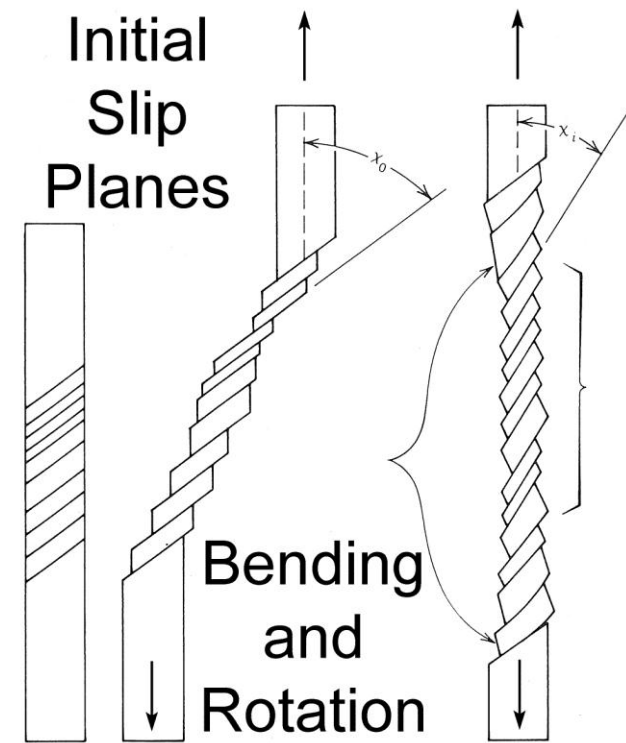


# Refining Crystal Plasticity Finite Element Model for Deformation of Single Crystal Niobium

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Farhang Pourboghrat, Chris Compton  
Michigan State University

# Motivation

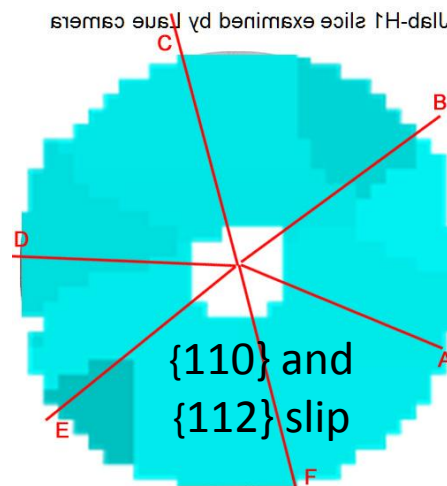
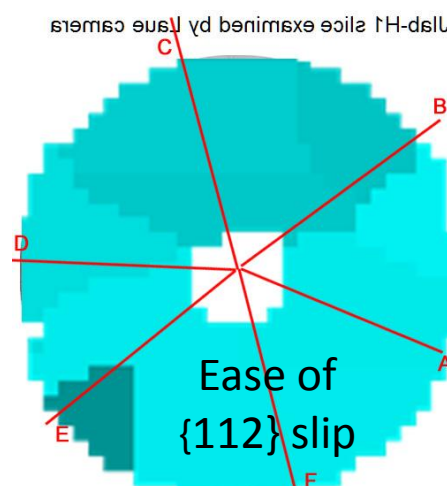
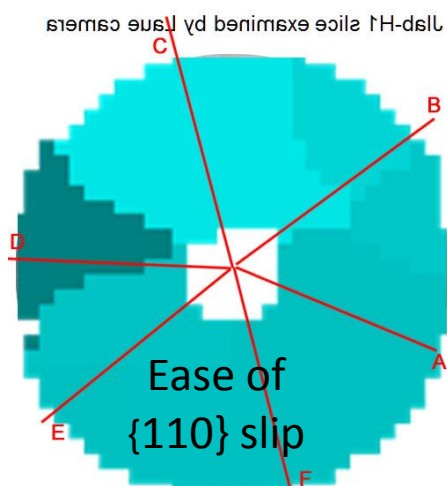
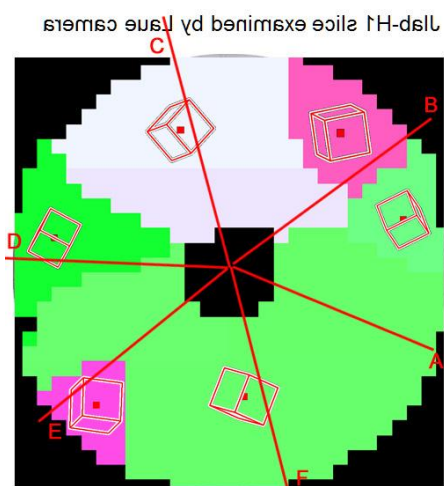
- Heterogeneous deformation caused by crystallographic slip makes forming of complex shapes challenging
  - Uniform thickness, uniform shape does not naturally occur due to effects of crystal slip systems; crystals rotate about an axis perpendicular to the slip direction, at rates that depend on the rate of shear strain, and dislocations present on other slip planes that cause hardening (stress increase).
  - With deformation, the resolved shear stress and resistance to shear evolves differently on each slip system, leading to varying amount of shear in different slip systems and crystal orientations, and hence, heterogeneous deformation (Orange Peel Effect)



# Example of effects of heterogeneous slip in deep drawn cavity half – differential thinning led to dragging, forming an ear, and a strange etch pit condition

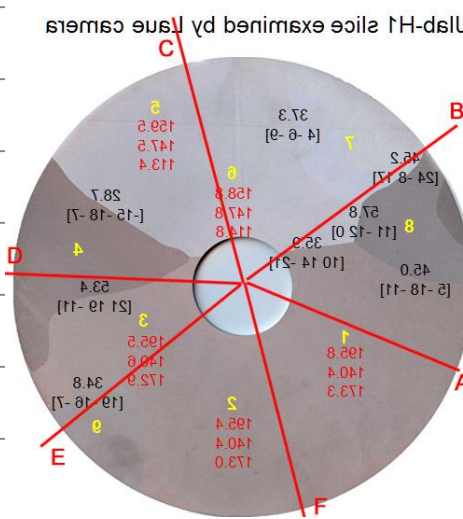
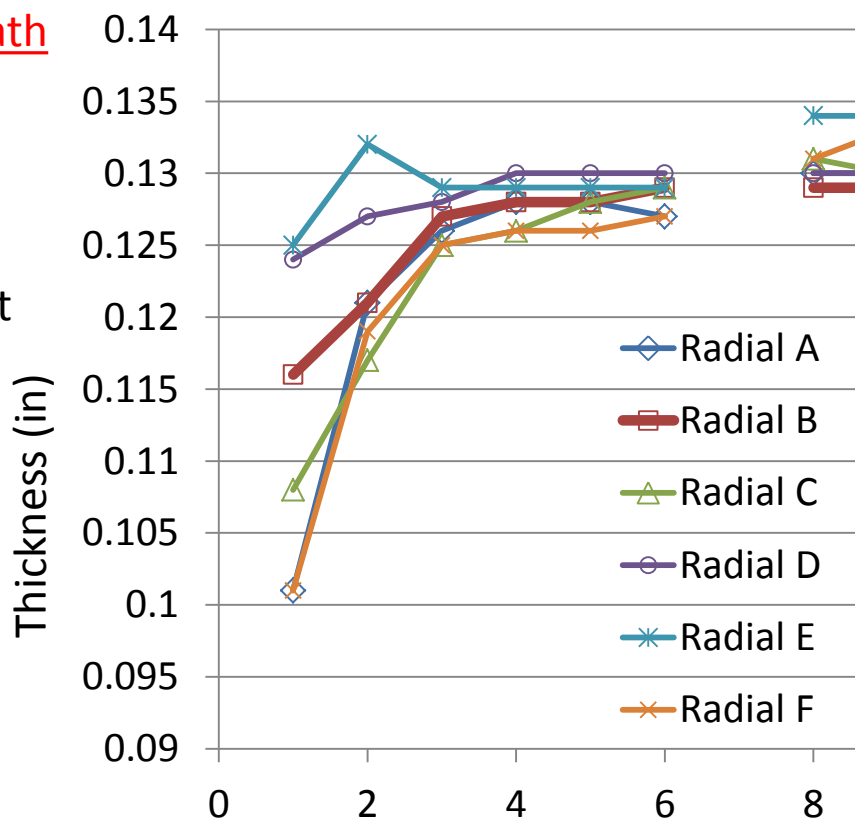
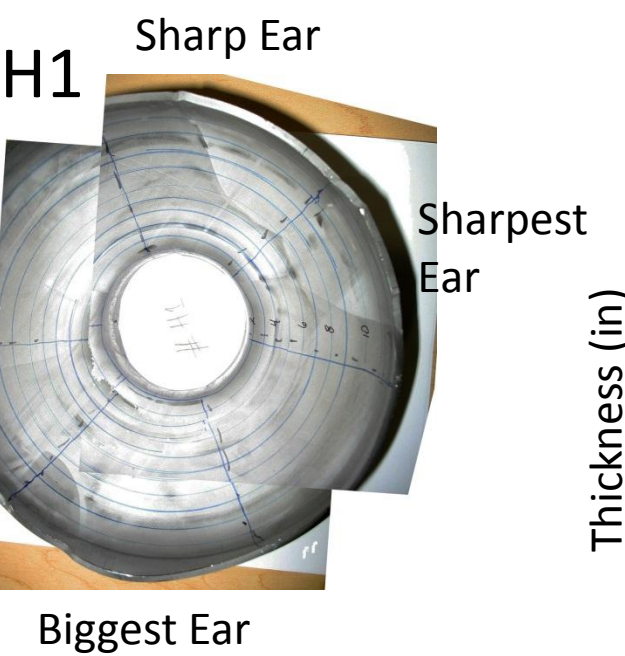
Burnish marks indicate lesser thinning rate, grabbing die, leading to bizzare etch pit pattern



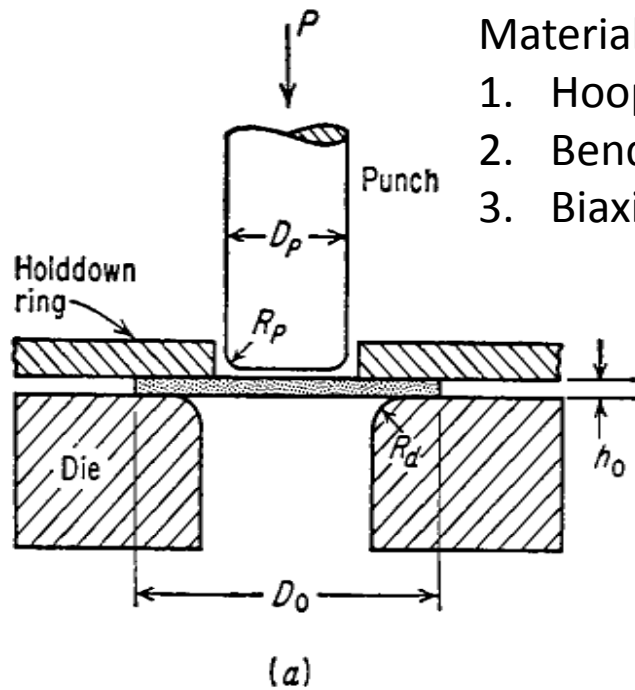


No obvious trends/correlation between crystal orientation, thickness, **biaxial** stress, thickness

→ Simulate complex strain path

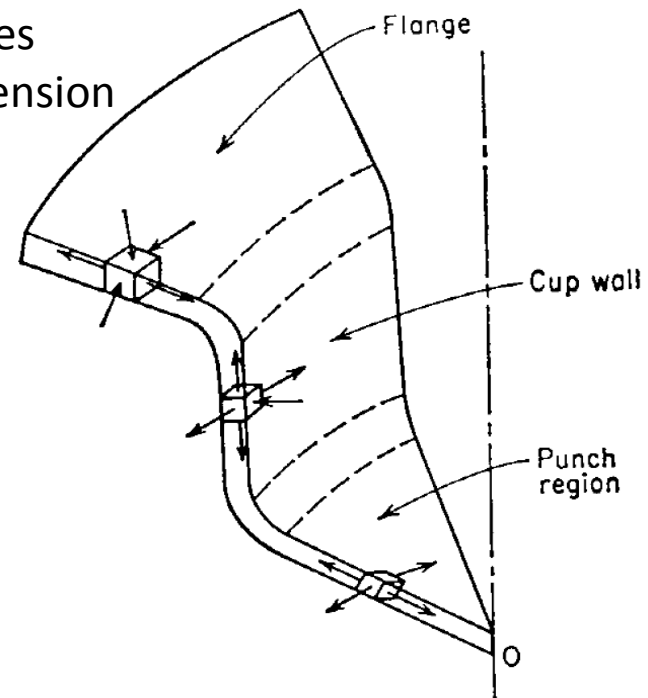
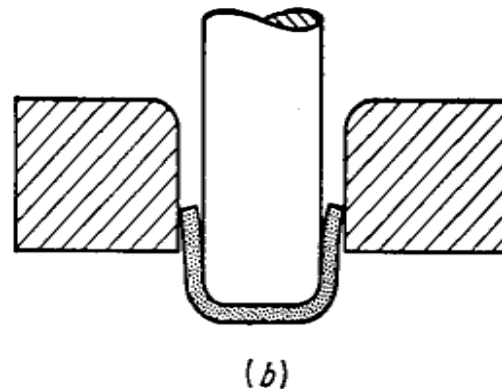


# Strain path for drawing is complex, Kinematics of Crystal plasticity model OK



Material in Equator / Weld Experiences

1. Hoop Compression hoop, radial tension
2. Bending + unbending
3. Biaxial stretching (not balanced)



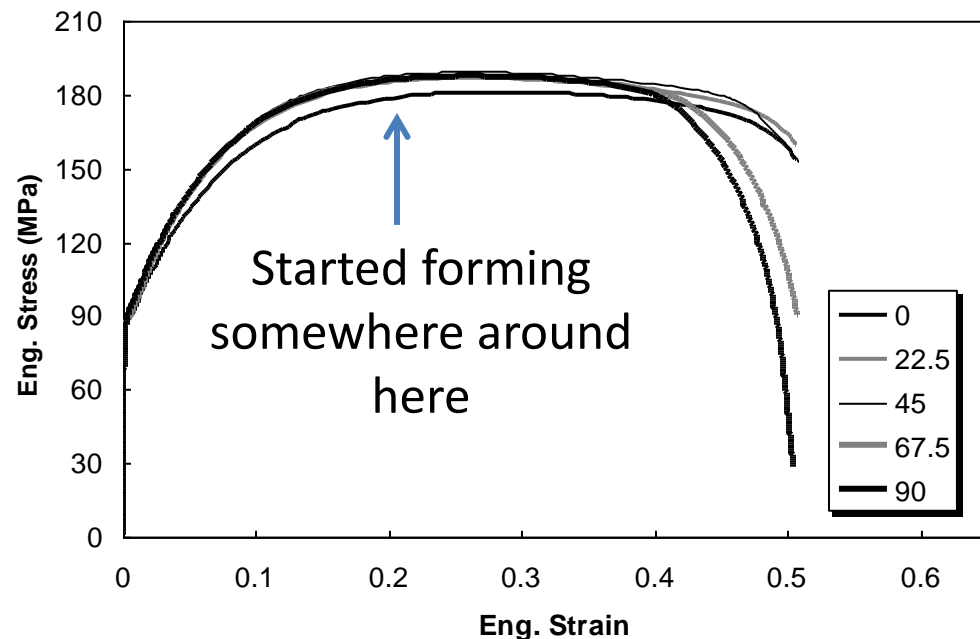
- Crystal plasticity models can simulate complex paths, and anisotropic slip, in general, the shape change is qualitatively modeled, but to be predictively quantitative, refining the stress-strain relationship is needed (as that affects how much strain can occur for a given increment of deformation)



# 1<sup>st</sup> attempt to bulge / inflate a non-optimal Nb tube

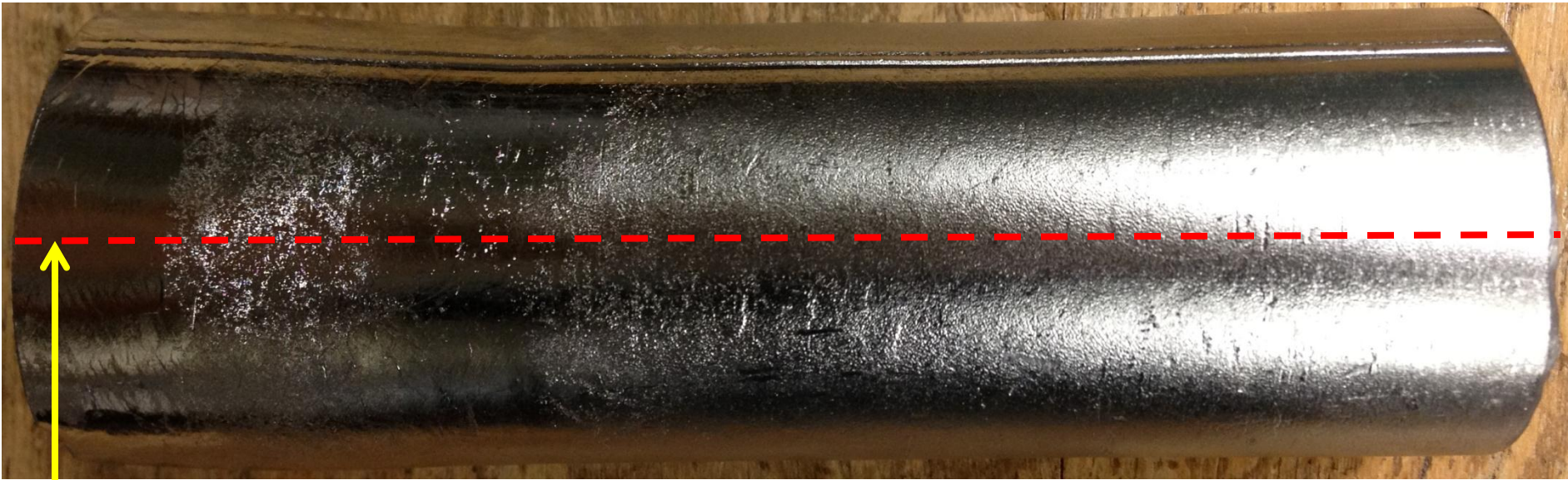


As expected, failed at weld



- Bent sheet metal to tube, welded along seam
  - Put in a lot of cold work by the bending process, then made large recrystallized grains
  - Tube was just over required dimension, so surface was machined (put even more cold work on surface)
- Such welded tubes sent to Jim Murphy at University Nevada Reno to convert into single crystal/large grain tubes

# Tube processed by Jim Murphy, University of Nevada at Reno



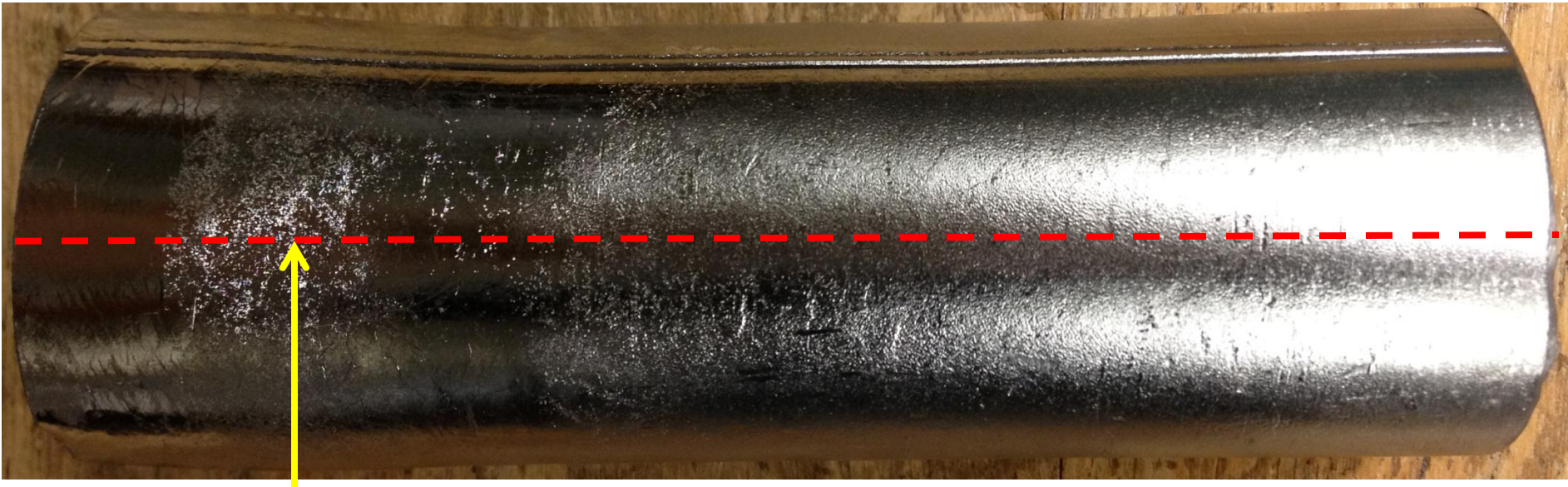
1 inch

Indicates the  
line all scans  
followed

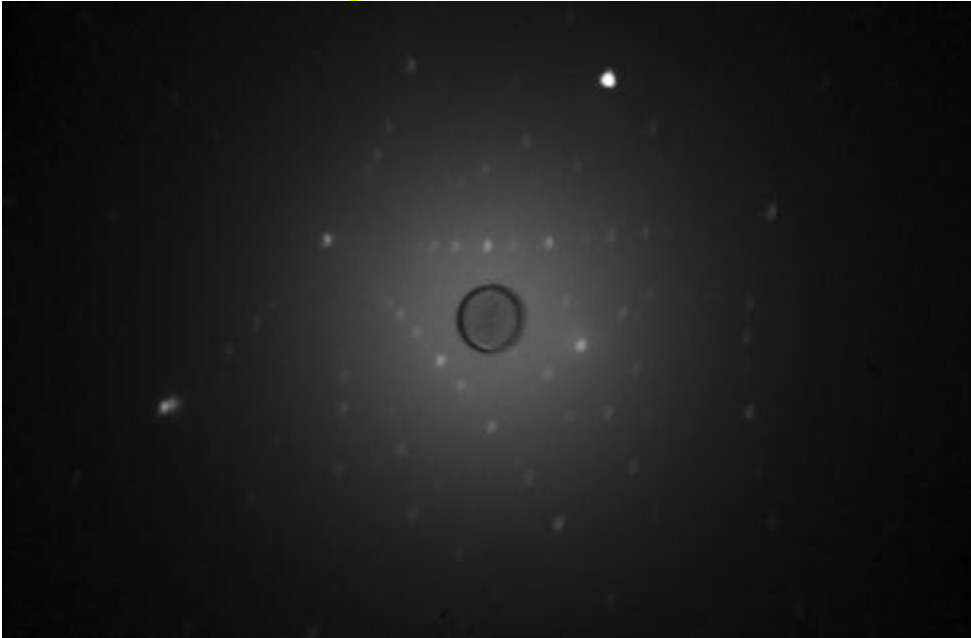
Where roughly  
each scan was  
done



First tube (with an opening at left end)

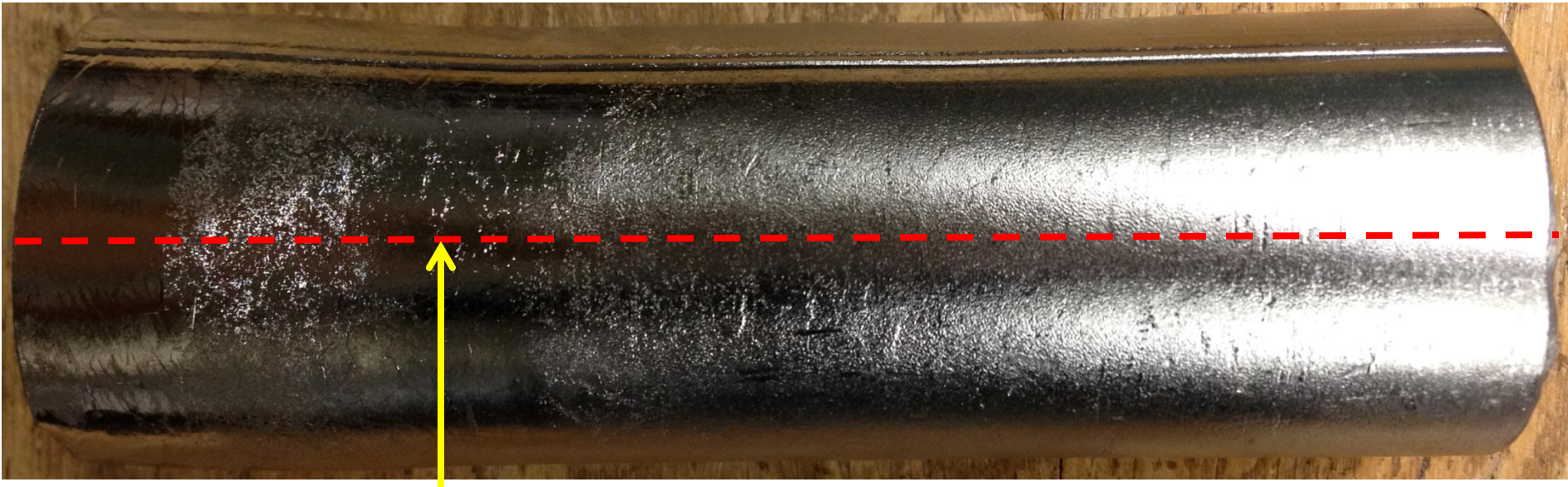


1 inch

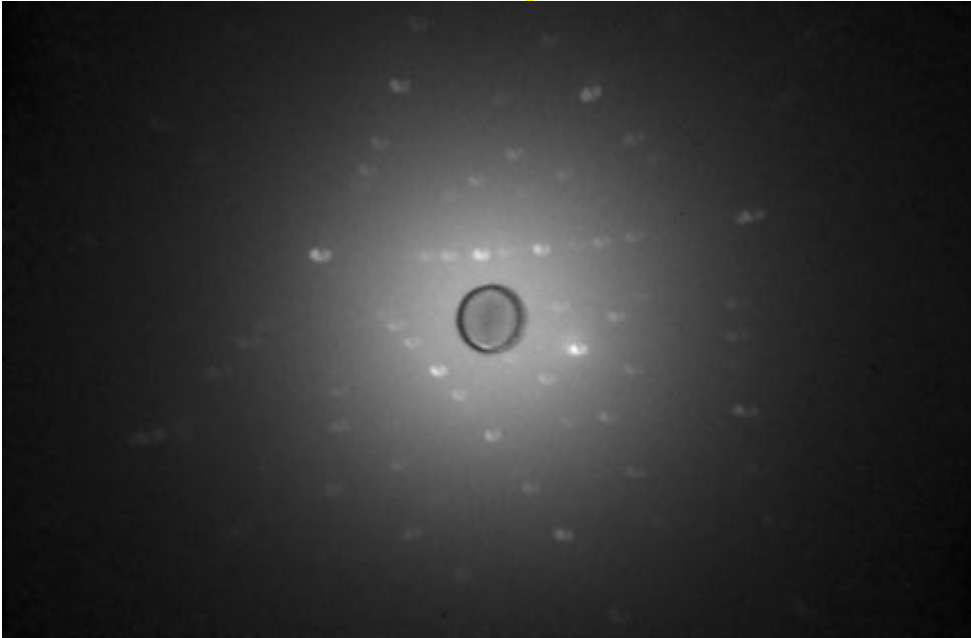




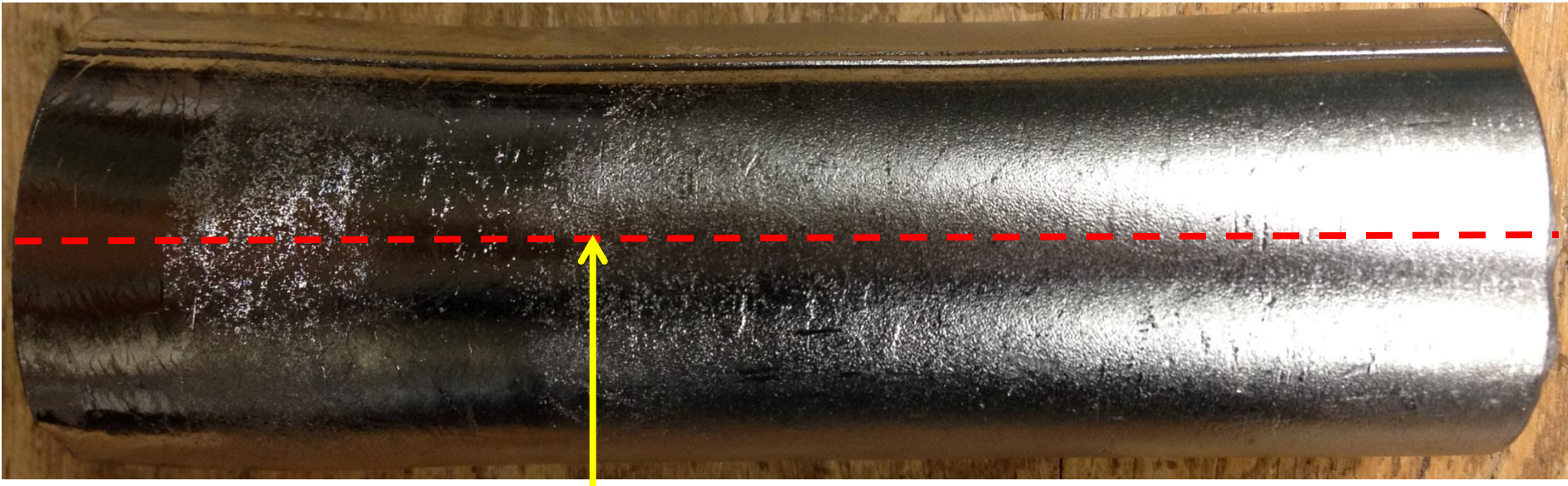
First tube (with an opening at left end)



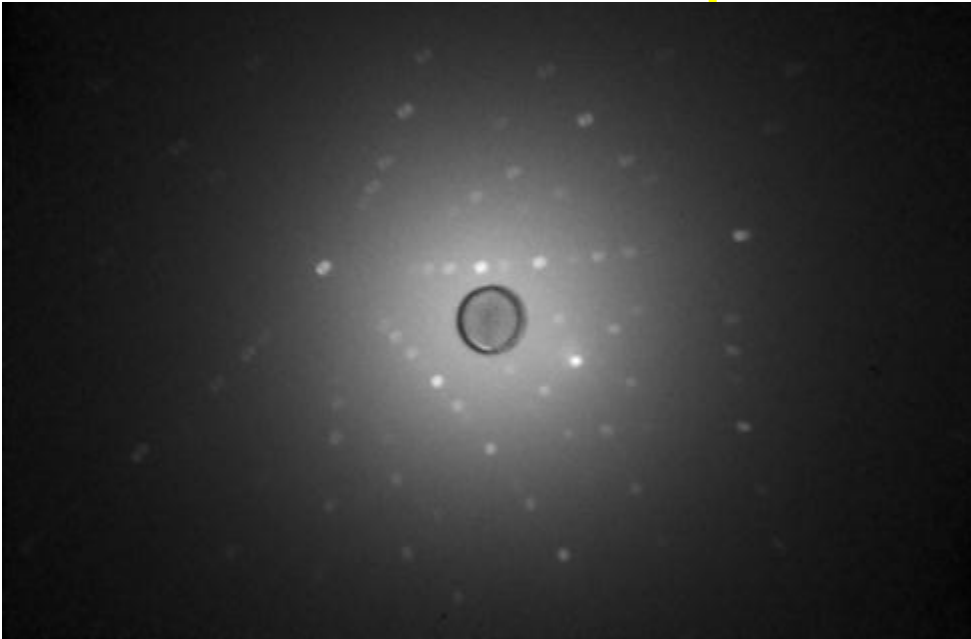
1 inch



First tube (with an opening at left end)

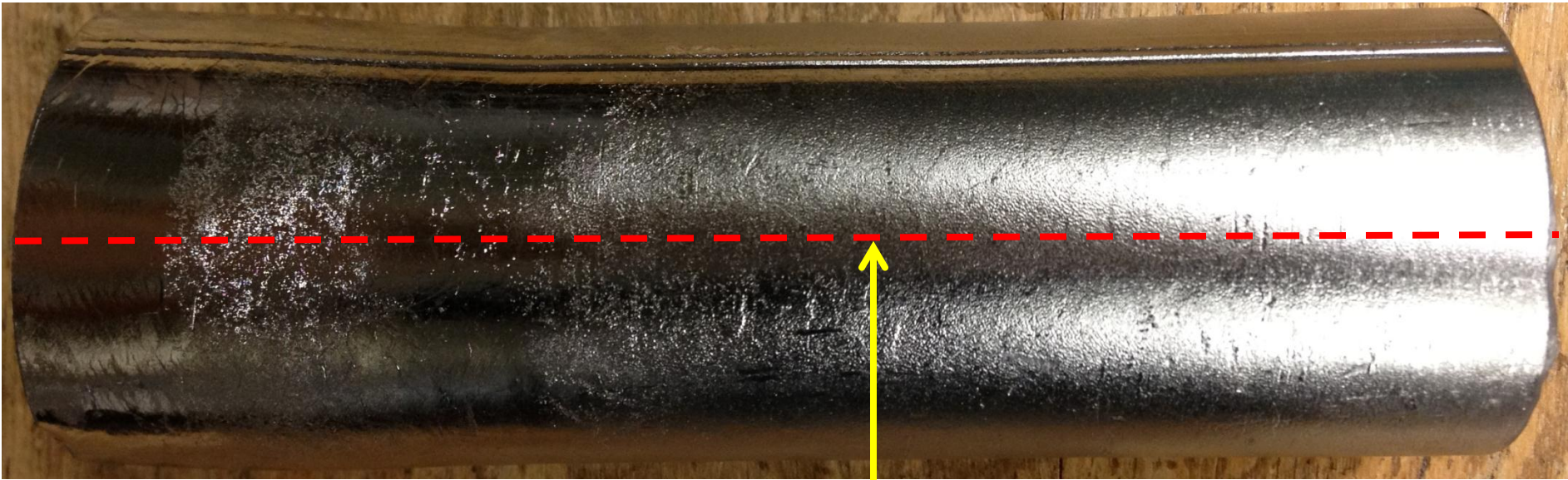


1 inch

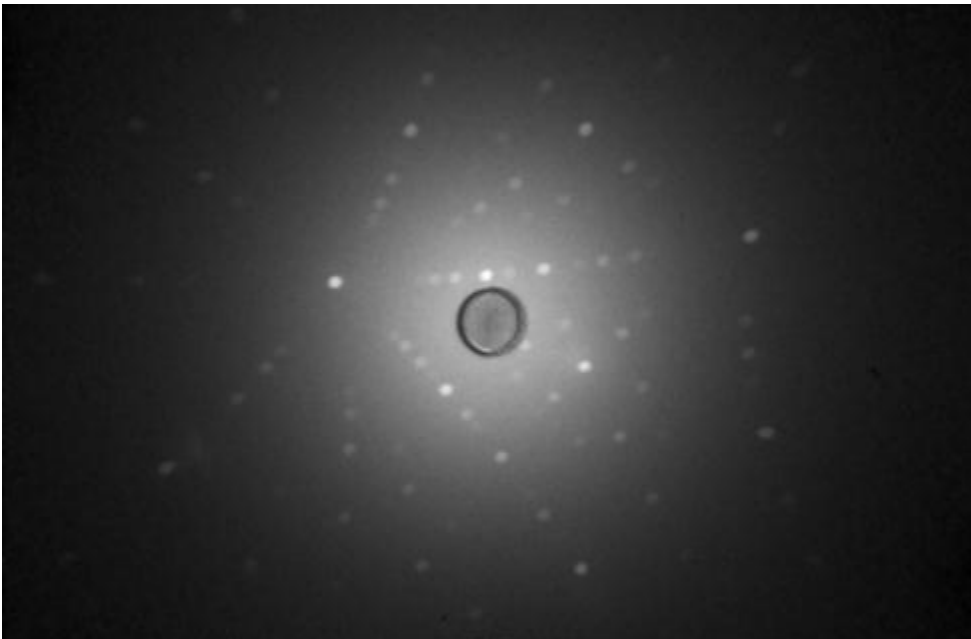




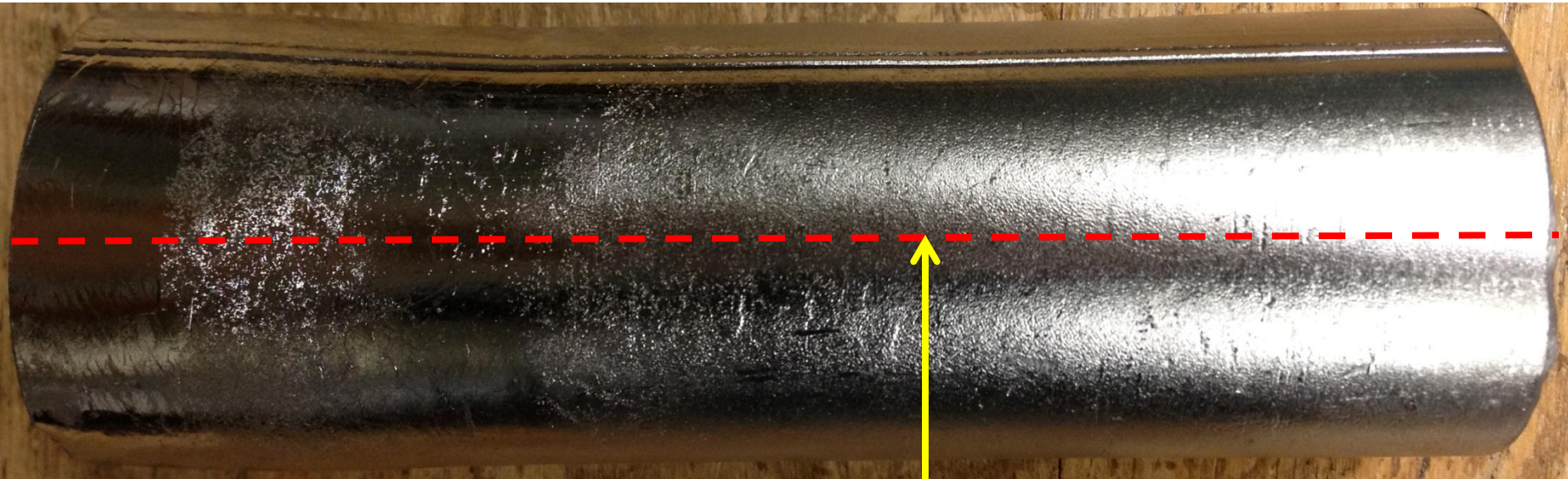
First tube (with an opening at left end)



1 inch



# First tube (with an opening at left end)



1 inch

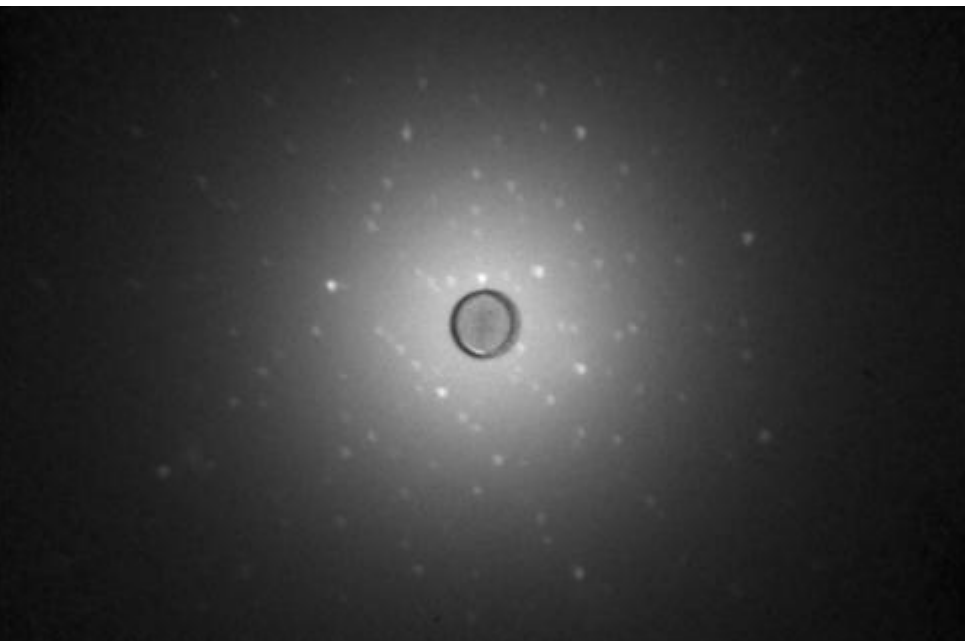
Here is the first grain  
boundary, ~2.6 inches  
from left end

Orientation 1: 161.9049 152.6249 165.5003

Orientation 2: 307.4421 179.2676 172.9297

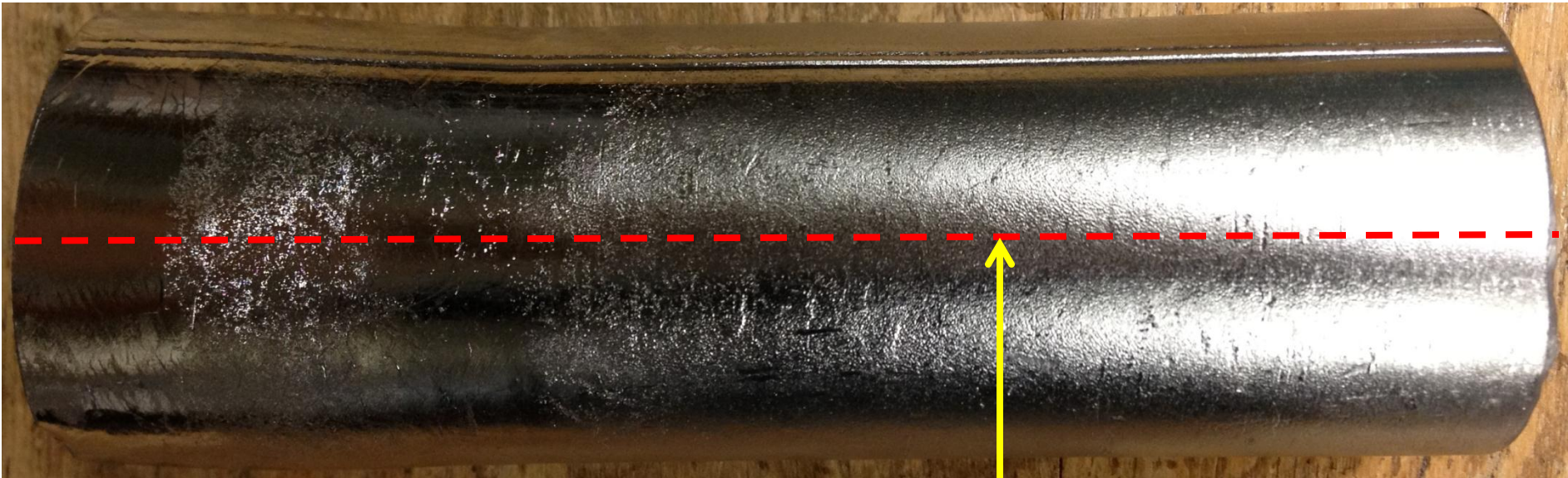
Misorientation @ rotation axis

50.1° @  $\langle 11 \bar{1} \bar{16} \rangle$



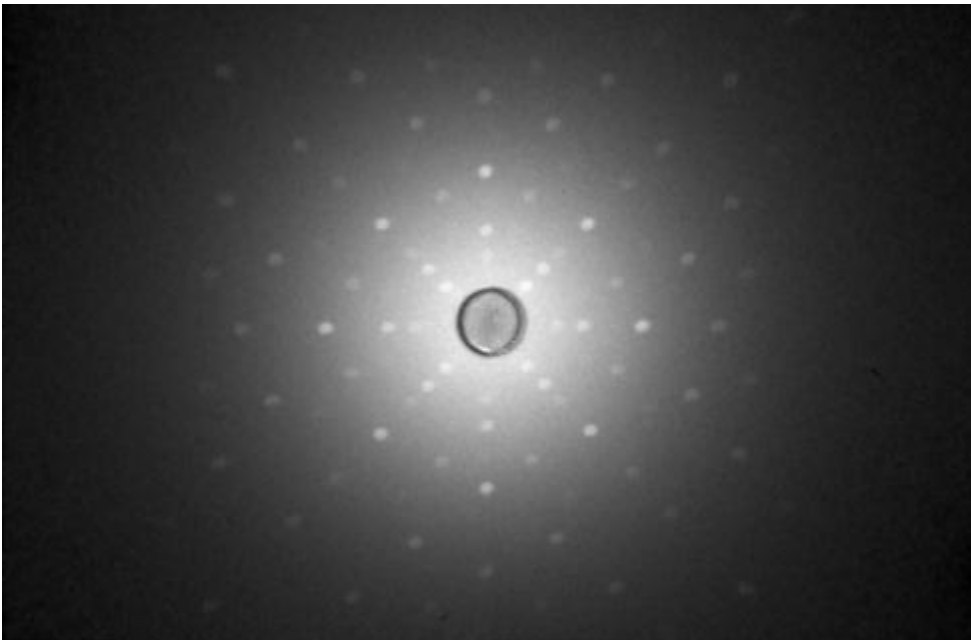


# First tube (with an opening at left end)

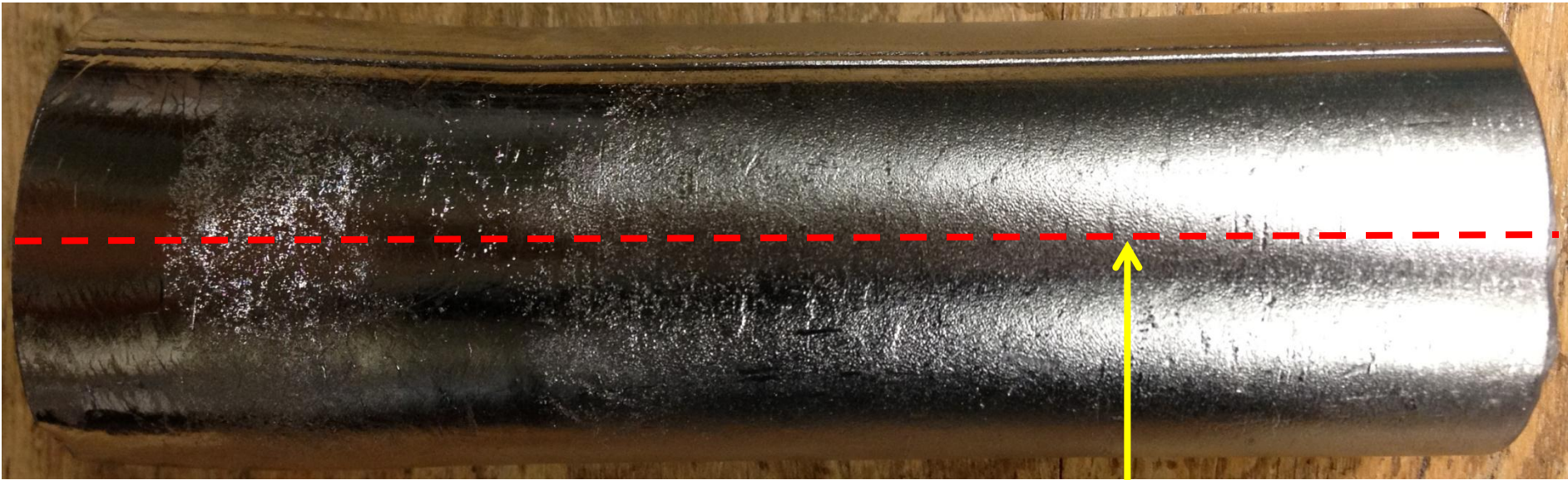


1 inch

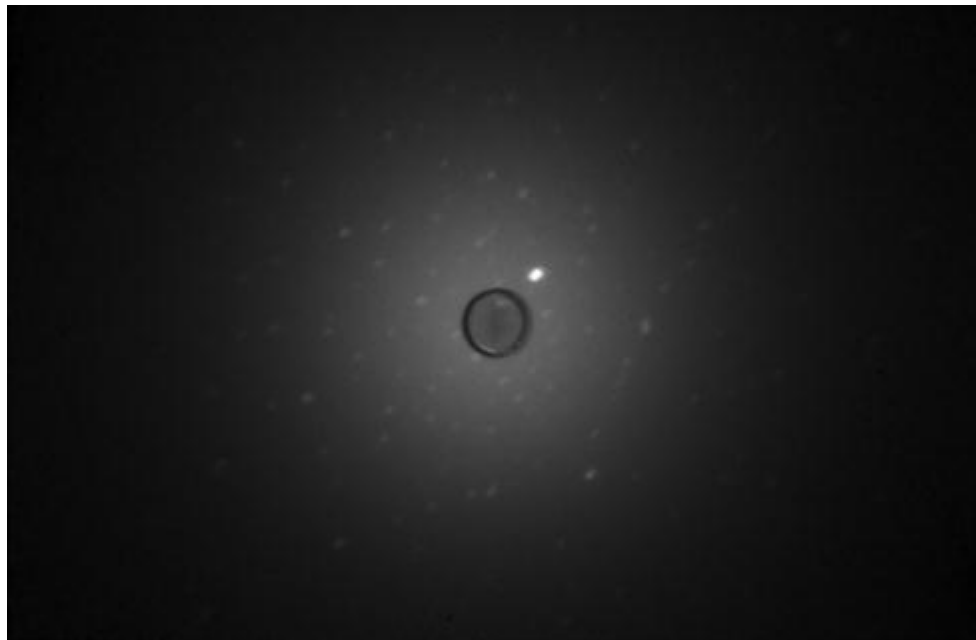
The remaining grains  
are smaller compared  
to the first



First tube (with an opening at left end)

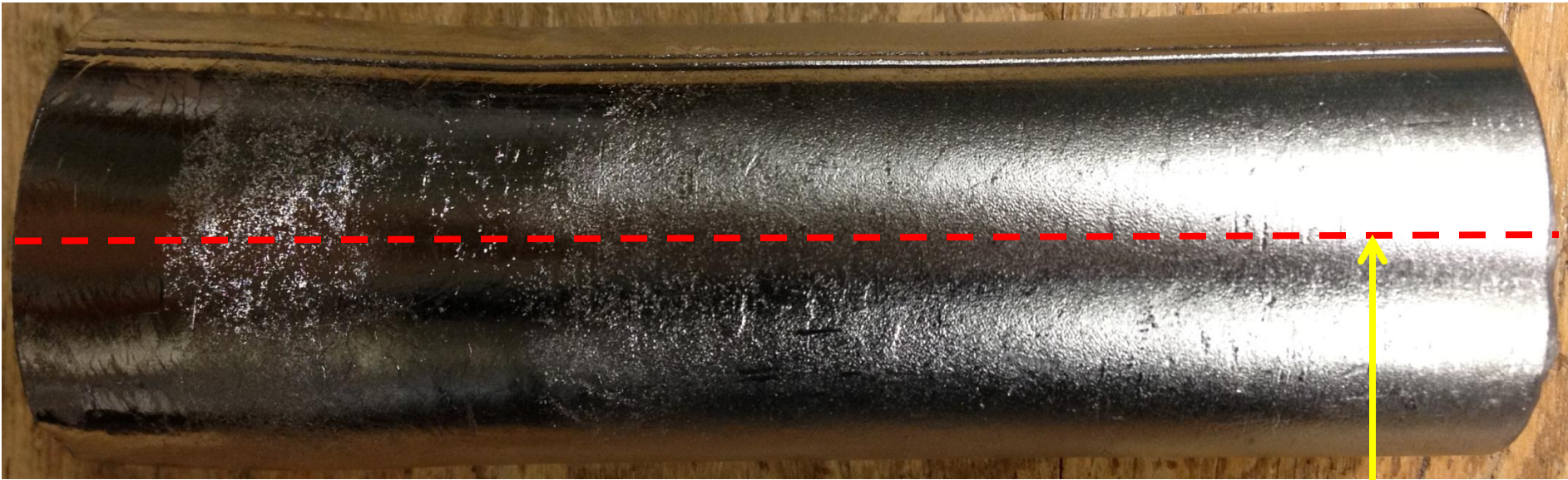


1 inch

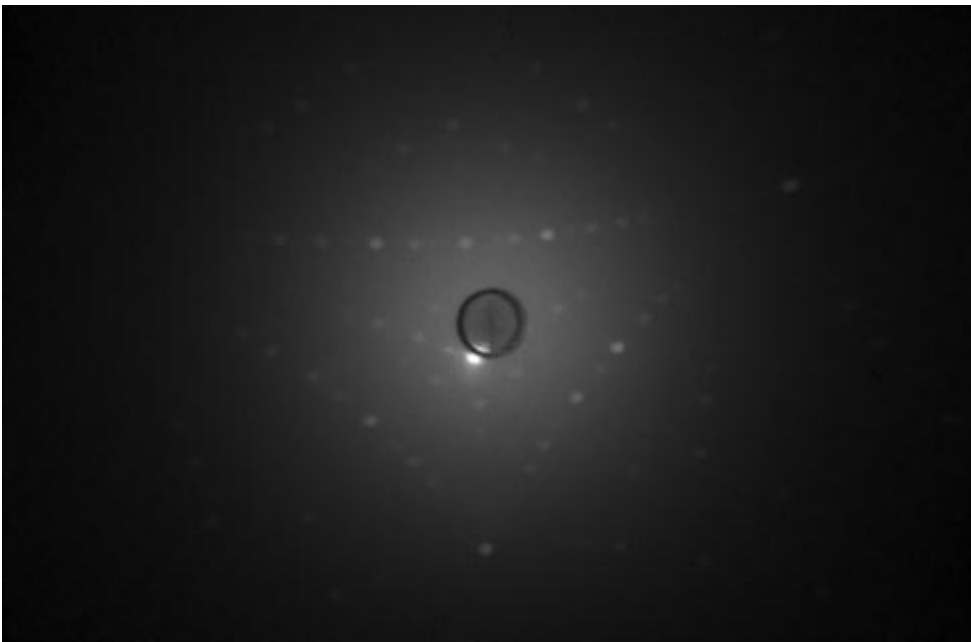




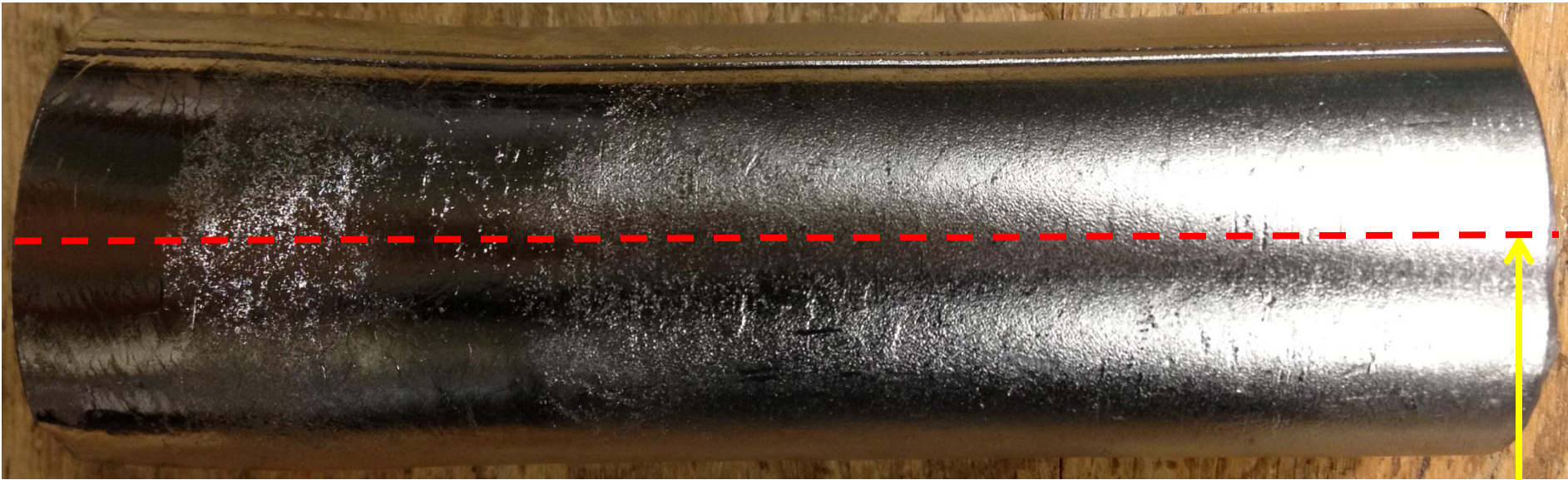
First tube (with an opening at left end)



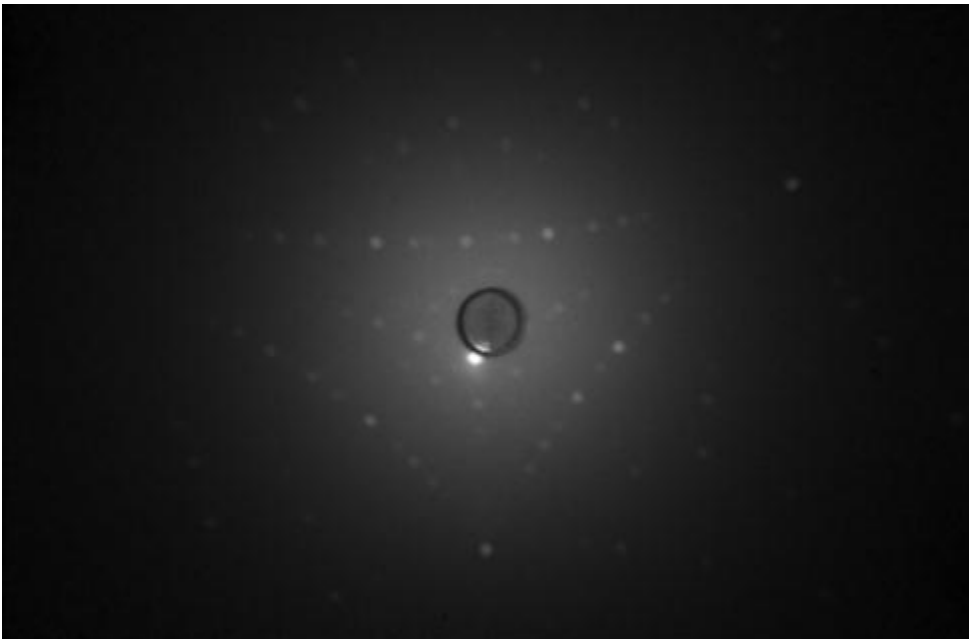
1 inch



First tube (with an opening at left end)

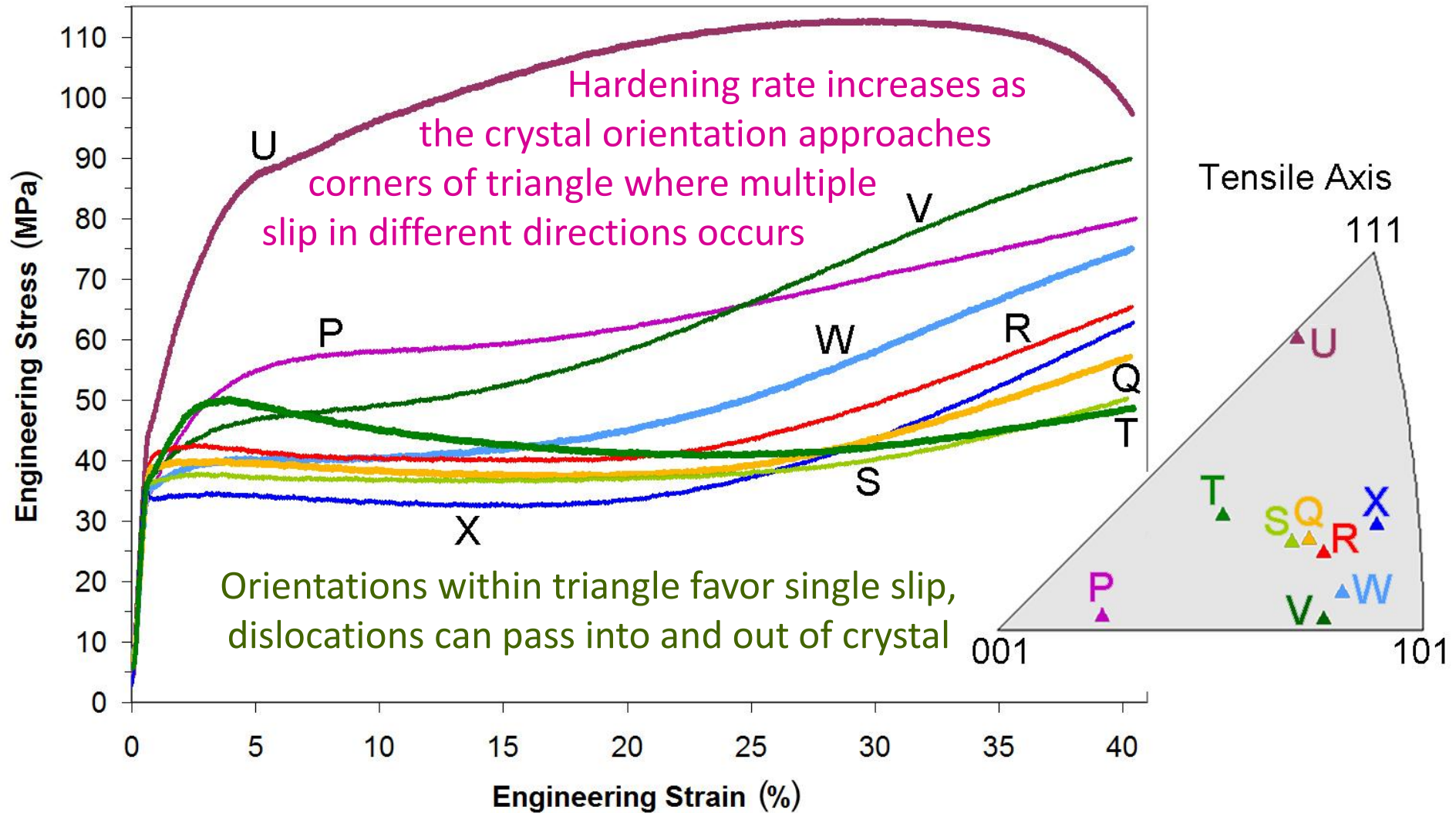


1 inch



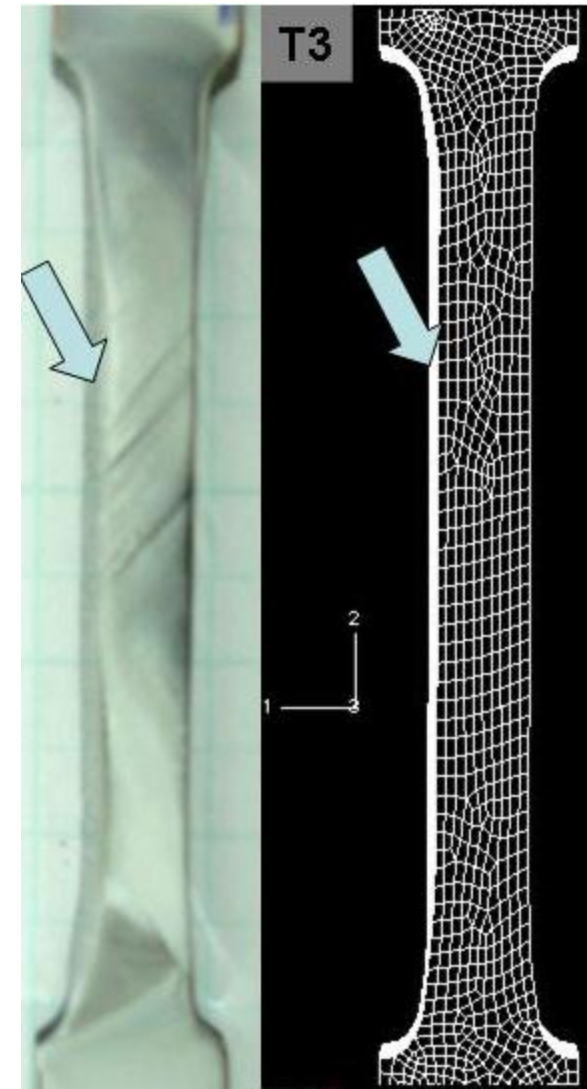
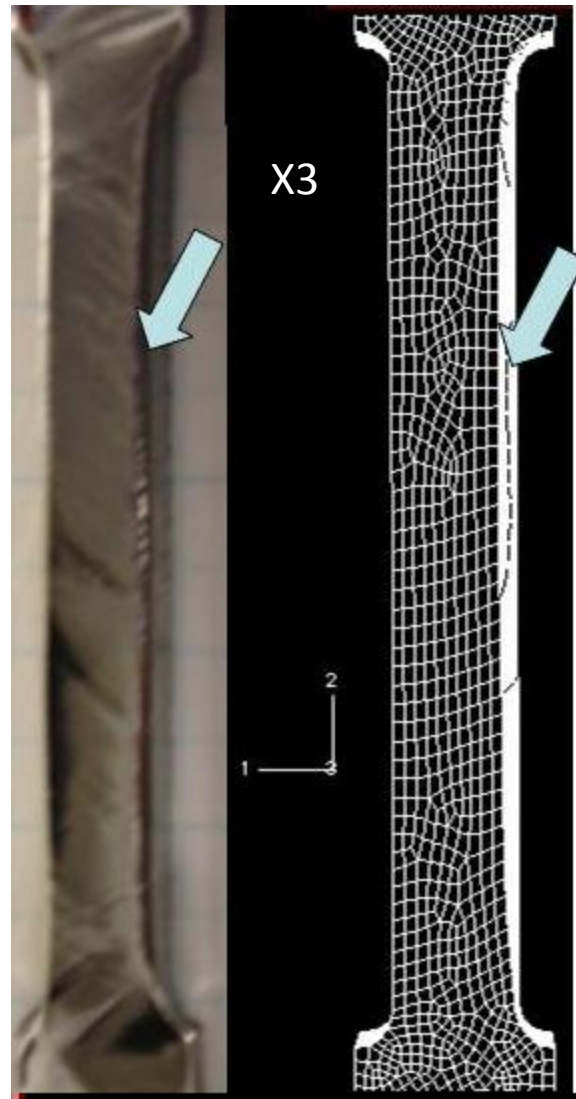
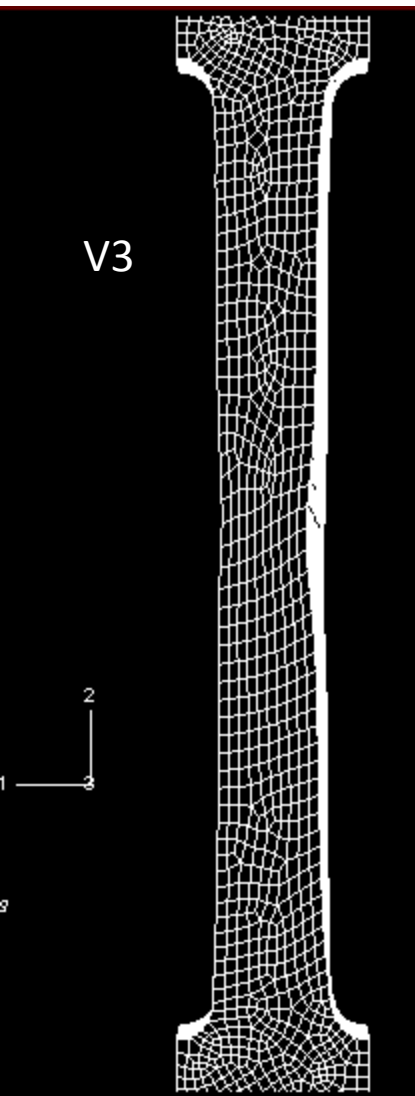


# Single crystal stress-strain, lattice rotation from 3-D X-ray diffraction, related to crystal orientation



Some orientations can become unstable , R, X, Q, T orientations show softening!

In prior work, asymmetric shape changes come out right, but the stress history did not...



# Hardening rule parametric study to simulate stress...

$$\dot{\tau}^{\alpha} = \sum_{\beta=1}^N h^{\alpha\beta} |\dot{\gamma}^{\beta}|$$

$$h^{\alpha\beta} = h^{\beta} Q$$

$$h_{\beta} = h_0 \left(1 - \frac{\tau_0^{\beta}}{\tau_s^{\beta}}\right)^a$$

$$\dot{\gamma}^{\beta} = f(\text{evolving yield surface})$$

$$Q = \begin{bmatrix} 1 & 1.4 & \dots & 1.4 & 1.4 \\ 1.4 & 1 & & & 1.4 \\ \vdots & & \ddots & & \vdots \\ 1.4 & & & 1 & 1.4 \\ 1.4 & 1.4 & \dots & 1.4 & 1 \end{bmatrix}$$

$\tau^{\alpha}$ : is the current slip resistance on slip system  $\alpha$  which evolves from the critical resolved shear stress  $\tau_0^{\alpha}$  with plastic slip on the active slip systems

$\dot{\gamma}^{\beta}$  is the plastic slip rate on the active slip system  $\beta$

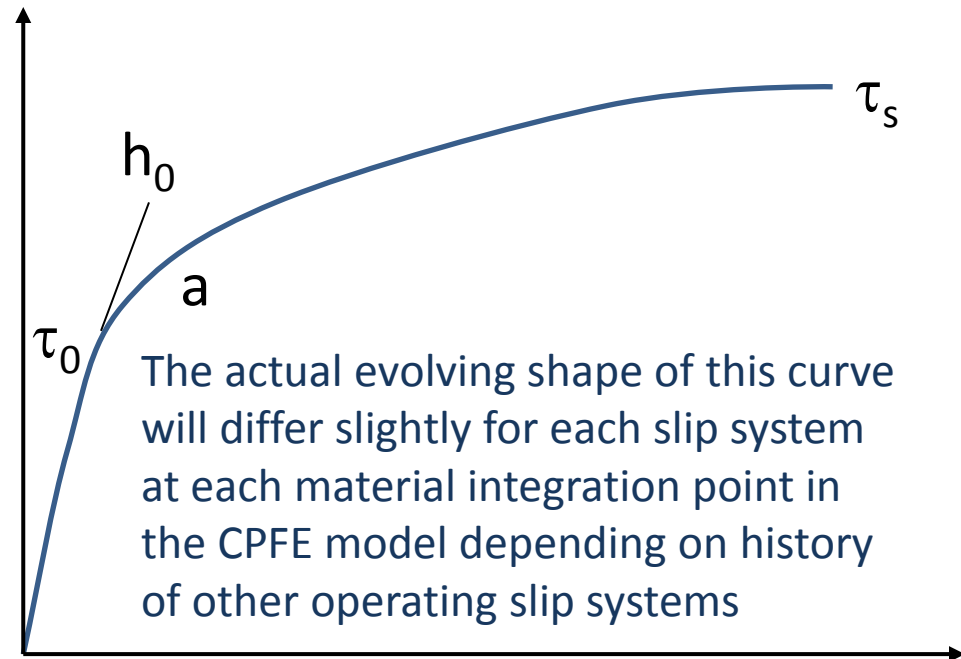
$h^{\alpha\beta}$  the components of the hardening matrix

$q$  is the so-called latent-hardening ratio

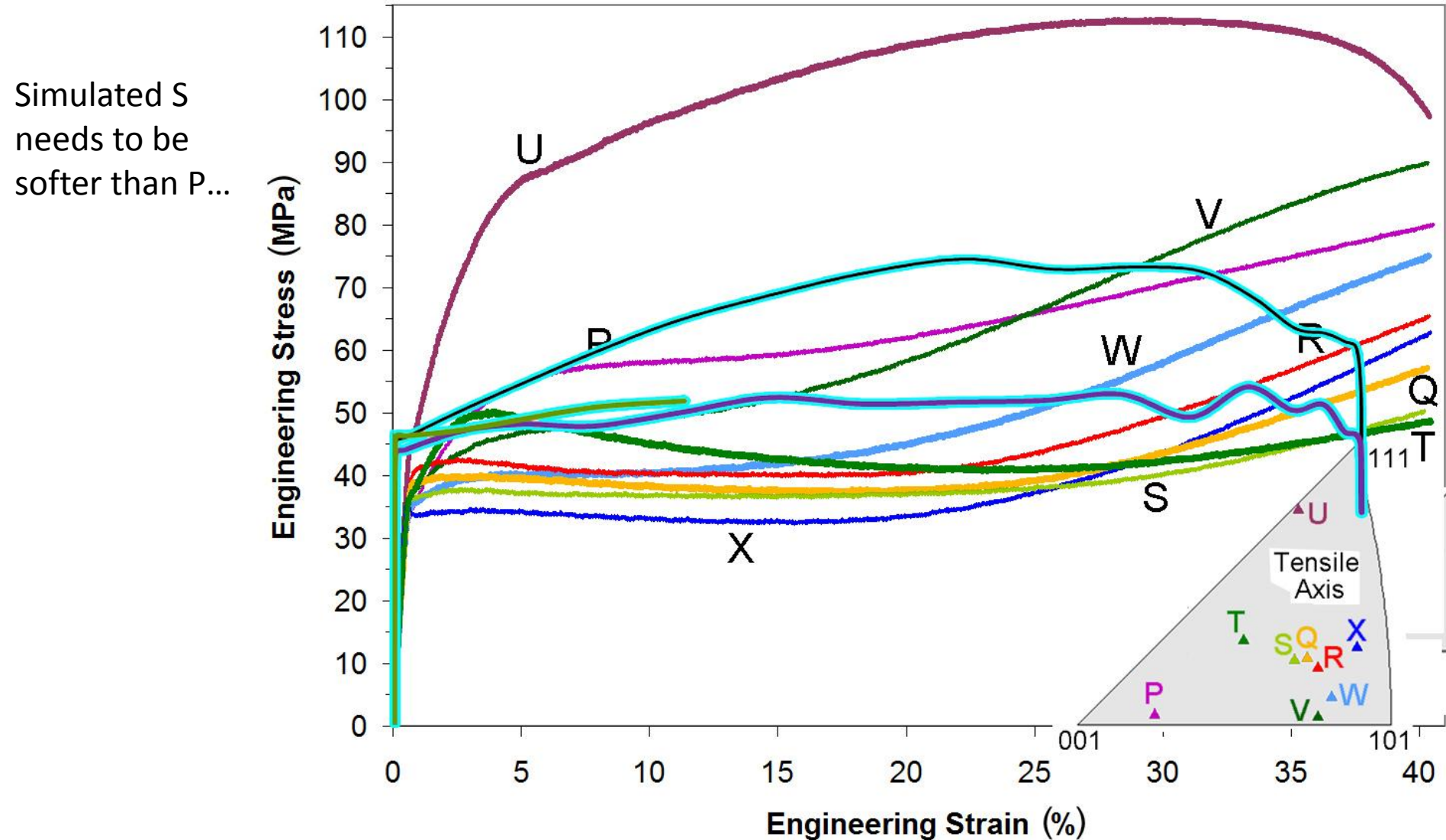
$h_0$  denotes the initial hardening rate

$\tau_s^{\beta}$  the saturation value of the slip resistance on slip system  $\beta$

$a$  is the exponent describing the shape of the function



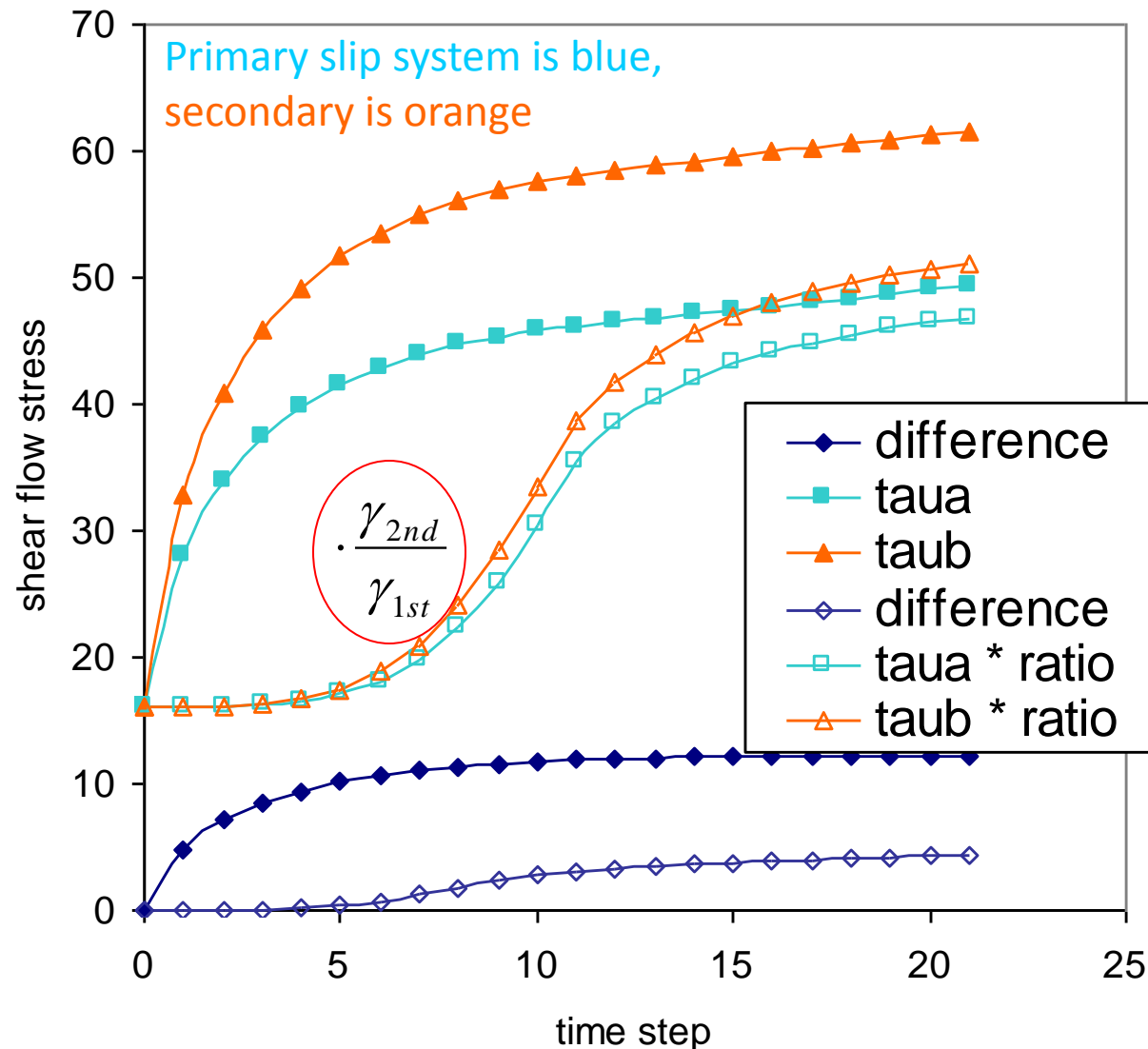
Recent simulations have the hardening rate a bit closer to reality, but not the later hardening process





# Thought experiment to examine effect of hardening law modification on sxl slip

- Two slip systems, one is highly favored at first, and dislocations pass **through** the specimen
  - No latent hardening
- When crystal rotates to favor other slip systems, normal hardening behavior develops, i.e. when shear on the secondary (unhardened) slip system becomes sizeable
- This coding is installed, and being adjusted



# Crystal plasticity simulations needed for quantitative prediction of material flow

- Single crystal models needed for large-grain cavity deformation simulations since much of the crystal will slip without seeing a grain boundary
  - Different hardening strategy needed from polycrystal
  - A good single crystal model should work in a polycrystal too
- Role of favored  $\{112\}$  slip needs to be installed, too
- Grain boundary slip resistance (Hall-Petch Effect) is challenging to install in CPFEM models – related research projects are pursuing this