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TEXTURE GRADIENT EFFECTS IN TANTALUM

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ABSTRACT

The effects of inhomogeneities in texture on the mechanical response of a tantalum plate were investigated. Through-thickness compression samples exhibited an hourglass shape after deformation. The compression tests were modeled using a finite-element approach. A polycrystal plasticity model is embedded at each element of the mesh enabling the simulation to account for the spatial distribution of texture and its evolution. The texture was characterized using spatially specific individual lattice orientation measurements. The orientations were measured using automatic analysis of electron backscatter Kikuchi diffraction patterns. The influence of the spatially nonuniform distribution of texture on the experimental and simulated results is discussed. This work demonstrates the capability of currently available tools for characterizing inhomogeneous microstructures and modeling the effects of variations in texture on mechanical behavior.

INTRODUCTION

In a previous paper[1], the characterization of the texture gradient in a tantalum plate was described. The spatial distribution of texture was characterized using individual lattice orientation measurements obtained through automatic analysis of backscattered electron Kikuchi diffraction patterns[2, 3, 4]. The plate exhibited a $\{100\}\langle 001 \rangle$ (cube) texture at the surface and a $\{111\}\langle 110 \rangle$ texture at the centerline. This paper described compression tests of through-thickness cylindrical specimens. After compression, these samples possessed an hourglass shape. The hourglass shape was ascribed to the through-thickness texture gradient present in the plate. The shape was effectively modeled using a Taylor polycrystal plasticity model where strain is assumed to be uniform throughout the polycrystal. To model the hourglass shape, two hypothetical samples were constructed. One sample possessing the texture at the surface of the plate and the second the texture at the centerline. The same amount of work in compression was numerically applied to both samples. The hypothetical sample with the plate surface texture strained more than the sample with the centerline texture. The ratio of the area at the surface of the sample to the area at the midplane was predicted to within a few percent of the measured value. However, the paper suggested that a more complete approach to modeling the effect of the variation in texture on the mechanical response could be achieved using the finite-element approach developed by Beaudoin and coworkers[5, 6].

The present work reviews some of the experimental details of the compression testing and the microtextural characterization presented in more detail in the previous paper. The finite-element modeling technique employed is also reviewed. This study details the mapping of the individual orientation measurements into the finite element model. Results of the simulation are presented and discussed.

EXPERIMENTAL DETAILS

The material for this study was cross-rolled and annealed arc-remelted tantalum plate. The nominal chemistry is reported in table I.

Table I – Chemical analysis of the test material (weight percent in PPM).

O	N	C	H	Fe	Ni	Cr	Ca	Cu	Si	Ti	Mo	W	Nb	Ta
38	24	5	<1	27	39	18	<2	<1	<8	<5	<5	<40	<10	Bal.

Through-thickness cylindrical test specimens (diameter = 5.0mm, length = 6.2mm) were electrodischarge machined from the plate. The specimens were compressed at strain rates of 0.001s^{-1} at room temperature. After straining, the samples were slightly hourglass shaped rather than remaining cylindrical or barreling slightly as commonly observed in compression samples.

A section plane passing through the center axis of a compression sample prior to deformation was prepared for the orientation measurements. Approximately 11,000 orientation measurements were made using an automatic technique based on computer analysis of electron backscatter diffraction patterns[2, 3, 4]. The measurements were made on a $1\text{mm} \times 4\text{mm}$ regular hexagonal grid with $20\mu\text{m}$ spacing between measurement points as shown in figure 1.

Figure 1 Schematic of region from which orientation measurements were obtained.

Numerical simulation of the compression deformation was carried out using a finite element code which derives material properties from polycrystal plasticity theory. In this approach, element constitutive properties are derived from an idealized polycrystal aggregate situated in the element. The polycrystal aggregate is typically represented by hundreds of orientations. The code utilizes massive parallel computations to carry out the numerous computations inherent in such a formulation.

An octant of the test specimen was discretized using a mesh of 5184 brick elements. Symmetry was assumed along specimen mid-planes with normals in the through-thickness, rolling, and transverse plate directions. The mesh consisted of twelve layers, each of which was comprised of 432 elements. Correspondingly, the experimental orientation measurements were partitioned into twelve groups of roughly 900 measurements. Symmetry operations were applied to each

measurement so as to achieve an orthorhombic sample description in agreement with the symmetries and boundary conditions prescribed in the mesh definition. This resulted in a set of approximately 3600 orientations assigned to each layer of the finite element mesh. The assignment, providing an initialization of material state, was carried out by taking a random selection of 256 orientations for each finite element from the appropriate layer measurement set.

A polycrystal viscoplasticity approach was used where the single crystal slip system constitutive behavior was assumed to follow a power law relationship as follows:

$$\dot{\gamma} = a |\tau / \hat{\tau}|^{1/m} |\tau| / \tau \quad (1)$$

where $\dot{\gamma}$ is the slip system shear rate, τ is the resolved shear stress and $\hat{\tau}$ is a scaling parameter that defines the hardness of the slip systems. The rate sensitivity m was taken as 0.06 based on compression test data[1]. The hardening was described using a Voce law formulation[7] where the strain-hardening rate for a crystal is given as a function of the resolved stress τ as follows:

$$d\hat{\tau} / dt = \theta_0 [1 - (\hat{\tau} - \tau_0) / \tau_v] |\dot{\gamma}^*| \quad (2)$$

This definition requires three material constants to parameterize the hardening behavior: the reference stress τ_0 at yield, the rate of decrease of $d\hat{\tau} / dt$ with $\hat{\tau}$, characterized by the Voce stress τ_v and an adjustable parameter θ_0 that sets the rate of hardening in the evolution equation. $\dot{\gamma}^*$ is the sum of shear rates on all slip systems in the crystal. The parameters used in the simulation were 66 MPa for τ_0 , 170.8 MPa for θ_0 and 90 MPa for τ_v .

The simulation was conducted using uniform time steps of 10s. As detailed above, each crystal was associated with the state variables describing orientation (three Euler angles) and hardness $\hat{\tau}$. The evolution of these state variables was computed for over 1.3 million crystals. The simulation was carried out to a strain of 0.26. The simulation was conducted on the Thinking Machines CM-5 computer at the Advanced Computing Laboratory at Los Alamos National Laboratory. The calculations were completed in four hours using one-eighth of the CM-5 processing power.

RESULTS

Figure 2 shows the distribution of {100} and {111} type grains in the sampling region. Orientation measurements having {111} poles within 15° of the plate normal are highlighted in black in the left hand figure and measurements having {100} poles within 15° of the plate normal are highlighted in the right figure. Clearly, the centerline of the plate is primarily composed of grains having {111} poles normal to the surface of the plate and the {100} type grains are primarily located at the surface of the sample. This is the cause of the hourglass shape after deformation of the compression samples. The {100} type grains are in a "softer" orientation than the {111} grains. Thus, more of the strain is accommodated by the grains at the surface of the sample than the grains at the center. The boundaries in figure 2 were formed by drawing a line segment between neighboring measurement points when the misorientation between the measurement points exceeded 15°. The measurements are too coarse to adequately reconstruct the grain boundary map as has been done from automatic orientation measurements in previous works[3, 4]. However, a nonuniform grain size distribution is evident in the figure and confirmed by metallographic observations.

Figure 2 Grain boundary maps reconstructed from the orientation measurements. Measurements are highlighted having (111) (left) and (100) (right) poles normal to the plate surface.

An interesting feature in the modeling effort was the correlation between the distribution of strain (and strain rate) and the distribution of orientation in the sample. Figure 3 shows the distribution of strain rate at a strain of 0.13 and later at a strain of 0.26.

Figure 3 Distribution of strain rate in the simulation at strains of 0.13 and 0.26.

At earlier stages of the deformation, elements lying along the transverse direction at the top surface of the specimen exhibit the highest deformation rate. The maximum deformation rate is located at the extreme position along the transverse axis – this will be the position of the most extreme hourglass effect. At a strain of 0.26, the position of maximum deformation rate has moved to the specimen through-thickness mid-plane at the extreme position of the rolling direction axis. The inhomogeneity of the deformation field is a result of texture gradients along the specimen axis; the strain rate would be uniformly distributed in a sample without texture variations.

Figure 4 shows a profile of a section plane in the compression sample. The particular plane shown is normal to the rolling direction of the plate. The symmetrized-experimental curve was formed by averaging the experimental curve with its mirror image (through the vertical). The experimental curve is not symmetric because either the texture gradient is not symmetric about the midplane of the plate or the midplane of the sample is not coincident with the midplane of the plate.

In addition to the hourglass shape of the compression specimen, there was also measurable ovaling. The ovaling measured on the experimental specimen at the mid-section was 98.0%. The ovaling predicted by the simulation was 97.9%, in close agreement with the experimental result. The ovaling measured at the surface was 98.3% and predicted by the simulation was 98.9%.

Figure 4 Experimental and predicted profiles of the compression sample.

DISCUSSION

The simulation captures the sense of the hourglass effect. However, the simulation results do not precisely match the experimental results. One cause is that the texture not only varies through the thickness of the plate but in the plane of the plate as well. Thus, each sample will differ in mechanical behavior simply due to in-plane variations in texture. Another cause for discrepancies is the description of the work hardening behavior used in the simulation. Polycrystalline plasticity models of this type generally require good single crystal work hardening data to achieve optimum results. In this case, the work hardening behavior was obtained from polycrystalline measurements and the single crystal data inferred using the polycrystal texture.

Nonetheless, the observed trends are well predicted by the simulation. The coupling of spatially specific orientation measurements with polycrystalline plasticity modeling within the finite-element regime provides an excellent way of using the orientational aspects of microstructure to quantitatively model the mechanical response of polycrystalline materials.

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