformation state near the surface where the rolls contact the sheet is usually different than in the center [20]. Consequently, many of the models for texture evolution applied in prior works on monotonic deformation would not be well suited to treat texture development during rolling. Furthermore, because α -U is a relatively strong metal that is hard to work at ambient conditions, rolling is carried out at elevated temperatures. Up to now, a fundamental analysis of texture development during large strain, elevated temperature rolling of α -U has not been carried out.

In this work, we study texture formation in α -U during simple compression and rolling using a combination of experiments and multi-scale crystal plasticity based modeling. We explore the effects of initial texture by fabricating samples with approximately the same grain size but different initial textures on the rate of texture formation and concomitant material response in compression. The fabricated material is subsequently rolled at 573 K to various strain levels and gradients in texture through the thickness of the sheet are characterized. The chief underlying deformation mechanisms responsible for the evolution of texture in α -U during compression and rolling to large reductions are identified to be as follows: (001)[100] and $1/2\{110\}\langle\bar{1}\bar{0}\rangle$ slip models are active during both through-thickness compression (TTC) and rolling at 573K with slightly different ratios, $\{130\}\langle\bar{3}\bar{1}0\rangle$ twinning is not active in TTC compression but profuse during rolling. Analysis shows that during rolling, (001)[100] results in the formation of two pronounced (001) texture peaks tilted 10 – 15° away from the normal toward the rolling direction. We demonstrate that the multi-scale coupled with finite elements can capture the development of texture gradients in α -U, a metal with a highly anisotropic plastic response.

2. Multiscale modeling approach

Linking the activation of slip and twinning within individual crystals to the imposed deformation conditions, such as rolling, requires linking deformation models from the subgrain scale to the sample scale [21–37]. To this end, we employ a multi-scale model to relate heterogeneous texture evolution at the scale of the sheet material to the deformation mechanisms occurring within a crystal. At the largest scale, we model the deformation of the sample as it is rolled using finite elements (FE). For the constitutive response at each integration point, we use a polycrystal plasticity model called the visco-plastic self-consistent (VPSC) scheme [38]. VPSC relates the deformation of the individual constituent crystals to that of the polycrystal. At the grain scale, we use crystal plasticity theory to relate the deformation of the individual crystal to its active slip and twinning modes. In this work, the shearing action provided by slip and twinning is modeled using a rate-sensitive flow rule [39–42]. To model lattice reorientation due to deformation twinning at the grain scale, we employ the composite grain model (TW) [43–45]. At the subgrain scale, the threshold stresses for activating slip and twinning on individual systems are calculated. For slip, the threshold stresses are governed by the evolution of stored dislocation density (DD) on the slip system according to thermally activated rate laws and hence are explicit functions of temperature and strain rate [18,46–54]. For twinning, the threshold stresses to first form twins also evolve with strain [46]. The stored dislocation density within the same grain, however, may indirectly affect the expansion of twin lamellae.

2.1. Sample scale: linking finite element method and VPSC

In the present model, each FE integration point is a polycrystal whose stress–strain response and microstructure evolution, such as crystallographic and morphologic texture and hardening evolution, are provided by the VPSC model. This model has been implemented as User Material Subroutine (UMAT) for the FE software Abaqus [55–58].

Inside the UMAT, the strain increment from Abaqus, $\Delta\epsilon^{FE}$, stress from the previous increment, σ^t , and a set of state variables are provided as the input at each material point at each trial time increment, $t + \Delta t$. The strain increment results from the applied loading and the associated nodal displacement increments. As the output, the updated stress, $\sigma^{t+\Delta t}$, and tangent stiffness matrix (Jacobian), $\mathbf{C}^{tg} = \partial\Delta\sigma/\partial\Delta\epsilon$, are calculated and returned. Once the stress field corresponding to the currently applied displacement field is calculated, equilibrium is checked. If not satisfied, increments in displacement are iteratively modified by the Jacobian until equilibrium is achieved. Finally, the same set of state variables are updated and returned.

In our formulation, at each polycrystalline integration point only the corotational increment in stress, $\Delta\sigma$ [59], needs to be calculated since the rigid body rotation is performed within ABAQUS on stress at start of the time increment as $\sigma^t = \Delta\mathbf{R}\sigma^{t,unrotated}\Delta\mathbf{R}^T$ [60–62]. Here, the stress–strain relationship at an integration point follows Hooke's law:

$$\sigma^{t+\Delta t} = \sigma^t + \Delta\sigma = \sigma^t + \mathbf{C} : (\Delta\epsilon - \Delta\epsilon_{vp}), \quad (1)$$

where \mathbf{C} is the elastic stiffness tensor, $\Delta\sigma$ is the corotational increment in the Cauchy stress (calculated in the corotational material frame and then transformed to the fixed global frame), and $\Delta\epsilon_{vp}$ is the increment in visco-plastic strain calculated by the VPSC model. The elastic stiffness, \mathbf{C} , is calculated using the elastic self-consistent (ELSC) code where the textural changes are also accounted for. The single-crystal elastic constants used for α -U are

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