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Temperature dependence of work hardening in sparsely twinning zirconium

Jaiveer Singh [a], S. Mahesh [b,*], Shomic Roy [a,c], Gulshan Kumar [a], D. Srivastava [d], G.K. Dey [d], N. Saibaba [e], I. Samajdar [a]

[a] Department of Metallurgical Engineering & Materials Science, Indian Institute of Technology Bombay, Powai, Mumbai 400 076, India
[b] Department of Aerospace Engineering, Indian Institute of Technology Madras, Chennai 600 036, India
[c] Scientific Services, Tata Steel Limited, Jamshedpur 831 001, India
[d] Materials Science Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400 085, India
[e] Nuclear Fuel Complex, Hyderabad 500 062, India

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ABSTRACT

Fully recrystallized commercial Zirconium plates were subjected to uniaxial tension. Tests were conducted at different temperatures (123 K - 623 K) and along two plate directions. Both directions were nominally unfavorable for deformation twinning. The effect of the working temperature on crystallographic texture and in-grain misorientation development was insignificant. However, systematic variation in work hardening and in the area fraction and morphology of deformation twins was observed with temperature. At all temperatures, twinning was associated with significant near boundary mesoscopic shear, suggesting a possible linkage with twin nucleation. A binary tree based model of the polycrystal, which explicitly accounts for grain boundary accommodation and implements the phenomenological extended Voce hardening law, was implemented. This model could capture the measured stress-strain response and twin volume fractions accurately. Interestingly, slip and twin system hardness evolution permitted multiplicative decomposition into temperature-dependent, and accumulated strain-dependent parts. Furthermore, under conditions of relatively limited deformation twinning, the work hardening of the slip and twin systems followed two phenomenological laws proposed in the literature for non-twinning single-phase face centered cubic materials.

1. Introduction

Work hardening, which seeks to explain the mechanical response of materials under arbitrary loading paths, poses many important unresolved problems in materials science and engineering [1–4]. A detailed theory that builds up from the microscopic mechanisms and predicts the macroscopic stress-strain curve along a prescribed loading-path remains non-trivial. This has led to a search for reliable phenomenological work hardening models [4]. Among other aspects, such models seek to capture the influence of working temperature and strain-rate on material mechanical response. As early as 1953, it was recognized [5] that this dependence was controlled by a microscopic phenomenon termed dynamic recovery.

Slip and deformation twinning are accommodative microscopic mechanisms that are activated during plastic deformation in a number of materials. Both mechanisms are simultaneously activated in low stacking fault energy fcc (face centered cubic) materials, such as $\alpha-$ brass, and in hcp (hexagonal close packed) materials such as zirconium. While twinning does contribute to accommodate the imposed deformation, it is now well established [6–8] that its contribution is small. Even so, the significance of deformation twins in material work hardening is great because of the interaction between twins and slip systems. Formation of deformation twins significantly alters the critical resolved shear stresses of slip systems in the grains, due to latent hardening, and reduction of the saturation stress of slip systems [8]. This, in turn, affects the activation of slip processes markedly [9].

Work hardening models that account for both slip and deformation twinning are often built upon polycrystal plasticity models or crystal plasticity finite element models. In plastically deformed hcp Zircaloy-4, Lebensohn and Tomé [10] pioneered the application

* Corresponding author.
E-mail address: smahesh@iitm.ac.in (S. Mahesh).

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of polycrystal plasticity models to predict texture and mechanical response. Tomé et al. [11] applied the viscoplastic self-consistent model to explain the work hardening of uniaxially deformed specimens cut along both the in-plane and through thickness directions from a strongly textured zirconium plate. In order to fit the experimental work hardening response, they assumed a strong latent hardening interaction between each extension twinning system and all slip systems and all other twinning systems. Using this framework, Kaschner et al. [12] could explain the mechanical response in pure zirconium during temperature change tests. Using distinct hardening parameters for the slip and twin systems at the two temperatures studied, they could capture the experimental mechanical response with the viscoplastic self-consistent polycrystal plasticity model. The internal variable controlling the hardening law of grains in Refs. [11,12] was the total accumulated slip and twinning shear in grains. Beyerlein and Tomé [13] proposed a model wherein dislocation densities were the internal variables. Temperature dependence enters into the Beyerlein and Tomé [13] model through the assumption of dislocation annihilation following the modified activation theory of Gilman [14]. Assuming that twin nucleation is thermally activated and therefore, probabilistic, and that twin propagation involves considerably less resistance than nucleation, the model of Beyerlein and Tomé [13] explains the temperature-dependent mechanical response under uniaxial loading both in-plane, and through the thickness of a clock rolled Zr sheet. An elastic-viscoplastic self-consistent model for Zircaloy capable of accounting for thermal strains was proposed by Qiao et al. [15]. A crystal plasticity finite element model of Zircaloy-2 incorporating both slip and twinning accommodation modes is due to Abdolvand et al. [16]. In this model, twins are not explicitly represented as parts of grains. Instead, a twin volume fraction is determined at each integration point, following a method similar to that used in the crystal plasticity models noted above. The twin volume evolves with deformation. Assuming the same deformation rate in both twin and matrix closes the system of equations at the integration point. As in the polycrystal plasticity models, slip-twin interactions are accounted for, using suitable latent hardening parameters.

Slip-twin interactions represent an important but complex aspect of polycrystal plasticity based work hardening models for hcp materials. While in Refs. [11,12,15,16], this interaction is modeled as a uniform latent hardening, a more complex scheme involving the intercept made on the slip direction by the twinning habit planes was adopted by Beyerlein and Tomé [13]. In contrast to all the aforementioned models, wherein twinned volumes are not explicitly represented, the conjugate grain model proposed by Proust et al. [17] treats twinned volumes as bands within the grains, deforming following compatibility conditions with the matrix. The interaction between twin and matrix in the physical grain, however, appears to be more complex than that suggested by Proust et al.'s simple compatibility condition [17,18].

It is clear from the foregoing, on one hand, that deformation twinning significantly affects the work hardening in hcp metals and alloys. Therefore, no simple relationship between the work hardening responses at different temperatures may be expected. On the other hand, a simple phenomenological work hardening model exists for fcc materials deforming by slip only, which adequately captures the temperature and strain-rate dependence of the work-hardening [4]. It is natural to ask if the temperature and strain-rate dependence of work hardening known in fcc materials will carry over to hcp polycrystalline materials, for the case of limited deformation twinning. It is the central objective of the present work to address this question.

In the present work, twinning is suppressed during uniaxial tension by loading samples cut from a highly textured Zircaloy-4 sheet along directions that are nominally unfavorable for extensive deformation twinning. The work hardening behavior, texture and microstructure evolution in the temperature range of 123 K–623 K has been characterized. Both yield stress and work hardening are found to depend strongly on the working temperature [12,17,19–21] and on sample orientation or strain mode [20,22–25]. The experimental observations are interpreted through polycrystal plasticity modeling based on the binary tree model [26]. This model has been employed in previous works on Zircaloy-4 [22,27] also. The model directly accounts for the intergranular interactions, and grain boundary accommodation. It is found that for moderate volumes of deformation twinned regions, a surprisingly simple dependence of the hardness of slip and twinning systems in the grain bulk on temperature and accumulated strain is obtained: The slip system hardness can be multiplicatively decomposed into temperature-dependent and strain-dependent parts. Furthermore, the temperature dependent part follows phenomenological scaling laws proposed in the literature for fcc materials [4,28].

2. Experimental method

In this study commercial Zirconium alloy (Zircaloy-4), rolled and then fully recrystallized sheet of 1.5 mm thickness, was used. The chemical composition of the Zircaloy-4 sheets is given in Table 1. Tensile test specimens were prepared according to ASTM E8 standards in two different sample orientations (RD and TD). A range of working temperatures, 123 K–623 K was used for direct and indirect observations. Tensile deformations were performed on servo-hydraulic Zwick-Roell™ tensile testing machine at the strain rate of 5×10^{-4} mm/s. Direct observations were taken for the working temperatures of 123 K–298 K. At 623 K temperature, direct observations on the specimen surface is not possible due to surface oxidation. The true stress-true strain ($\sigma - \varepsilon$) data were further analysed to extract information on work-hardening behaviours ($\frac{d\sigma}{d\varepsilon}$ versus σ). Interrupted tensile deformations, at different true strains, were used for detailed characterization for bulk texture and microstructural analysis.

Both X-ray diffraction and EBSD (electron backscattered diffraction) measurements were performed. For X-ray diffraction and microstructural characterization through EBSD, specimens were polished through standard metallography and electropolishing in a 20:80 solution of perchloric acid and methanol by volume at −20 °C and 20 V dc [29]. For the latter, a Struers™ Lectopol system was used. All the microstructural measurements were made in the RD-TD section, containing rolling (RD) and transverse (TD) directions. The EBSD measurements were made on a FEI™ Quanta 3D-FEG (field emission gun) SEM (scanning electron microscopy), using TSL-OIM™ EBSD software. Multiple EBSD scans were made to cover large areas with identical beam and video conditions. EBSD measurements were done with step size of 0.2 μm. EBSD data above 0.1 CI (CI – confidence index is a statistical measure of automated indexing, >0.1 CI data representing > 95% success [30]) were taken for further analysis.

X-ray bulk textures of four incomplete (maximum tilt angle: 85°) pole figures ((0002), $(10\bar{1}0)$, $(10\bar{1}2)$, and $(10\bar{1}3)$) were measured on a PANalytical™ X'Pert PRO MRD system. A monochromatic Cu Kα beam of 2 mm × 2 mm and Standard Schulz method in reflection mode [31] were used for these measurements. Combinations of highly accurate Eulerian cradle (0.0001° reproducibility) and multi-channel solid-state area detector (Pixel™) used for these pole figure measurements. ODFs were then calculated by inversion of the pole figures using the Arbitrarily Defined Cells (ADC) Method [32]. Commercial software, LaboTex from LaboSoft™, was used for the ODF calculations and plotting.