LA-UR-97-4469

Title: TEXTURE EVOLUTION IN UPSET-FORGED P/M AND WROUGHT TANTALUM: EXPERIMENTATION AND MODELING

CONF-971168--

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Submitted to: 1997 INTERNATIONAL CONFERENCE ON TUNGSTEN REFRACTORY METALS AND ALLOYS BY METAL POWDERS INDUSTRIES FEDERATION TO BE HELD AT ORLANDO, FL ON NOVEMBER 17-19, 1997

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TEXTURE EVOLUTION IN UPSET-FORGED P/M AND WROUGHT TANTALUM: EXPERIMENTATION AND MODELING

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ABSTRACT

Preferred orientations in polycrystalline materials can significantly affect their physical and mechanical response through the retention of anisotropic properties inherent to the single crystal. In this study the texture evolution in upset-forged P/M and wrought tantalum was measured as a function of initial texture, compressive strain, and relative position in the pressing. A <001>/<111> duplex fiber texture parallel to the compression axis was generally observed, with varying degrees of a radial component evident in the wrought material. The development of deformation textures derives from restricted crystallographic slip conditions that generate lattice rotations, and these grain reorientations can be modeled as a function of the prescribed deformation gradient. Texture development was simulated for equivalent deformations using both a modified Taylor approach and a viscoplastic self-consistent (VPSC) model. A comparison between the predicted evolution and experimental results shows a good correlation with the texture components, but an overly sharp prediction at large strains from both the Taylor and VPSC models.

INTRODUCTION

Tantalum has received significant attention for defense and civilian applications due to its high density and high melting point. For some of these applications an upset-forge, or free uniaxial compression, fabrication step is performed. This forging operation may be desired or required for refining the microstructure, homogenizing non-random microstructures, or shaping the part for subsequent deformation steps. Accompanying this deformation step is an evolution of the microstructure; this paper specifically addresses changes in the crystallographic texture as a function of compressive strain, initial texture, and relative position in the forging. Experimental observations of the texture development are compared with simulations applying two different models.

The core impetus of this work was to determine the requisite amount of compressive deformation to evolve a uniform texture with axial (compression axis) symmetry from two initial product forms, and the degree to which previously developed plasticity models could be employed to predict the evolution of this texture at large strains, assuming ideal deformation conditions. In this study, the powder metallurgy (P/M) material represented an initially random texture, while the round-rolled bar introduced an initial preferred orientation before the upset deformation. The possible effect of tool-workpiece friction on heterogeneous texture development was examined by sampling from various areas within the upset forging.

The plasticity models applied in this study, namely the Taylor-Bishop-Hill[1-3] (Taylor) and viscoplastic self-consistent[4-5] (VPSC) models, operate on the principle of restricted crystallographic slip as simple shears that induce rotation of grains; the proclivity of a greater than average number of grains to rotate toward equivalent orientations results in macroscopic textures. Differences between the models manifest themselves in the possible selection of different sets of slip systems, and different strains apportioned to each system, to accommodate a given increment of prescribed strain. The Taylor model enforces strain compatibility such that the deformation path of each grain is equivalent to the polycrystal as a whole. This is in effect an upper-bound solution for yield stress, the grain with the 'hardest' orientation must deform equivalently to the 'softest', and the single crystal yield surface must be closed for each grain. The selection calculation of the operative slip systems was improved by Bishop and Hill[2-3] on the principle of 'maximum external work' rather than Taylor's 'minimum internal strain' criterion. A modified Taylor approach is employed for this work, in which a small rate sensitivity is applied to avoid ambiguity in slip system selection, and a relaxed constraint[6] treatment is activated as grains flatten at greater strains. Relaxed constraint amounts to a reduction in the number of required slip systems for plastic flow from five to three within highly aspected grains.

In contrast, the VPSC model utilizes the concept of a homogeneous effective medium (HEM) representing the average properties of the polycrystalline matrix surrounding each specific grain. The interaction of a grain and the HEM can be solved explicitly by the Eshelby inclusion formulation[7], and this results in enforcement of local stress compatibility. The overall effect is to account for anisotropy between the grain and matrix, and provide for the accommodation of global strain by a range of strains in individual grains, unlike the rigid constraints of the Taylor model. An increment of plastic deformation can be accommodated by a given grain more or less than the HEM, depending on its orientation. The net result is the requirement of fewer active systems for arbitrary plastic flow, and a more realistic range of plasticity among the grains as compared to the Taylor model. The VPSC model is therefore generally more effective for application to low-symmetry materials with a minimal number of independent slip and/or twinning systems, and for large deformations as is the case for the upset forging in the current study.

EXPERIMENTAL

Two initial tantalum product forms were fabricated from powder and wrought processing routes. The P/M part was produced by hot isostatically pressing (HIP'ing) standard grade (841 ppm oxygen) tantalum powder into a cylindrical form at 1600°C and 210 MPa for one hour, followed by machining three cylindrical forging blanks of 2.5 cm diameter from the pressing. Wrought bar stock was obtained in the as-rolled condition from Cabot Corp., then annealed at 1150°C for 1 hour in vacuum to improve its formability. The long axis of the bar stock was made to coincide with the compression axis. Upset-forgings were performed on three samples from each product form, compressed to nominal true strains of -0.5, -1, and -2, for a total of six conditions. The forgings were performed on an MTS hydraulic load frame at room temperature and quasi-static strain rates, between steel platens lubricated with MoS_2 grease. Deformation was interrupted for relubrication at increments of approximately 0.25 strain.

Samples were sectioned from each of the six conditions at various positions in the forgings, followed by a tantalum-specific metallographic preparation[8]. X-ray texture measurements were performed on a Huber four-circle goniometer and Scintag X-ray system using Fe K-α radiation. Texture data were reduced to orientation distribution functions (ODFs) using the *popLA* software package[10]. Grain files comprised of 1000 weighted orientations, used for input to represent the texture in simulation codes, were discretized from the ODF[9]. The *popLA* software (program DIOR) was also employed to graphically represent the discrete simulation output as density plots.

The Taylor model was accessed through *LApp*[11-13], a polycrystal plasticity code developed at Los Alamos National Laboratory, while the VPSC model was provided in a special version of code supplied by one of the authors (CT) and R. Lebensohn. Relaxed constraint conditions were activated in the Taylor model at a rate such that 2% (by volume) of the grains were relaxed at a strain of -0.55, 32% at $\varepsilon = -1$, and 82% at $\varepsilon = -2$. Either two deformation modes, {110}<111> and {112}<111> slip, or one mode, {110}<111> slip, were allowed to accommodate the deformation. In the case of two modes, the critical resolved shear stress (CRSS) was equivalent. The uniaxial compressive strain was accomplished for both models in steps of 0.025 to $\varepsilon = -0.5$, steps of 0.05 to $\varepsilon = -1$, and steps of 0.1 to $\varepsilon = -2$. The models were implemented by computer simulation on a Pentium-based PC. The typical run-time, depending on the number of strain-steps and model employed, ranged from 3 to 15 minutes.

RESULTS

Both experimental and simulation results are presented as (100) compression axis-normal pole figures (PFs) or compression axis inverse pole figures (IPFs, which plot the distribution of a sample axis on a crystal reference frame, in this case the standard triangle for cubic crystals), each calculated from the ODF. Figure 1 shows the experimental and simulation results as IPFs for the P/M material in matrix format; rows correspond to strain and columns to source (experimental and model type). The IPF alone adequately represents the evolving P/M texture, since it commences random and retains sample symmetry about the compression axis during processing. The experimental results in the left-hand column (Fig. 1j, 1n, and 1r) display the evolution of a nearly equally weighted duplex <001>/<111> fiber texture parallel to the compression axis. This has developed to a strength of nearly 8 multiples of random distribution (m.r.d.) by $\varepsilon = -0.5$, and moderately sharpens to nearly 16 m.r.d. by $\varepsilon = -2$. This sharpening is accompanied by a draining of orientations from non-<001> or <111> regions. Simulation results from the relaxed constraints Taylor model with two slip modes, shown in the second column of Fig. 1, accurately predicts an equivalent bifurcation of texture components into the <001> and <111> regions, but with pronounced over-sharpening at larger strains. Draining of texture components from the <101> region into <001> and <111> is predicted to begin at small reductions, and the <001> component develops somewhat earlier than the <111>. The VPSC prediction with two operative modes (Fig. 1, third column) is very similar to the Taylor results, but with somewhat earlier development and sharpening of the <001>/<111> texture. The VPSC model utilizing only the {110}<111> deformation mode (Fig. 1, fourth column) is less accurate in predicting the texture at intermediate strains, as the <111> component is skewed near <112> until $\varepsilon = -2$, a condition not experimentally validated. This one-mode condition for bcc metals is equivalent to fcc metals in tension under full constraints.

Figure 2 shows the experimental texture from the recrystallized round-rolled bar before upset forging, in the form of a recalculated (100) bar axis-normal PF and bar axis IPF. The complexity of the texture arises from the asymmetric nature of the radial forging and round-rolling process steps used in its manufacture. The experimental texture of the upset-forged bar is displayed at $\varepsilon = -1$ in Figure 3 and $\varepsilon = -2$ in Figure 4, both as a function of position in the forging. Although the upset process is axisymmetric, texture symmetry cannot be assumed since the initial texture is asymmetric about the bar axis. Indeed, the PFs in Fig. 3 show this lack of symmetry at all positions. Although the development of the <001>/<111> texture is present, more so in the periphery of the forging (Fig. 3a and 3c) than in the center, it is not a fiber texture. That is, a preferred direction exists in the plane normal to the compression axis (forging plane) for both the <001> and <111> components, as

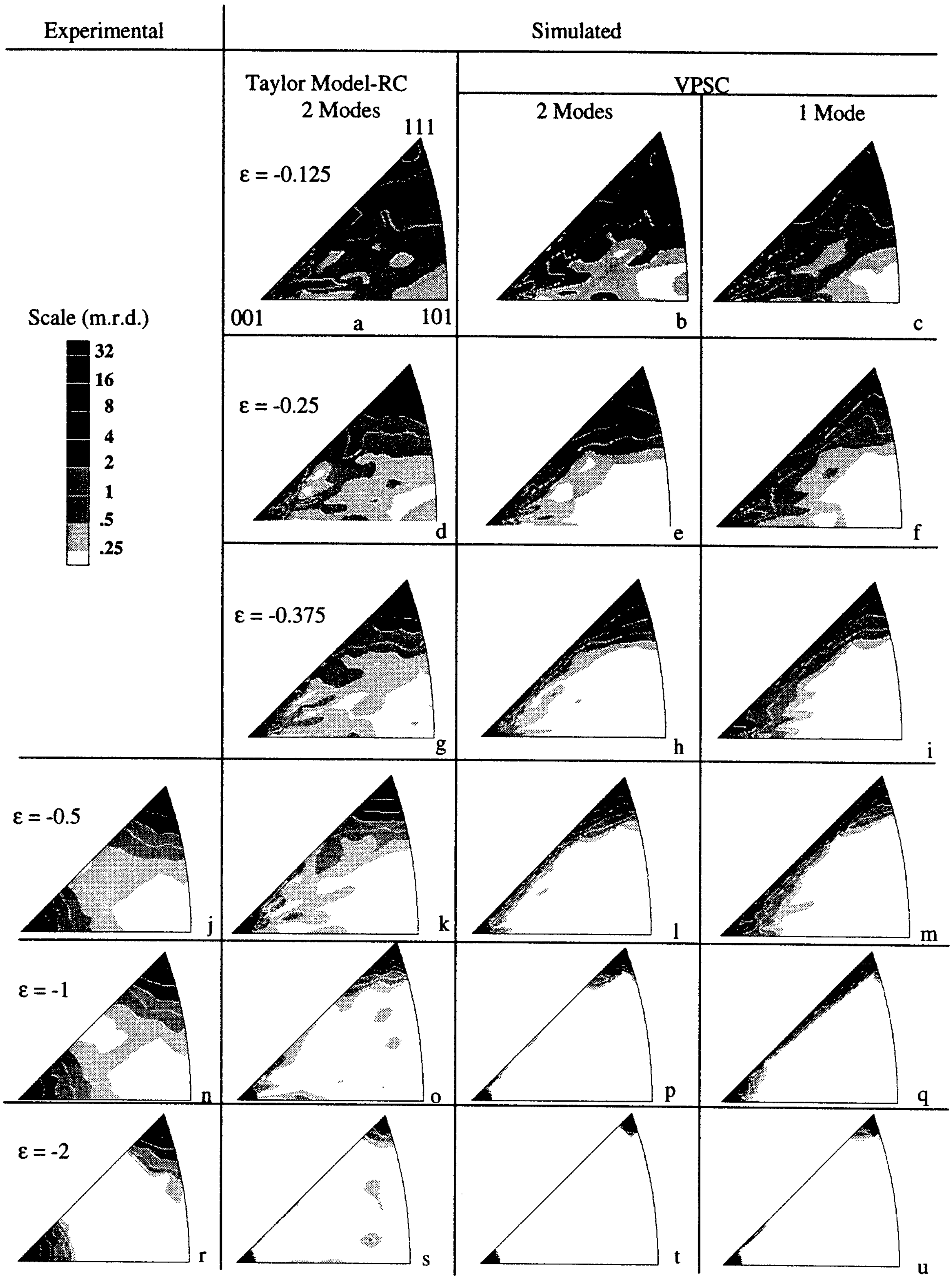

Figure 1: Texture evolution in upset-forged P/M tantalum as a function of compressive strain as shown by compression axis inverse pole figures. Experimental and simulated results sorted by column, strain sorted by row; a-c) ε = -0.125, d-f) -0.25, g-i) -0.375, j-m) -0.5, n-q) -1, r-u) -2.

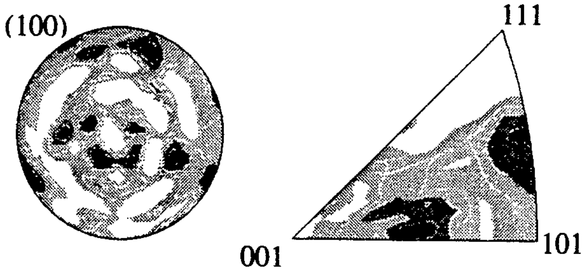

Figure 2: Initial texture of as-recrystallized (no upset strain) tantalum round-rolled bar. Bar axis-normal (100) recalculated pole figure and bar axis inverse pole figure.

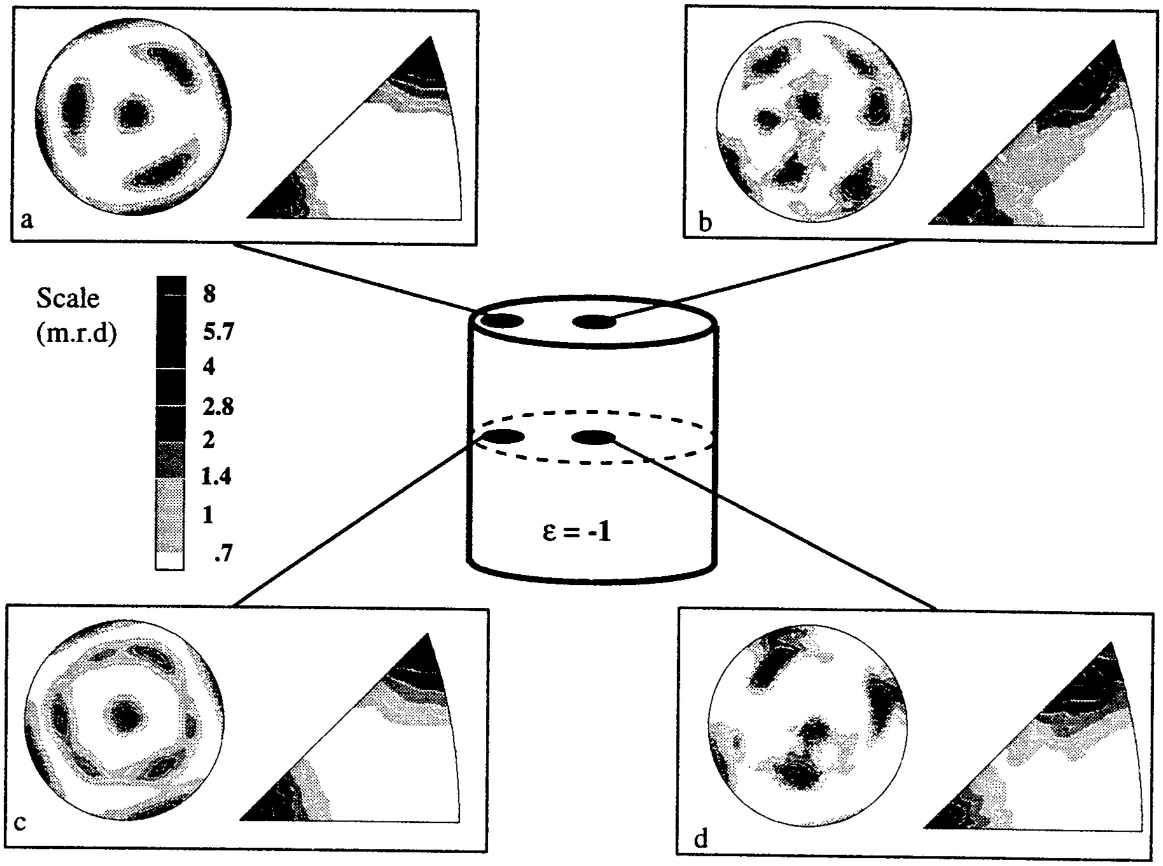

Figure 3: Upset-forged (ε = -1) tantalum texture (recalculated (100) compression axis-normal pole figure and compression axis inverse pole figure) as a function of position in the forging: a) surface (workpiece-tool interface), outer radius, b) surface, inner radius, c) midplane, outer radius, and d) midplane, inner radius.

evidenced by the three-fold and four-fold symmetry in the PFs, respectively. At ε = -2 (Fig. 4) the texture is trending toward axisymmetry, especially at the midplane. This indicates significant upset forging strain is required to fully break down remnants of the original bar texture. Simulation results for the bar material are displayed for the Taylor and VPSC models, both with two operative slip modes, in Figure 5. Once again, the predictions between the models are similar, with the VPSC resulting in a slightly accelerated sharpening of the compression texture. Both models fail to capture the detail of the preferred direction in the forging plane, and evolve symmetry about the compression axis to produce a near-fiber texture earlier in the strain history than the experimental results.

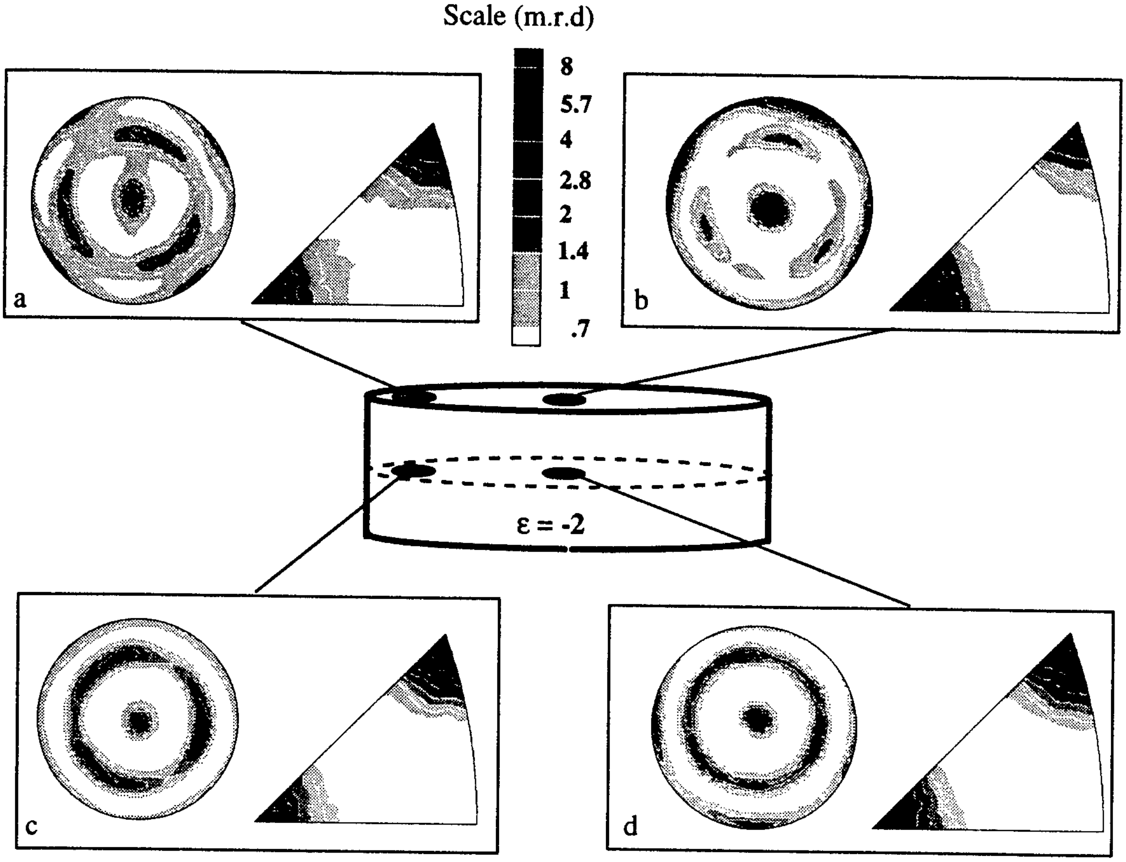

Figure 4: Upset-forged (ε = -2) tantalum texture (recalculated (100) compression axis-normal pole figure and compression axis inverse pole figure) as a function of position in the forging: a) surface (workpiece-tool interface), outer radius, b) surface, inner radius, c) midplane, outer radius, and d) midplane, inner radius.

DISCUSSION

The evolution of a duplex <001>/<111> texture in uniaxially compressed tantalum is observed both experimentally and by simulation. However, the development of this texture was dependent on the initial texture, and its simulation qualitiatively correct but overly sharp compared to experiment. Predictions for the P/M material (Fig. 1) show that two slip modes more accurately portray texture evolution in tantalum than only {110}<111> slip, in agreement with Wright et al[14]. Figure 6a shows a plot of the relative activity of {110}<111> and {112}<111> slip modes for both the Taylor and VPSC simulations. A preference for slip on {112} planes is observed for both models, especially by VPSC at large strains; this result was anticipated for Taylor simulations by Kocks[15]. Changing the relative CRSS's would affect the relative slip activity, and may influence the predictions. Figure 6b shows the distribution of grain sizes for the VPSC two-mode simulation by a plot of the relative grain dimension along the compression axis as a function of upset strain. The large variance in grain flattening is not surprising; <111> is a 'hard' orientation in compression and <001> is relatively 'soft'.

The effect of relative position in the forging on texture (Figs. 3 and 4) is dominated by the frictional conditions at the tool-workpiece interface. Under ideal conditions, all regions of a compressed disk would undergo equivalent strains. In practice, a friction hill exists diametrally across the surface as

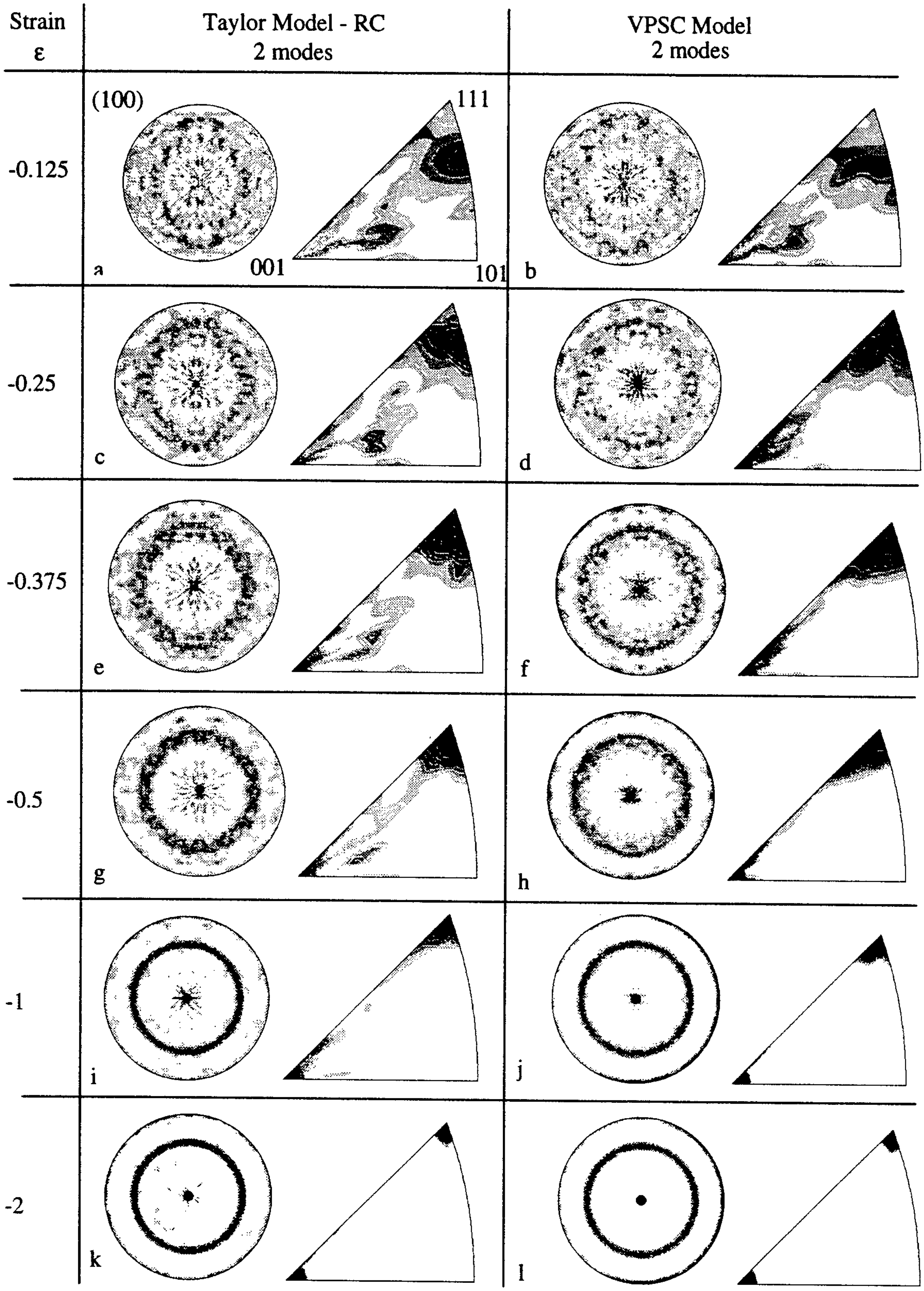

Figure 5: Simulated texture evolution in upset-forged round-rolled bar tantalum as a function of compressive strain as shown by compression axis-normal (100) pole figures and compression axis inverse pole figures. Taylor and VPSC model results (both 2 slip modes) sorted by column, strain sorted by row; a-b) $\varepsilon = -0.125$, c-d) -0.25, e-f) -0.375, g-h) -0.5, i-j) -1, k-l) -2. Scale equivalent to Figs. 3 and 4.

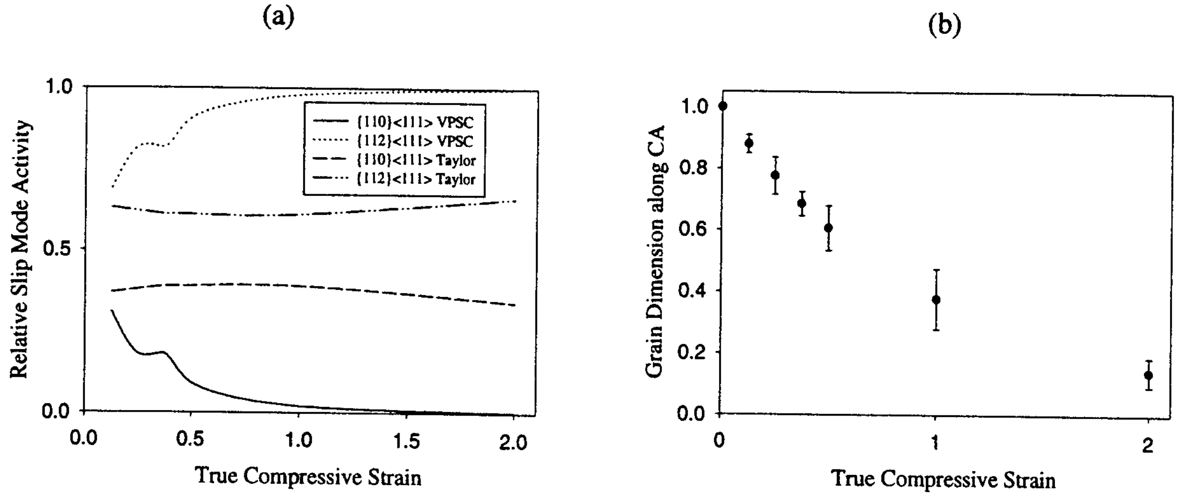

Figure 6: Statistics from P/M tantalum compression simulations with two slip modes as a function of compressive strain, showing a) the relative activity of the two slip modes for the VPSC and Taylor calculations, and b) the standard deviation of the mean relative grain dimension along the compression axis (CA) for the VPSC calculation.

depicted in Figure 7, with its maximum at the center. The effect of this gradient is to increase the hydrostatic stress and decrease the deviatoric stress component toward the center of the disk. Therefore, the effective strain in a given element is dependent on both its radial and axial position. For the bar stock at $\varepsilon = -1$ (Fig. 3), the greatest texture evolution and symmetry enhancement is found at the edge. This can be attributed to the larger effective strain in these regions. Continued reduction leads to greater texture homogeneity (Fig. 4), as the 'dead zone' of low deviatoric stress is eventually reduced. However, the surface region retains more asymmetry, a probable result of continuing to experience somewhat less strain than other regions as the forging stress increases. In any event, it is observed that compressive strains on the order of $\varepsilon = -2$ are required to sufficiently eliminate textural heterogeneities. Predictions of texture evolution in the rolled bar (Fig. 5) assume ideal deformation conditions, and therefore do not capture information on heterogeneity within the forging. The over-sharpening phenomenon probably results in predicting axial symmetry in the forging plane sooner than is realistic even if ideal conditions could be obtained.

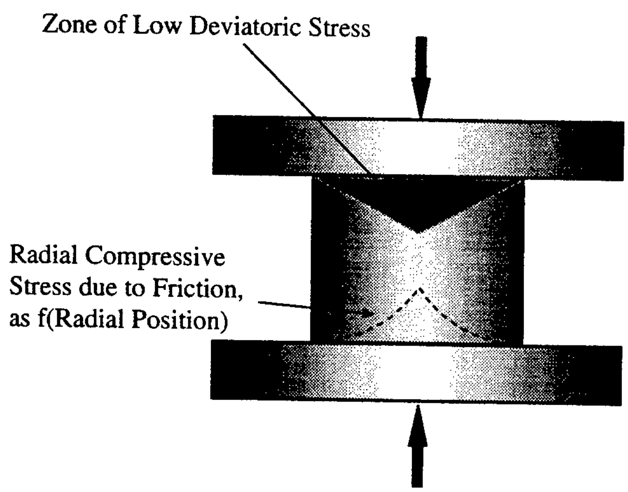

Figure 7: Schematic showing effect of tool/workpiece friction on stress state during upset forging.

The issue of overly intense texture predictions from plasticity models at large strains has been a general observation for many years, and can be attributed to stochastic effects not captured by the computation; these effects may be divided into those creating an ambiguity in the selection of slip systems and those due to spatially specific interactions with neighboring grains[16]. Previous work on an 'effective-cluster' modification[17] to the Taylor model resulted in somewhat more dispersed texture distributions at large strains. In this approach each grain is considered together with its immediate environment as a cluster, the cluster is embedded in an elastic medium representing the entire polycrystal, and stress compatibility is enforced between the two. The somewhat surprising result from the present work was that the VPSC model did not ameliorate the over-sharpening as compared to the Taylor results. This may be due to the nature of the deformation texture in this case, with the two end orientations displaying such a large misorientation. Perhaps the texture, once drained into <001> and <111> regions, is constrained to rotate toward its endpoint more rapidly than if a spread of orientations were produced such as during plane-strain deformation. A converse way of interpreting the results is how well the Taylor model, with all of its assumptions, was able to predict the texture evolution in upset tantalum.

CONCLUSIONS

Upset forging of P/M produced a nearly balanced <001>/<111> fiber texture with a maximum strength approaching 16 times random by $\varepsilon = -2$. Round-rolled tantalum bar produced similar textures, but retained some asymmetry about the compression axis up to $\varepsilon = -2$. Heterogeneities in texture as a function of position were especially noticeable at $\varepsilon = -1$, but substantially reduced by $\varepsilon = -2$.

Simulations of the upset forging using the Taylor and VPSC models successfully predicted the <001>/<111> texture development, although both similarly over-sharpened the texture as the compression progressed. The use of two deformation modes, {110}<111> and {112}<111> slip, resulted in better predictions than applying only the former mode.

ACKNOWLEDGMENTS

The assistance of P.C. Mombourquette, W.W. Roybal, and V.D. Vargas for P/M processing, S.J. Atencio and S.W. Quintana for thermomechanical processing, and A.M. Kelly for metallographic preparation is gratefully acknowledged. This work was conducted under the auspices of the U.S. Department of Energy under contract W-7405-ENG-36.

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M98002924

Report Number (14) LA-UR--97-4469
CONF-971168--

Publ. Date (11) 199711
Sponsor Code (18) DOE/DP, XF
UC Category (19) UC-704, DOE/ER

DOE