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Title: Local and Polycrystalline Textures in BCC Metals; Their
Evolution and Effect on Mechanical Response

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Local and Polycrystalline Textures in BCC Metals; Their Evolution and Effect on Mechanical Response

J.F. Bingert, B.L. Henrie, C.M. Cady, G.T. Gray III, and P.J. Maudlin
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Los Alamos, NM 87545

ABSTRACT

Texture development in BCC metals follows from the active deformation mechanisms and imposed strain path. Tensile, compressive, plane strain, and shear deformation induce different crystal rotations and thus resultant textures at both the macroscale and mesoscale. This work investigates the interaction of texture and bulk plasticity with regards to constitutive behavior, strain localization, and damage initiation in BCC metals. Tantalum and low-carbon steel were analyzed by electron backscatter diffraction to determine the crystallographic mesostructure, while mechanical testing was performed over a range of strain rates and temperatures. Polycrystal plasticity modeling was used to predict texture evolution for a suite of strain paths and to calculate multi-dimensional yield surfaces. The calculated yield surfaces were then applied to estimate texture effects on mechanical properties. Measuring the plastic anisotropy associated with experimental compression samples enabled validation of these simulations. The impact of relative slip system activity on anisotropic plasticity will also be explored.

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Outline

- Introduction
 - Texture Analysis and Visualization
- Tantalum
 - Rod
 - 5D Yield Surface
 - Effect of Texture on Mechanical Response of 2 Different TMP
 - Plate
 - Bar
 - Instability Analysis
- Nb in Cu/Nb Nano-composite
 - Interface-Controlled Plasticity
- Low-Carbon Steel
 - Superimposed Morphological Anisotropy



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Introduction

- Pure Transition Metals vs. Alloys
 - Deformation Textures – $f(\text{Imposed Deformation Gradient})$
 - Annealing Textures
 - Recovery
 - Recrystallization
- Texture Evolution
- Quantitative Texture Analysis
- Property Modeling and Prediction
- Through-Thickness Heterogeneities



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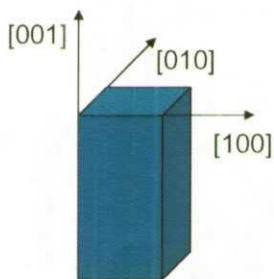


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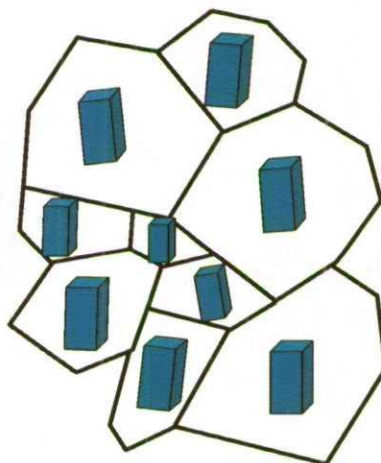
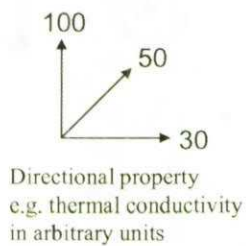
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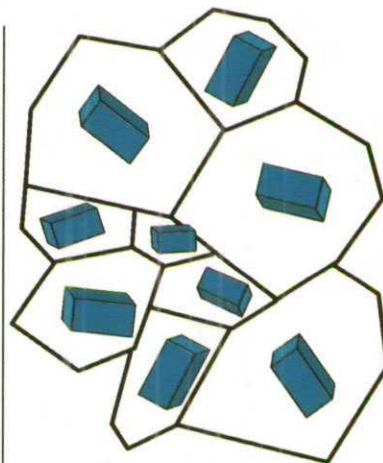
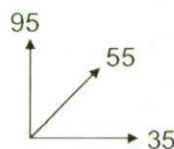
Transfer of Single Crystal Properties to Polycrystal



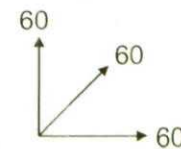
Single Crystal
(orthorhombic system)



Sharply Textured Polycrystal



Randomly Textured Polycrystal



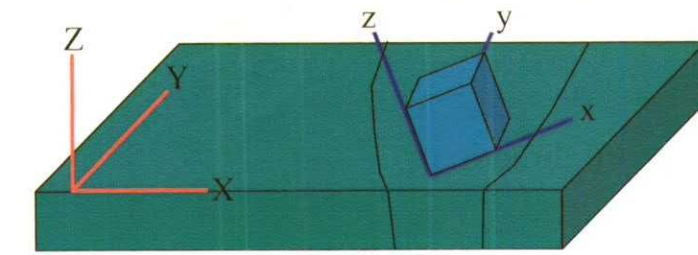
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Basis for Bunge Euler Angle Orientation Description



Sample Coordinate System

e.g. Rolled Plate

X = RD

Y = TD

Z = ND

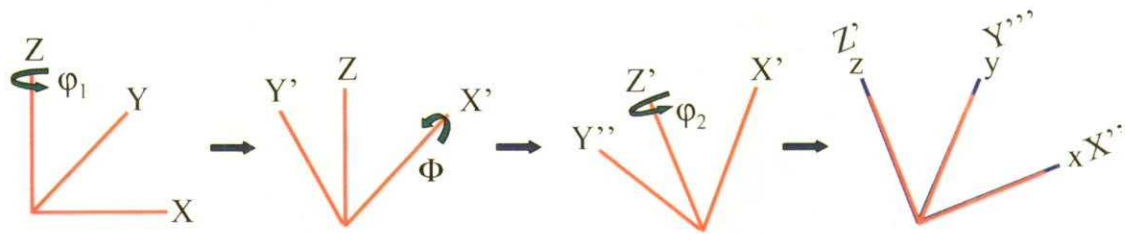
Crystal Coordinate System

e.g. Cubic

x = [100]

y = [010]

z = [001]



Position (x,y)

Discrete orientation $g = (\phi_1 \Phi \phi_2)$



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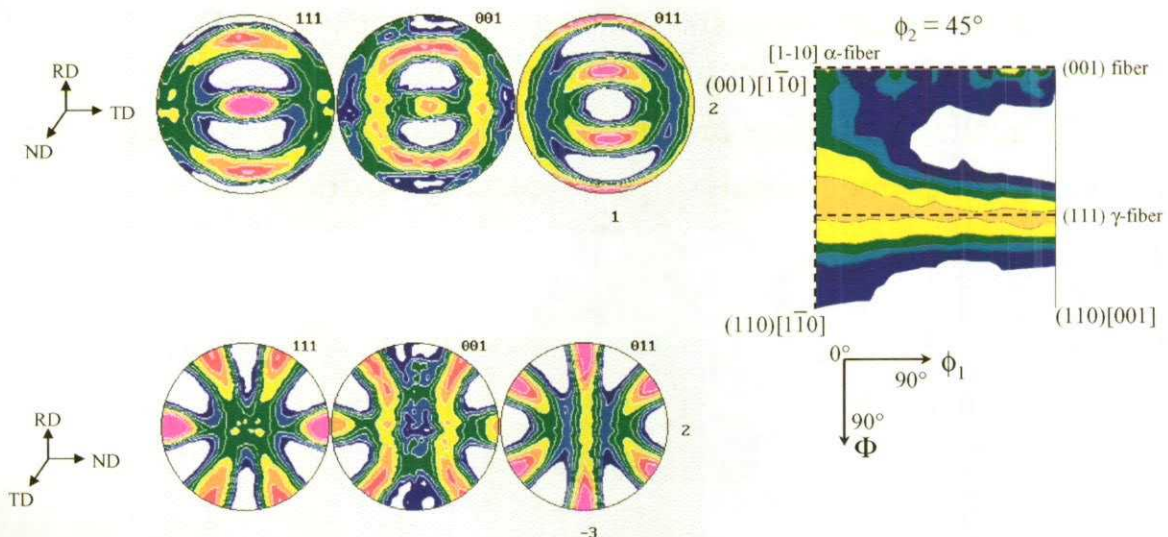
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Typical bcc plane strain texture

Rolled bcc X-ray Bulk Textures



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bcc Texture Rules of Thumb

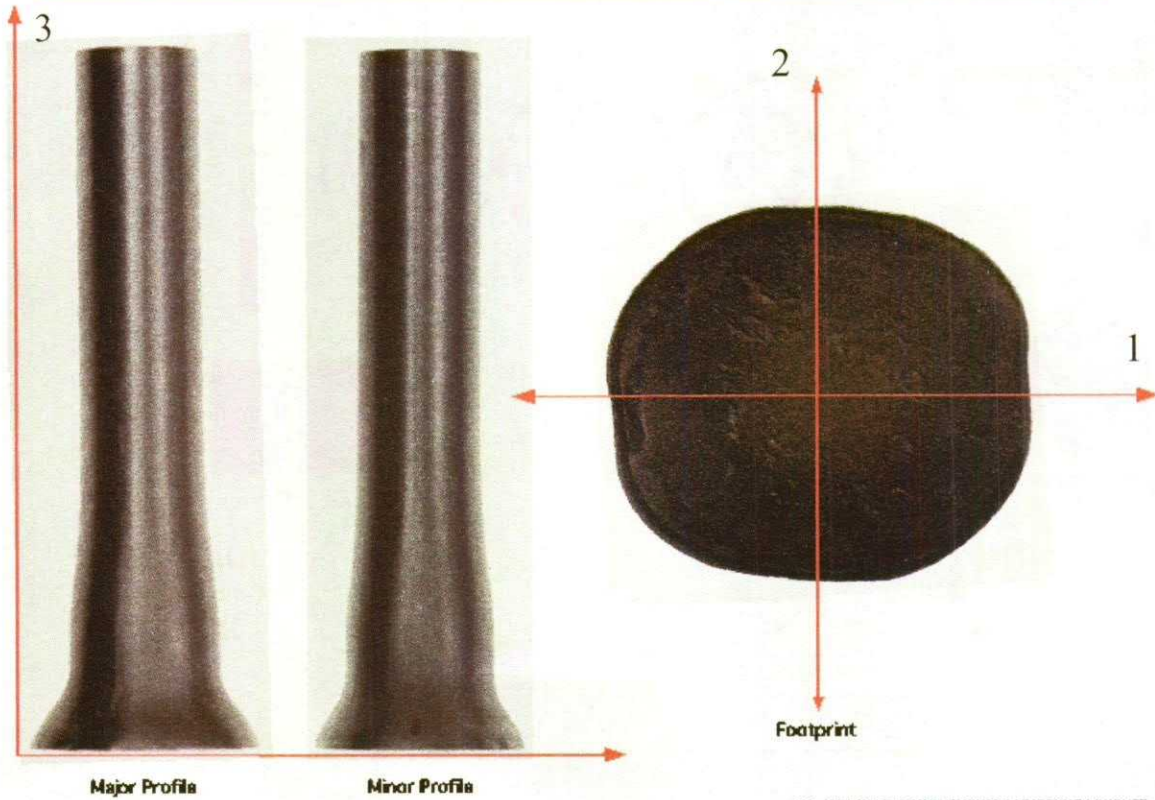
- Tension $\rightarrow$ $\langle 110 \rangle$
- Compression $\rightarrow$ $-\langle 111 \rangle + \langle 001 \rangle$
- $\langle 001 \rangle$ soft direction
- $\langle 111 \rangle$ and $\langle 110 \rangle$ hard directions

Ta Rod

- $\langle 110 \rangle$ texture suggests orthotropic symmetry at first glance, but not upon further inspection
- Calculated Pi-plane of yield surface predicts near-isotropy
- Taylor cylinder result surprise: rectangular footprint(!)

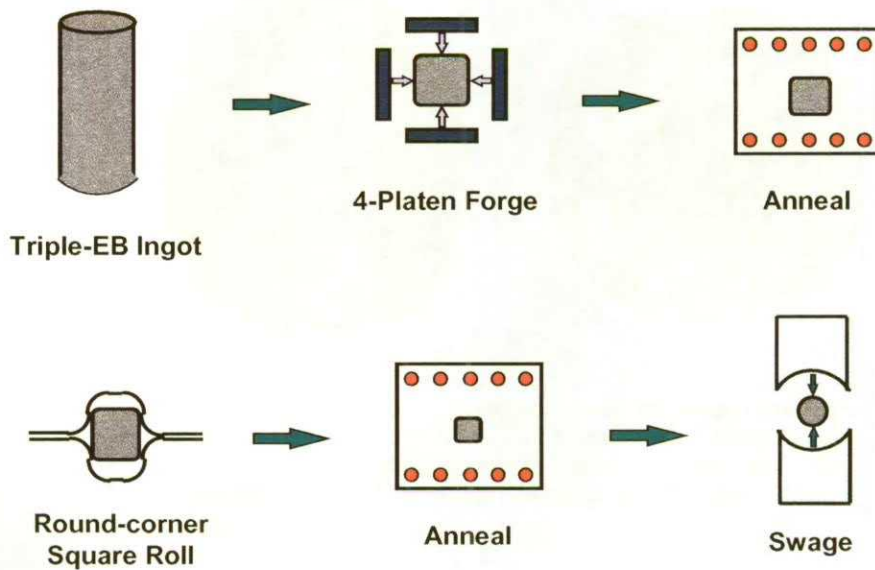
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Ta Rod: Final Taylor Specimen Shapes (139 m/s)



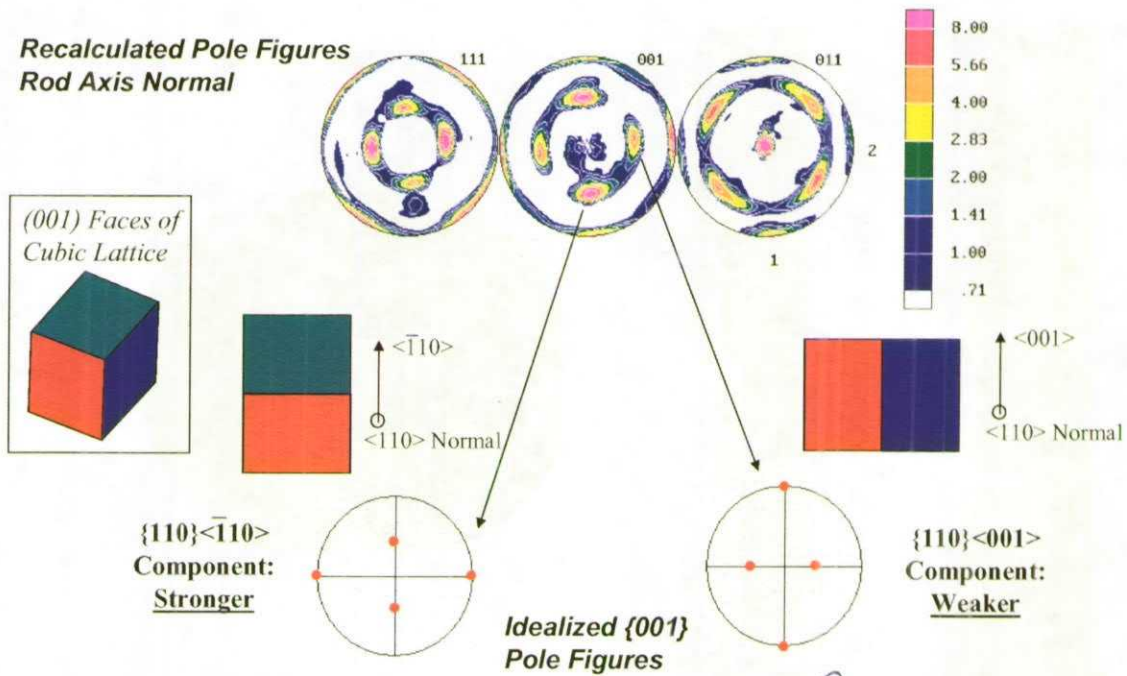
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Generic Ta Rod Processing

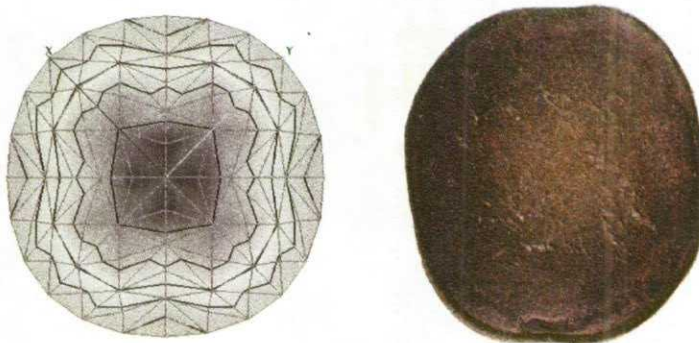


Ta Rod Texture

Recalculated Pole Figures Rod Axis Normal



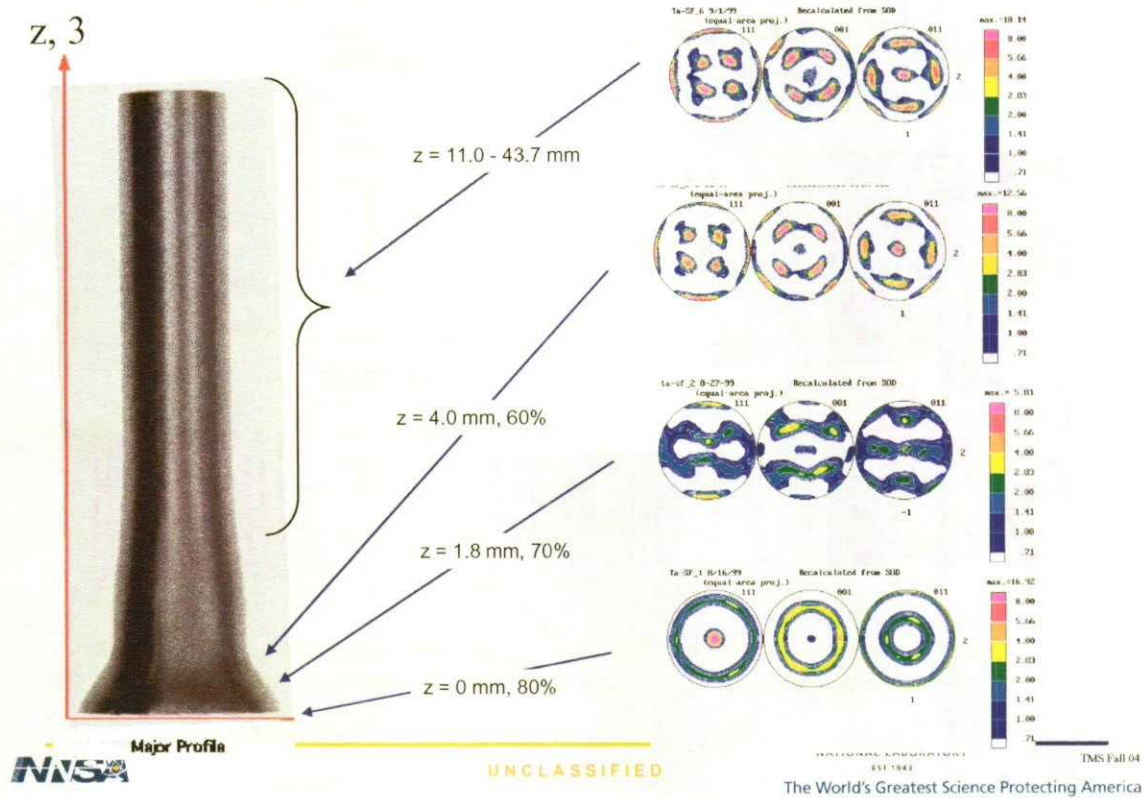
Orthotropic Yield Surface Calculation: Inaccurate Simulation



Potential causes for poor simulation:

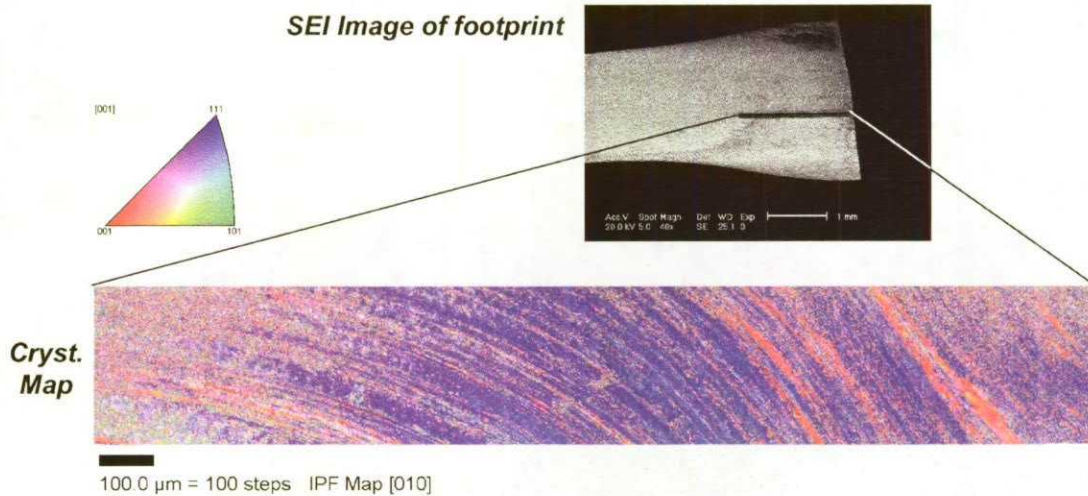
- Heterogeneous texture
- Effect of highly aspected grain morphology
- Yield surface does not capture important interactive terms

Measured Texture Evolution for Ta Rod

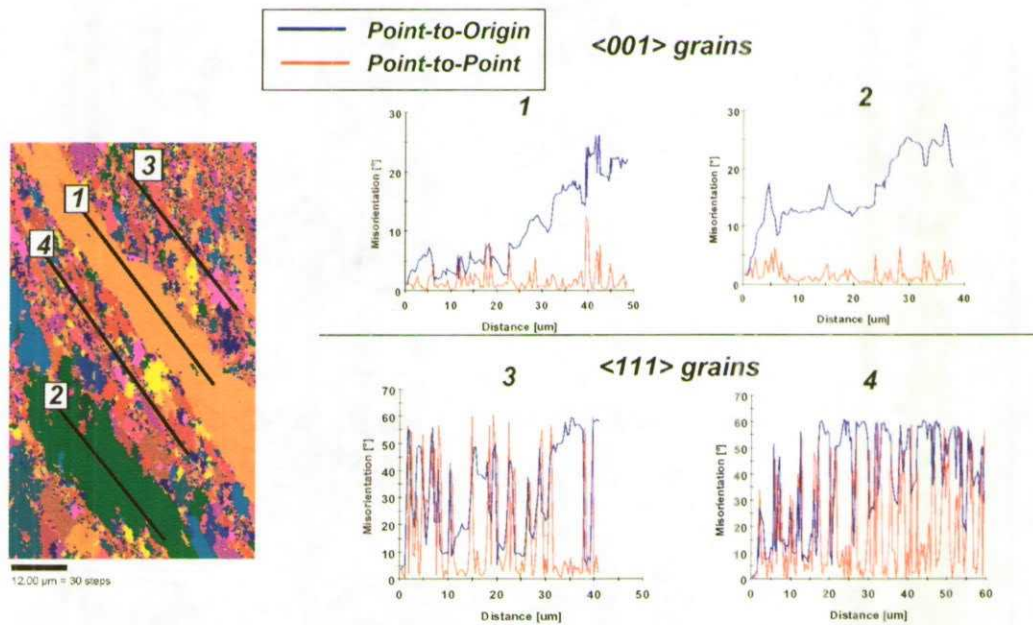


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Microtexture Map of Near-Footprint Region of Ta Rod

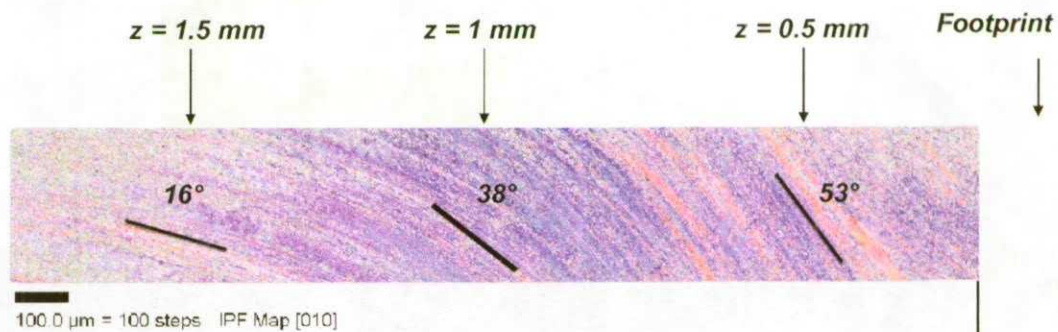


Misorientation Profiles

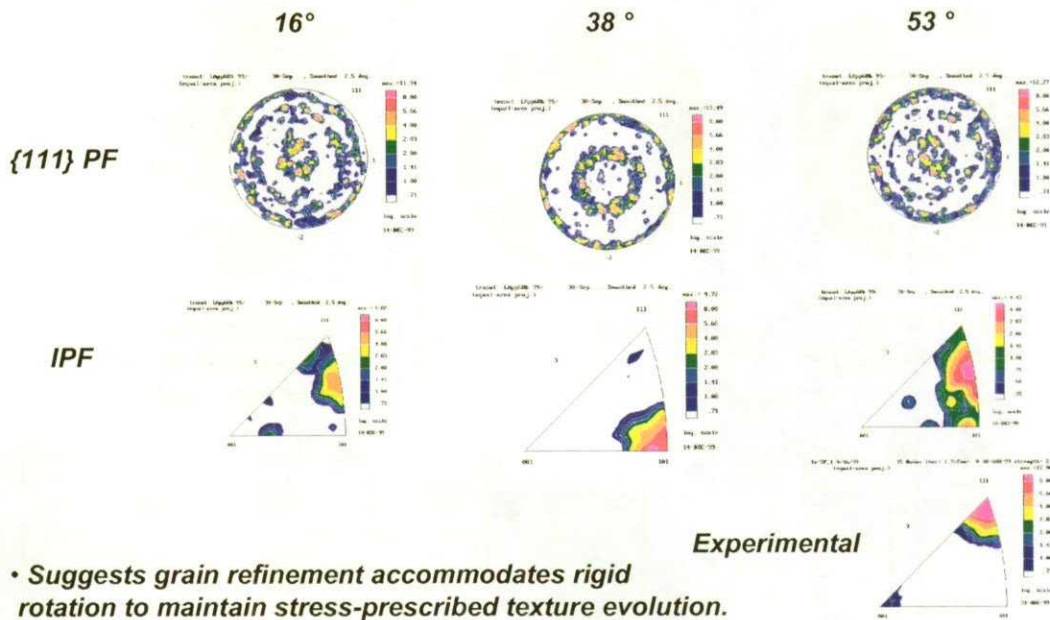


- **<001> grains evolve through gradual and cumulative misorientation changes.**
- **<111> grains evolve through small- and high-angle boundary networks.**

Observed Rotations from Grain Flow Paths

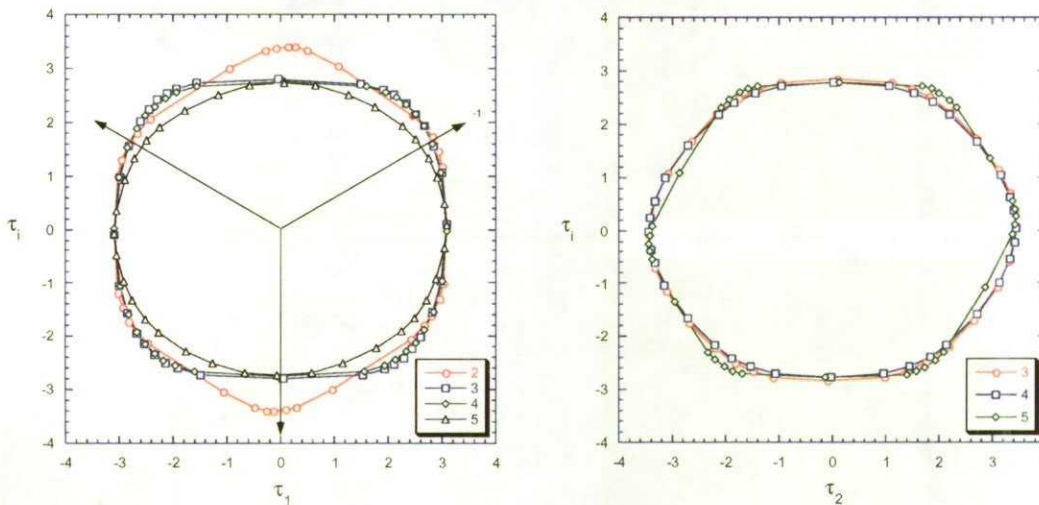


Suggested Texture Evolution with Imposed Rotation

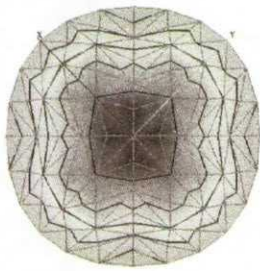


Ta Rod Yield Surface Projections

Pi-plane (τ_1 - τ_2) and Cross-terms



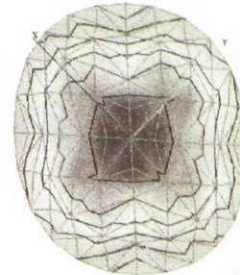
Ta Rod Taylor Cylinder Impact Interface: Predicted vs. Exptl.



Simulated:
Orthotropy Enforced



Experimental



Simulated:
No Symmetry Enforced
(Generalized YS)

$$\alpha \Rightarrow \begin{bmatrix} 2.06 & -1.08 & -0.975 & 0 & 0 & 0 \\ -1.08 & 2.13 & -1.04 & 0 & 0 & 0 \\ -0.975 & -1.04 & 2.02 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3.81 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4.05 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4.23 \end{bmatrix}$$

$$\alpha \Rightarrow \begin{bmatrix} 2.06 & -1.08 & -0.975 & 0.058 & 0.2 & 0.134 \\ -1.08 & 2.13 & -1.04 & 0.0155 & -0.224 & -0.0359 \\ -0.975 & -1.04 & 2.02 & -0.0735 & 0.0245 & -0.098 \\ 0.058 & 0.0155 & -0.0735 & 3.81 & -0.33 & -0.27 \\ 0.2 & -0.224 & 0.0245 & -0.33 & 4.05 & -0.06 \\ 0.134 & -0.0359 & -0.098 & -0.27 & -0.06 & 4.23 \end{bmatrix}$$

Interaction between normal stresses and shears accounted for



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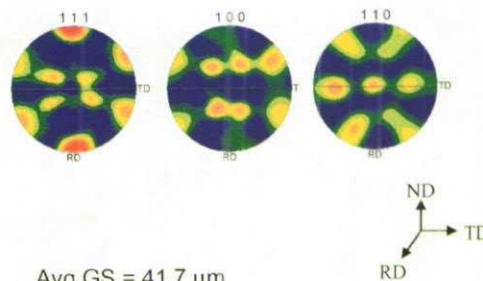
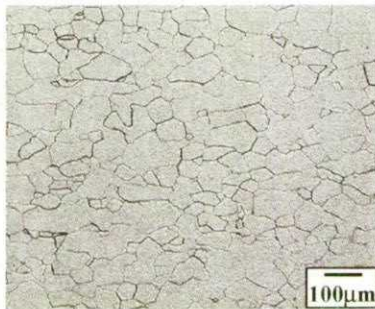
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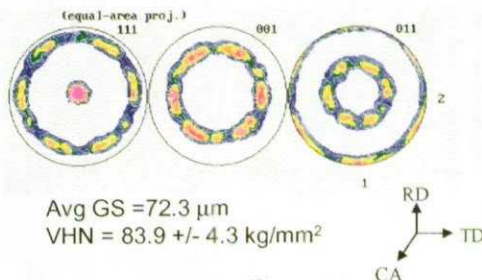
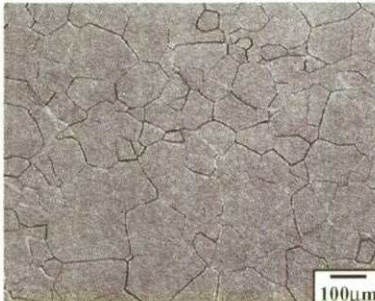
Thermomechanically Processed Tantalum

Plate



Avg GS = 41.7 µm
VHN = 95.0 +/- 7.1 kg/mm²

UF Bar



Avg GS = 72.3 µm
VHN = 83.9 +/- 4.3 kg/mm²



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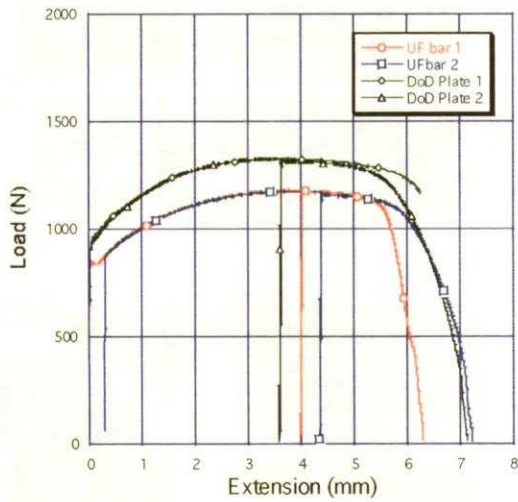


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Chemistry and Mechanical Properties Similar



QS Tensile Testing

Element (ppm)	Plate	Bar	HIP
C	10	<10	-
O	64	<10	680
N	10	<10	46
H	4.4	2.1	16.3
Nb	<20	127	<20
W	50	<50	200

Chemical Analysis



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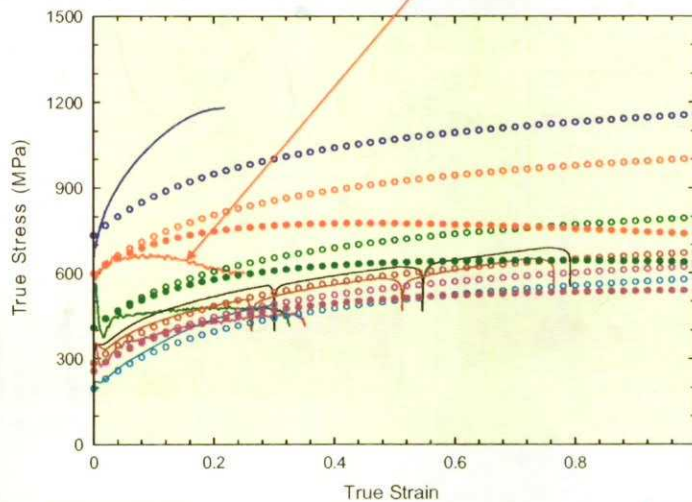
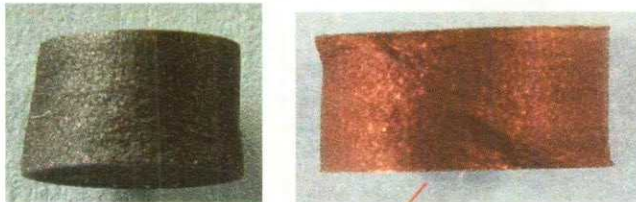


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Ta UF Bar Uniaxial Compression: Unstable Behavior in TT Dir.



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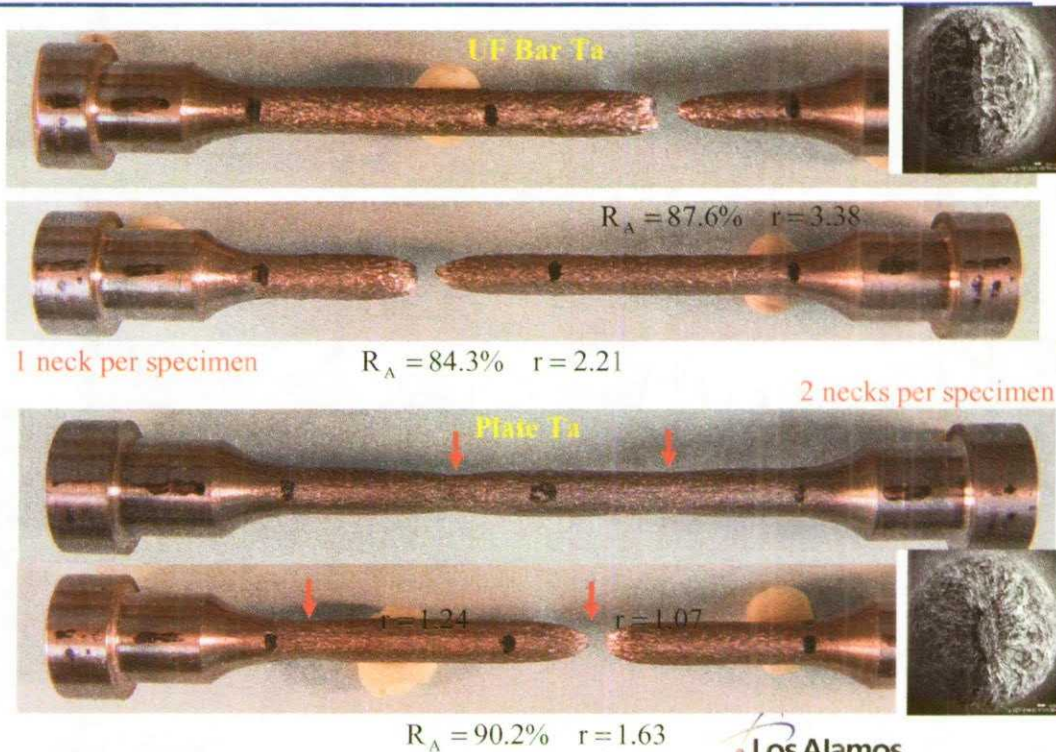


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Quasi-Static Strain-to-Failure Tensile Testing



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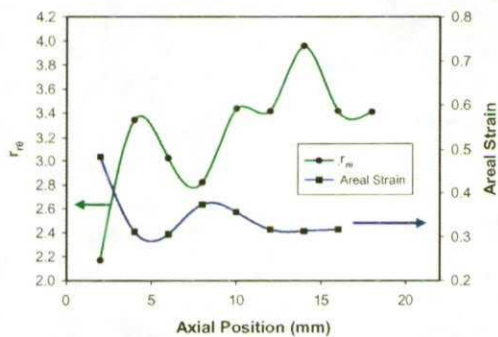
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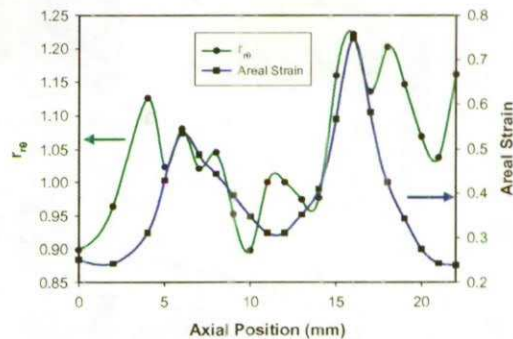
Ta Plastic Anisotropy: In-Plane QS RT Tensile Samples

Ta Upset-Forged Bar



UF Bar

Ta Plate



Plate



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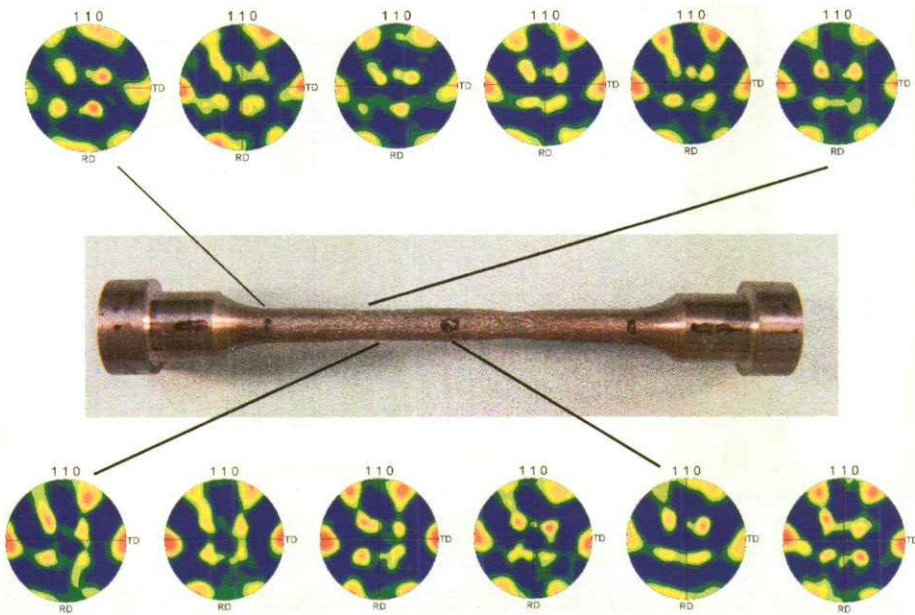


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Ta Plate IP QS RT Tensile Textures as f(Position)



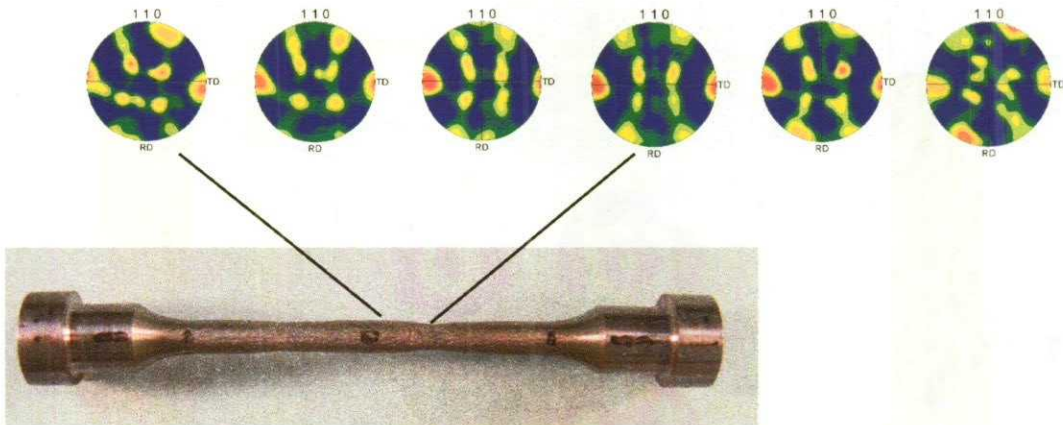
NISA

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Ta Plate IP QS RT Tensile Textures as f(Position)

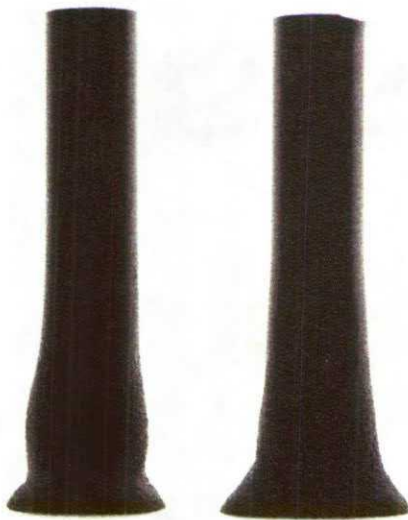


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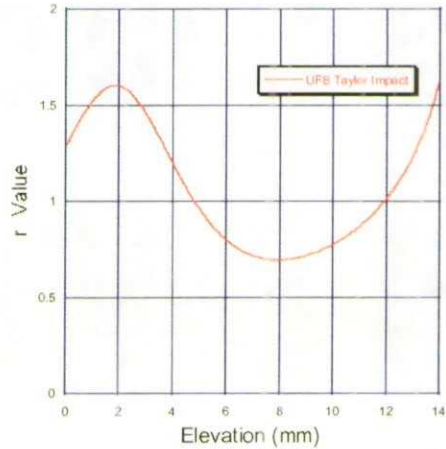
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Oscillatory Anisotropy in Ta UF Bar Taylor Sample



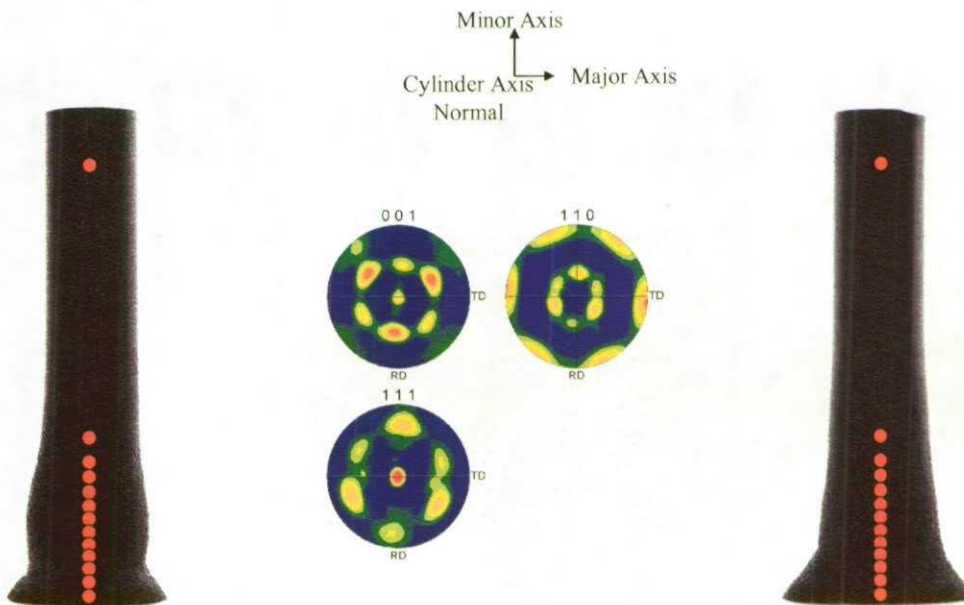
Minor

Major



- *r-value decreases toward impact interface until direction of major and minor axes reverse.*
- *Does plasticity modeling predict this?.....*

Texture wrt Axial Position in UF Bar Taylor



Minor

Major

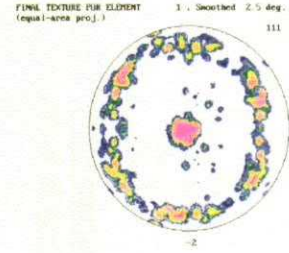
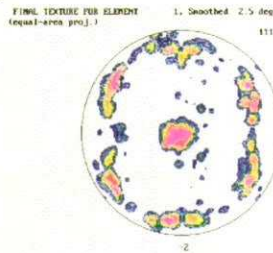
VPSC from EPIC deformation paths – UF Bar Ta

Major Axis
Minor Axis
Normal
Cylinder Axis

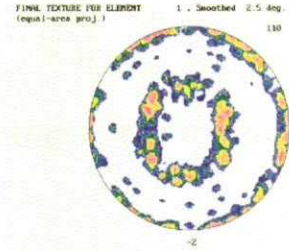
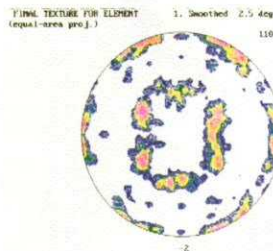
$z = 3 \text{ mm}$

$z = 8 \text{ mm}$

(111)



(110)



- *Plasticity simulation suggests little texture evolution.*
- *Monotonic r-value with strain predicted.*



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Possible Explanations

- Heterogeneous microstructure due to radial banding in upset forged blank.
- Plastic anisotropy so large in r - θ plane that $\langle 110 \rangle$ develops in originally soft direction of major axis due to straining in that direction.
 - Results in transition of relative anisotropy to orthogonal axis.
- *Plastic instability.*



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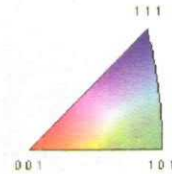
Tantalum Plate Through-Thickness Microstructural Heterogeneity



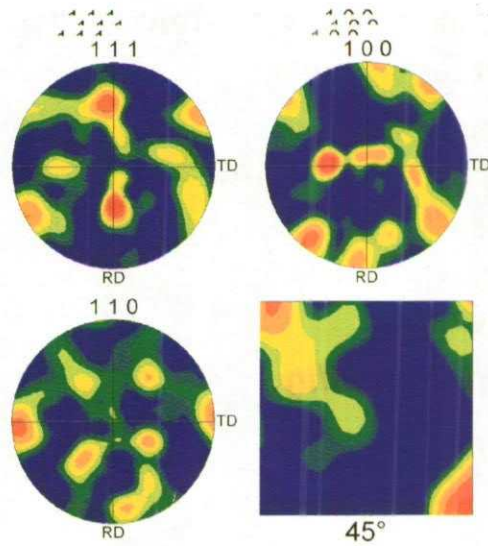
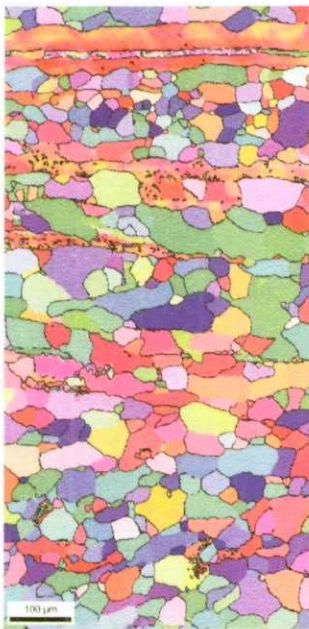
Each scan is .5mm by 1mm

Color Coded Map Type: Inverse Pole Figure [001]

Tantalum



Tantalum Plate Through-Thickness Microstructural Heterogeneity



Shear Bands/Flow Instabilities

– Classification

- Brass type – low SFE, twinning
- Cu type – med. to high SFE
- Adiabatic

– Potential Factors (affect microband and clustering)

- Strain, rate, texture, temperature, GS, microstructural heterogeneities
- Zener-Holloman

$$Z = \dot{\epsilon} \cdot \exp(Q / RT_D)$$

Sharp transition correlated w/ onset of dynamic recovery

– Potential Mechanisms at Microstructural Scale

- Slip asymmetry: activity of co-planar vs. co-directional slip
- Stress conc. at tips of microband groups
- Restricted glide on systems parallel to microbands
- Texture Softening

$$\frac{d\sigma}{d\epsilon} = M^2 \frac{d\tau}{d\Gamma} + \tau \frac{dM}{d\epsilon} \leq 0$$

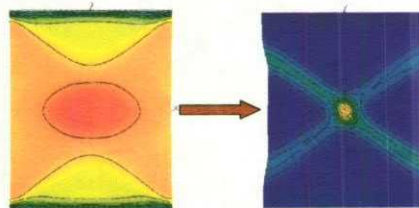
- Conditions that restrict dynamic recovery and equiaxed subgrains

Material Instability

Homogeneous deformation transitions into highly localized deformation, often in very thin (10 to 100 μm) planar bands. Inside the band, material is under intense deviatoric strain (mostly shear) and will possibly develop small voids or micro-cracks

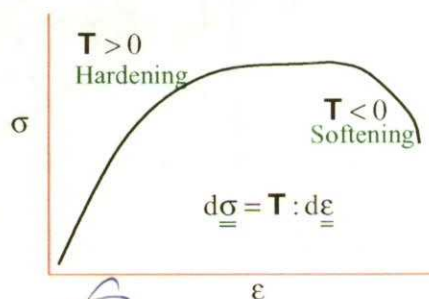
Needed Conditions for Localization

- Material instability
- Space and time defect structure



Mechanisms of Material Softening

- Thermal softening: shock heating & plastic work
- Damage (nucleation, growth of cracks & voids)
- Changes in microstructures (phase transition)
- Sudden strain-rate drops (after shock passage)
- Effects of texture; other non-associative effects



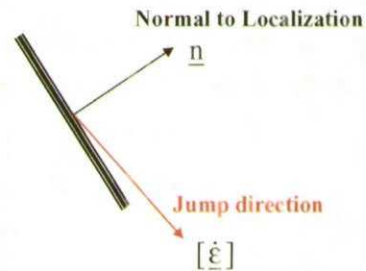
Material Instability Theory

Constitutive Form: $d\underline{\underline{\sigma}} = \underline{\underline{T}} : d\underline{\underline{\varepsilon}}$

Total Stiffness: $\underline{\underline{T}} = \xi : \left(\underline{\underline{P}}^d - \frac{(\underline{\underline{\sigma}} : \underline{\underline{\alpha}} : \underline{\underline{\xi}}) \otimes (\underline{\underline{\sigma}} : \underline{\underline{\alpha}})}{\underline{\underline{\sigma}} : \underline{\underline{\alpha}} : \underline{\underline{\xi}} : \underline{\underline{\alpha}} : \underline{\underline{\sigma}} + \frac{2}{3} \underline{\underline{\sigma}} \underline{\underline{\sigma}} : \underline{\underline{\alpha}} : \underline{\underline{h}}} \right) + 3K \underline{\underline{P}}^s$

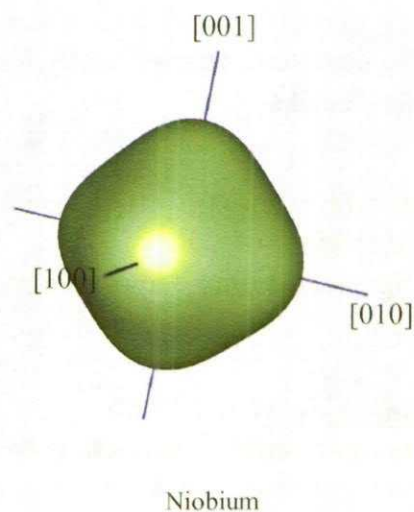
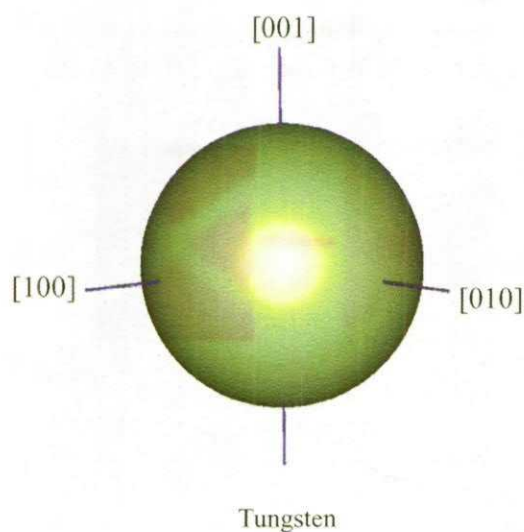
Acoustic tensor: $\underline{\underline{A}} \equiv \underline{\underline{n}} \cdot \underline{\underline{T}} \cdot \underline{\underline{n}}$

Bifurcation: $\text{Det}(\underline{\underline{A}}) = 0$

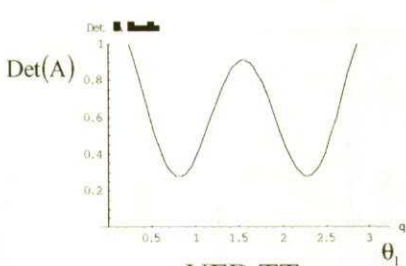


- 1) Onset of Localization
- 2) Orientation of localization plane
- 3) Straining jump direction

Elastic Anisotropy in bcc Metals

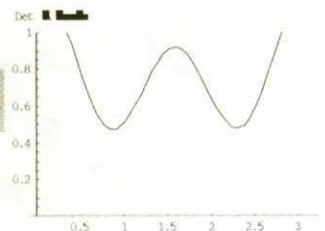


Bifurcation in the UF Bar & Plate Ta



UFB TT

$$\text{Det}(A)/\text{Det}(A)_{\text{iso}} = 92.0\%$$



UFB IP

$$\text{Det}(A)/\text{Det}(A)_{\text{iso}} = 160.0\%$$

Instability Ranking: UFB TT > Plate TT > Plate IP > UFB IP

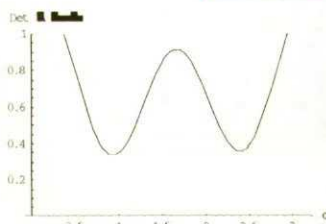


Plate TT

$$\text{Det}(A)/\text{Det}(A)_{\text{iso}} = 112\%$$

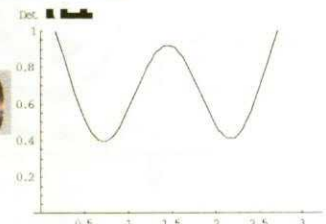
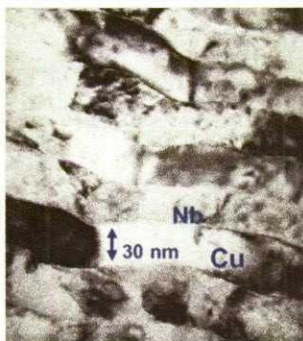


Plate IP

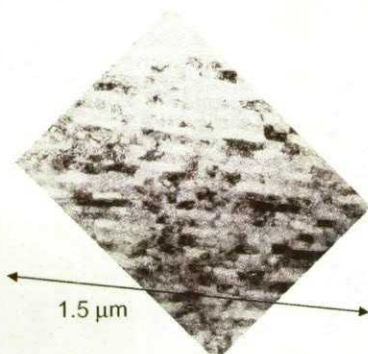
$$\text{Det}(A)/\text{Det}(A)_{\text{iso}} = 132.0\%$$

75 nm Cu-Nb multilayer rolled to $\epsilon_{\text{eff}} = 105\%$



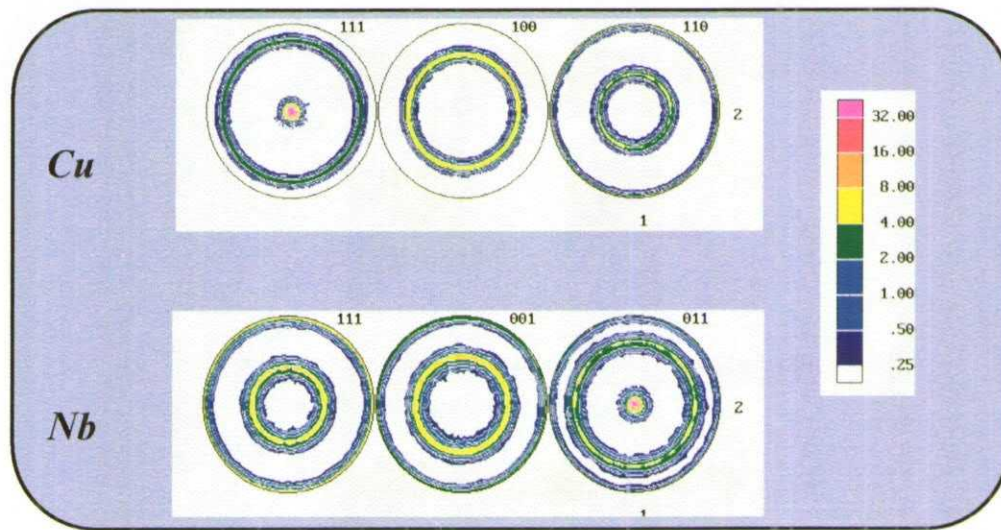
A. Misra, LANL

- No cell structure.
- $\{110\}\text{Nb}/\{111\}\text{Cu}/\text{interface}$ relationship ~ preserved.



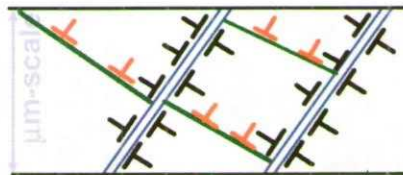
- Uniform reduction
- Bifurcation (sausaging) would be expected for composites with different σ_y and/or $d\sigma/d\epsilon$ behavior deforming under bulk plasticity.

Nb/Cu Nano-Composite As-Deposited Texture



Kurdjumov-Sachs OR
 $\{111\}\text{Cu} // \{110\}\text{Nb} // \text{interface}$
 $\langle 110 \rangle \text{Cu} // \langle 111 \rangle \text{Nb}$ locally preserved, but axisymmetric in bulk

Symmetric Slip

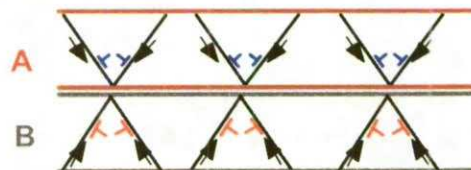


Pile-up behavior in micron-scale materials:

- dislocation cell structure forms
- crystal spin induced by slip → texture evolution

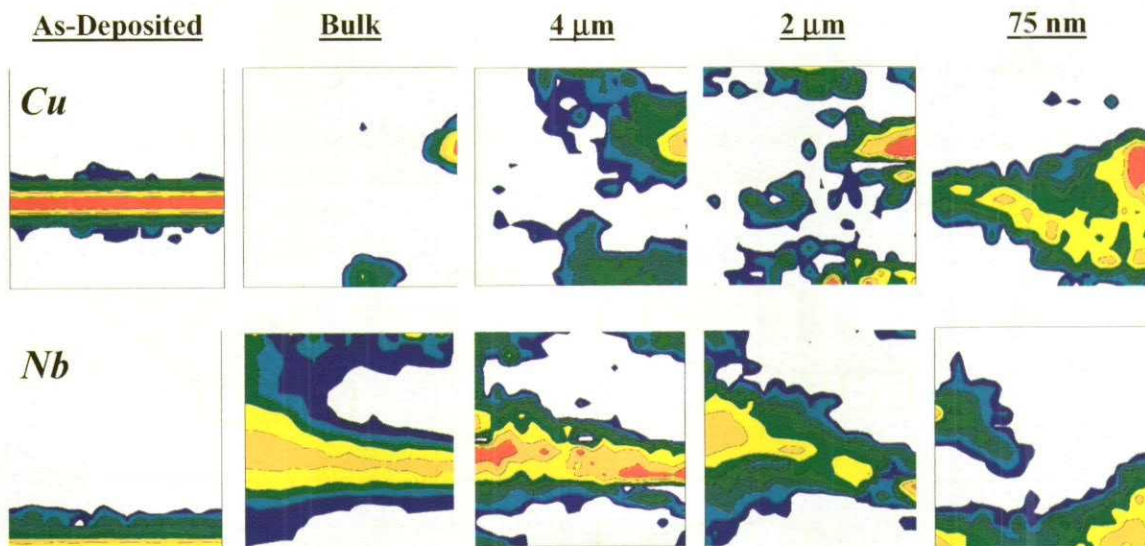
Anderson, P.M., Bingert, J.F., Misra, A., and Hirth, J.P., *Acta Mat.*, 51 (2003) 6059-6075.

Misra, A., et al., *Acta Mat.*, 52 (2004) 2387-2394.



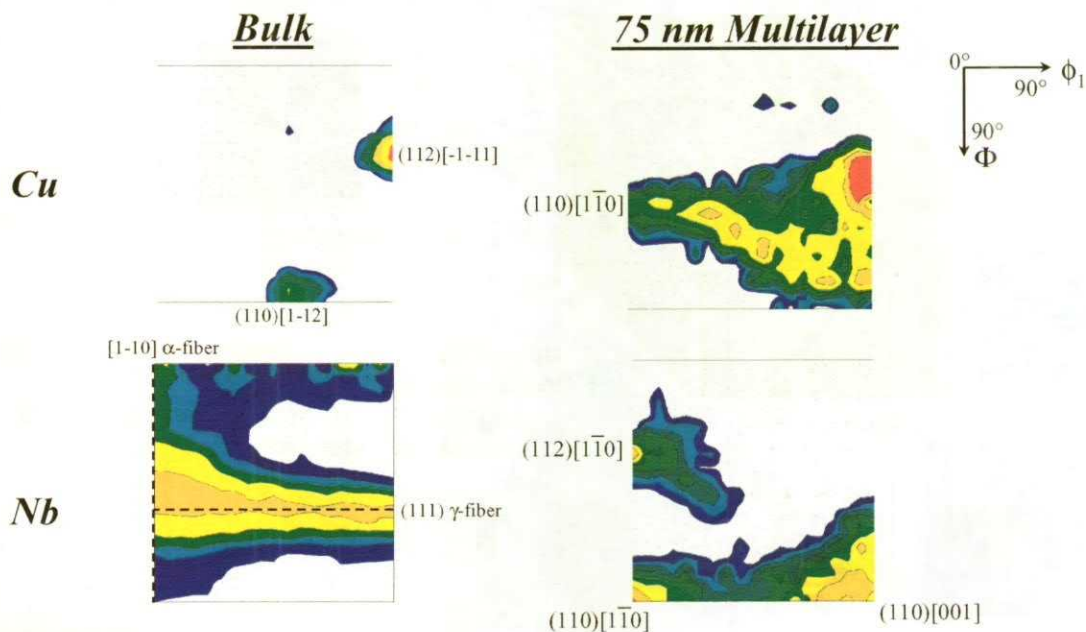
- Single dislocation slip is symmetric, with a fine distribution (hence, negligible out-of-plane lattice rotations)
- Deposition of dislocation segments at interfaces by the glide of single Orowan loops

Effect of Layer Thickness on Cu/Nb Composite Textures



- Continuous transition from bulk to nano-scale behavior.
- Multilayer texture development not inhibited from rotation by initial texture.
- Suggests full retention of as-deposited KS OR possible with finer layers.

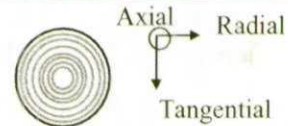
Rolling Texture Comparison in Cu/Nb



- Texture partitions to bulk and retained deposition components at nano-scale.
- Retained deposition component displays tendency for stable orientations.

Morphological and Crystallographic Texture

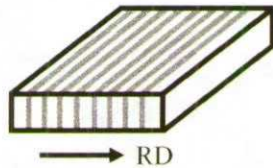
- Banded (ferrite-pearlite) 0.3C-1Mn-1Si steel round bar  Tanger
- Process so as to superimpose anisotropic effects of morphological banding and texture on mechanical properties and damage initiation and growth.
CWD = crystallographically weak direction



A) Rolling

RD = Radial

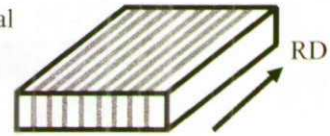
Band Spacing =
increased
CWD $\longleftrightarrow$



B) Rolling

RD = Tangential

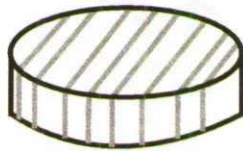
Band Spacing =
constant
CWD $\longleftrightarrow$



C and D) Compression

CA = Axial

Band Spacing = inc.
CWD $\longleftrightarrow$



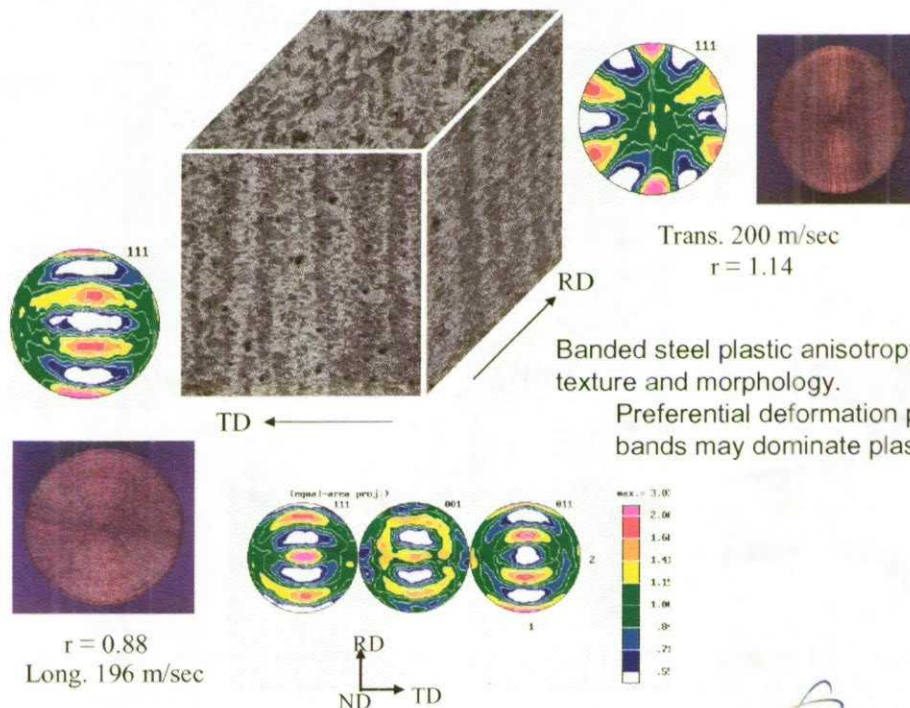
E) Compression

CA = Radial

Band Spacing = dec.
CWD $\longleftrightarrow$



Orientation A: RD = Radial_{Bar}



Banded steel plastic anisotropy affected by both texture and morphology.

Preferential deformation parallel to ferrite bands may dominate plastic anisotropy.

Summary

- Ta Rod: Generalized yield surface needed to capture non-orthotropic plastic anisotropy.
- Ta Plate and Rod: Mechanical response, both plastic anisotropy and localization, sensitive to microstructure.
 - Instability analysis potentially applicable to determine relative resistance to strain localization.
- Nb/Cu Nano-composite: Interface-controlled plasticity results in non-Schmid texture evolution.
- Banded Low-C Steel: Morphological texture (vs. crystallographic) may dominate plastic anisotropy.