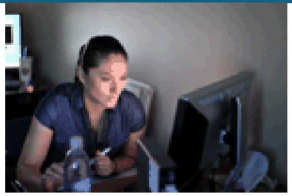
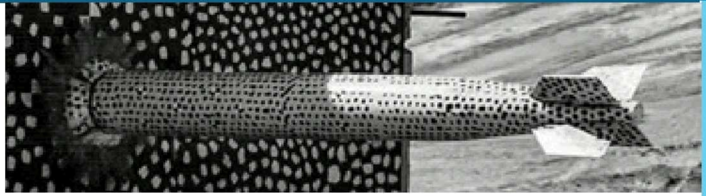
SAND2019-15444C

Investigating active slip planes in tantalum under compressive load





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[1]Sandia National Laboratories
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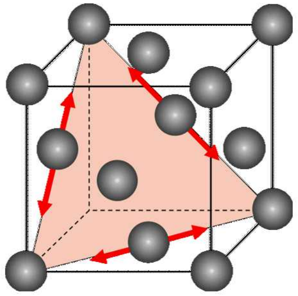
Introduction: Active slip planes in Ta

❖ **Tantalum**

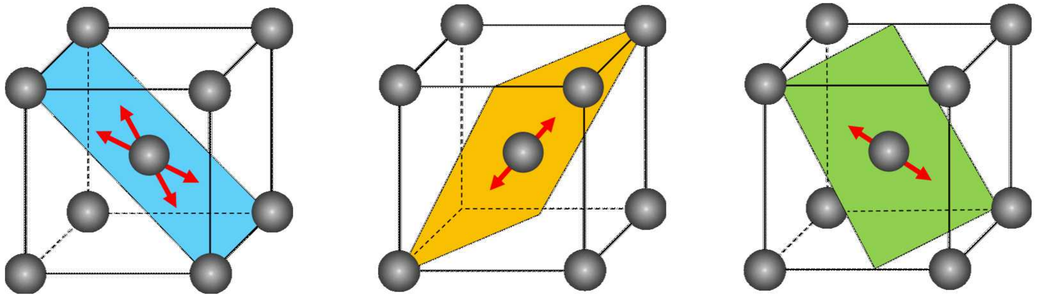
- High melting point (3290 K) & density (16.7 g/cm^3)
- Strong, ductile, high corrosion resistance
- ***Active slip planes in Tantalum?***

FCC



<110>{111}

BCC



<111>{110} <111>{112} <111>{123}

❖ **Previously…**

- Experiments – slip trace analysis
  - {110} slip – Shields et al. (1975), Mitchell & Spitzig (1965), Byron & Hull (1967), Hull et al. (1967)
  - {112} slip – Nawaz & Mordike (1975)
  - {110}+{112} slip –Nawaz & Mordike (1975)
  - Wavy slip – Smialek & Mitchel (1970), Takeuchi et al. (1972), Takeuchi & Maeda (1977)

{110} planes at low T

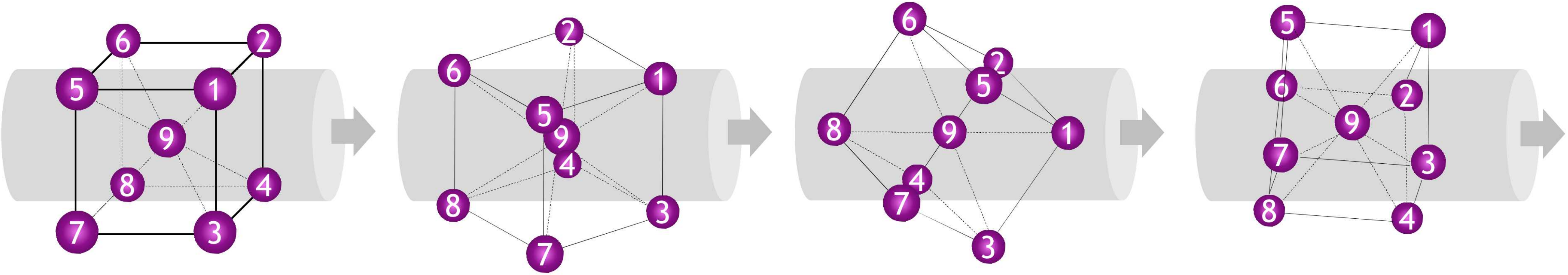
{112} planes at elevated T

- Atomistic simulations / DFT
  - {110} slip or {112} slip
  - Alternating {110} slips to form net {112} slip.

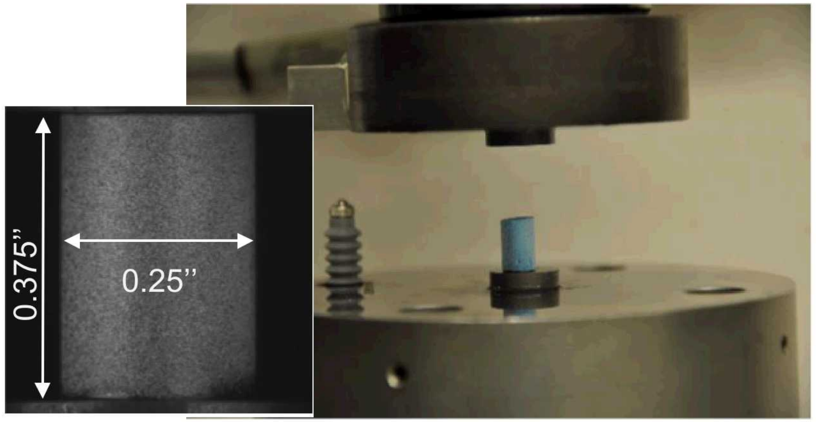
Previous experimental observations and modeling work are not sufficient to conclude the active slip planes in tantalum.

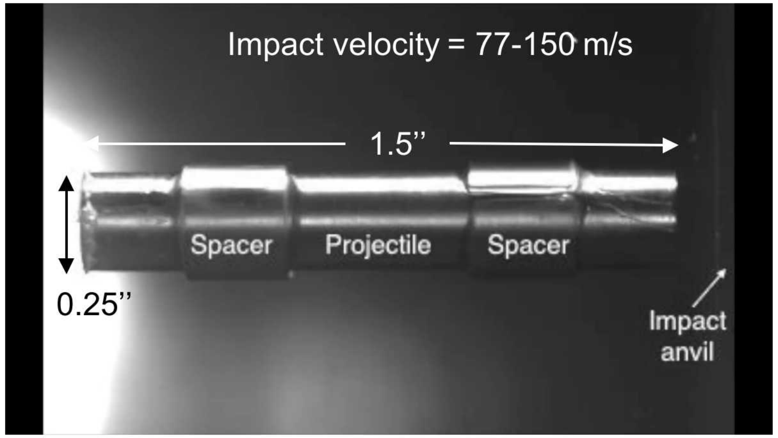
Overview

- Single crystals in 4 orientations: [001], [011], [$\bar{1}$11], [$\bar{1}$49]



- Two mechanical tests: Taylor impact tests & quasi-static compression tests



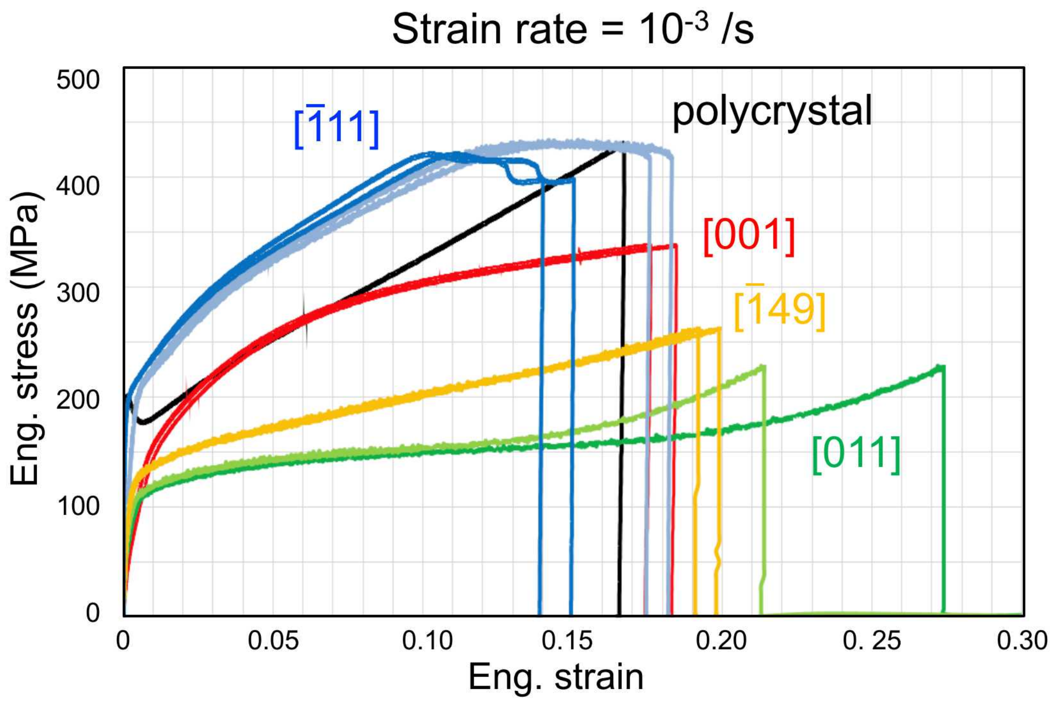


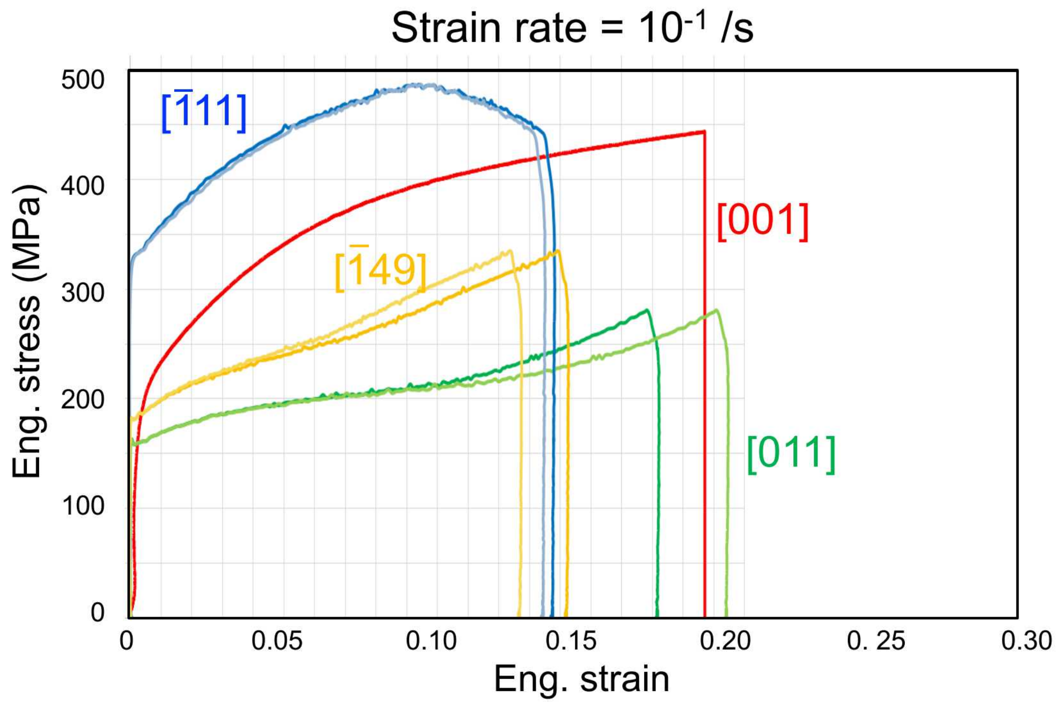
Quasi-static compression: $\dot{\varepsilon}$ =0.1 /s & 0.001 /s

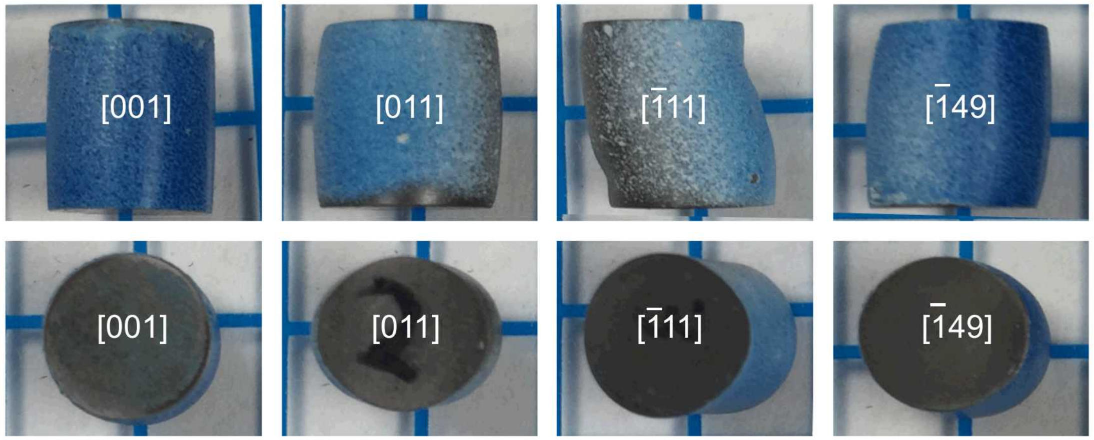
Taylor impact test (LANL): $\dot{\varepsilon} < 5 \times 10^4\ s^{-1}$

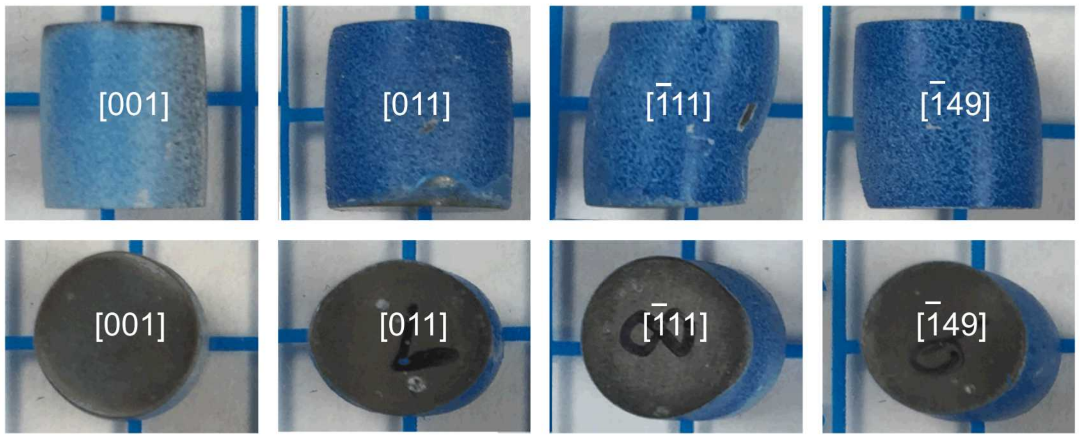
- Crystal plasticity finite element simulations + EBSD analysis

Quasi-static compression tests

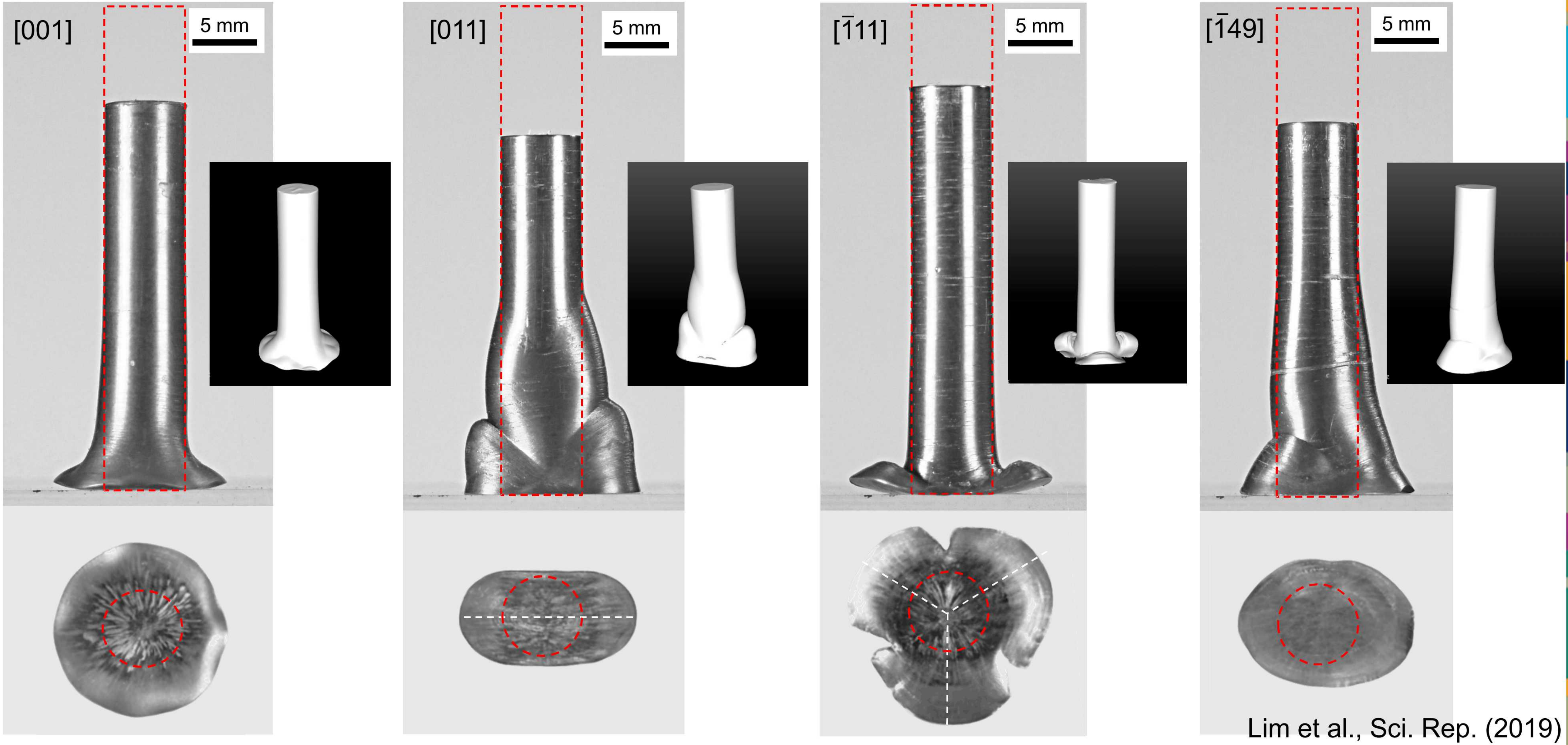








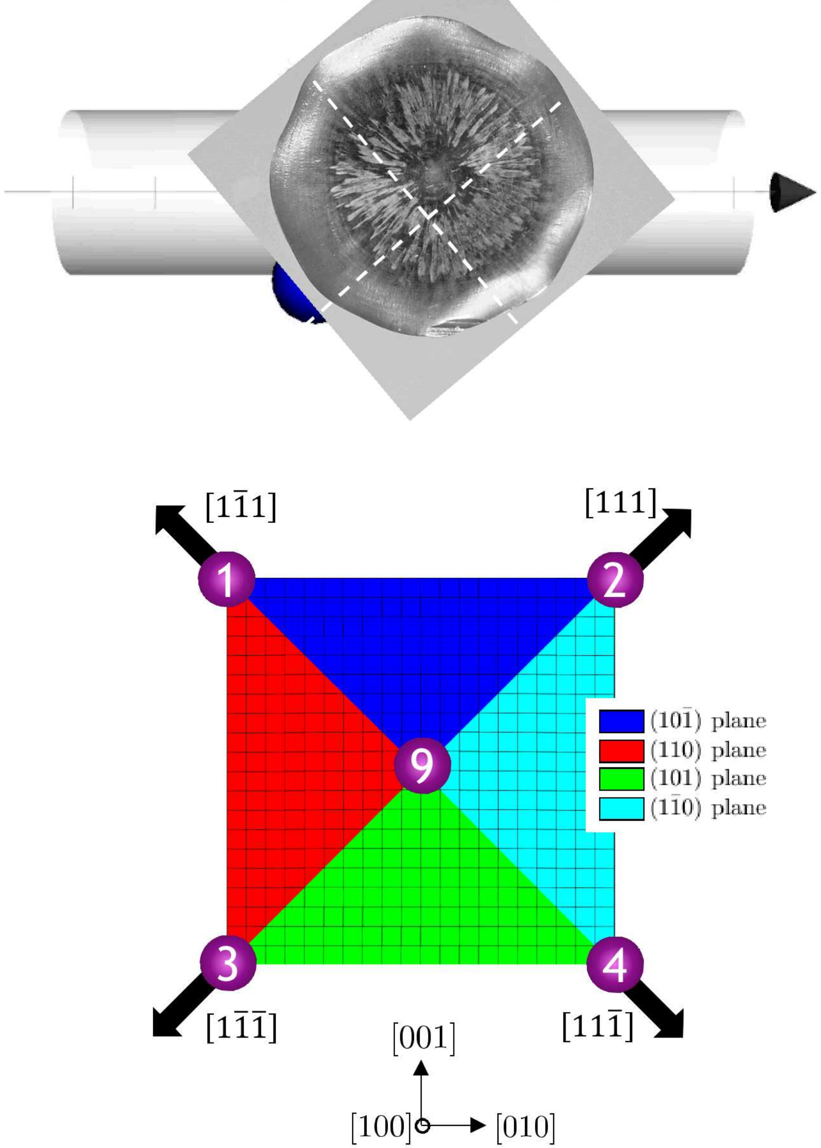
Taylor impact tests (impact velocity = 137 m/s)



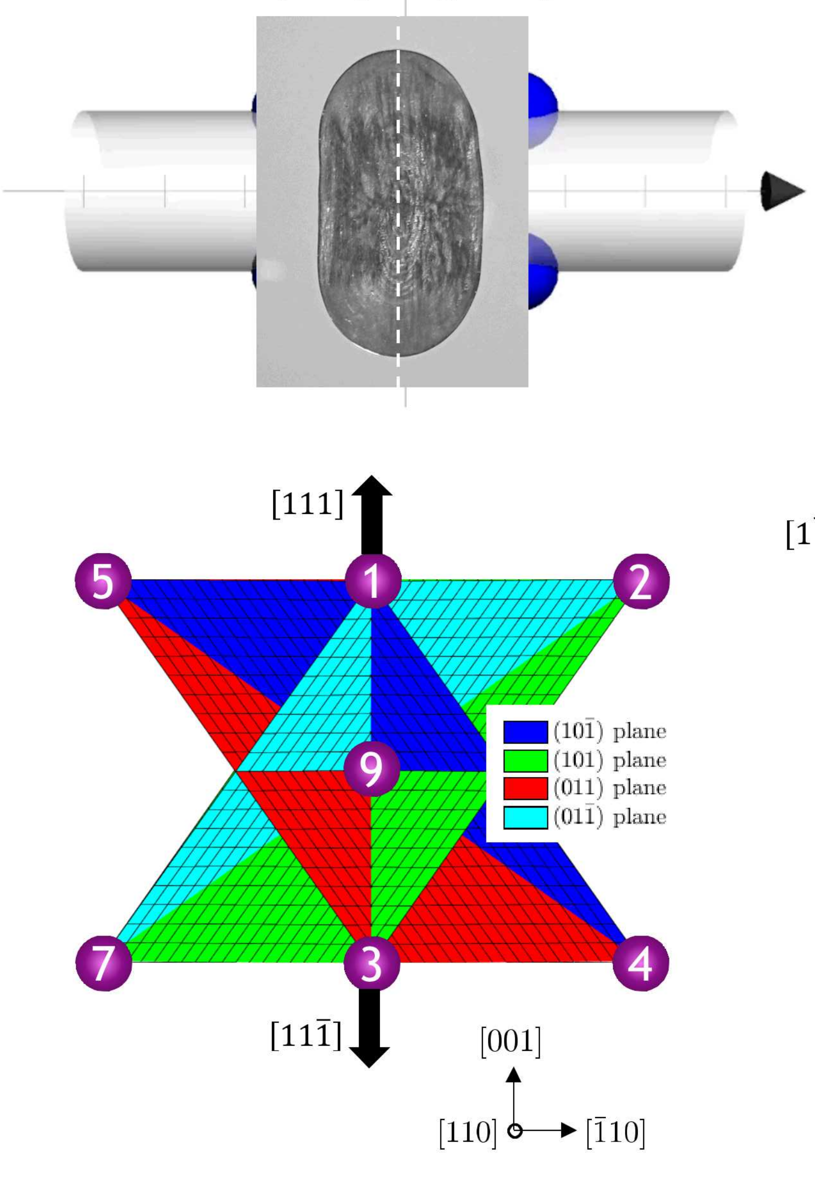
Lim et al., Sci. Rep. (2019)

Crystallographic analysis

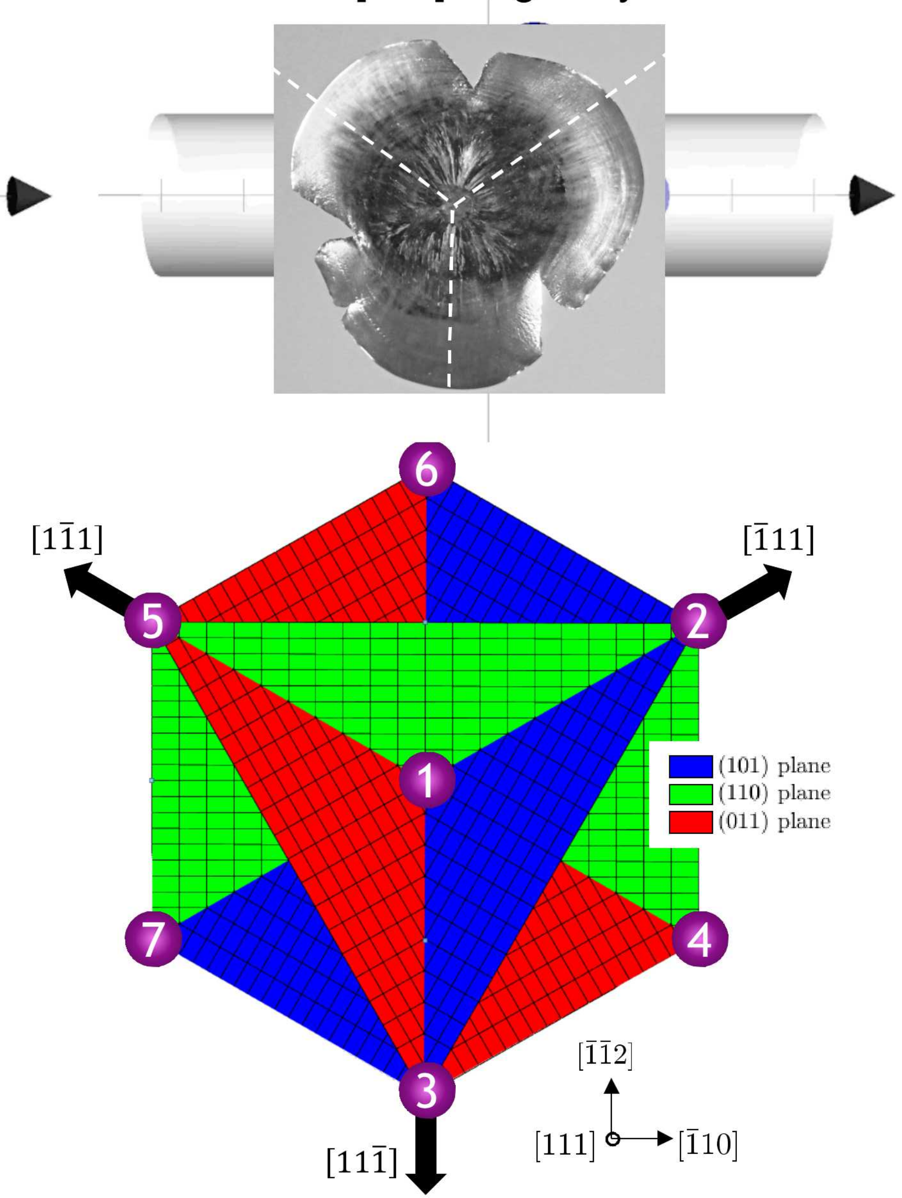
[001] single crystal



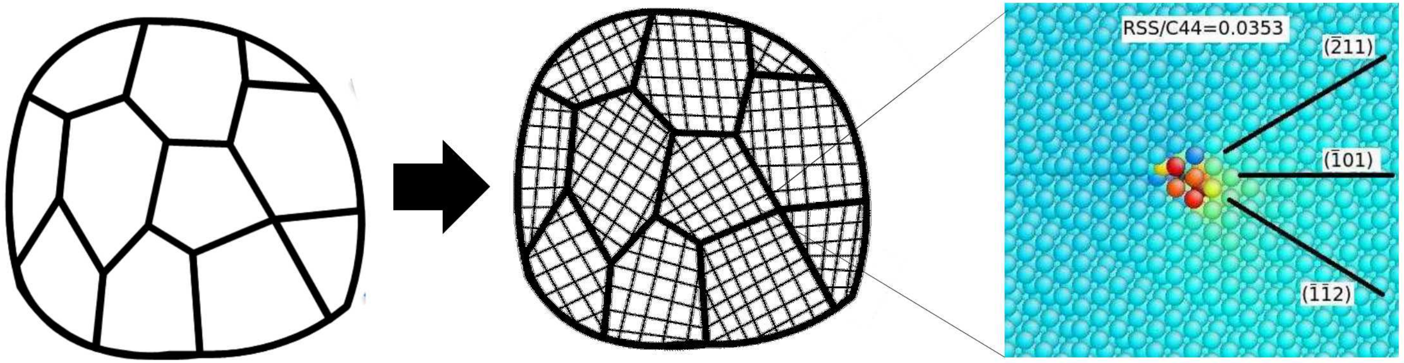
[011] single crystal



$[\bar{1}11]$ single crystal



Crystal Plasticity-Finite Element (CP-FE) method



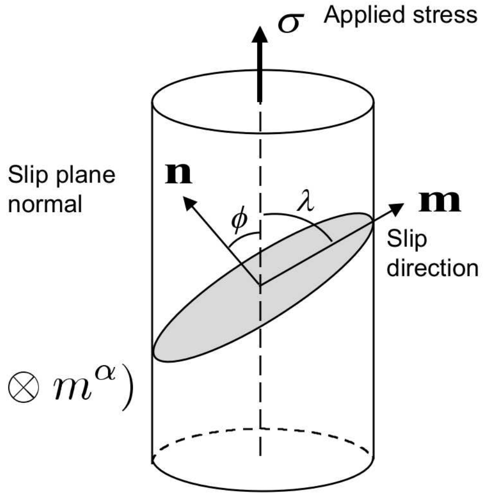
Polycrystalline body

FE discretization

$$\dot{\gamma}^{\alpha} = \dot{\gamma}^{0}\left(\frac{\tau^{\alpha}}{g^{\alpha}}\right)^{1/m}$$

$$\tau^{\alpha} = \mathbf{P}_{s}^{\alpha} : \sigma$$

$$\mathbf{P}_{s}^{\alpha} = \frac{1}{2}\left(m^{\alpha} \otimes n^{\alpha} + n^{\alpha} \otimes m^{\alpha}\right)$$



- Grain-level (mesoscale) approach to materials modeling using multiscale strategies – realistic length and time scales

- Explicitly model discrete grains and slip systems based on dislocation slip

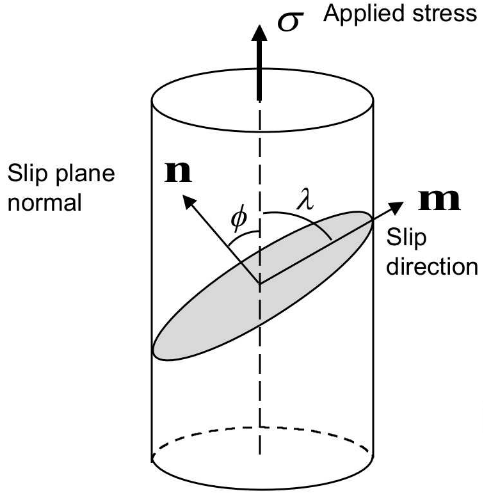
- Predicts heterogeneous material's responses resulting from microstructure.

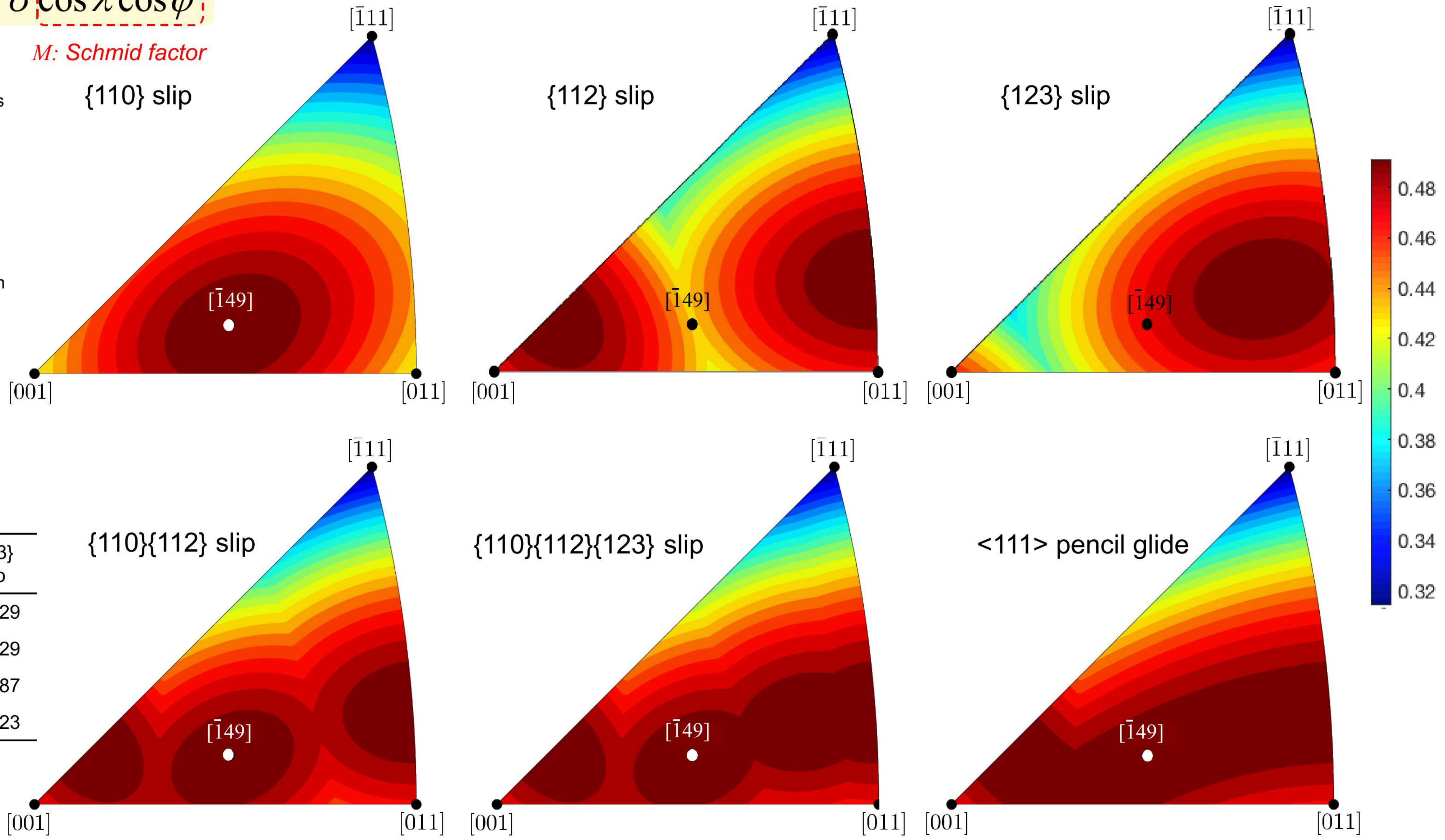
- More predictive than macroscopic plasticity models (i.e. texture evolution and elastic/plastic anisotropy)

Maximum Schmid factors

Schmid's law: $\tau = \sigma \boxed{\cos\lambda \cos\varphi}$

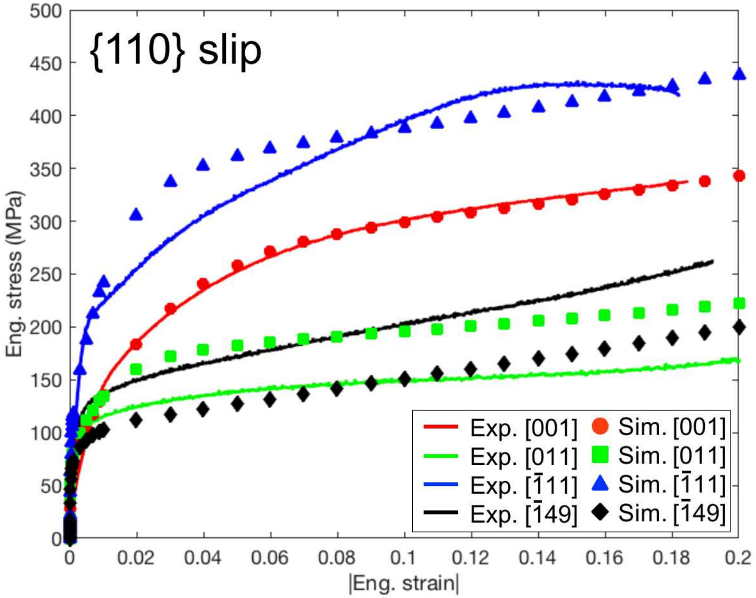
M: Schmid factor

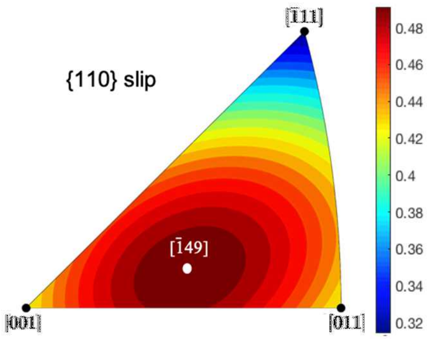


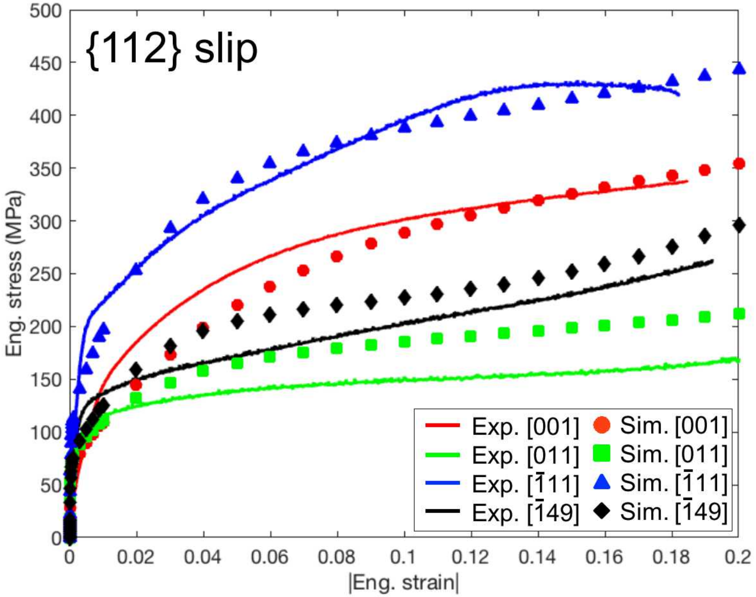


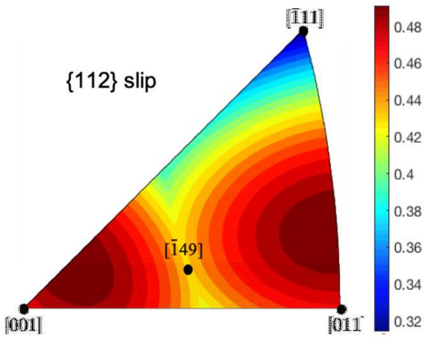
Directions	{110} slip	{112} slip	{123} slip
[001]	0.4082	0.4714	0.4629
[011]	0.4082	0.4714	0.4629
[111]	0.2722	0.3143	0.3087
[149]	0.5000	0.4377	0.4723

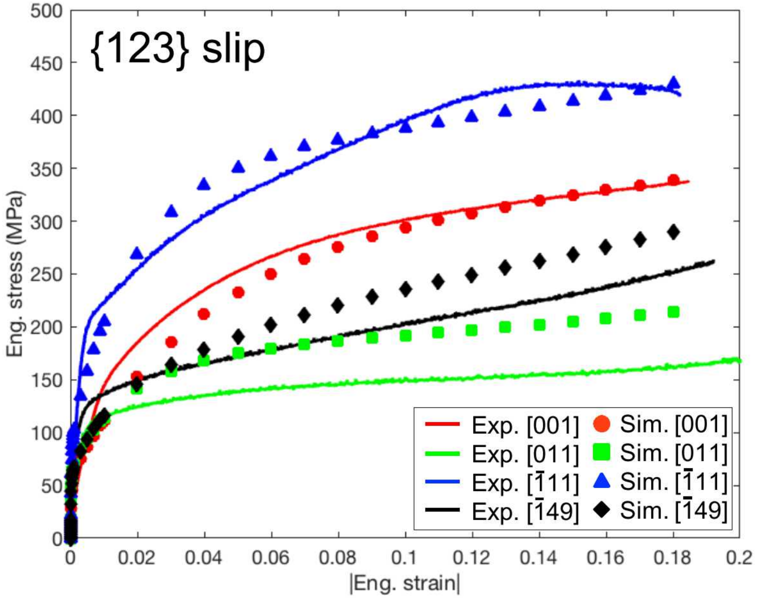
Quasi-static compression: Exp. vs CP-FE simulations

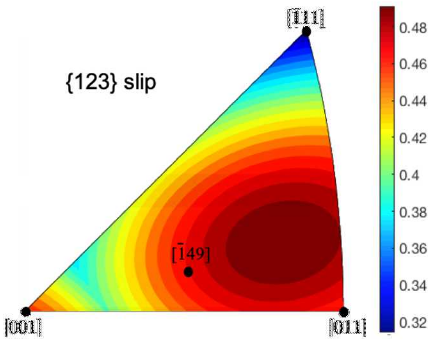


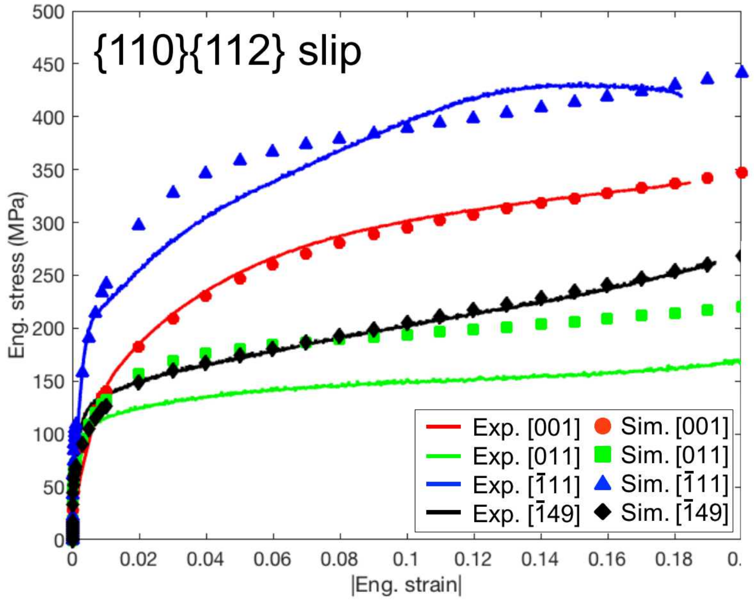


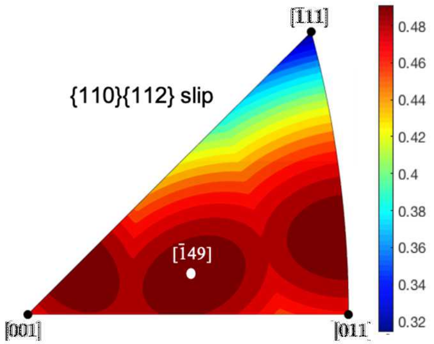






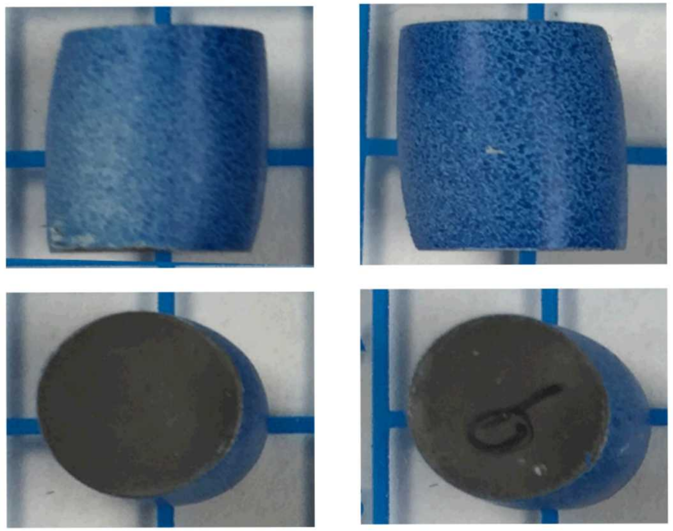


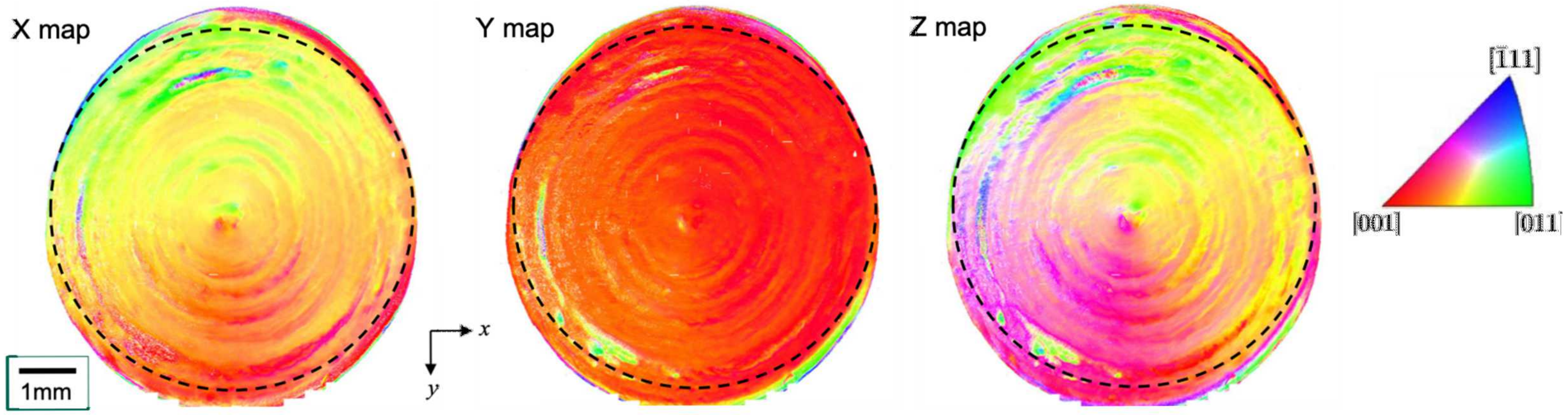




Deformation of $[\bar{1}49]$ single crystals

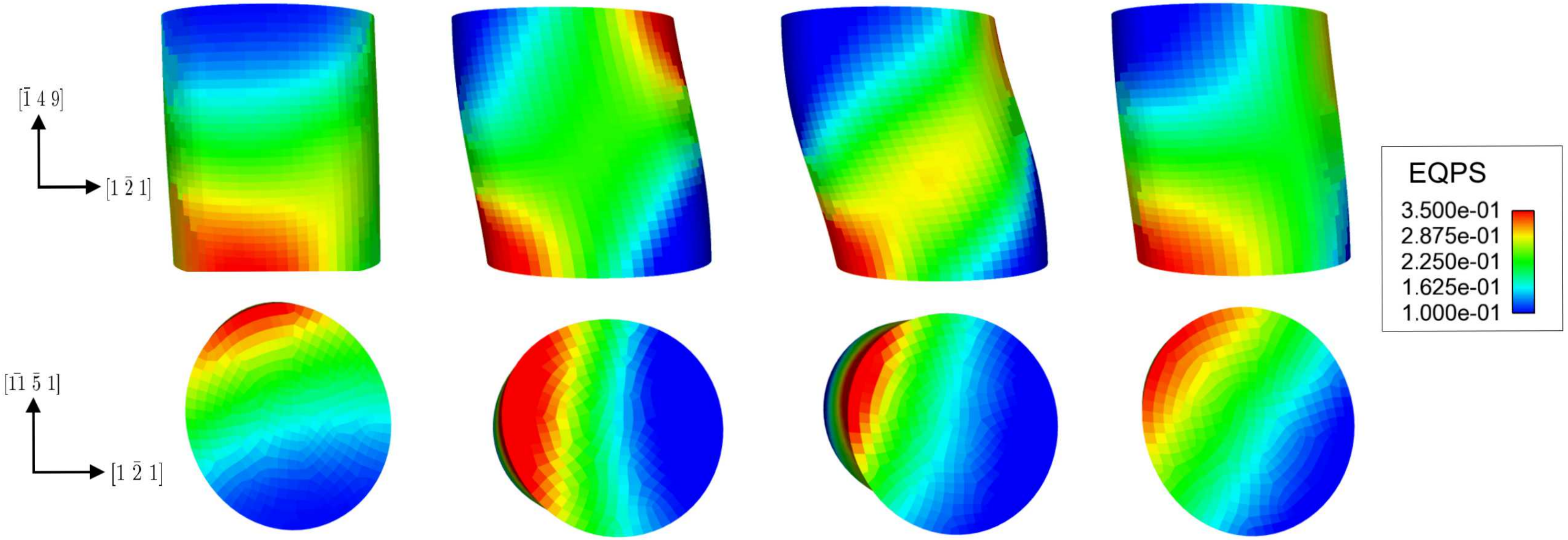
Strain rate = 10^{-3} /s | Strain rate = 10^{-1} /s



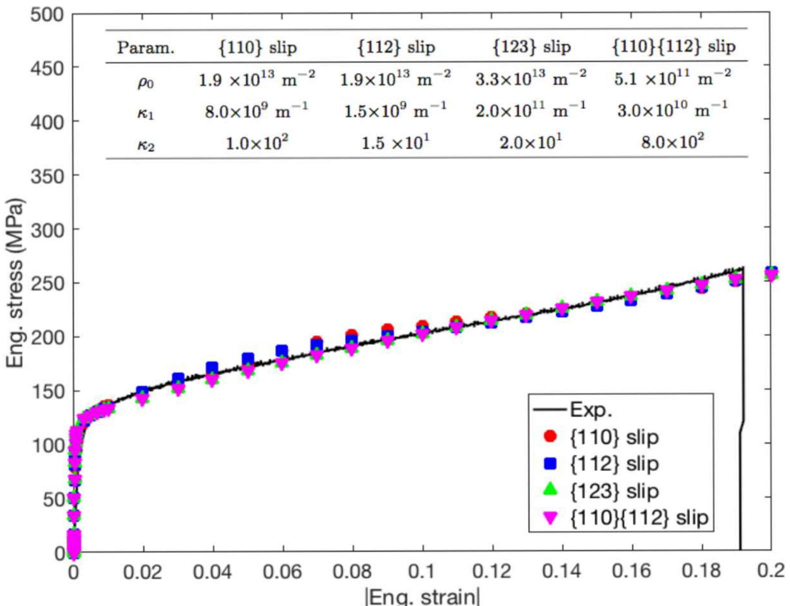


CP-FE simulations

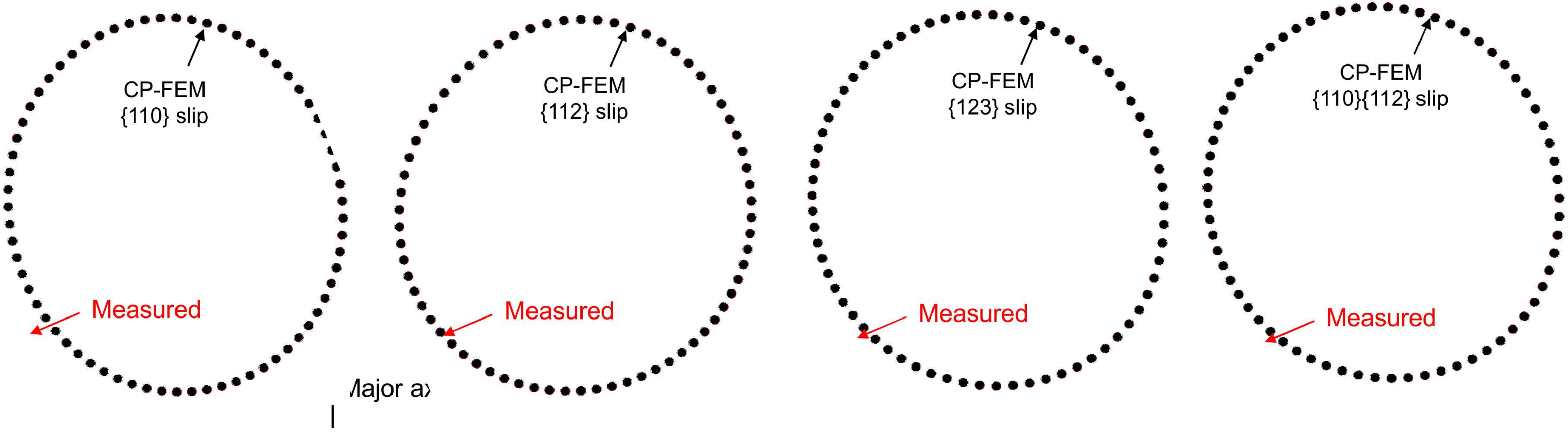
{110} slip | {112} slip | {123} slip | {110}+{112} slip

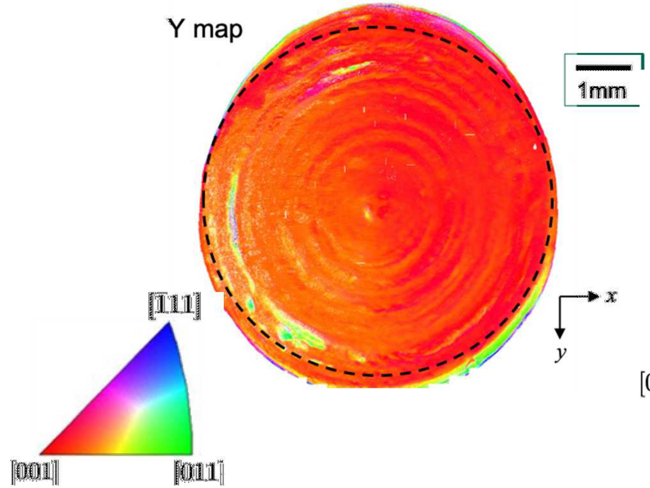


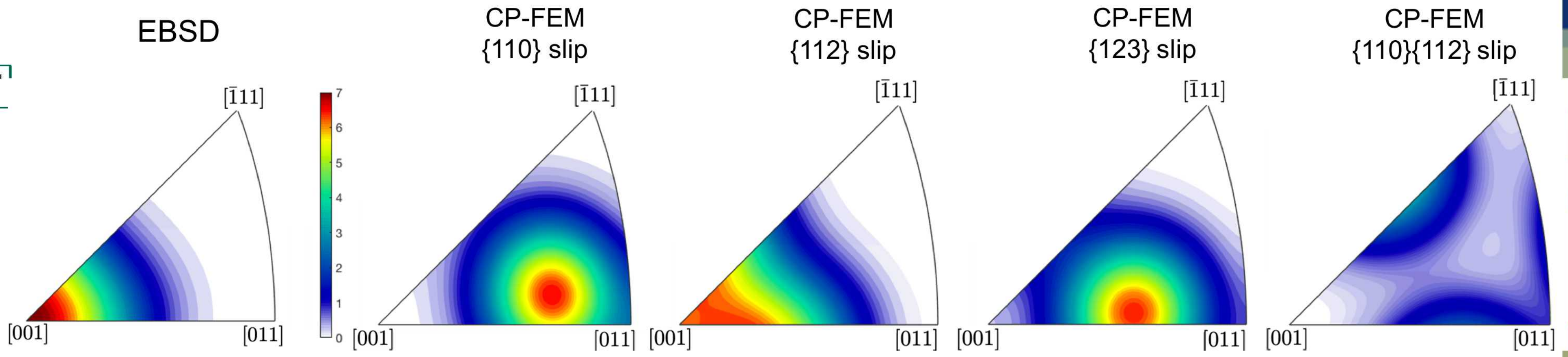
Param.	{110} slip	{112} slip	{123} slip	{110}{112} slip
ρ_0	1.9×10^{13} m^{-2}	1.9×10^{13} m^{-2}	3.3×10^{13} m^{-2}	5.1×10^{11} m^{-2}
κ_1	8.0×10^{9} m^{-1}	1.5×10^{9} m^{-1}	2.0×10^{11} m^{-1}	3.0×10^{10} m^{-1}
κ_2	1.0×10^{2}	1.5×10^{1}	2.0×10^{1}	8.0×10^{2}



[$\bar{1}$49] single crystal: CP-FEM vs. exp.

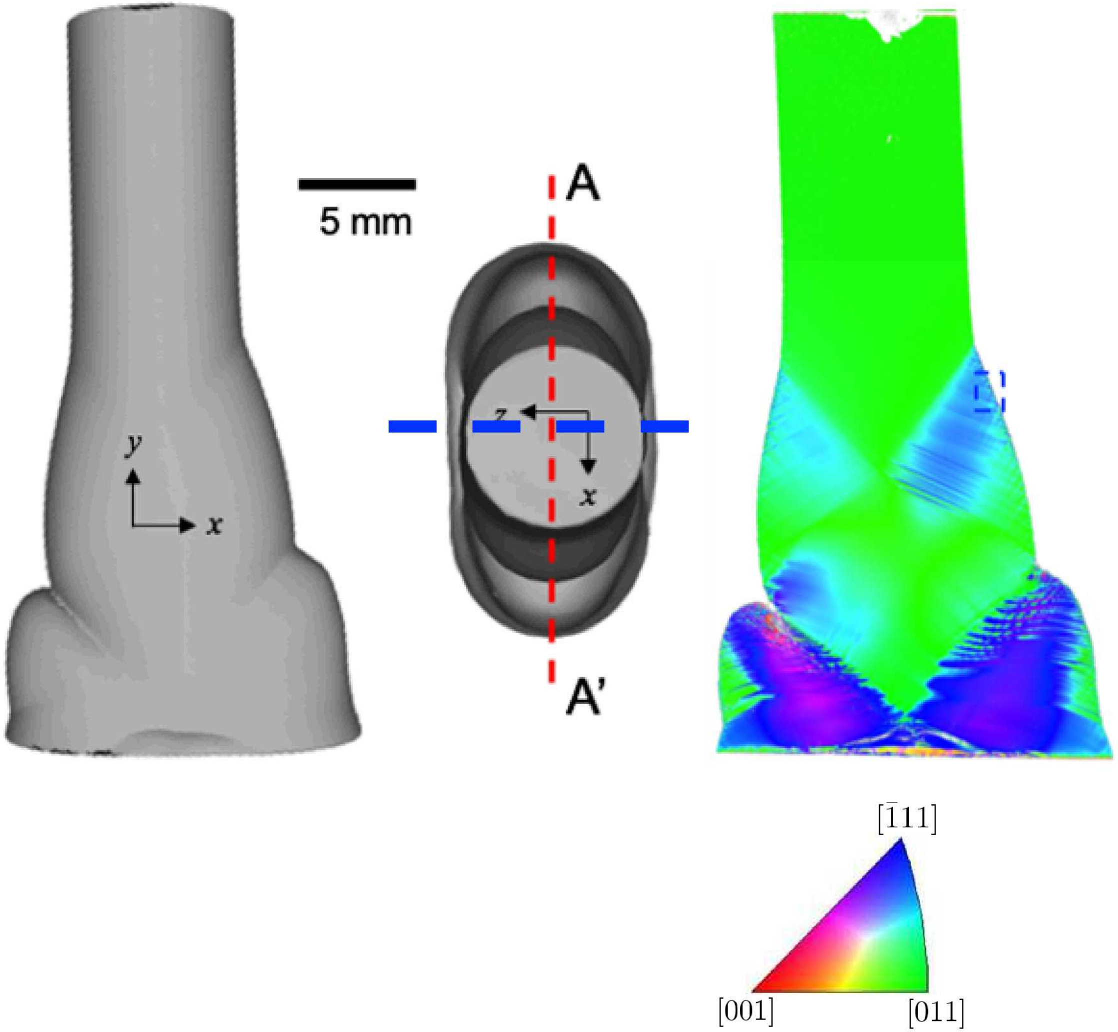


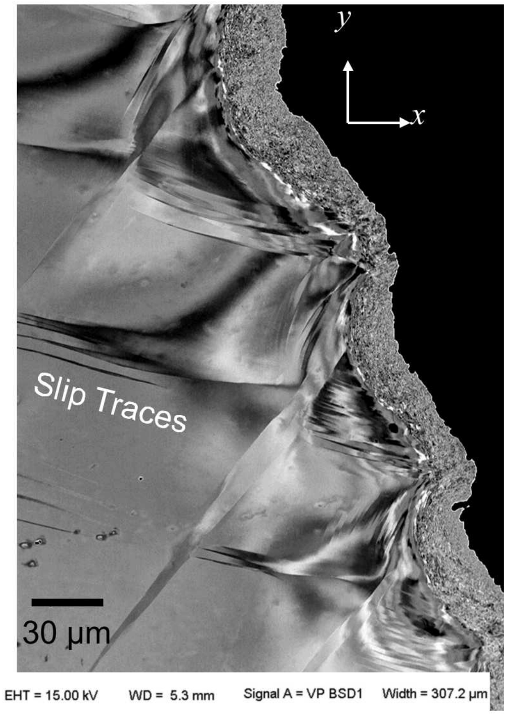


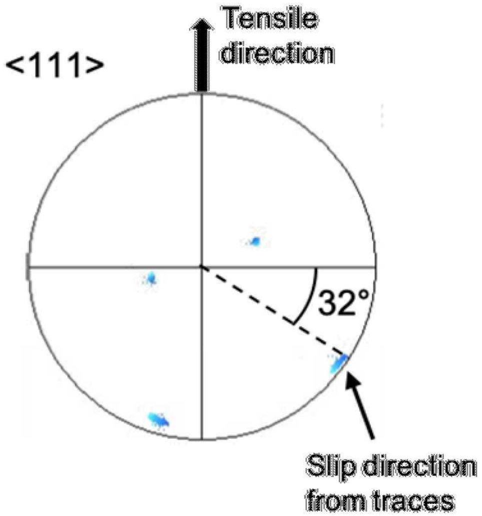


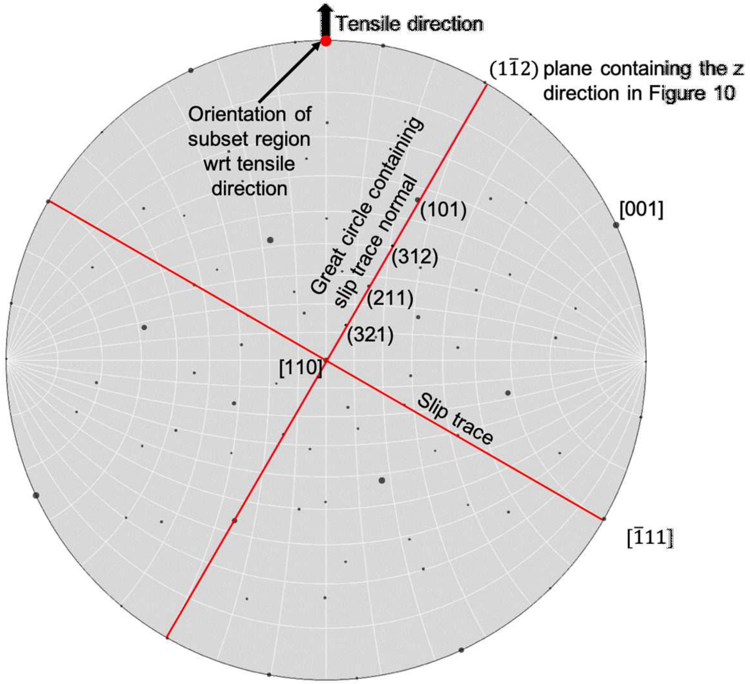
Slip traces in dynamically deformed [011] single crystal

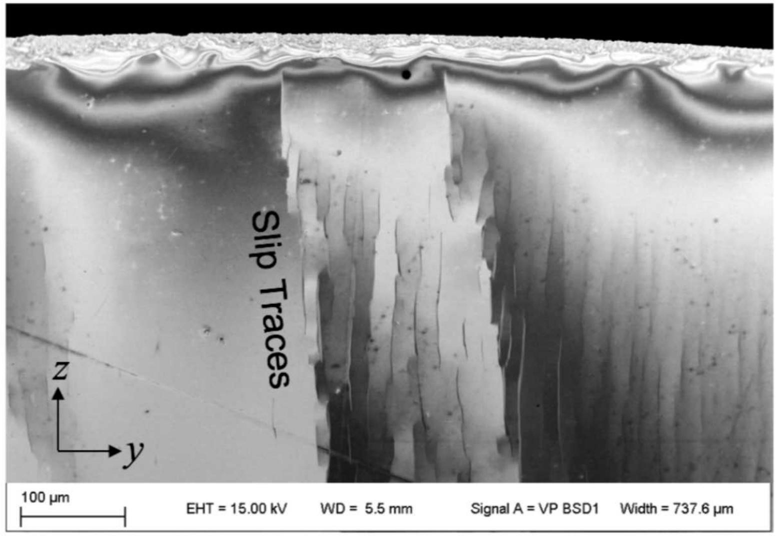
[011] single crystal
Impact velocity = 137 m/s



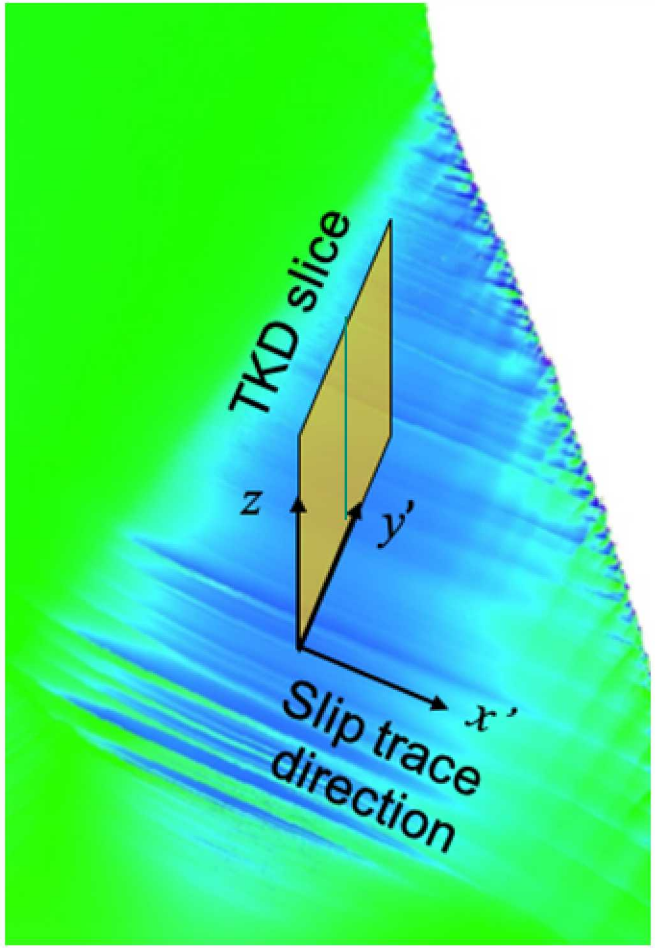


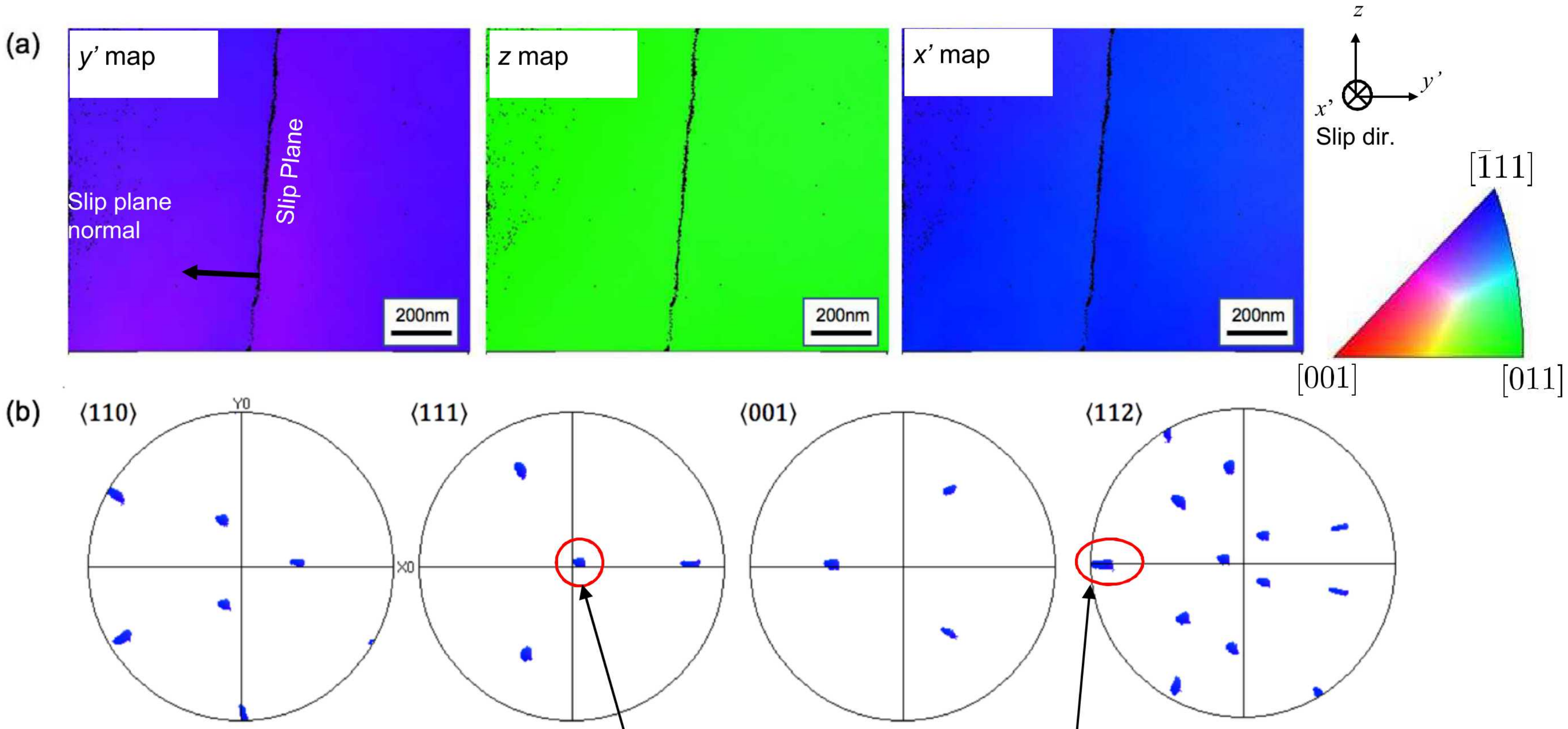






Transmission Kikuchi Diffraction Analysis of slip planes





No <110> directions on the perimeter and equator simultaneously

<111> slip direction is directly out of page

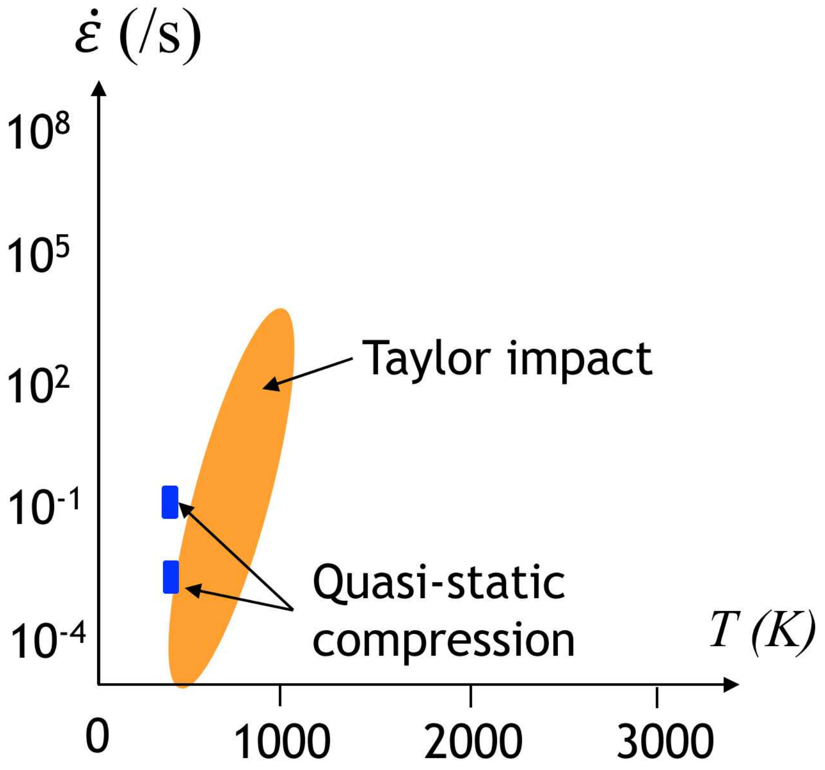
Normal direction of the slip plane is <112>

Summary

- Four tantalum single crystals along [001], [011], [$\bar{1}$11] and [$\bar{1}$49] directions are used to perform quasi-static compression tests and dynamic impact tests.

- Stress-strain response, deformed shape, texture and slip traces support {112} slip under compressive load.

- A follow-up study will focus on the investigation of fundamental slip mechanisms using TEM analysis and atomistic simulations at various temperature and strain rate regimes.



THANK YOU !

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- Materials Margins Assurance (MMA)
- **C**ampaign **2** (C2) Dynamic Materials Properties

(-1-12) Slip Pathway at zero stress