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The Role of Crystallography and Nanostructures on Friction in FCC Metals

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Materials Science &Technology
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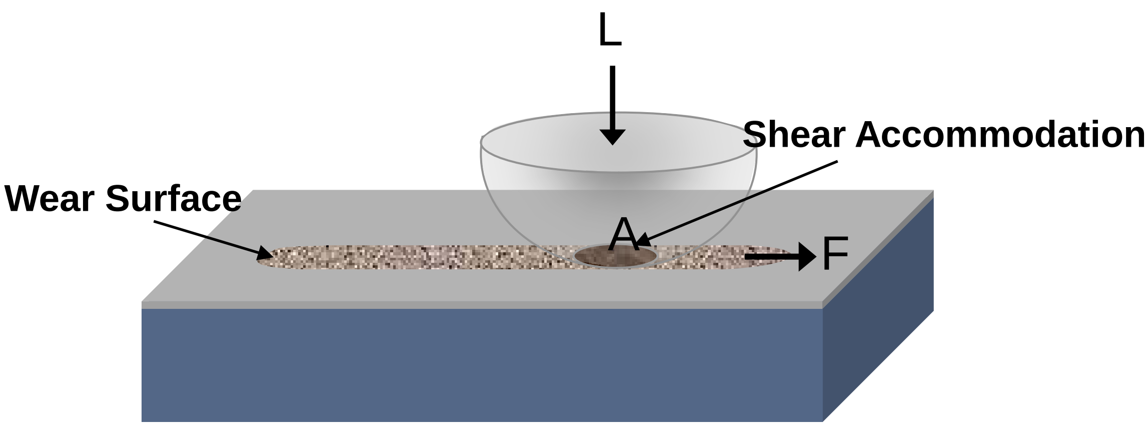
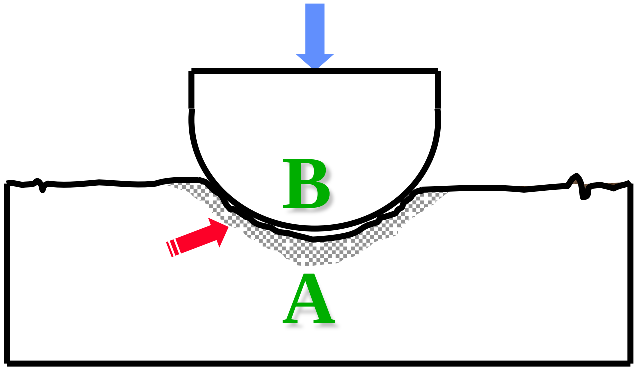
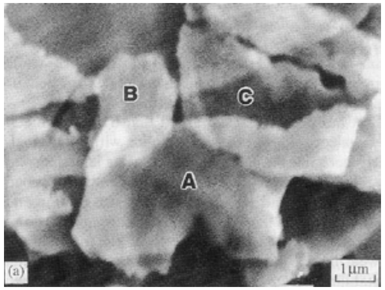
Tribology is a Systems Property

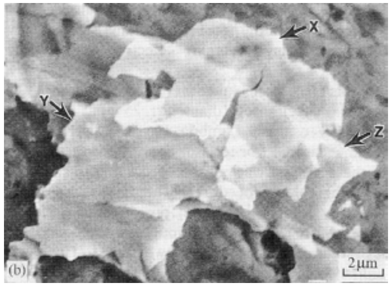




Fluids
Additives

Solid Lubricants (WS_2 on Steel)





Major Theme

Fundamental Understanding of the Evolution of Friction-induced grain structure in single crystals metals (Start from the Clean Slate)

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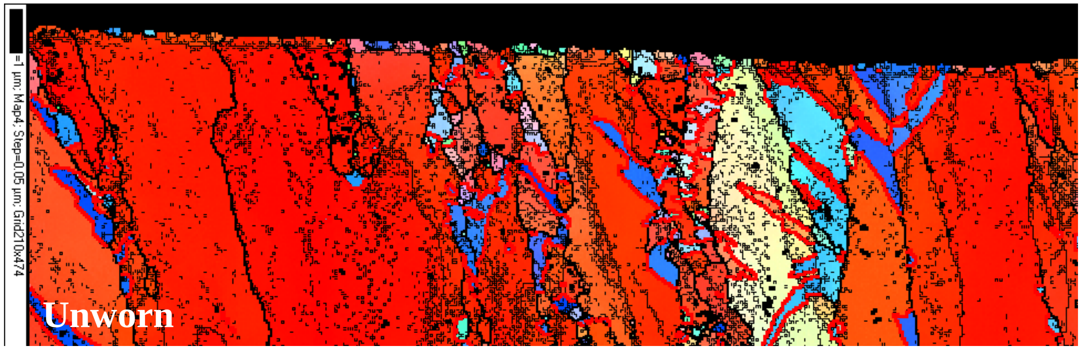
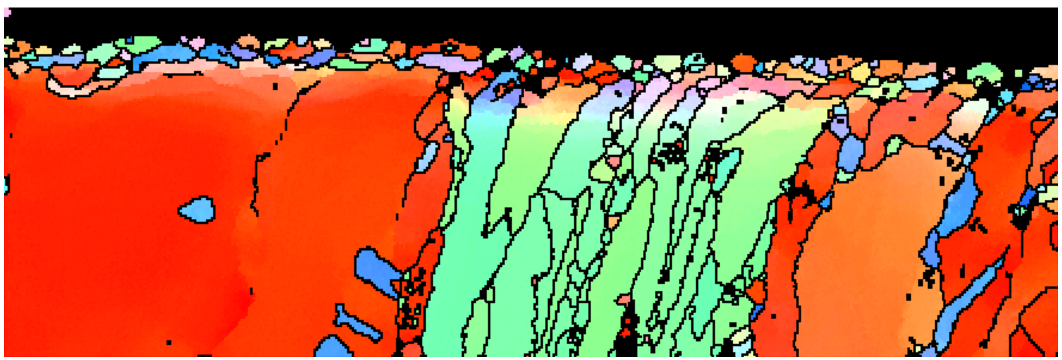
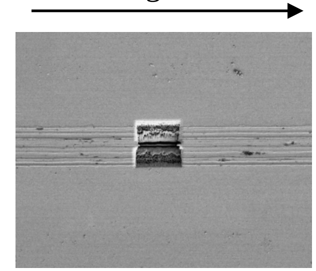
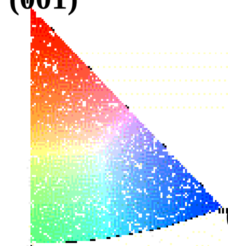
Modern Tools: FIB, Orientation Imaging, TEM

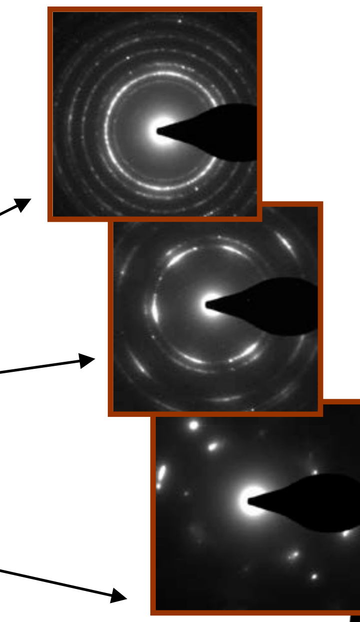




Cross sections through wear scars







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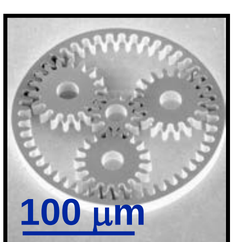

Prasad SV, Michael JR, Christen TR, *Scripta Materialia* 48 (2003) 255

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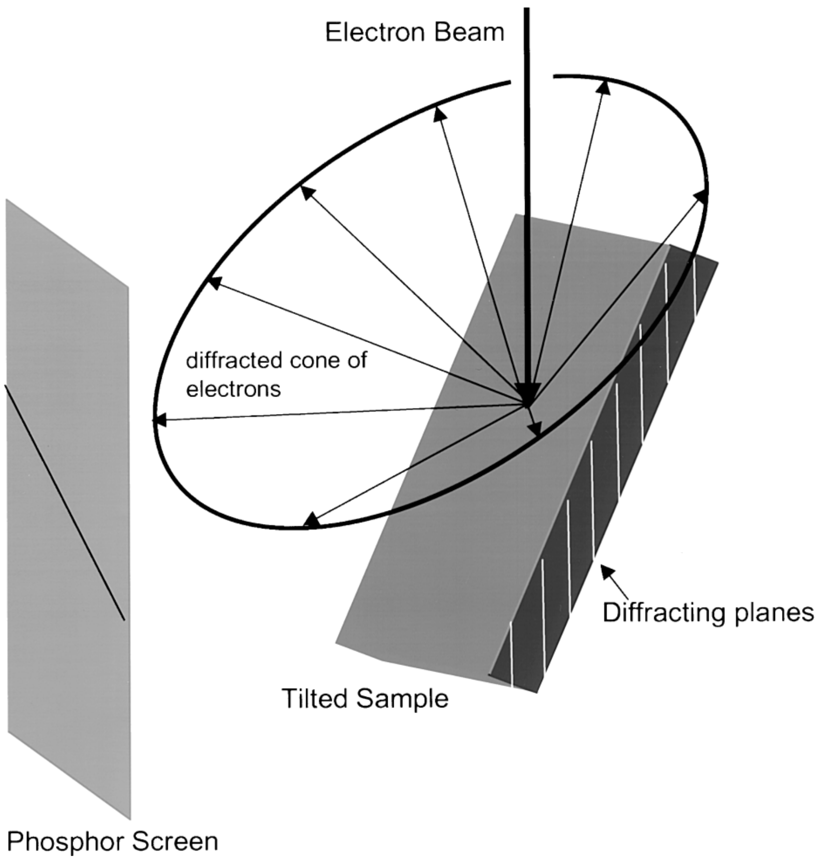
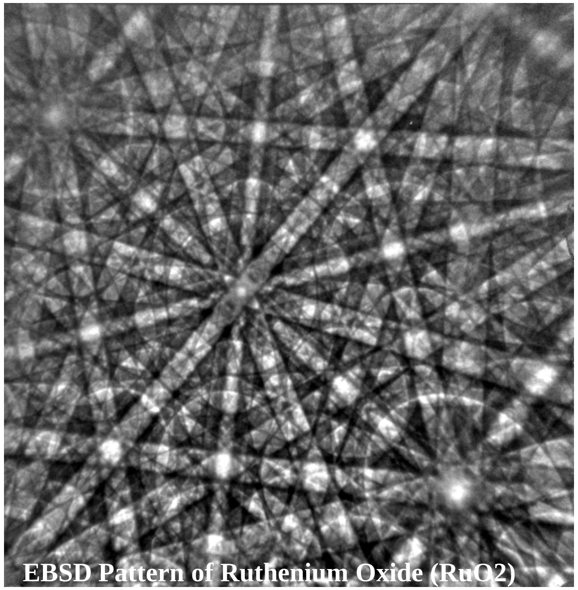
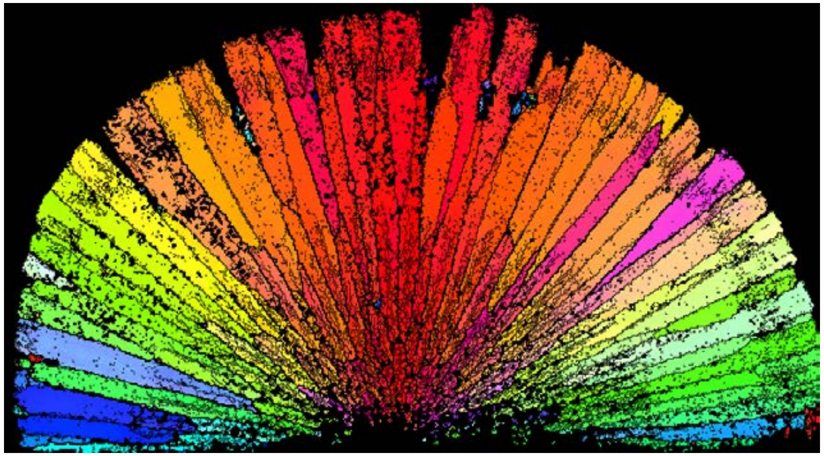
Electron Backscatter Diffraction (EBSD) in the SEM

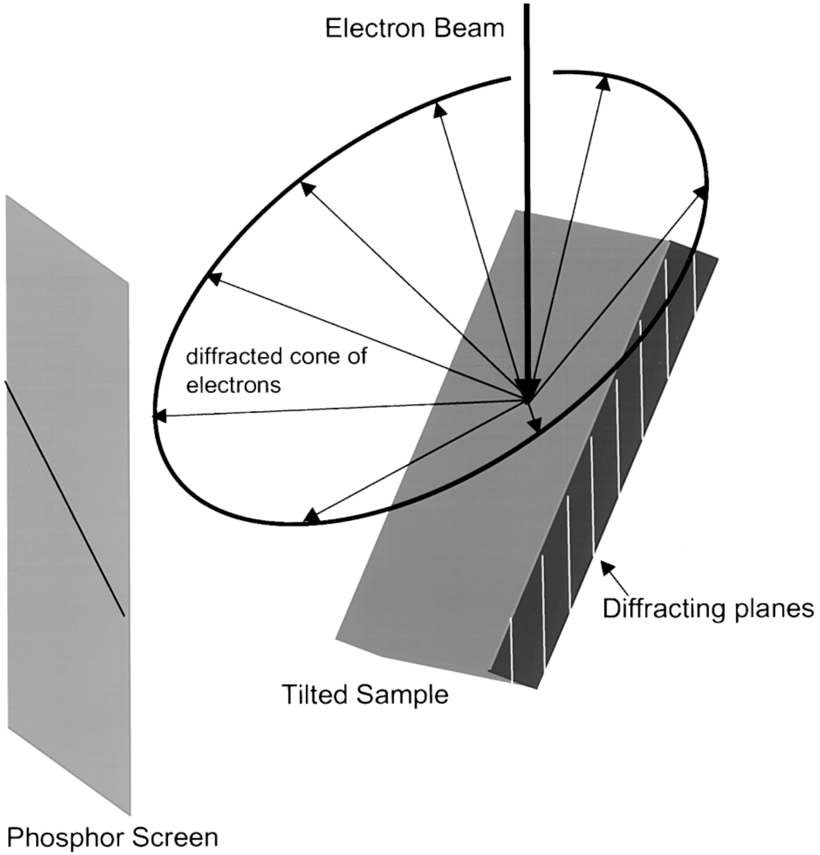


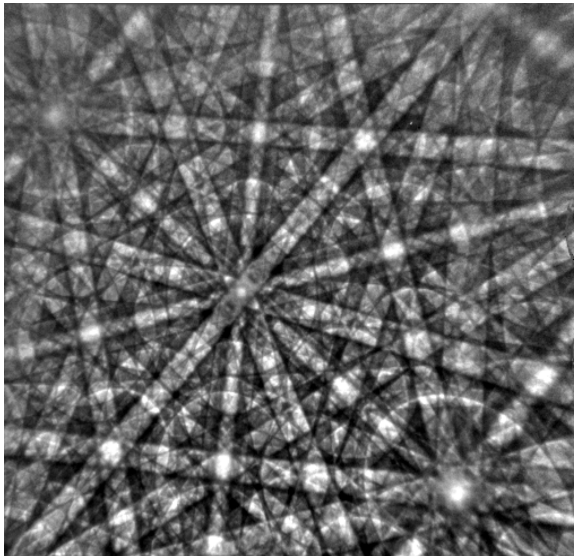


EBSD Pattern of Ruthenium Oxide (RuO2)

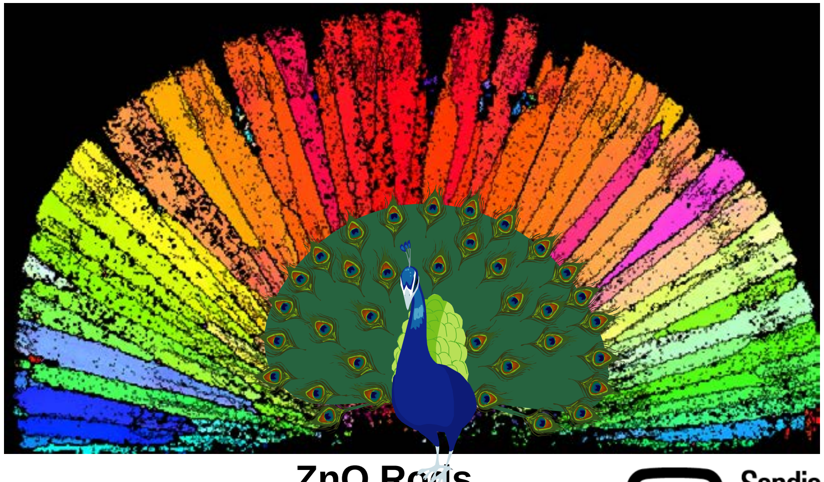


Electron Backscatter Diffraction (EBSD) in the SEM





EBSD Pattern of Ruthenium Oxide (RuO_2)



ZnO Rods

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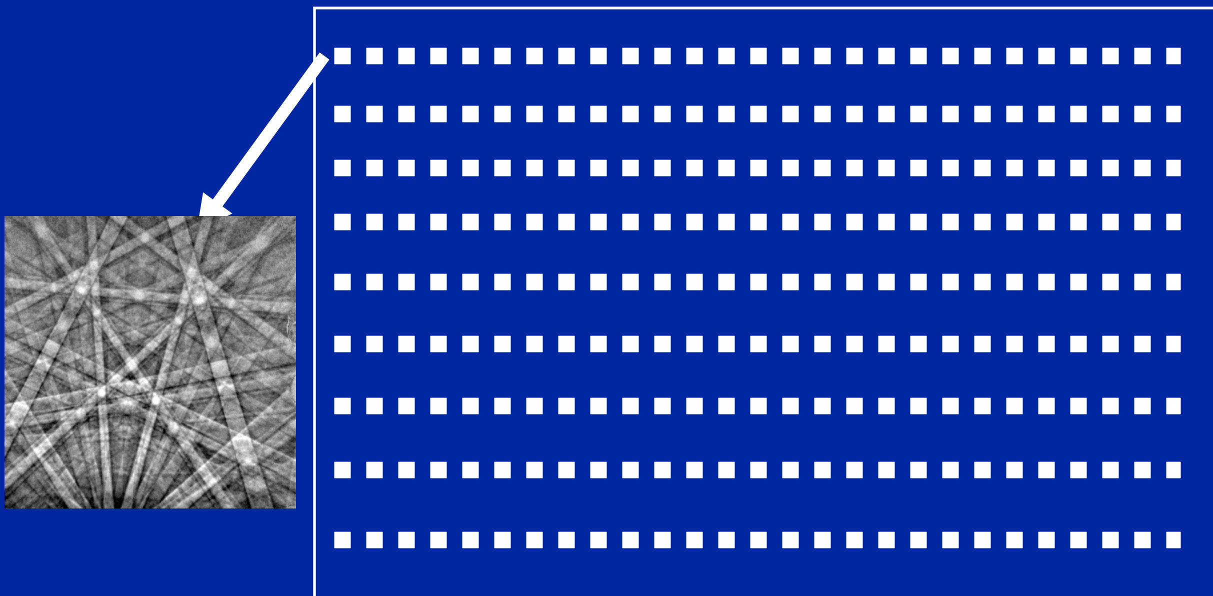
Automated EBSD Pattern Indexing



SEM image with pixels for EBSD

Step size dictated by microstructure and level of detail needed.

Minimum step size < 20nm!

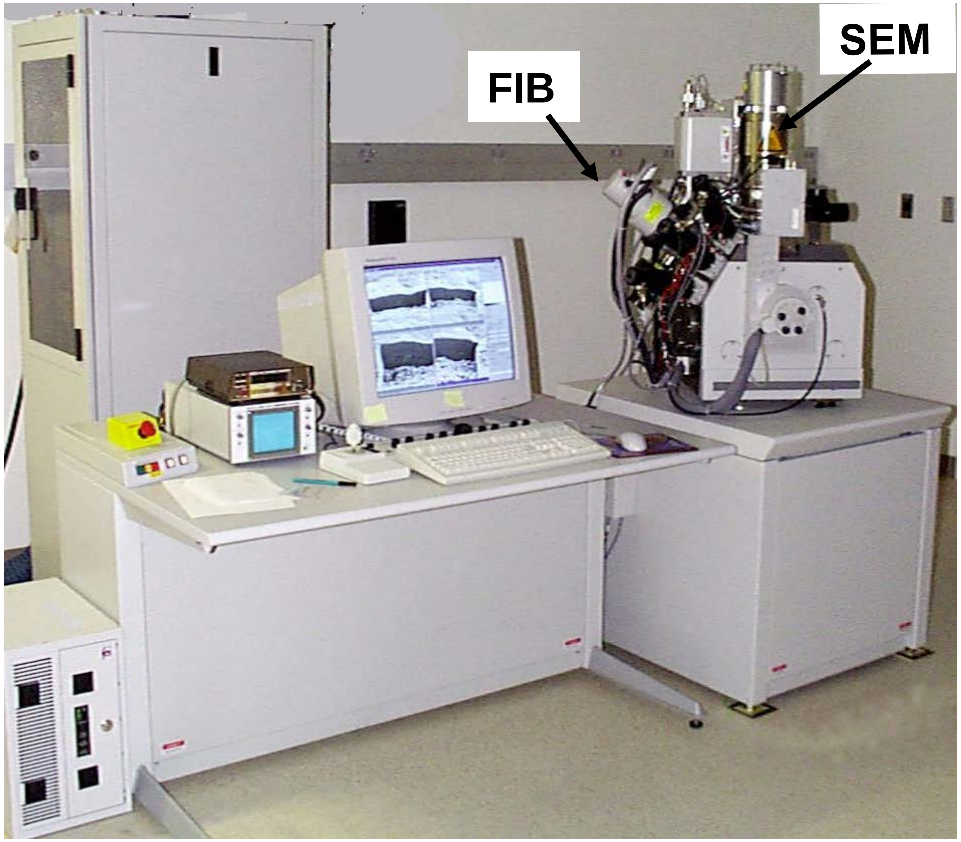
1. Scan area of interest pixel by pixel.
2. Collect EBSD pattern
3. Located 4 – 7 lines on pattern – Hough transform
4. Calculate angles between bands
5. Compare with known unit cells (short list)
6. Index pattern
7. Calculate orientation
8. Move to next pixel

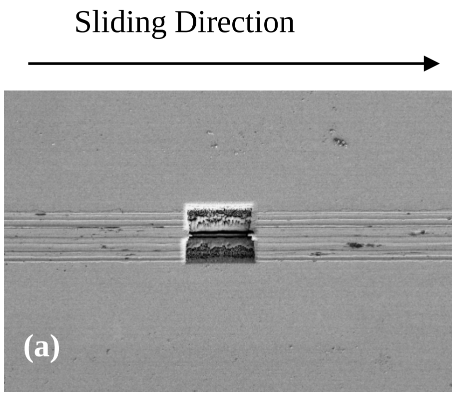
Modern systems can do this up to 50 times per second!

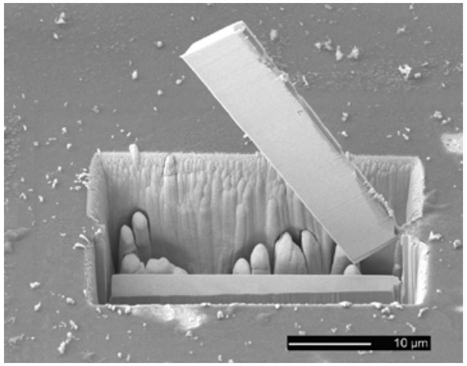
Typical FIB Configurations

Conventional Techniques
•Ion Milling (Dimpling)
•Electropolishing
•Ultramicrotomy

(-) (-) (-)
Not site specific







Dual-beam system from FEI: Both a FIB column and a SEM column are present on one sample chamber.

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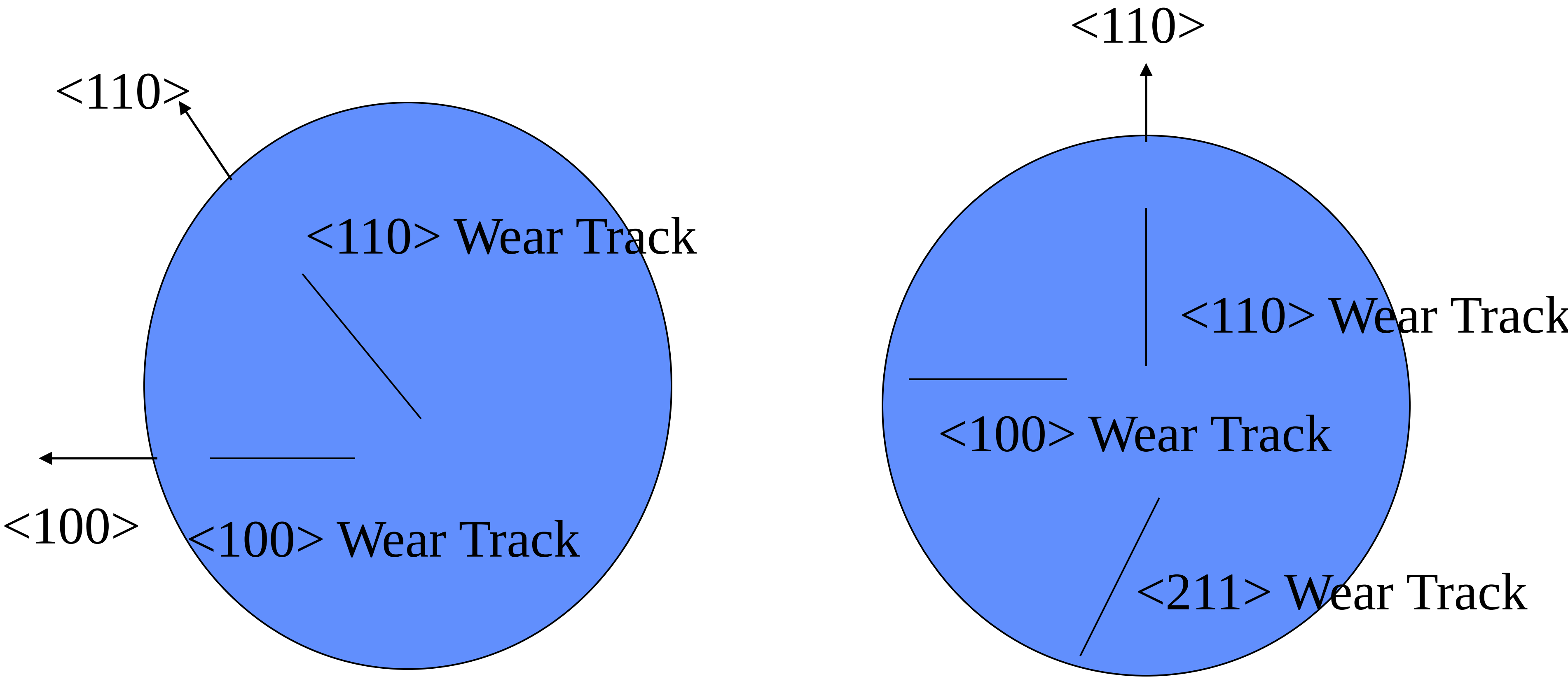
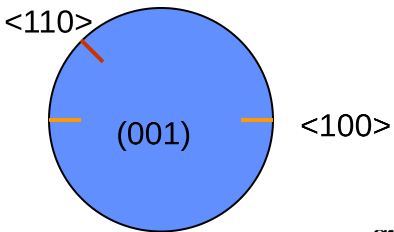
Crystallographic configurations for friction testing on single crystal Ni

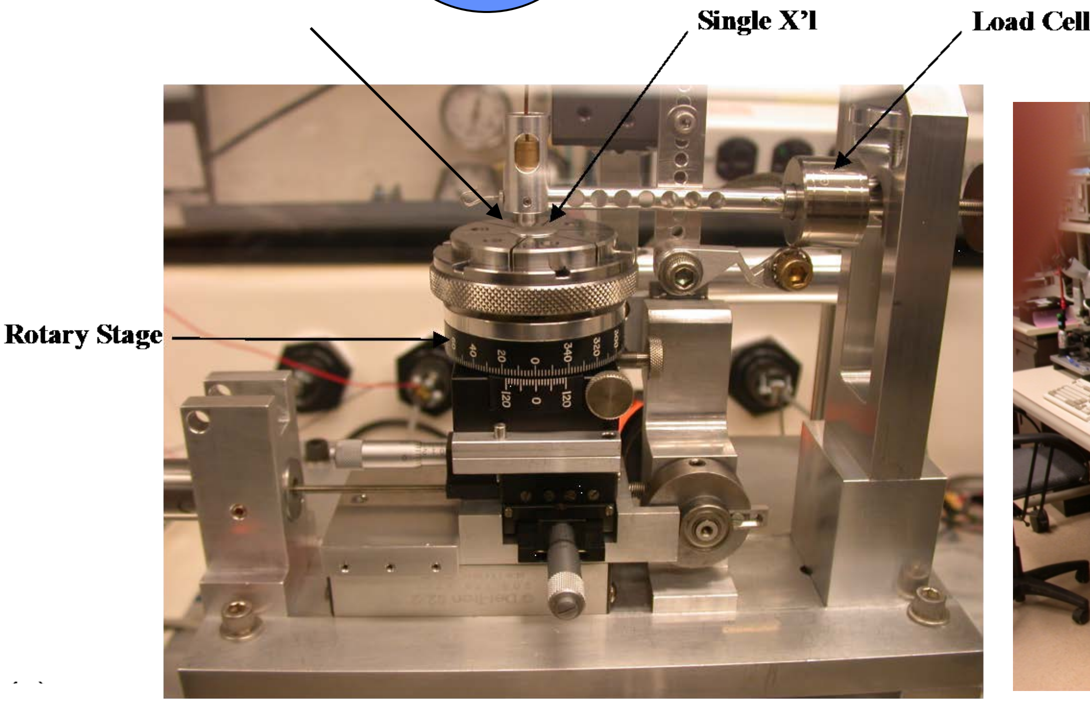


(001) Crystal Face

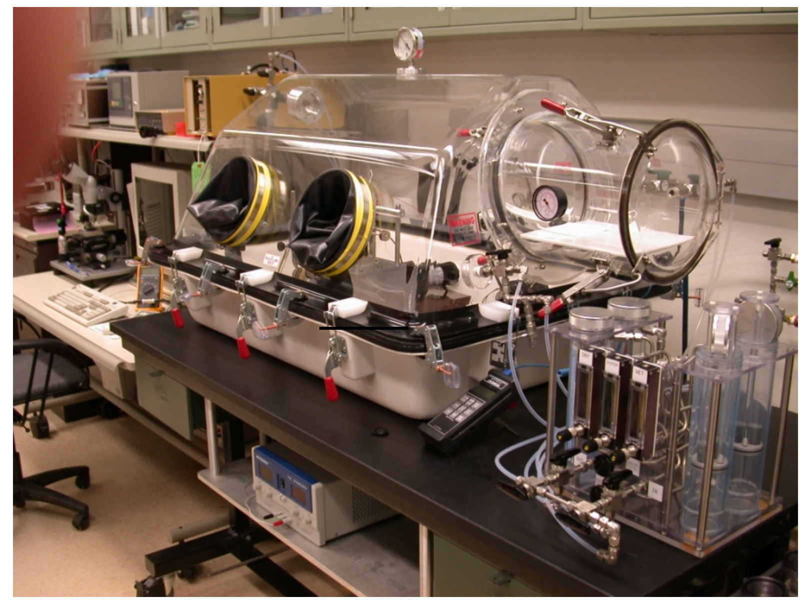
(011) Crystal Face

Rotary Friction Test Module



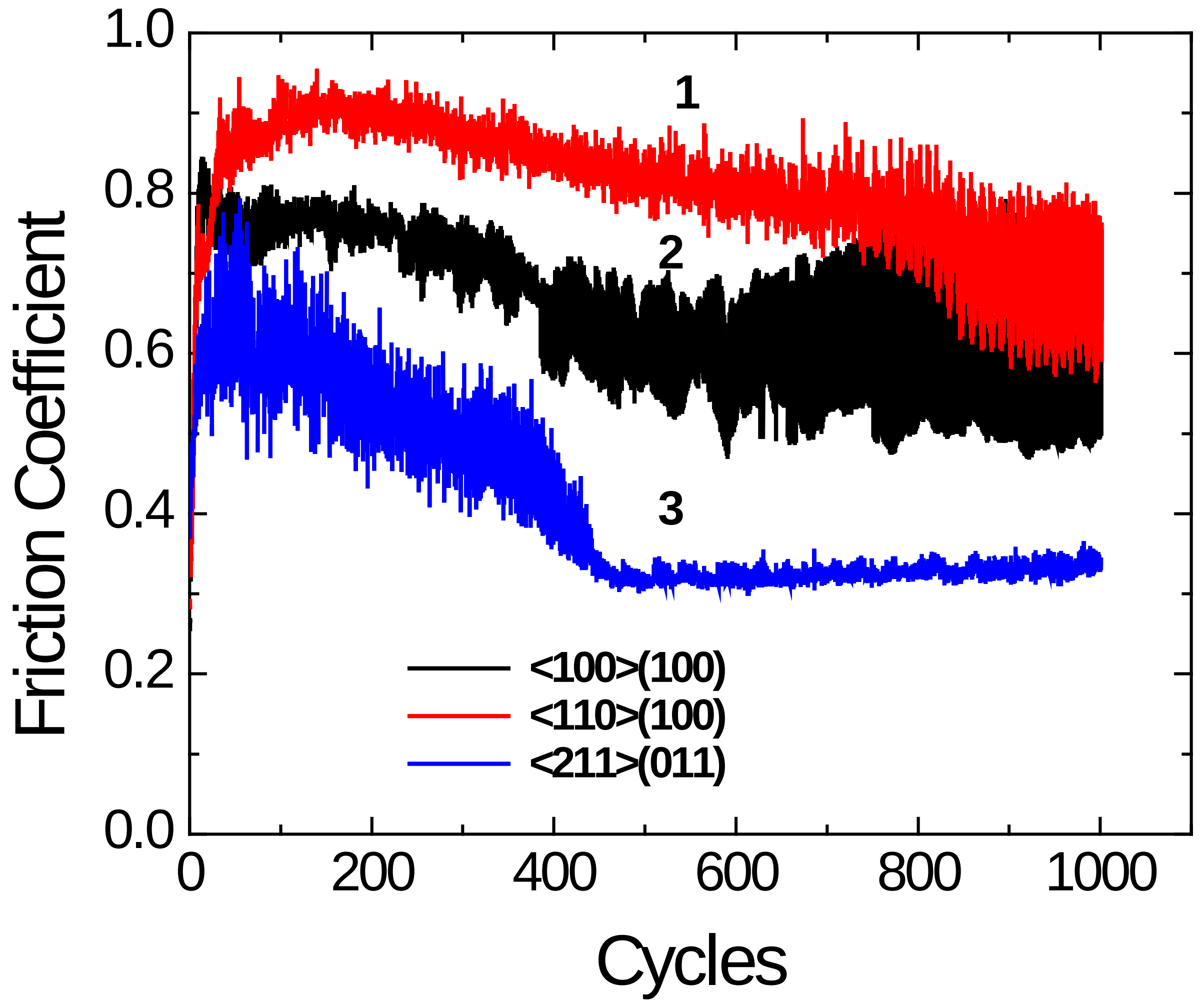


Rotary Stage for Single Crystal Alignment



Environmental chamber

Friction is dependent on crystallographic orientations



Normal load: 100 mN
Counterface: 1/8” Si_3N_4 Ball

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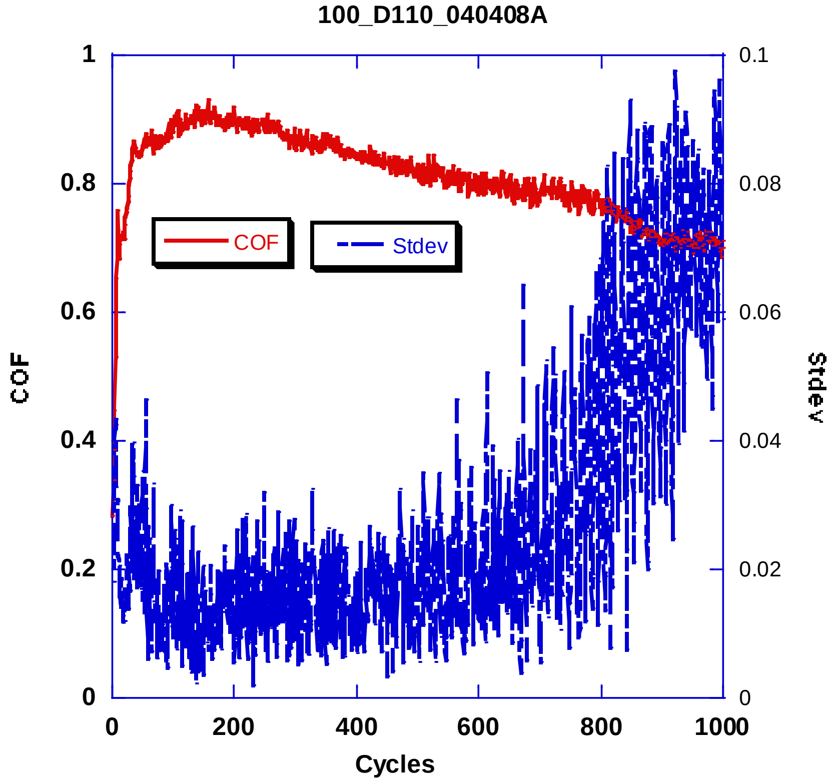
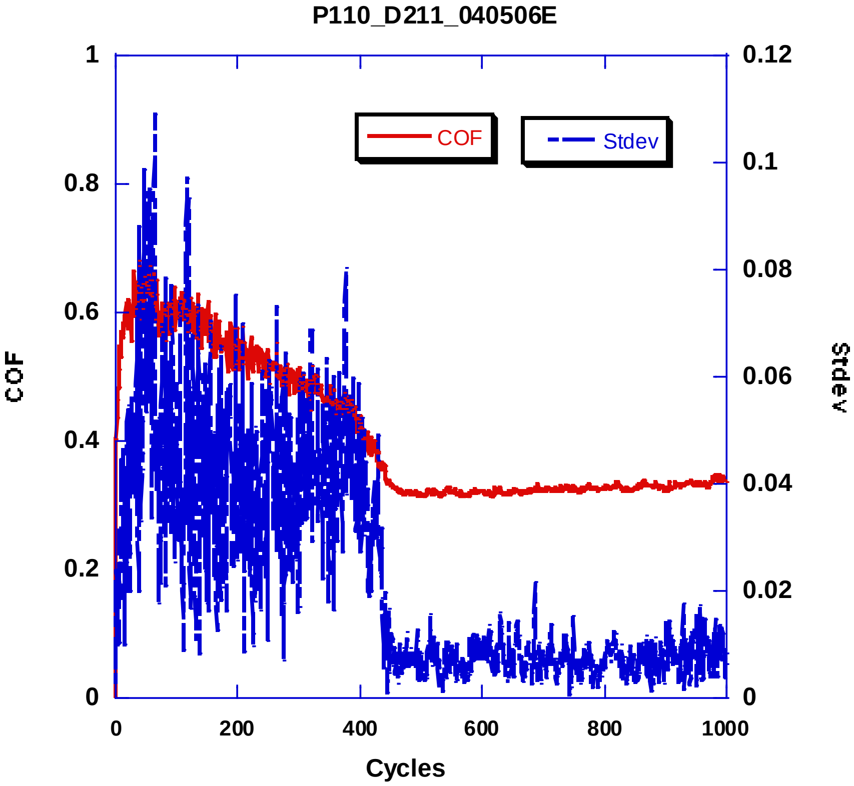
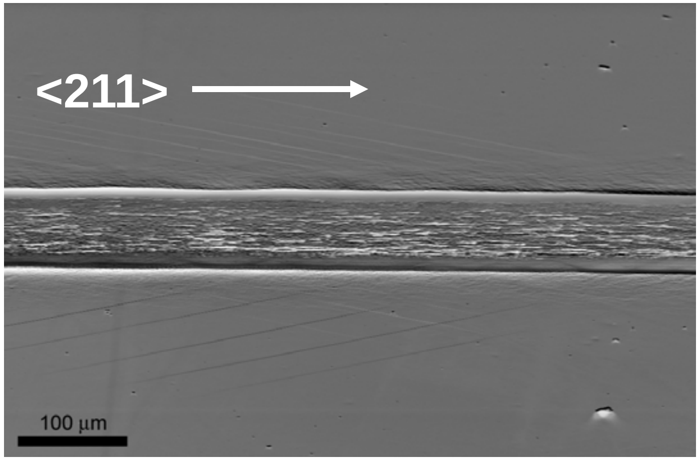
Friction data on two crystallographic directions

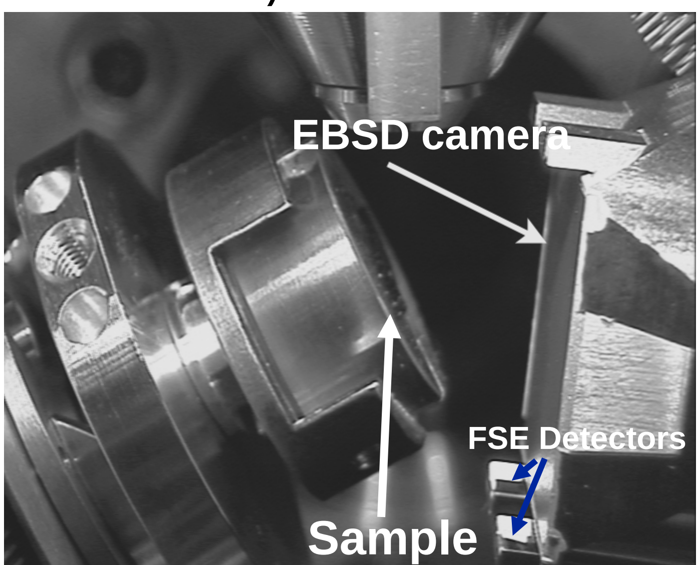


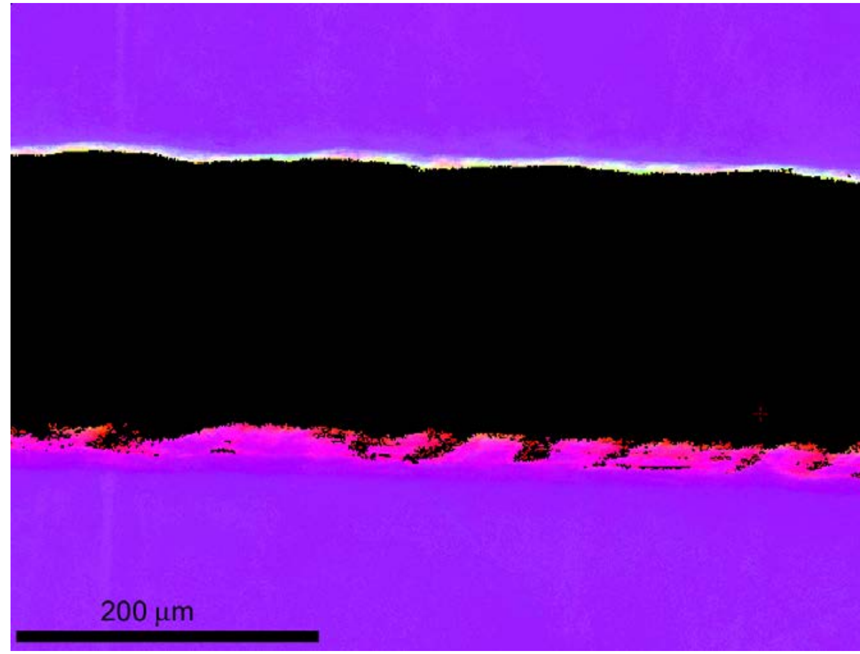


SEM imaging (FSE) and EBSD of wear scars in plan-view

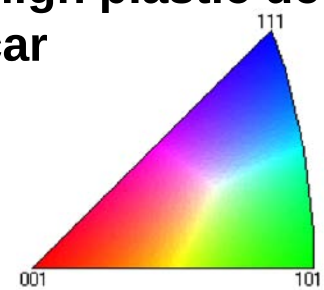


SEM image of forward scattered electrons (FSE). Note visibility of {111} slip traces. (Image not corrected for 70º tilt.)





EBSD IPF map with respect to the sliding direction. Note dark region due to high plastic deformation in wear scar



Larger tilts produce higher quality EBSD patterns

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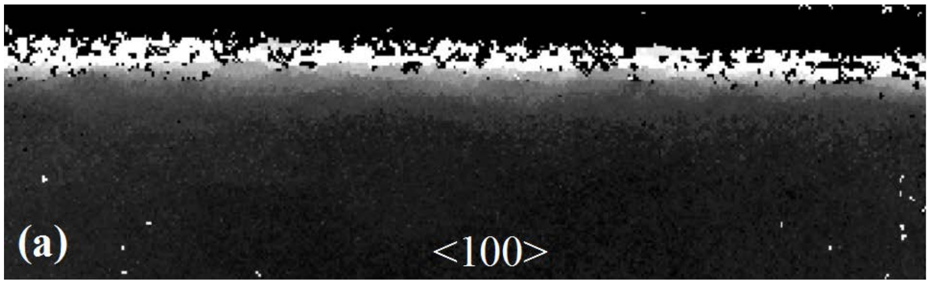
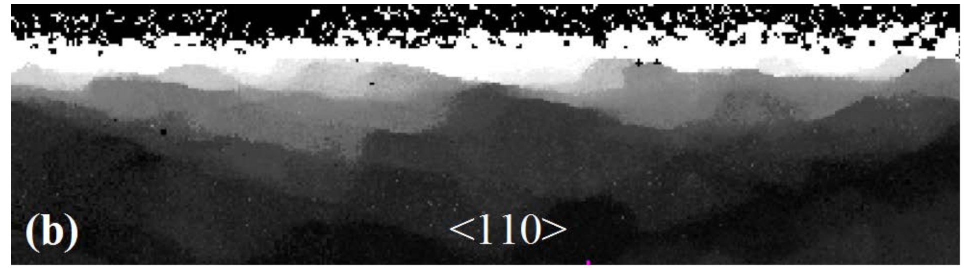
Depth of deformation is related to crystallography

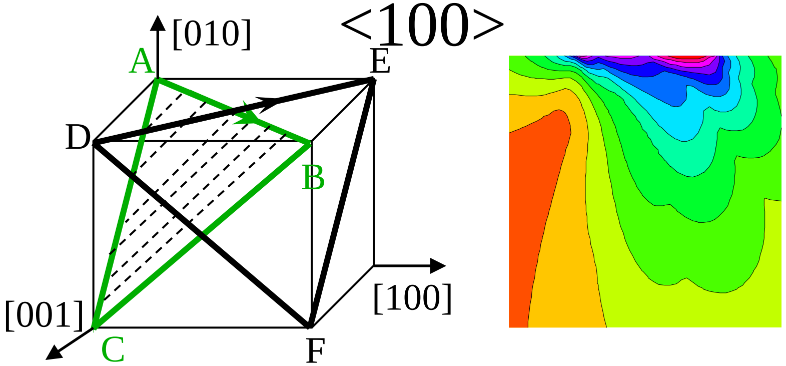




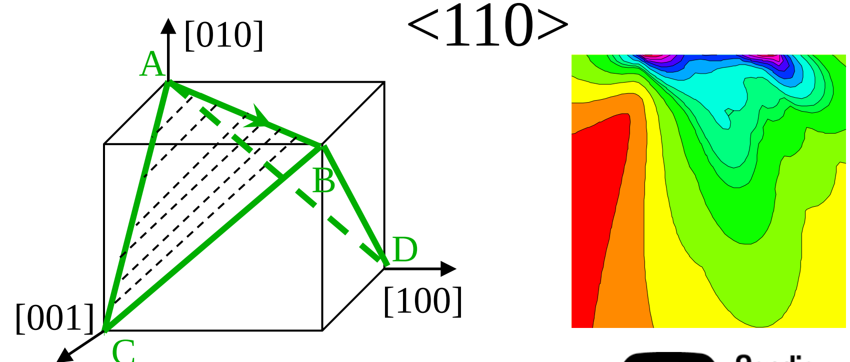
Maps showing the orientation changes relative to undeformed regions on (100) crystal surface. Brighter color represents larger orientation change. The magnitude of orientation change was about 6º total in for the friction track in the <100> direction and about 13 º for the track in <110> direction.

Slip system orientations show intersecting slip systems for <100> wear (ABC plane in AB direction, and DEF in DE), but not for <110> (ABC in AB and ABD in AB), suggesting more hardening for <100>. Color maps of resolved shear stress from analyses of plastic deformation show the strong asymmetry induced by sliding (as opposed to static) contact.

<100>



<110>



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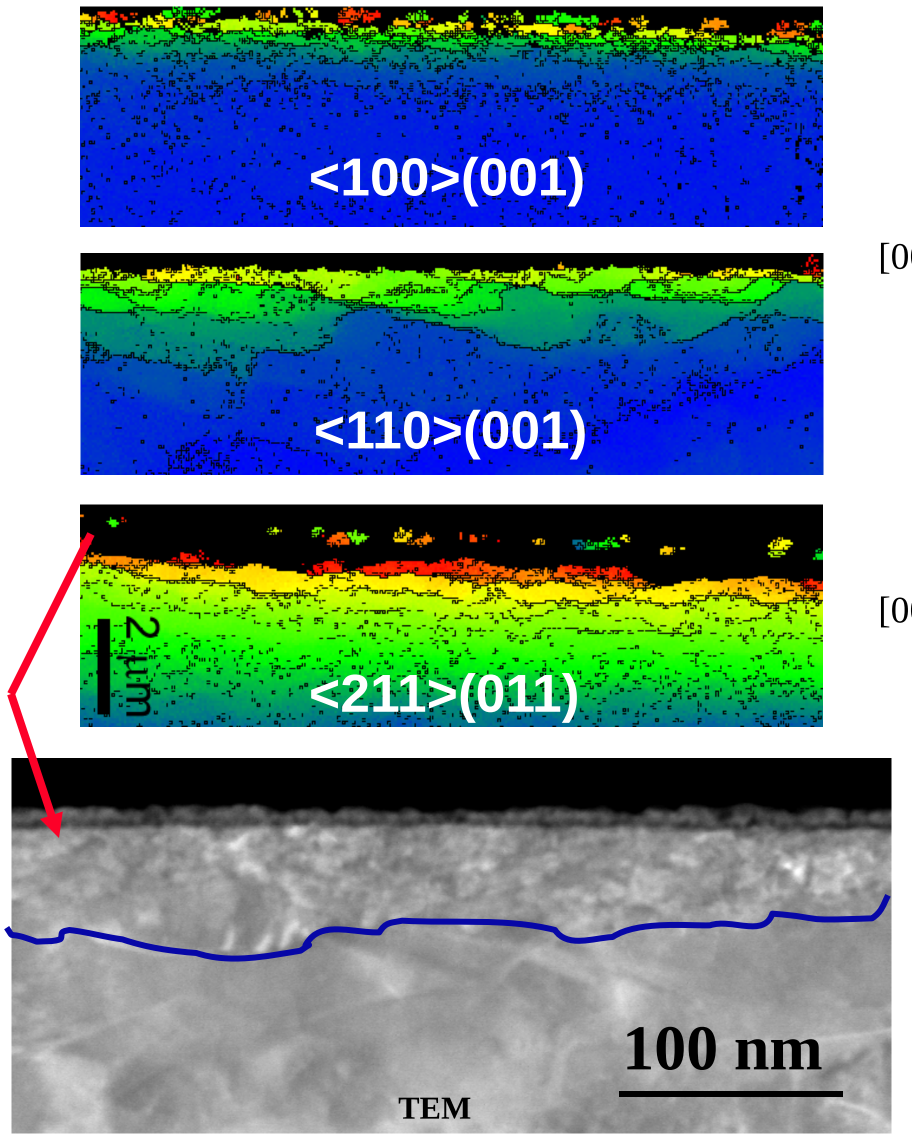
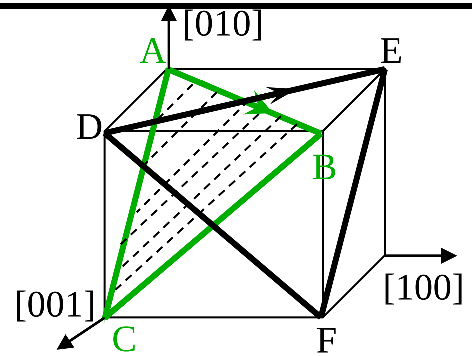
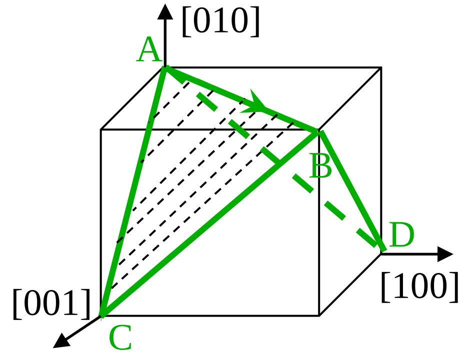
Depth of deformation is related to crystallography

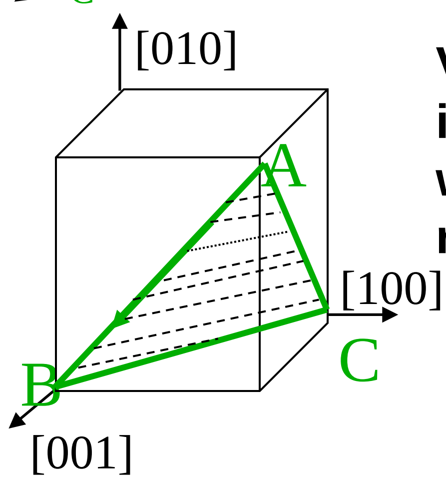




Strong dislocation interactions- high work hardening



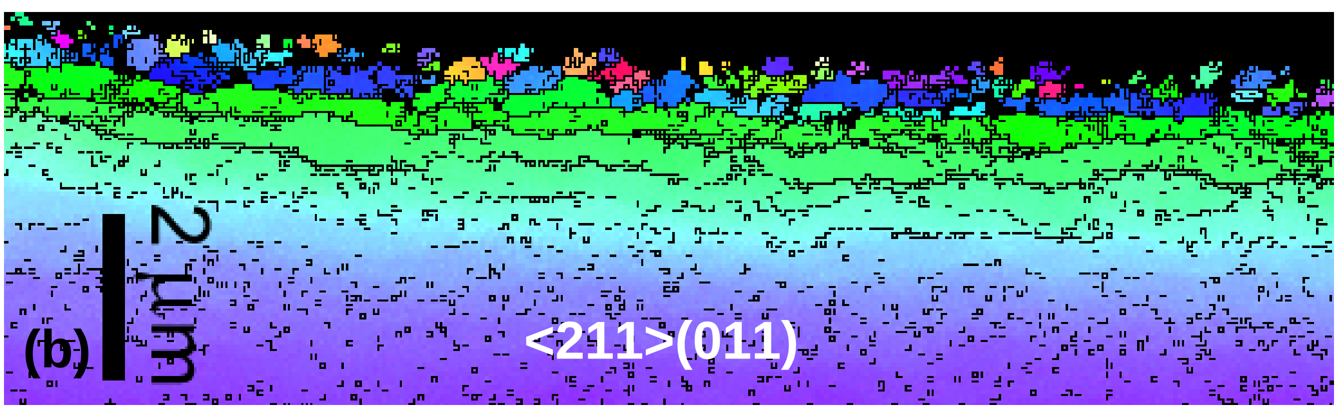
Weak dislocation interactions- low work hardening

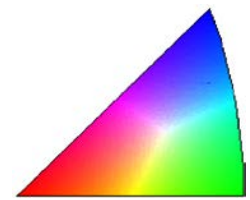


Very weak dislocation interactions- low work hardening – rapid recrystallization

EBSD: Crystallographic maps

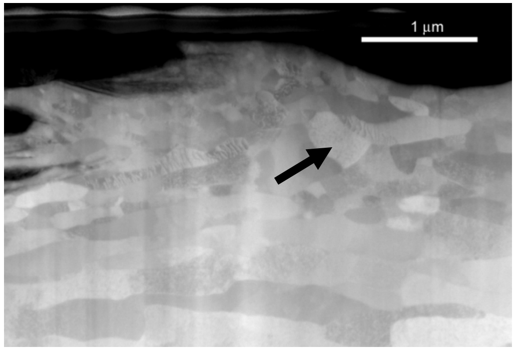
(a)





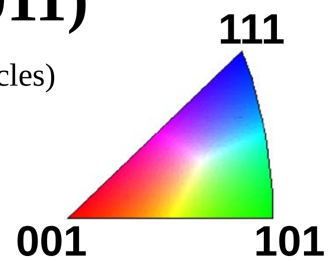
(c)

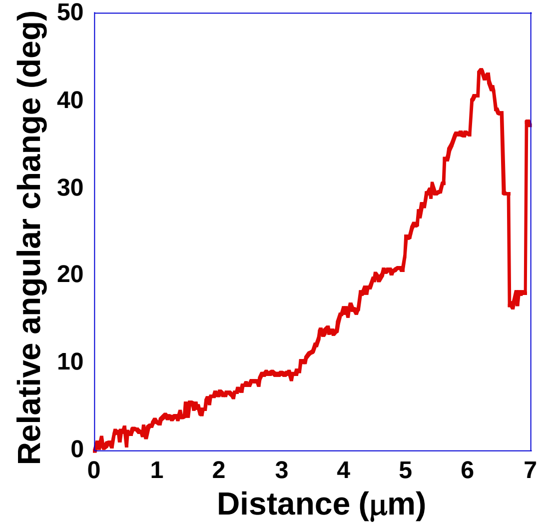
Relationship between crystallography and sliding-induced deformation

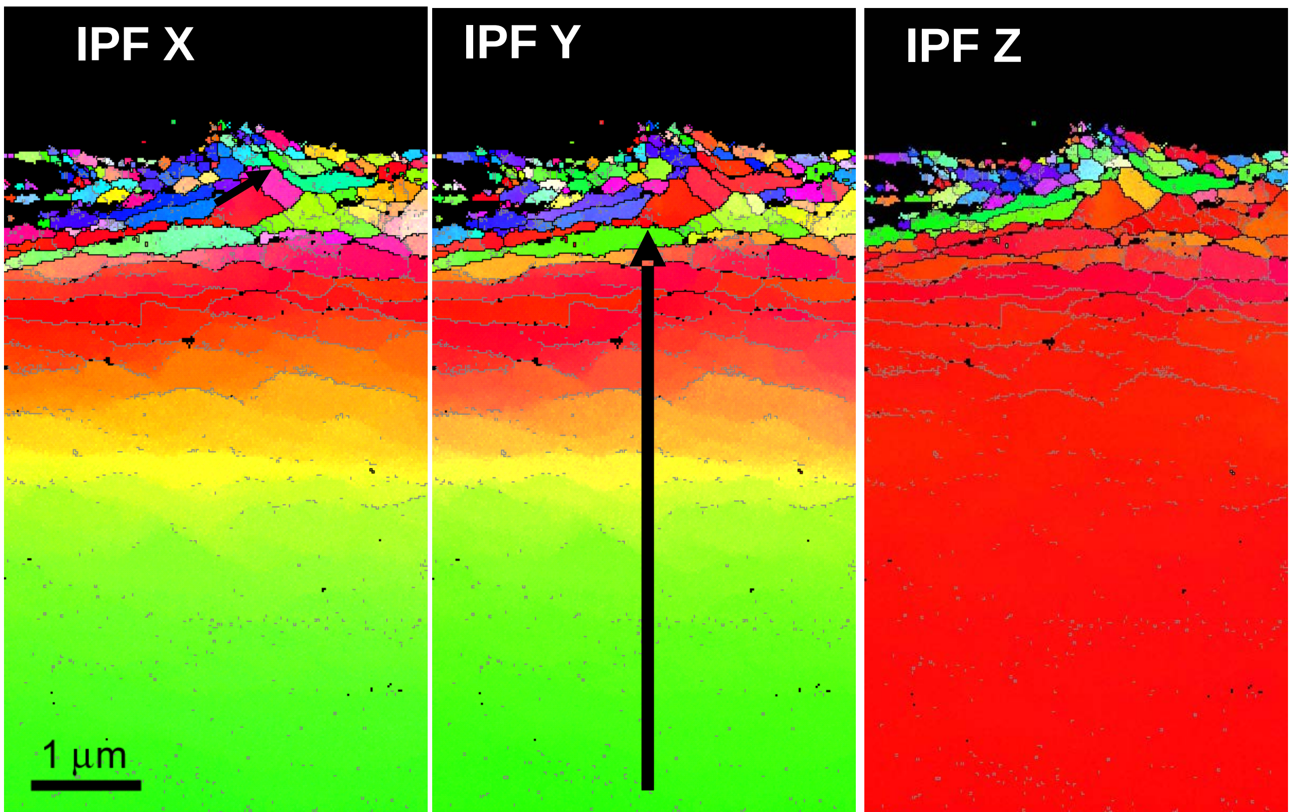


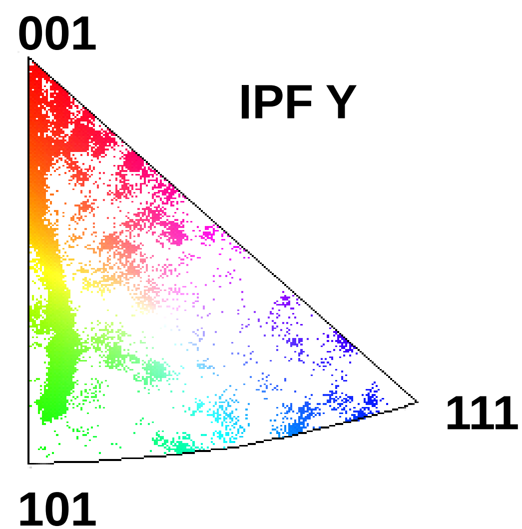
<110> on (011)

(100 grams for 200 Cycles)









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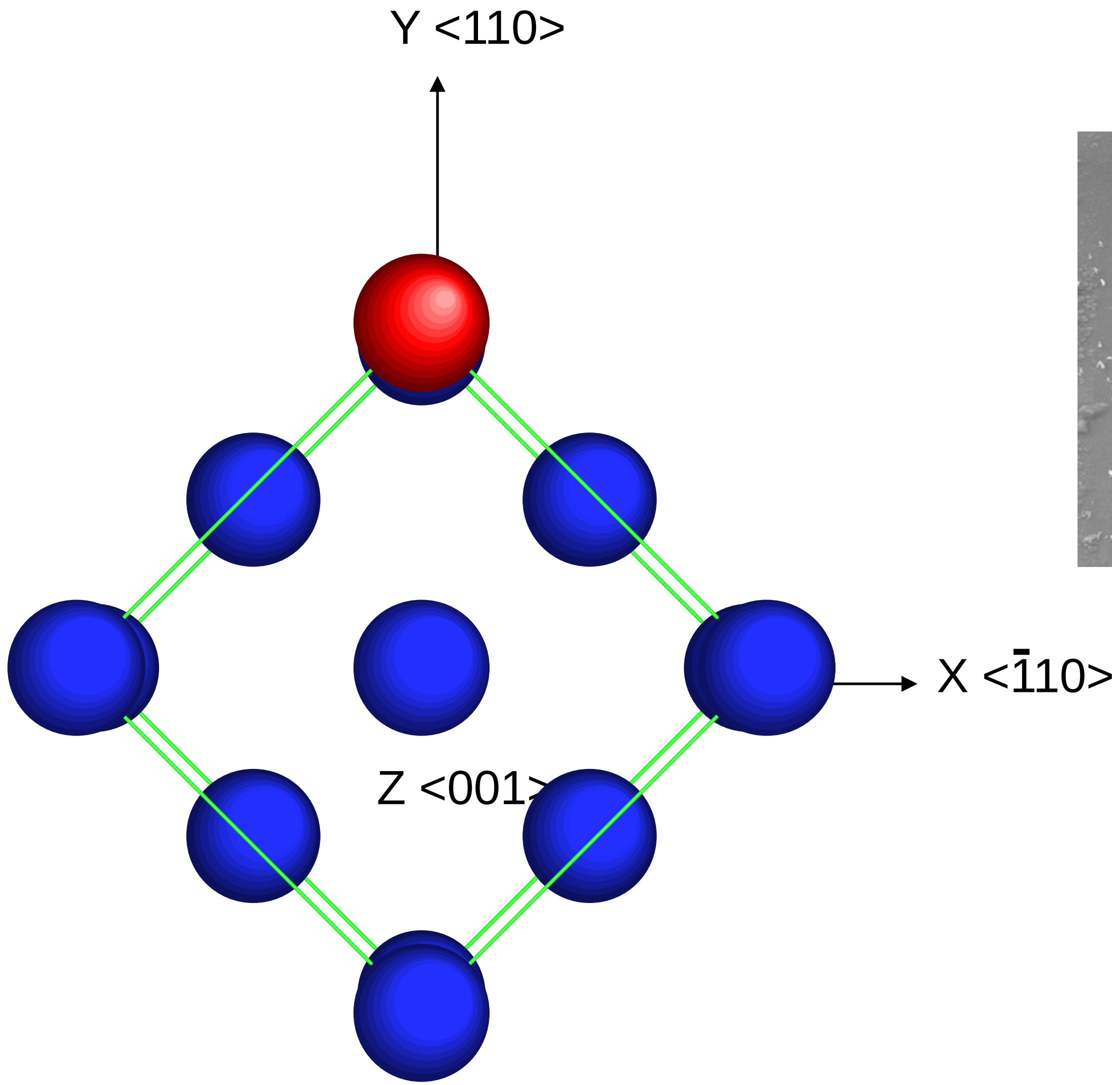
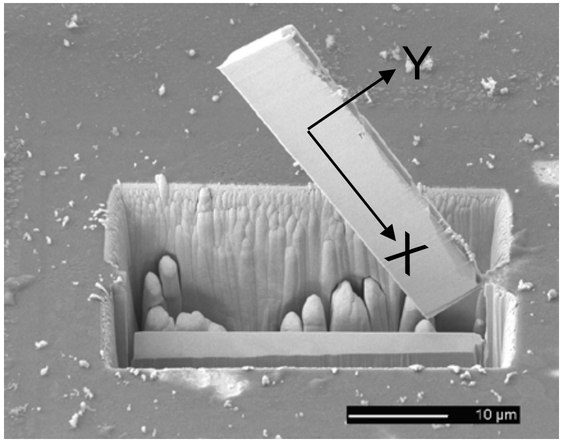
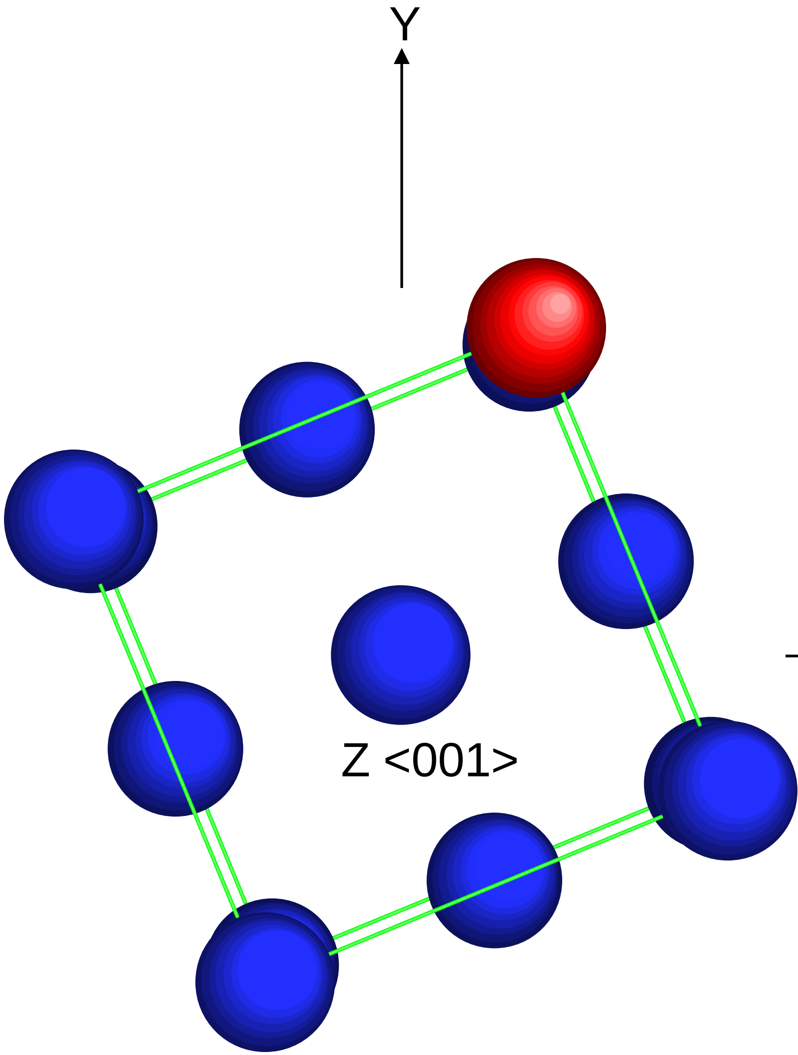
Schematic illustration of grain rotation. 1

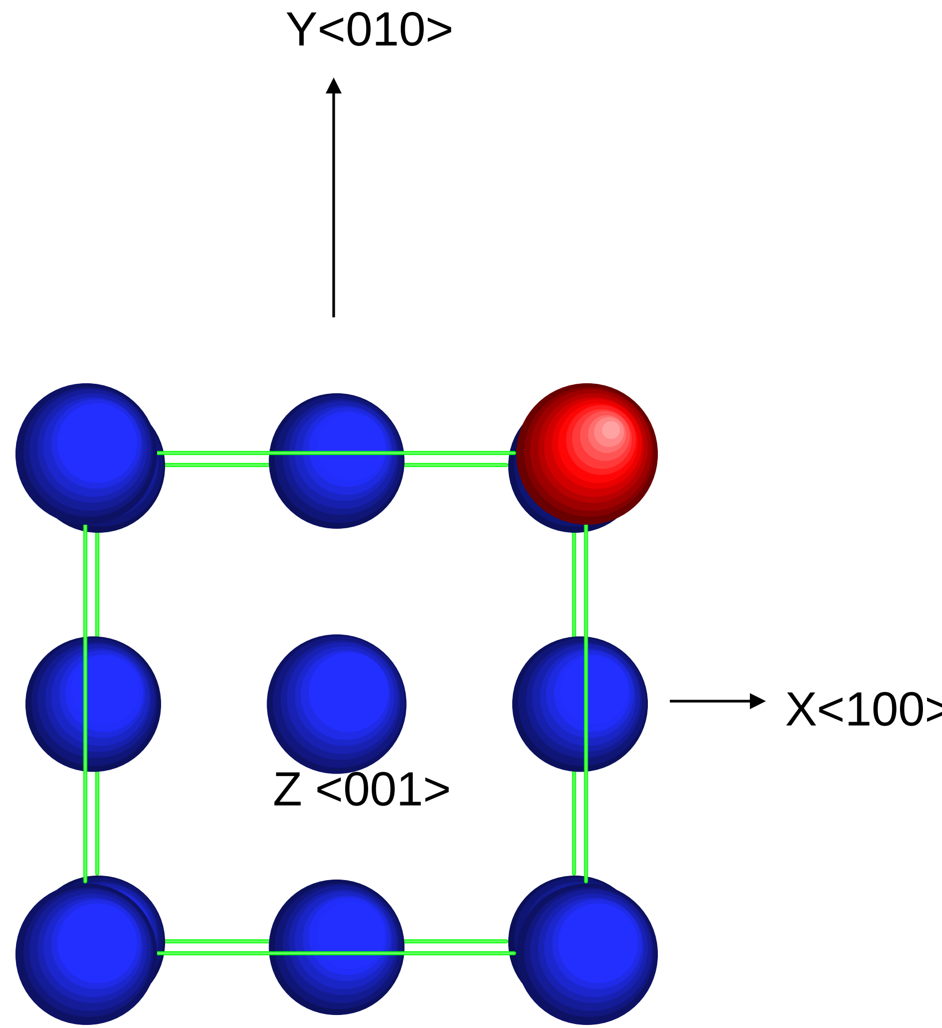




Schematic illustration of grain rotation. 2



22.5 degree rotation



45 degree rotation

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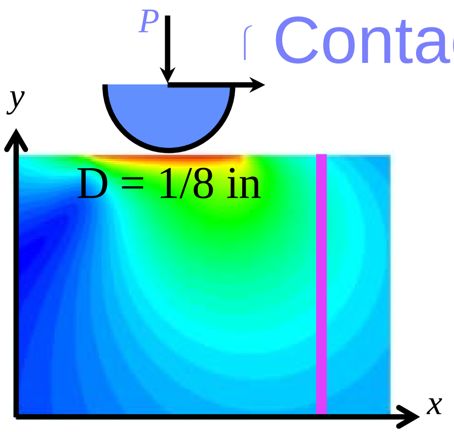
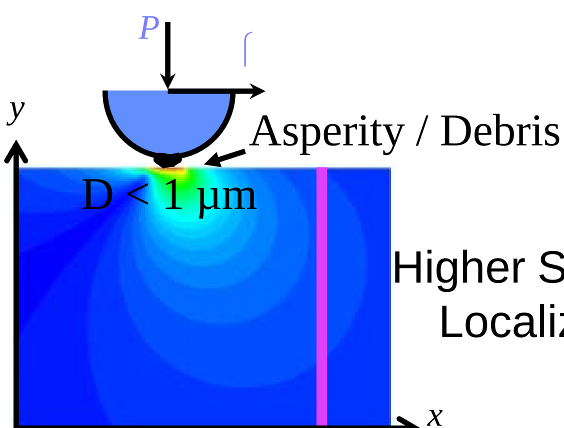
Contact Mechanics and Crystal Plasticity

Frictional Elastic Contact Stresses[3]



- or -



Higher Stress, Localized

Mechanical State

Material Properties

Deformation Model[1,2]

$$\tau_{rss} = \frac{1}{2}\boldsymbol{\sigma} : (\mathbf{d} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{d})$$

$$\dot{\gamma} = \dot{\gamma}_o \left(\frac{\tau_{rss}}{\tau_{crss}} \right)^m$$

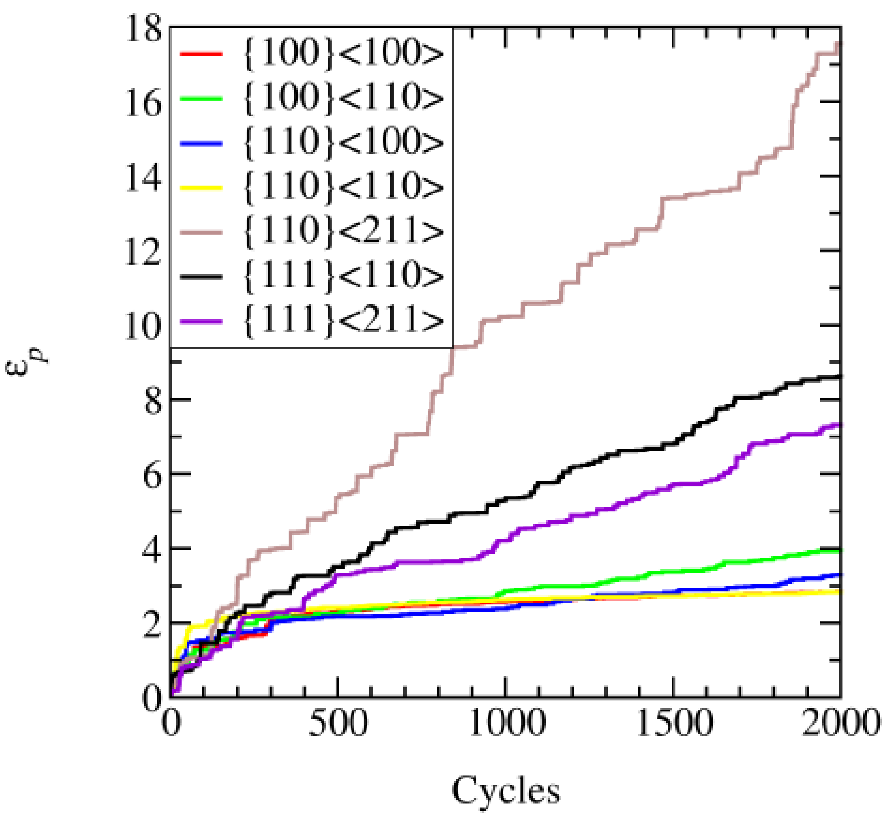
$$\dot{\mathbf{D}}_p = \frac{\dot{\gamma}}{2} (\mathbf{d} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{d})$$

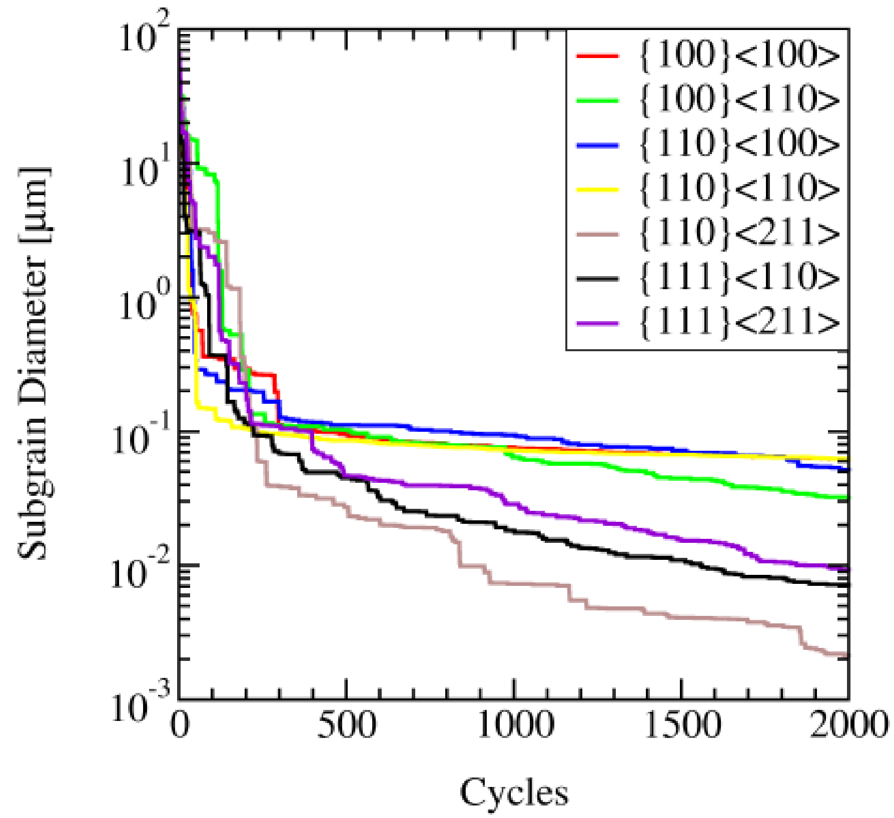
$$\Delta\varepsilon_p = \Delta t \sqrt{\frac{2}{3} (\dot{\mathbf{D}}_p : \dot{\mathbf{D}}_p)}$$

$$\tau_{crss} = \tau_o + A\left[1 - \exp\left(-\frac{n}{A}\varepsilon_p\right)\right]$$

1. R.J. Asaro and J.R. Rice, "Strain Localization in Ductile Single Crystals," *J. Mech. Phys. Solids* **25** (1977) 309-38.
2. E. Voce, "The Relationship Between Stress and Strain for Homogeneous Deformation," *J. Inst. Metals* **74** (1948) 53
3. D.A. Hills, D. Nowell, and A. Sackfield, *Mechanics of Elastic Contacts*, Oxford 1993.

Plastic Strain and Subgrain Formation (Model)





P = 1N μ = 0.8

$$d_{GNB} \approx \frac{0.724}{\varepsilon^{1.12}} \ \mu\text{m (for Al)}^{1}$$

1. A. Godfrey and D.A. Hughes, “Scaling of the Spacing of Deformation Induced Dislocation Boundaries,” *Acta Mater.* **48** (2000) 1897.

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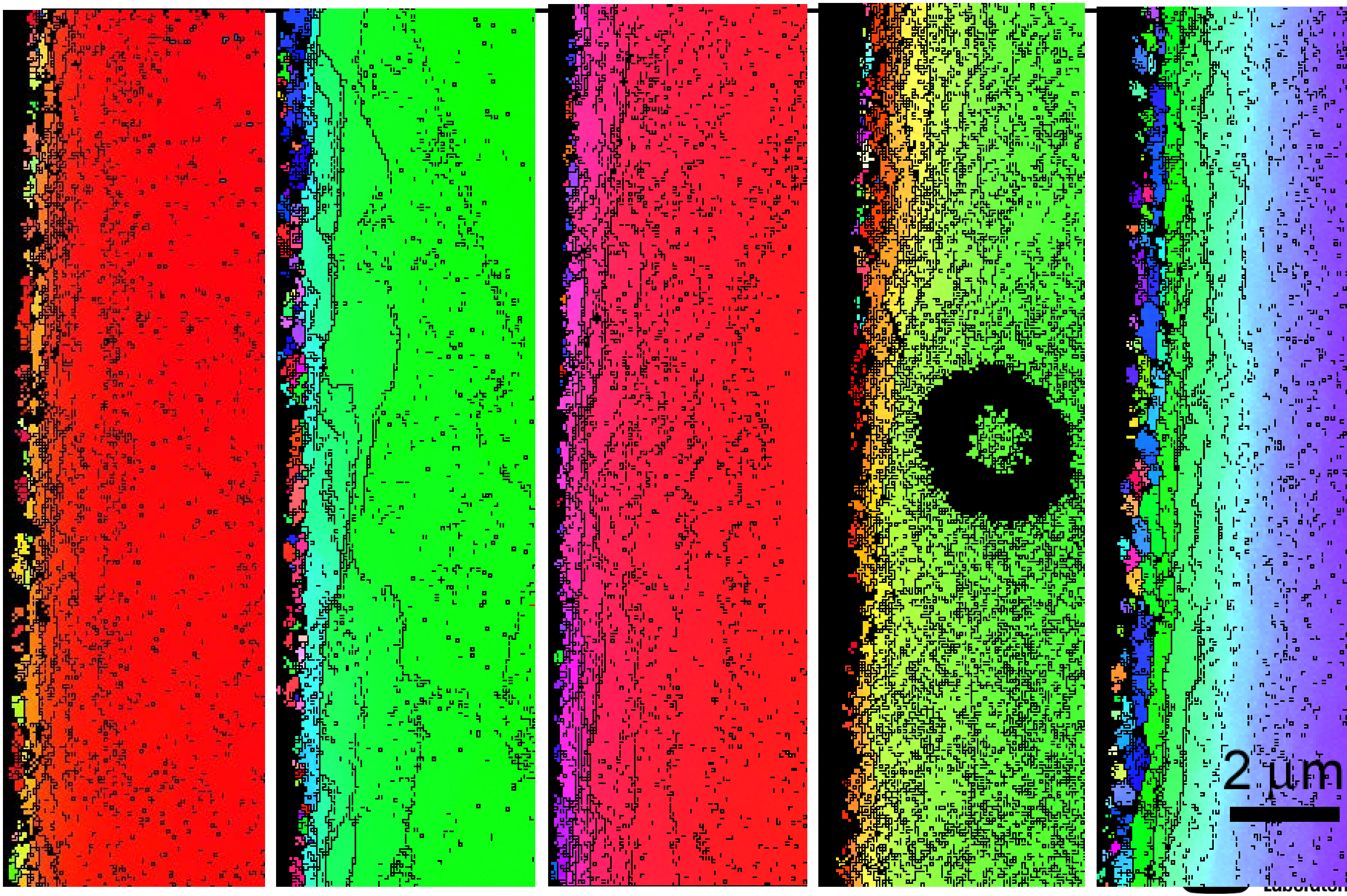
Model: Qualitative Validation

Increasing Plastic Strain ↓

Experimental Measurements	Model
{100}<100>	{110}<110>
{110}<100>	{100}<100>
{110}<110>	{110}<100>
{100}<110>	{100}<110>
{111}<110>	{111}<211>
{111}<211>	{111}<110>
{110}<211>	{110}<211>

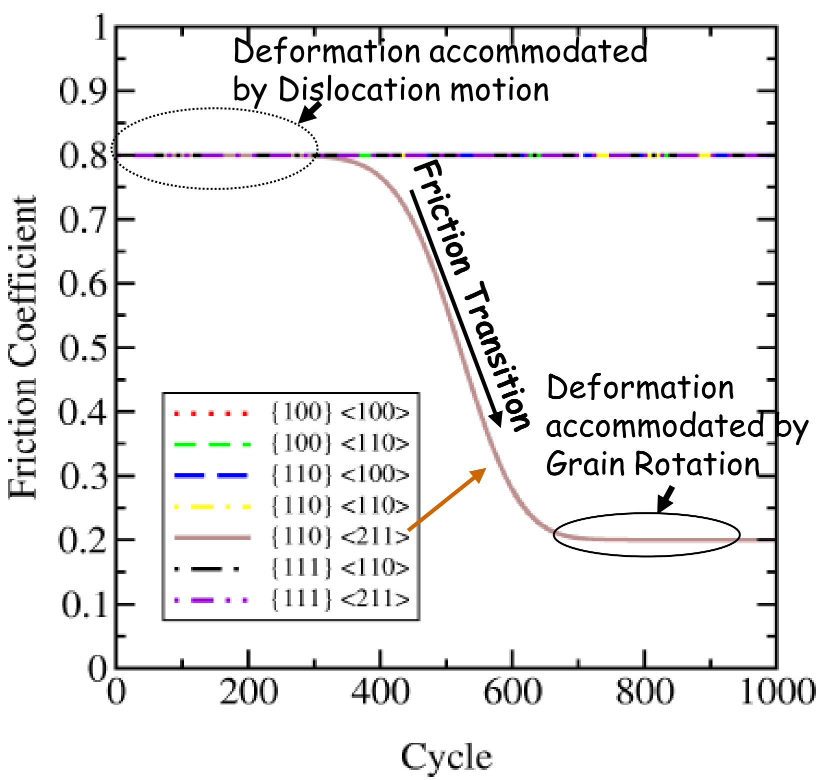
EBSD inverse pole figure maps of wear scars

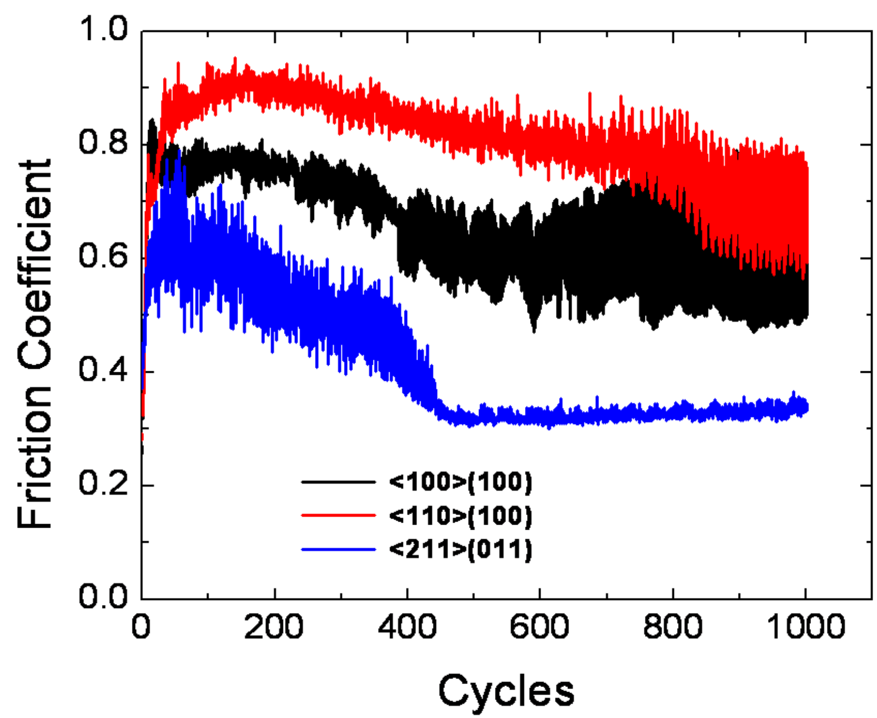
<100>(001) **<110>(001)** **<100>(011)** **<110>(011)** **<211>(011)**



Grain Boundary Sliding Model

$$\dot{\varepsilon}_{gb} = \tau \frac{160\Omega}{kT} \frac{1}{d^2}\left(1 + \frac{\pi\delta}{d}\frac{D_{\mathrm{gb}}}{D_{\mathrm{bk}}}\right) D_{\mathrm{bk}} \longrightarrow \mu = 0.2 + 0.6\exp\left[-2\left(\frac{\varepsilon_{gb}}{\varepsilon_p}\right)^2\right]$$





1. R. Raj and M.F. Ashby, "Grain Boundary Sliding and Diffusional Creep," *Met. Trans.* **2** (1971) 1113.

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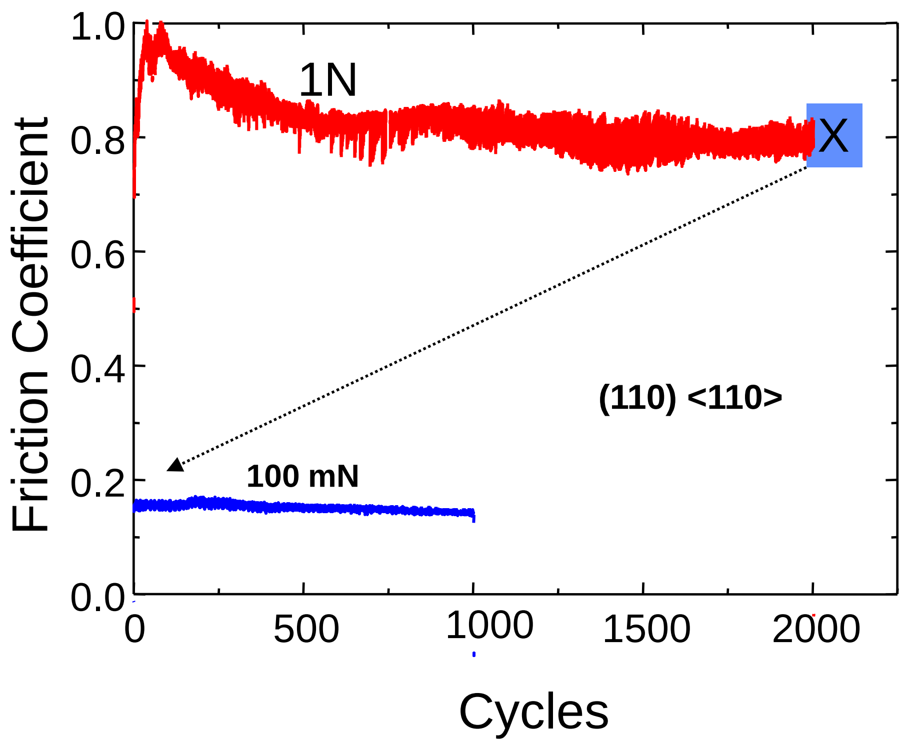
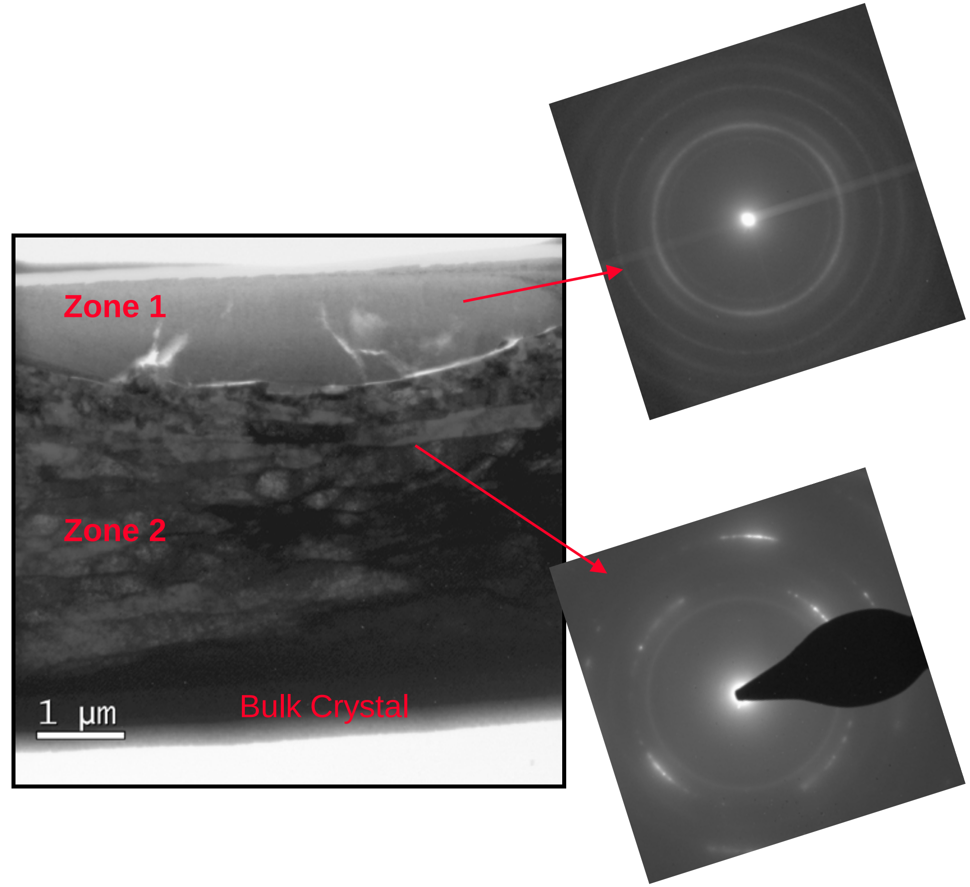
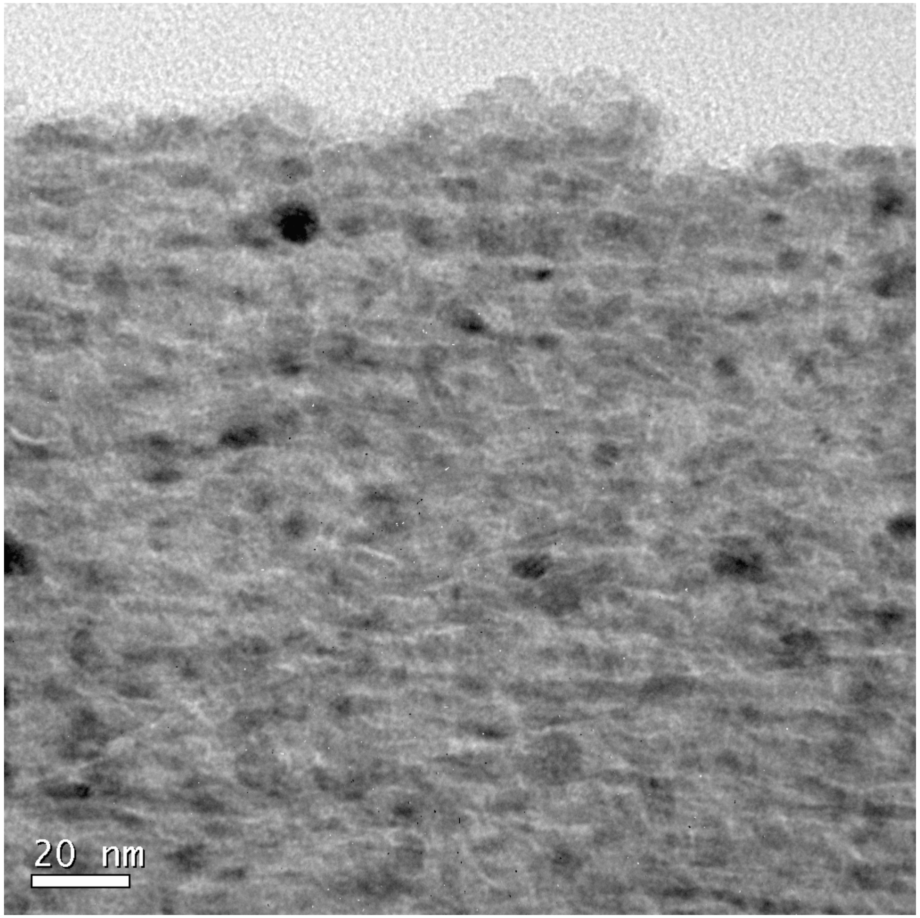
Higher normal loads (1N) produced unique substructures with interesting friction behavior

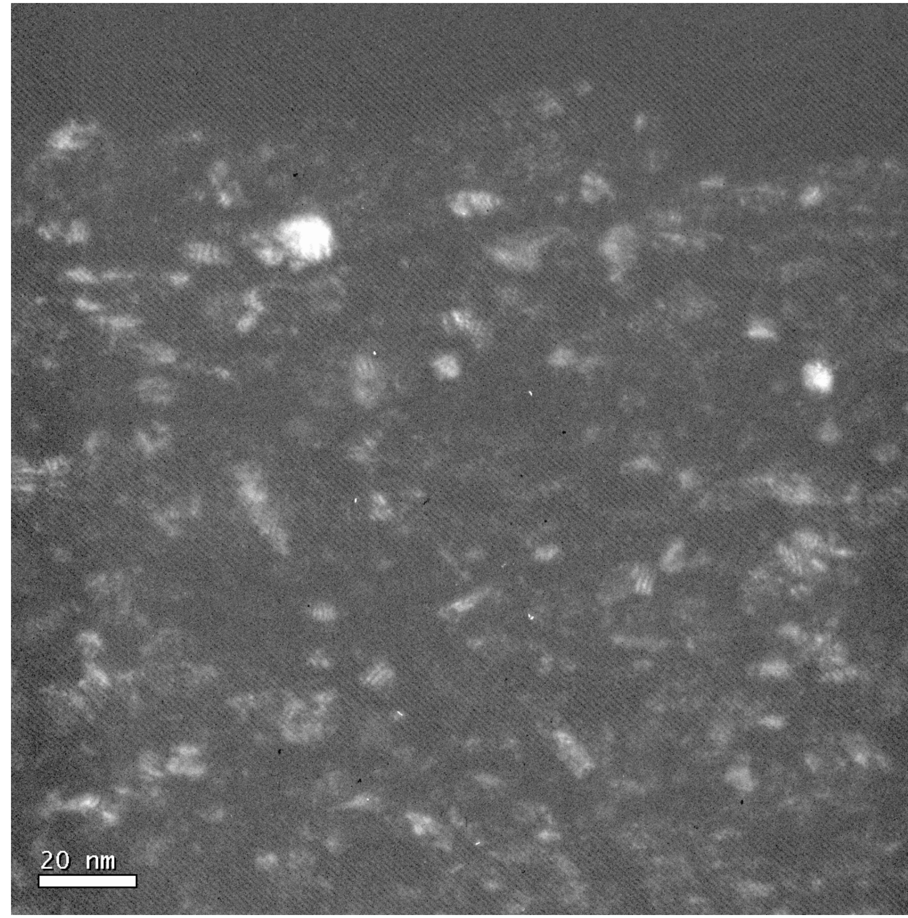




High resolution images of Zone 1



Bright-field TEM image



Dark-field TEM image

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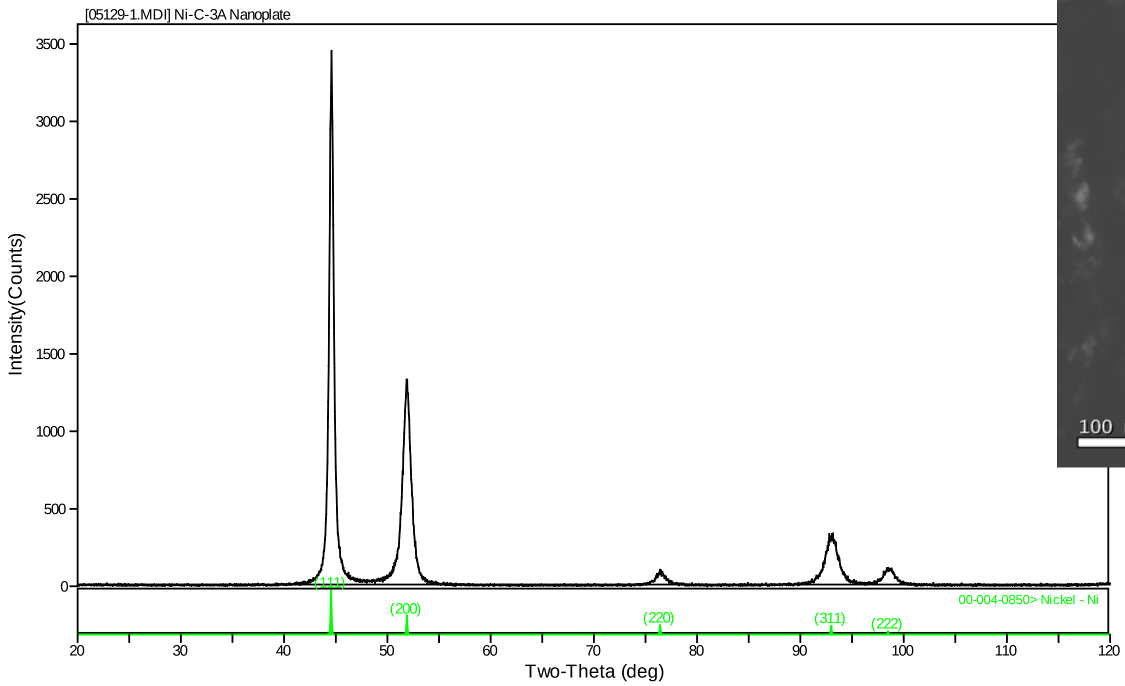
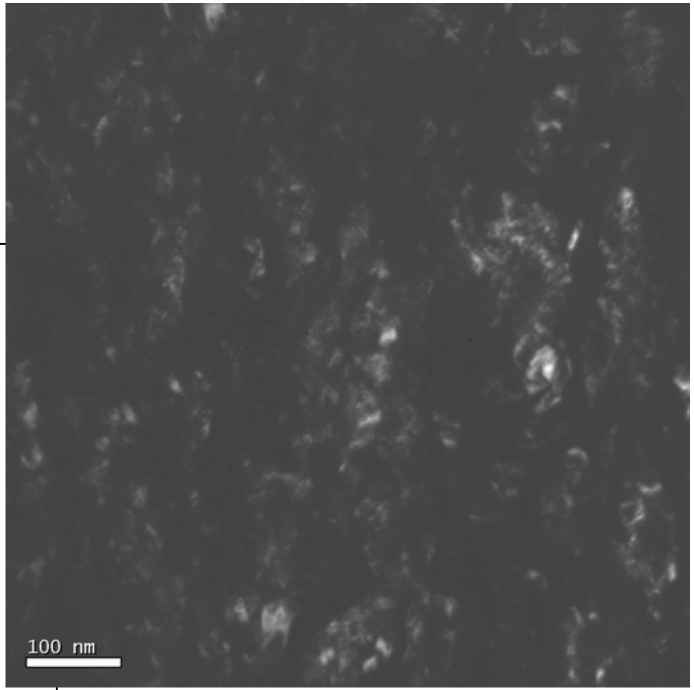
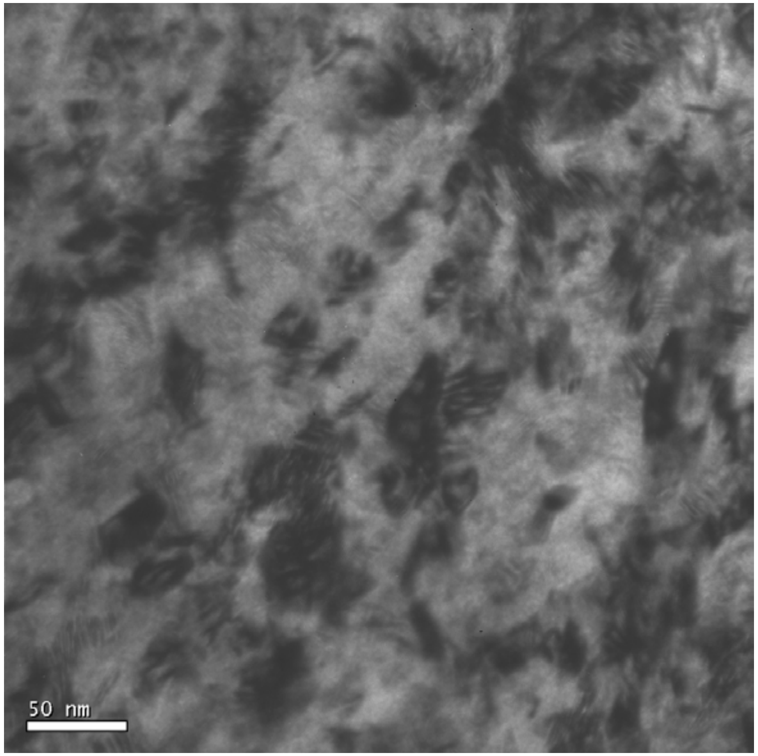
Part II:
Application to Nanocrystalline Thin Films



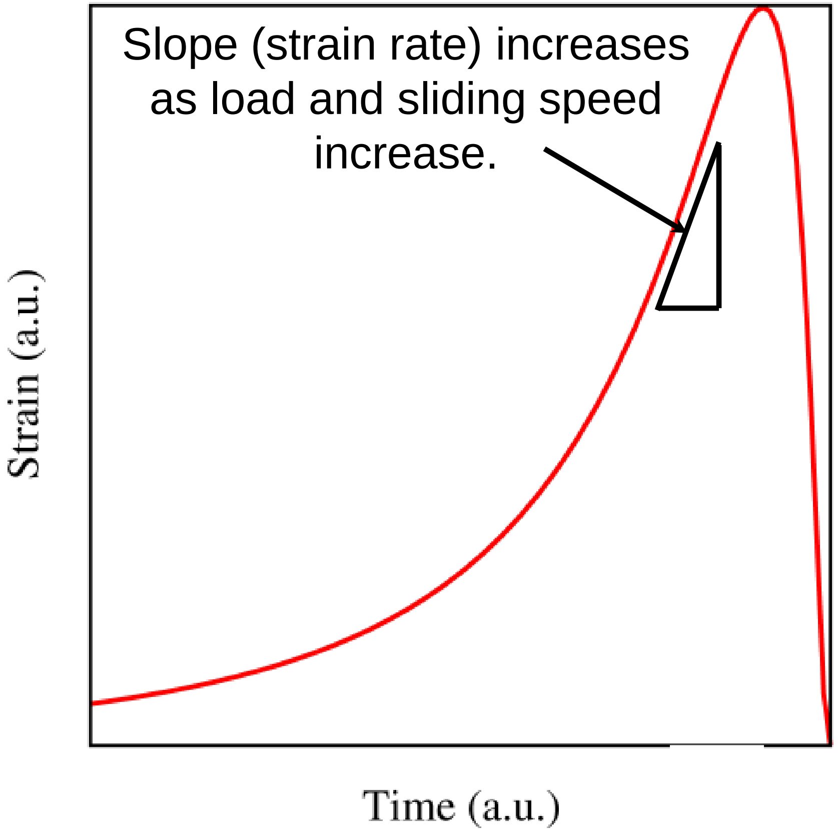


Nanocrystalline Ni Film: Strain Rate Effects

Load and sliding speed dictate subsurface strain rate

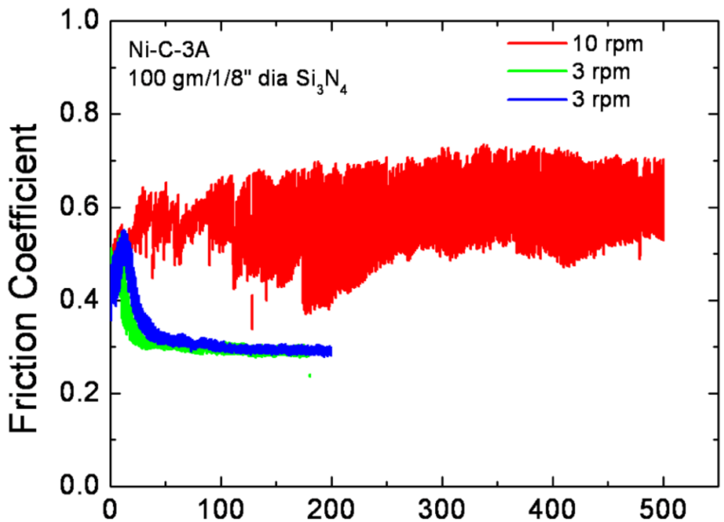


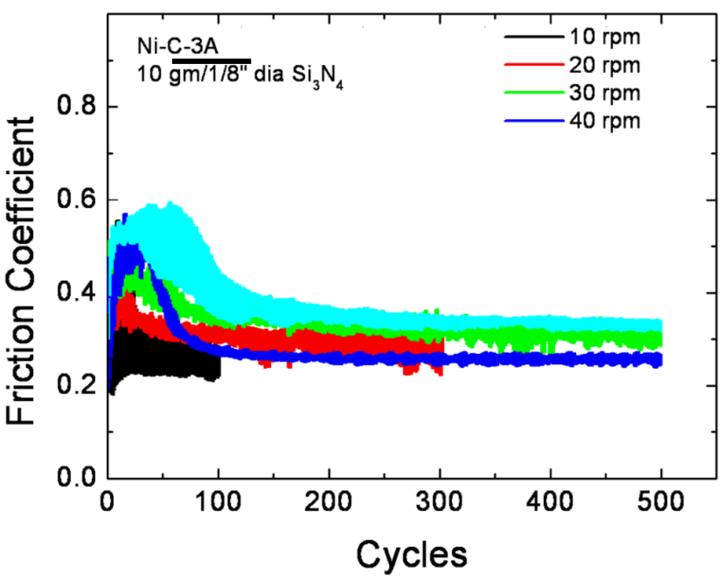
Bright-field TEM image



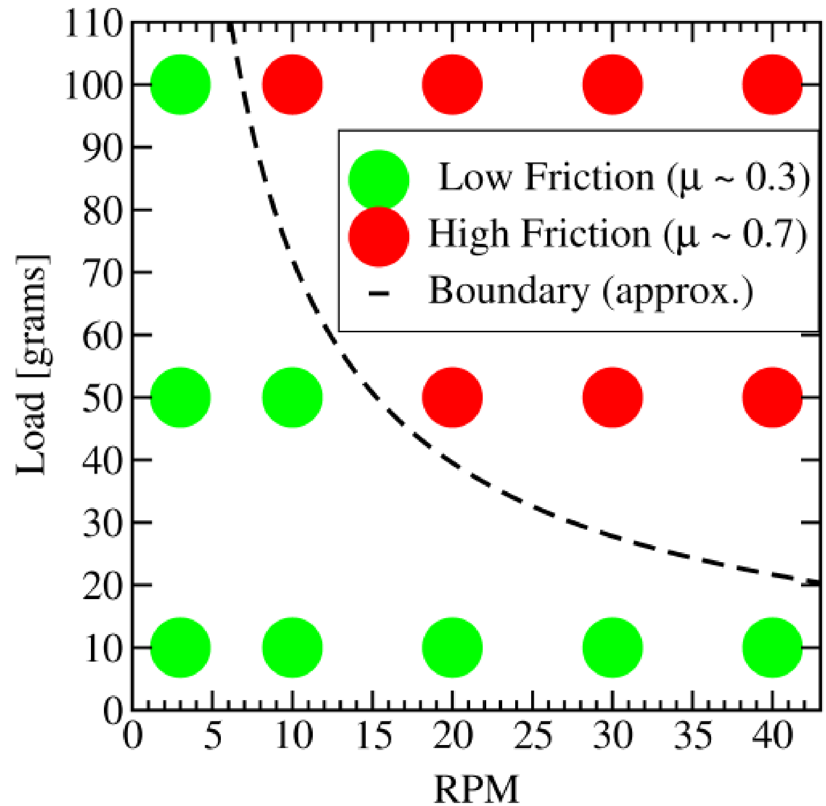
Schematic of the strain history experienced by the material below the worn surface.

Nanocrystalline Ni: Strain Rate Effects on Friction





Transition to low friction shows a clear dependence on strain rate.



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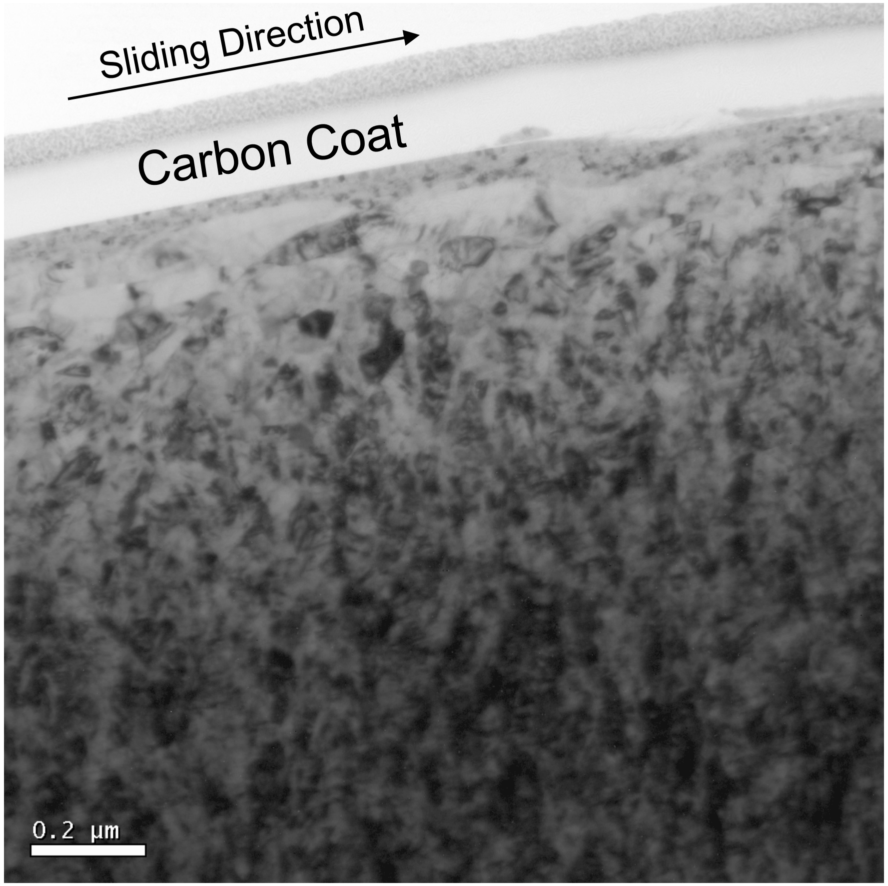
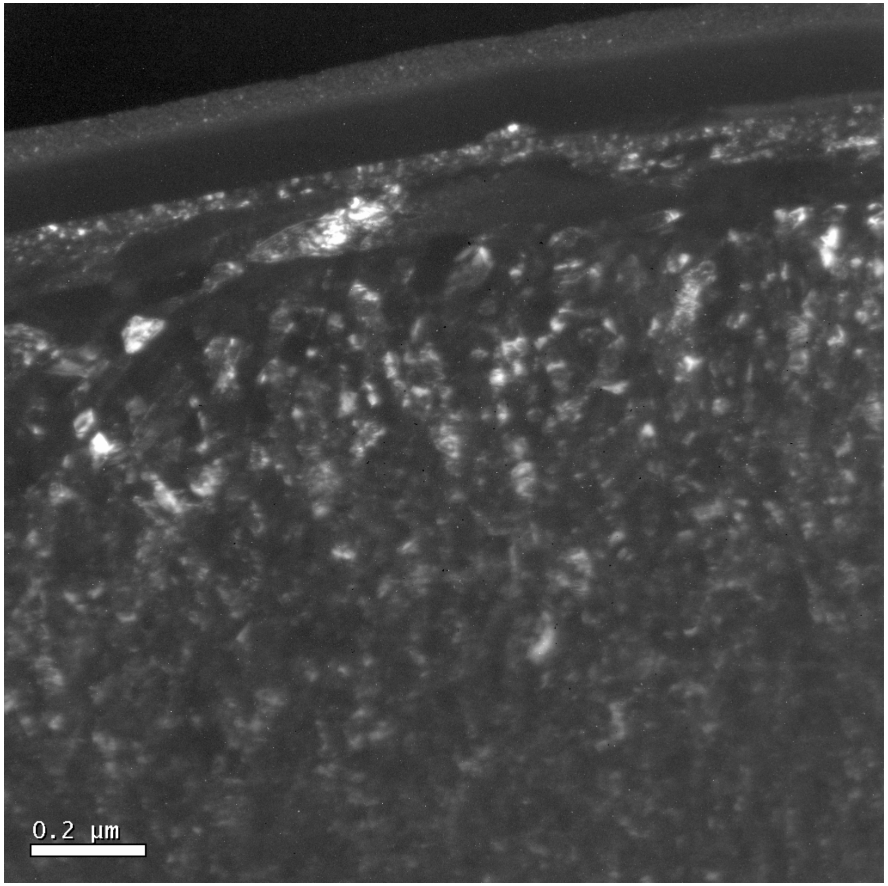
Transmission Electron Microscopy of Subsurfaces: Low Friction Case





BF-TEM

DF-TEM

Sample preparation: FIB microscopy with low KeV cleaning

Low magnification micrographs

Ni-3C-A1 #1 051202D Track 19, 10g, 20rpm, 600cycles

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Higher Magnification Micrograph

Ni-3C-A1 #1 051202D Track 19, 10g, 20rpm, 600cycles

Zone 1+

Zone 1

Ultra Nanocrystalline

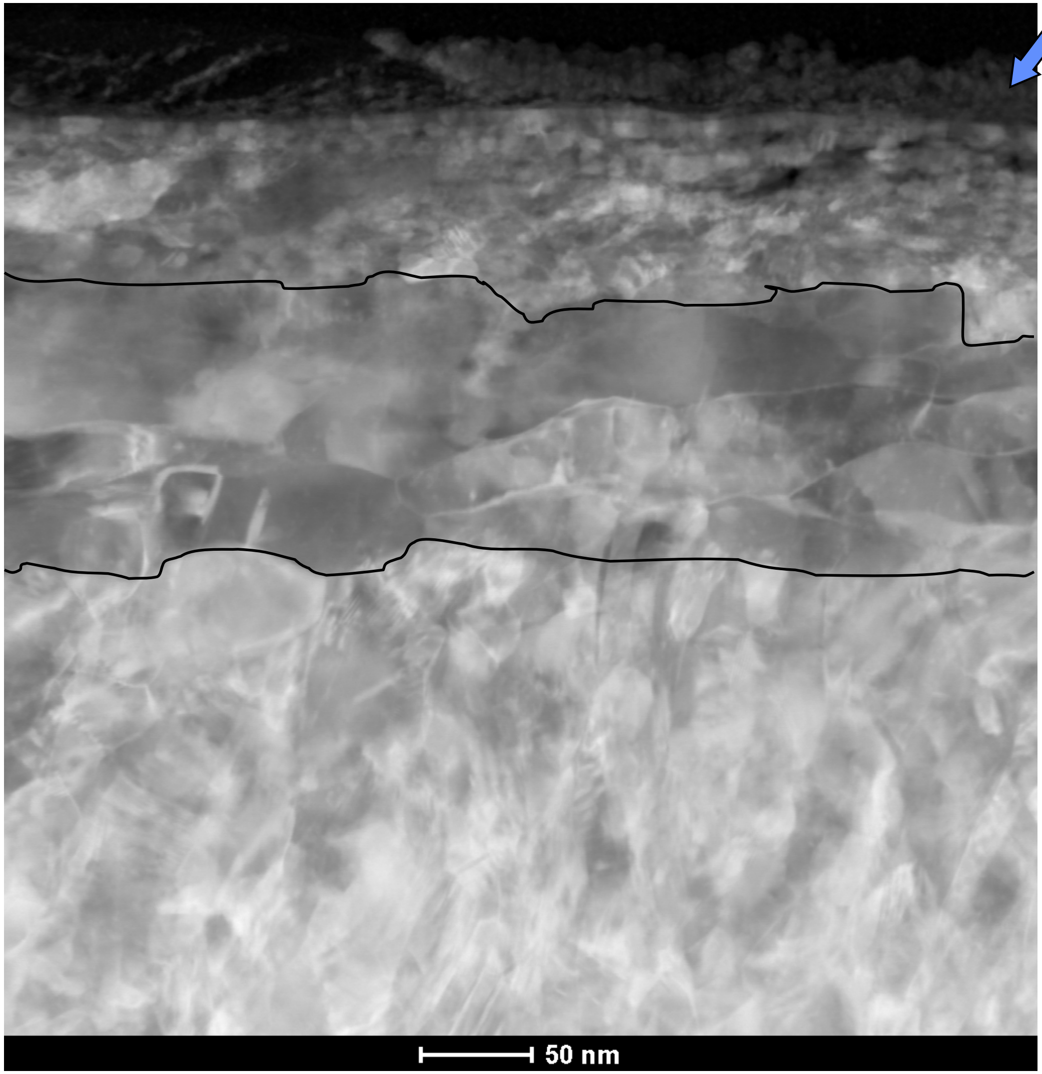
Zone 2

Grain Growth +
Texture

Zone 3

Bulk

Annular DF Image



Annular DF STEM Image

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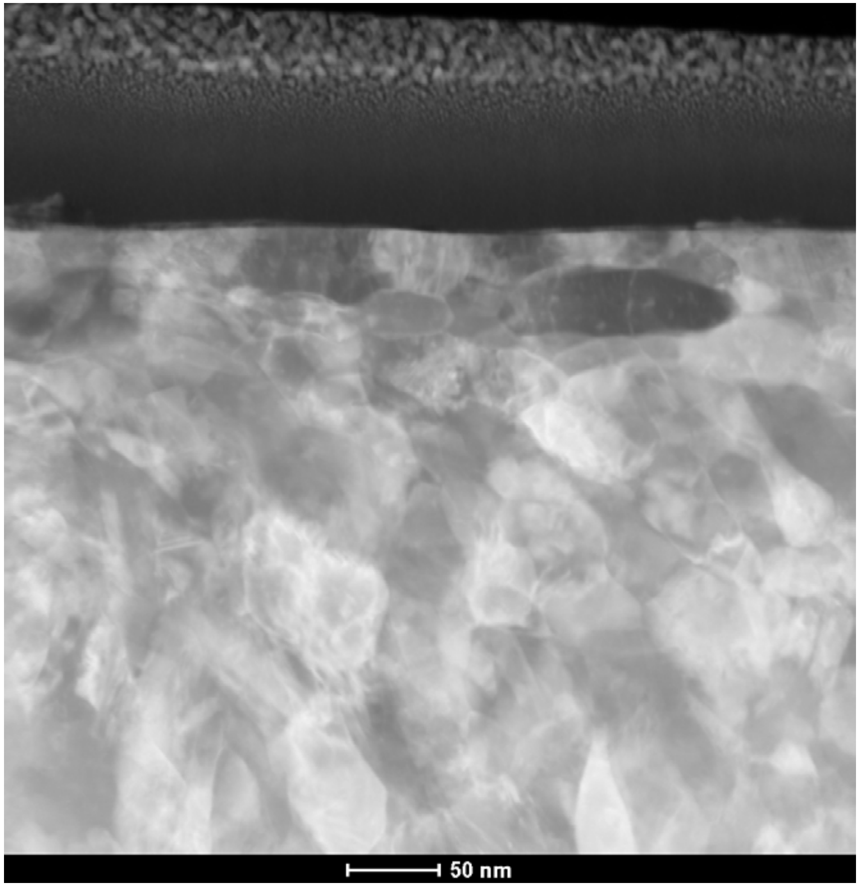
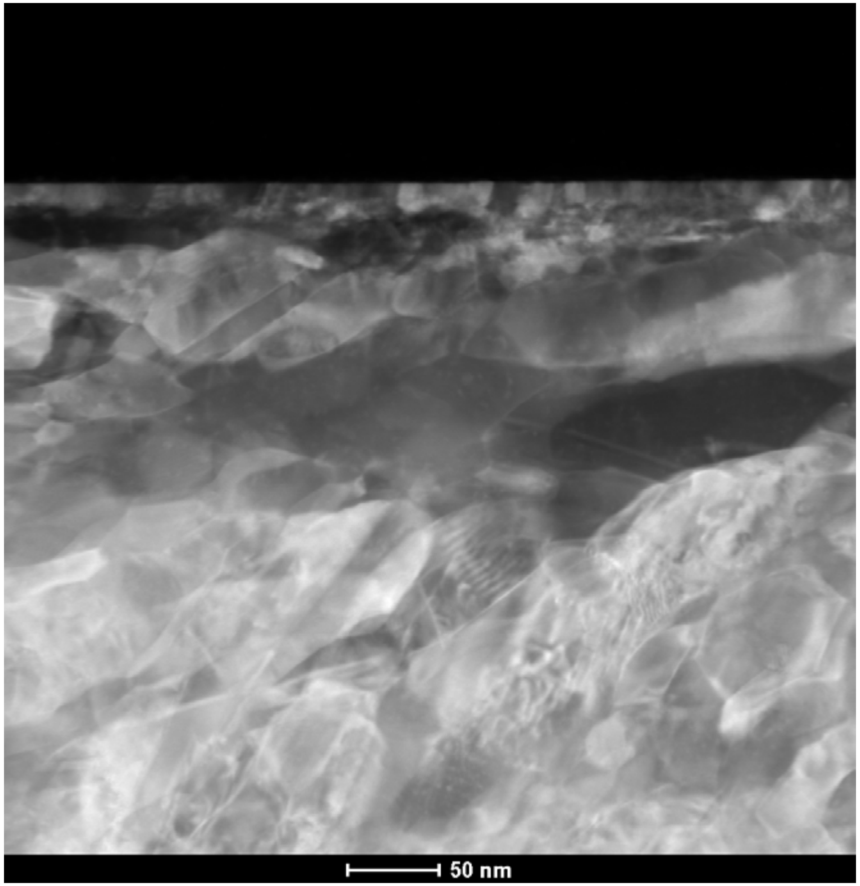
Comparison of Subsurfaces: High Friction (Red) and Low friction (Green)

20rpm

3rpm



No Zone 1



Zone 1 Present

Annular DF STEM Images

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Concluding Remarks

- Friction-induced deformation is related to crystallography
- Friction-induced deformation can generate nanostructures with unique friction characteristics
- Grain boundary sliding appears to be a viable deformation mechanism, and perhaps a route to mitigate metallic friction
- But the critical issues are: (a) friction-induced grain growth, and (b) stability of ultrananocrystalline zones.

Acknowledgements

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Rand Garfield for friction measurements

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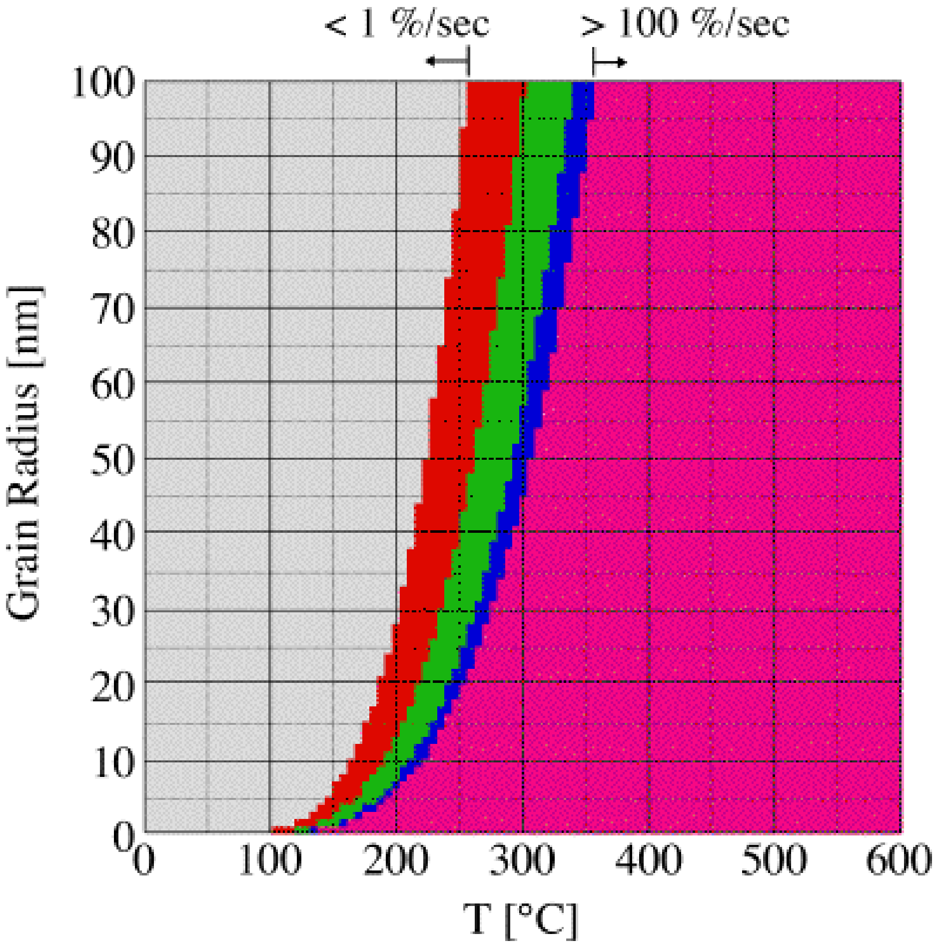
Supplementary Slides

Raj and Ashby suggest a dependence of the grain-boundary-accommodated shear on the inverse of the cube of the grain size. Thus, very small grains might be expected to slide or rotate, even at room temperature. If we postulate an exponential dependence of the friction coefficient on the ratio between grain boundary and dislocation straining, and we bound the functional form according to the experimentally observed friction limits, i.e. 0.2 and 0.6, then we qualitatively reproduce the friction behavior observed experimentally.

The material model for dislocation plasticity is based on a reduced form of continuum crystal plasticity. The stress tensor, sigma, is projected, i.e. resolved, onto each slip system. The resulting resolved shear stress, tau_rss, relative to the critical value, tau_crss, determines the rate of dislocation slip, gamma_dot. This, in turn, is projected onto the slip geometry to produce the plastic strain rate tensor. An invariant of this tensor, integrated in time, is used to calculate the plastic strain increment, and the total plastic strain is used to update the critical resovled shear stress for the next cycle.

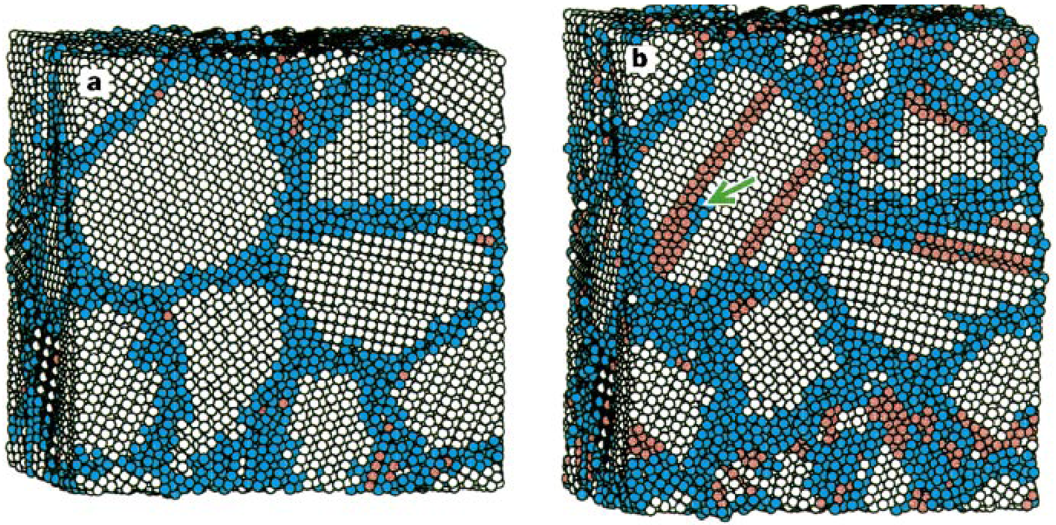
Grain Boundary Sliding and Diffusional Creep

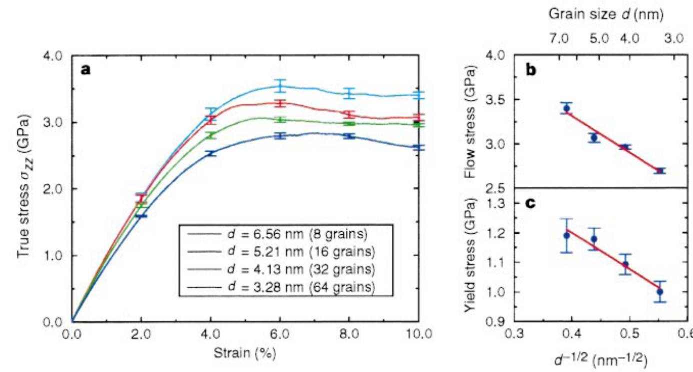


Contour Map of Shear Strain Rates From Grain Boundary Sliding[1]

$$\dot{\gamma} = \tau \frac{160\Omega}{kT} \frac{1}{d^2} \left(1 + \frac{\pi\delta}{d} \frac{D_{gb}}{D_{bk}} \right) D_{bk}$$

R. Raj and M.F. Ashby, "Grain Boundary Sliding and Diffusional Creep," *Met. Trans.* **2** (1971) 1113.

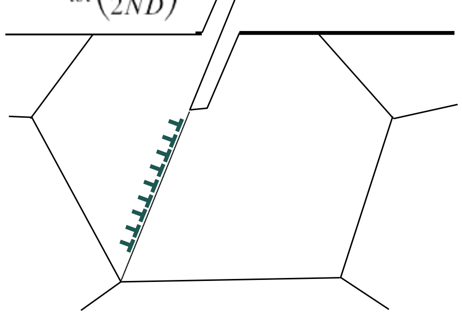

a
b


a
True stress σ_{zz} (GPa)
Strain (%)
d = 6.56 nm (8 grains)
d = 5.21 nm (16 grains)
d = 4.13 nm (32 grains)
d = 3.28 nm (64 grains)
Grain size d (nm)
b
Flow stress (GPa)
c
Yield stress (GPa)
$d^{-1/2}$ ($nm^{-1/2}$)

TWO KEY ENABLING MECHANISMS

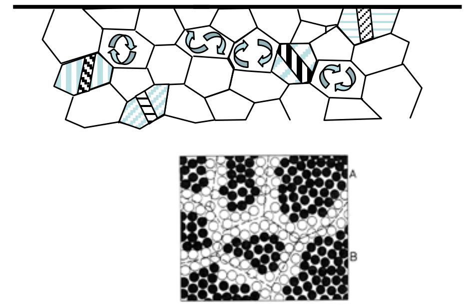
1. Suppress length-scale for dislocation-mediated plastic damage modes

$$h \approx a_{\mathrm{tot}}\left(\frac{b}{2ND}\right)$$



Conventional grain dislocation-based persistent slip band (PSB) crack initiation

$$\dot{\varepsilon} = \frac{\sigma\Omega\delta D_b}{d^3 kT}$$

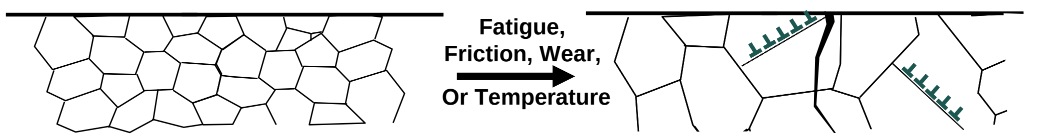


Nanocrystalline plasticity via grain rotation Or nanotwinning prevents PSB cracks.

2. Stablize beneficial nanodomains against thermal or mechanical coarsening

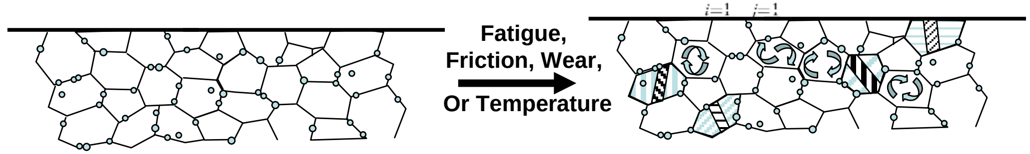
$$\frac{d\rho}{dt} = \frac{\mu_{BB}\gamma_{BB}}{2\langle R_B\rangle^2}\left\{\mathbf{M\Gamma}\left(a + (a-2)\frac{1}{\rho}\right) - \frac{\rho}{4}\right\}$$

(a) Unstable:



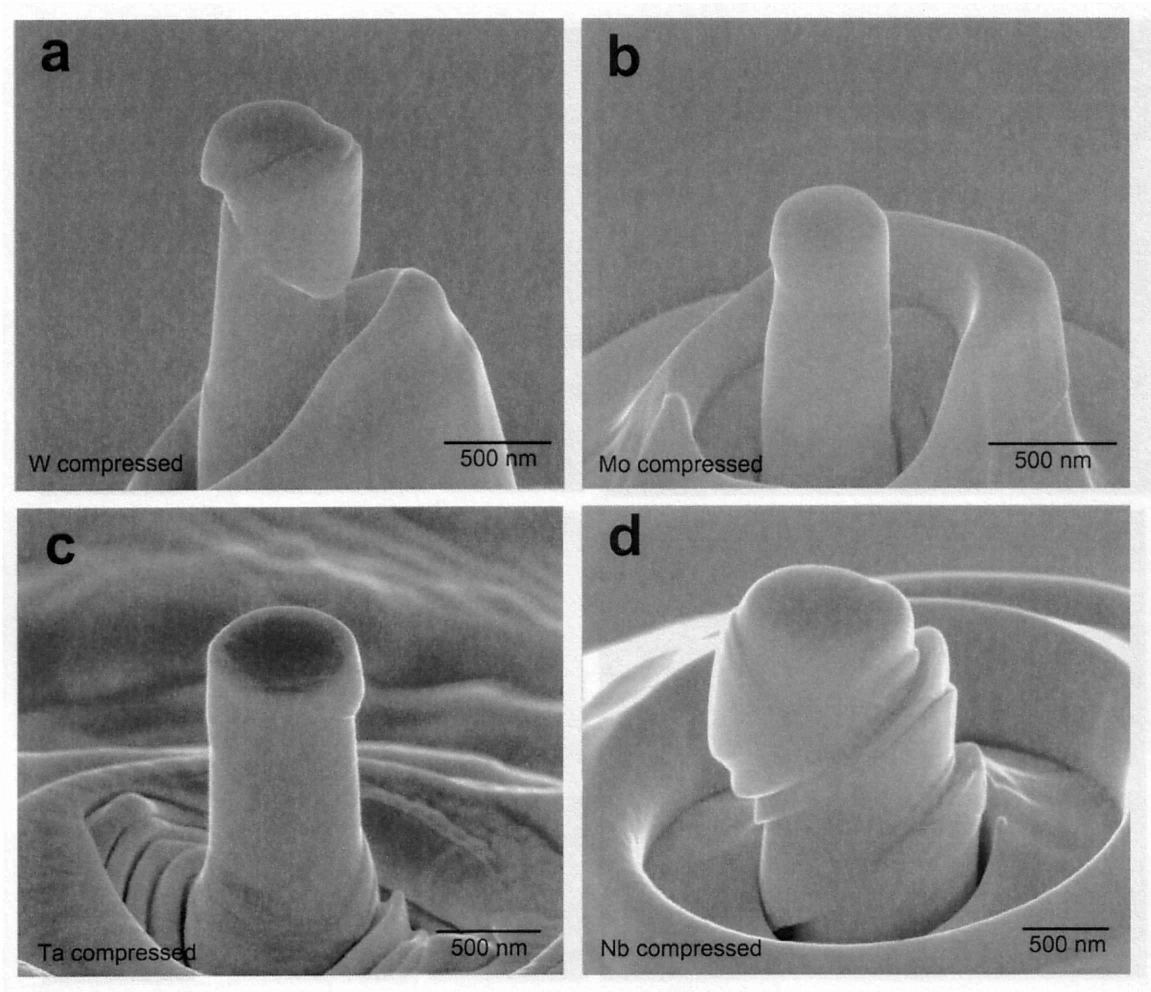
$$E = \sum_{i=1}^{N}\sum_{j=1}^{z}\gamma(O_i, O_j)$$

(b) Stable:



New Science:

(a) Exploit length-scale transition from dislocations to alternative nanoscale mechanisms (twinning, grain rotation).
(b) A nanoscale grain-growth model with incorporation of Zener pinning and solute drag to predict nanodomain stability.
(c) Grain-size effects predicted by MD-informed grain-boundary interactions in a dislocation dynamics framework
(d) Understand failure mechanisms (crack initiation, frictional accomodation) in dislocation-starved scenarios.



Kim, Jang, Greer, Acta Mater. 58 (2010) 2355

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