SAND2016-6106C

Microstructural Evolution and Friction Transitions in Nanocrystalline Alloys

Tim Furnish, Nic Argibay, Blythe Clark, Brad Boyce,
Mike Dugger, Mike Chandross

Materials Science and Engineering Center, Sandia National Laboratories,
Albuquerque, New Mexico USA

June 29, 2015

Coatings for Severe Environments, IC4N 2016

Sandia National Laboratories

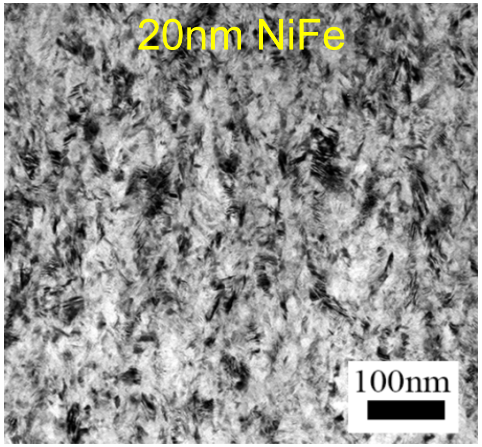
U.S. DEPARTMENT OF ENERGY | Office of Science

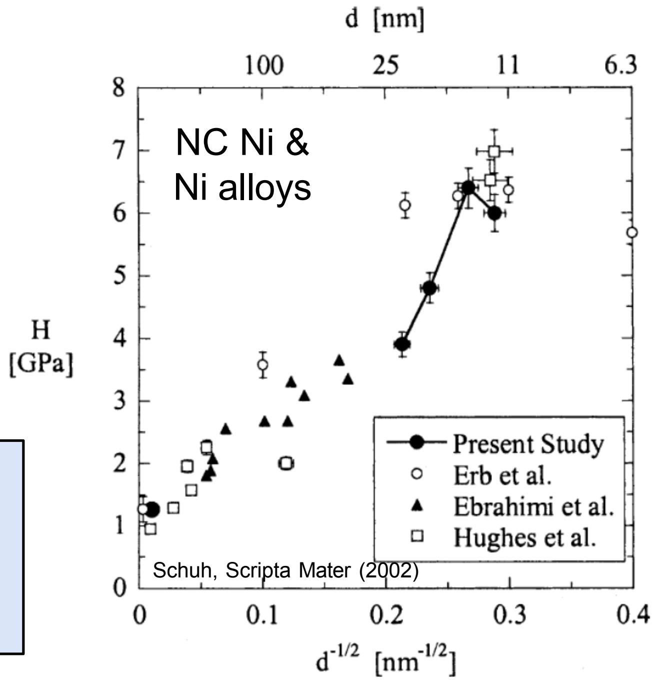
NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND2015-4425 C.

Nanocrystalline metals show unique mechanical behaviors and a potential for tunable properties

- **Nanocrystalline (NC)** materials are generally defined by having an average grain size of < 100nm
- When grains are at the nanoscale, **unique mechanical properties** and plastic responses are observed
- NC metals show a potential for:
  - ultra-high strength & hardness (up to 10+ times that of CG counterparts!)
  - high wear-resistance
  - high fatigue strengths

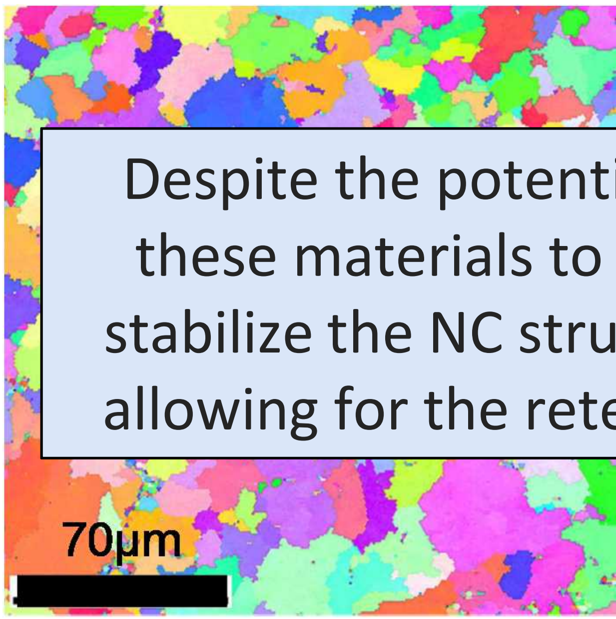




The ultrahigh strength and hardness in NC metals, and the pronounced grain size sensitivity, make them good candidates for tailored mechanical properties.

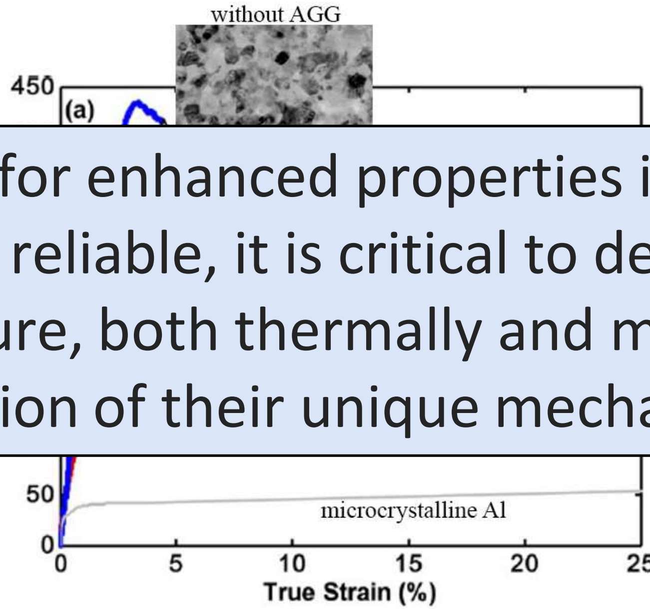
But… NC metals show a propensity for both **thermal** and **mechanical** grain growth at relatively low homologous temperatures (even room temp)!

NC Pd (originally 10nm grain size) after two months at RT



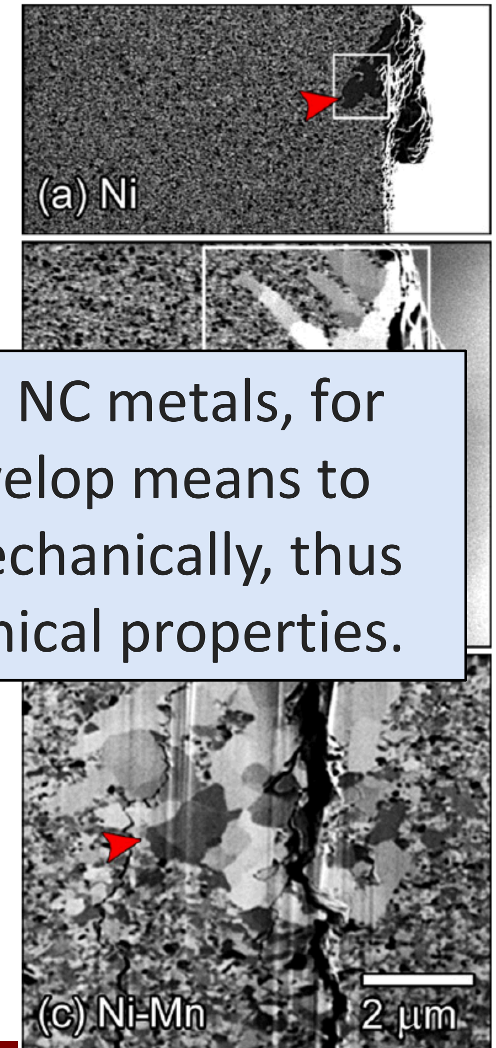
M. Ames, Acta Mater (2008)

Grain growth during **mononotic loading** leading to decreased strength



Gianola et al., Acta Mater. (2006)

Fatigue-induced grain growth leading to crack initiation



Boyce, Met. Mat. Trans. A (2011)

Despite the potential for enhanced properties in NC metals, for these materials to be reliable, it is critical to develop means to stabilize the NC structure, both thermally and mechanically, thus allowing for the retention of their unique mechanical properties.

Much research has been focused on improving thermal stability of NC metals via alloying

S. Simões, Nanotechnology (2010)

Two routes to stability – kinetic and thermodynamic

$$v = M \cdot P = M_o \exp\left(-\frac{Q_m}{kT}\right) \cdot \frac{2\gamma_o}{r}$$

M = grain boundary mobility

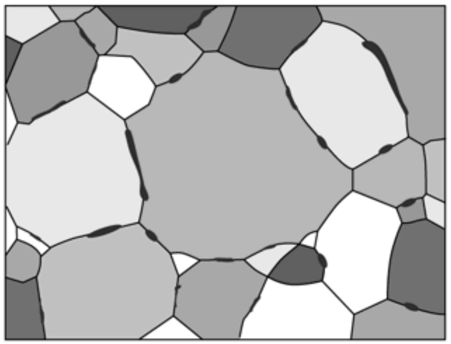
P = pressure on grain boundary

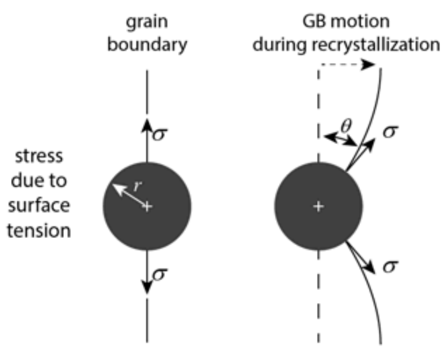
γ_o = interfacial energy per unit area

r = mean grain radius

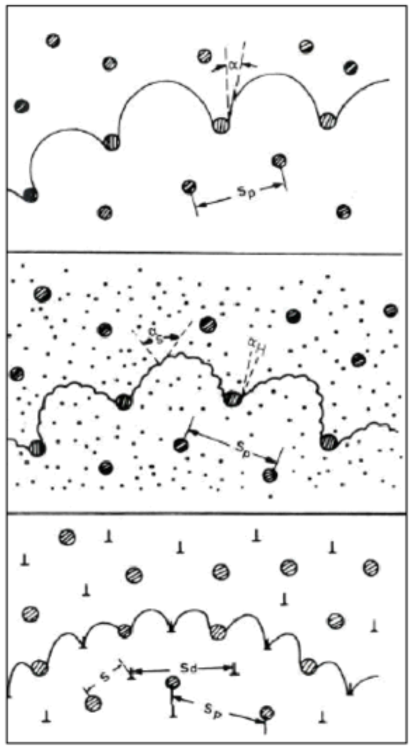
Limit the *kinetics* of recrystallization (traditional quasi-stability)

e.g. Zener pinning, solute drag, porosity





drag force: $f_D = 2\pi r \sigma \cos\theta \sin\theta$



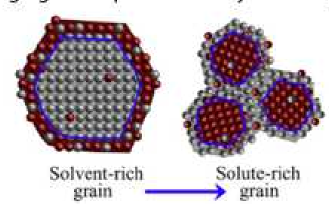
Weissmüller (1993), Kirchheim (2002), and Schuh (2012) have made significant contributions toward understanding and achieving ***thermodynamic*** stability by lowering grain boundary energy through solute segregation

Regular Nanocrystalline Solution (RNS) Model:
ref: Chookajorn et al., Science, 2012

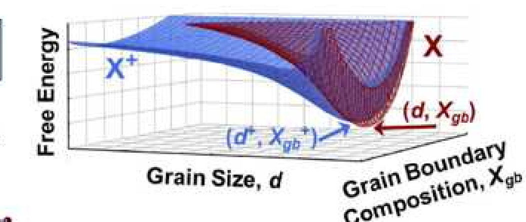
$$\Delta G^{mix} = (1 - f_{gb})\Delta G_c^{mix} + f_{gb}\Delta G_{gb}^{mix} + z\nu f_{gb}(X_{gb} - X_c)\left[(2X_{gb} - 1)\omega_{gb} - \frac{1}{zt}(\Omega^B\gamma^B - \Omega^A\gamma^A)\right]$$

$$dG = \left[\gamma - \frac{N_\beta}{A}\Delta G_{seg}\right]dA$$

Grain structure model:
segregated 2-phase metal system



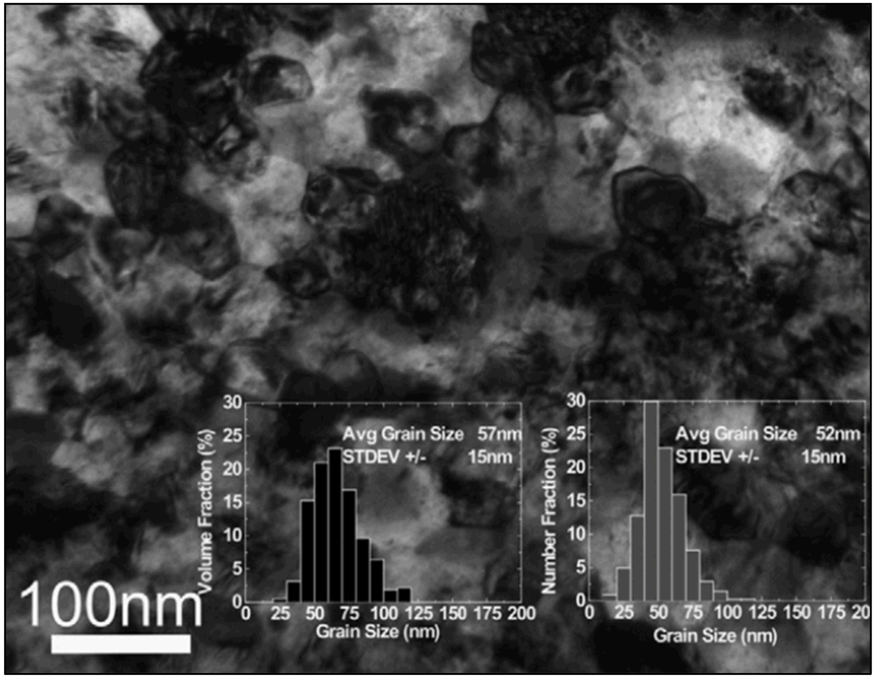
ref: Murdoch et al., Acta Mat. (2013)



ref: Murdoch et al., Acta Mat. (2013)

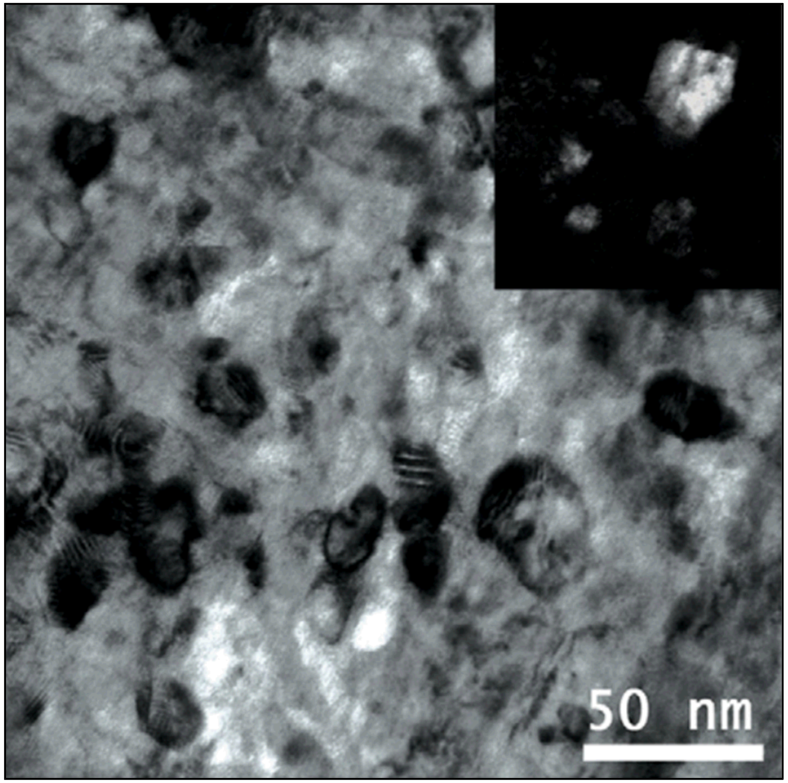
Progress has been made to impart **thermal stability** in NC metals via alloying – but, limited work on **mechanical** stability

Fe-4Zr, 913 C, 1 hr



K.A. Darling, Mat Sci & Eng A (2010)

W-20Ti, 1100 C, 1 week



T. Chookajorn & C.A. Schuh, Acta Mater. (2014)

…plus examples of improved thermal stability in other NC alloys: Ni-P, Cu-Ta, Ti-Cu, Pd-Zr, and Ni-W.

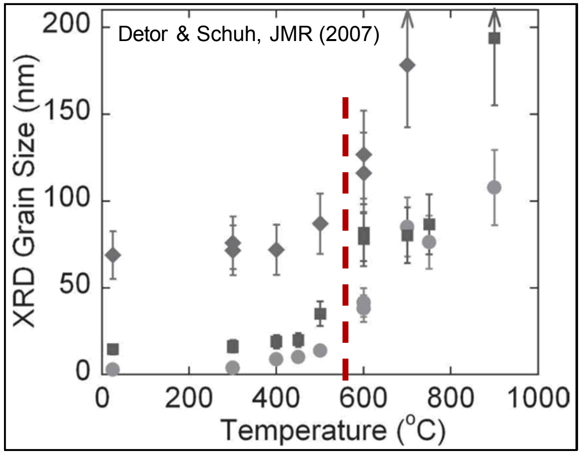
Why Ni-W? Researchers have developed an electroplating method for controllable compositions, grain sizes, and mechanical properties!

Microstructural and mechanical properties of Ni–W electrodeposits.

W content (at.%)	Average XRD grain size (nm)	Average TEM grain size (nm)	Hardness (GPa)	Wear volume (μm^3)	Friction coefficient
3.0	47		4.0	9.49×10^6	0.63
6.0	30		5.6	7.40×10^6	0.67
8.2	26	25	5.9	5.88×10^6	0.61
12.5	15		6.6	5.12×10^6	0.65
15.7	9		6.8	5.06×10^6	0.66
18.2	6	6	6.9	4.03×10^6	0.65
22.9	5		7.1	3.79×10^6	0.60
27.9	3	3	7.1	2.77×10^6	0.66

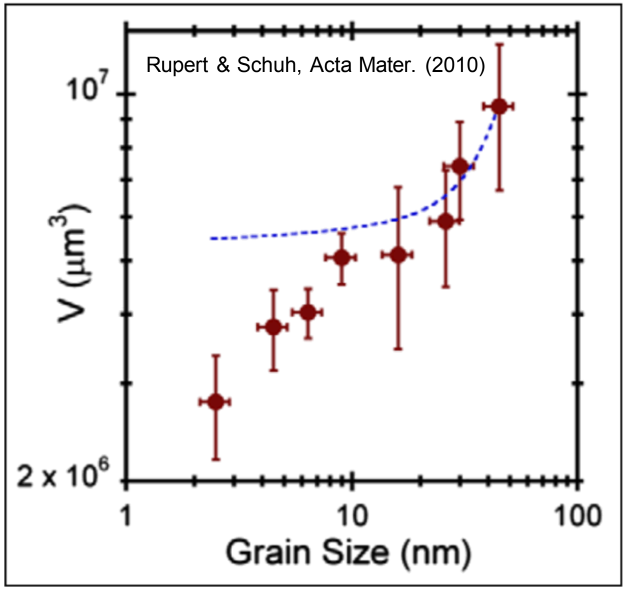
Detor & Schuh, JMR (2007)

24 hour anneals at various temperatures

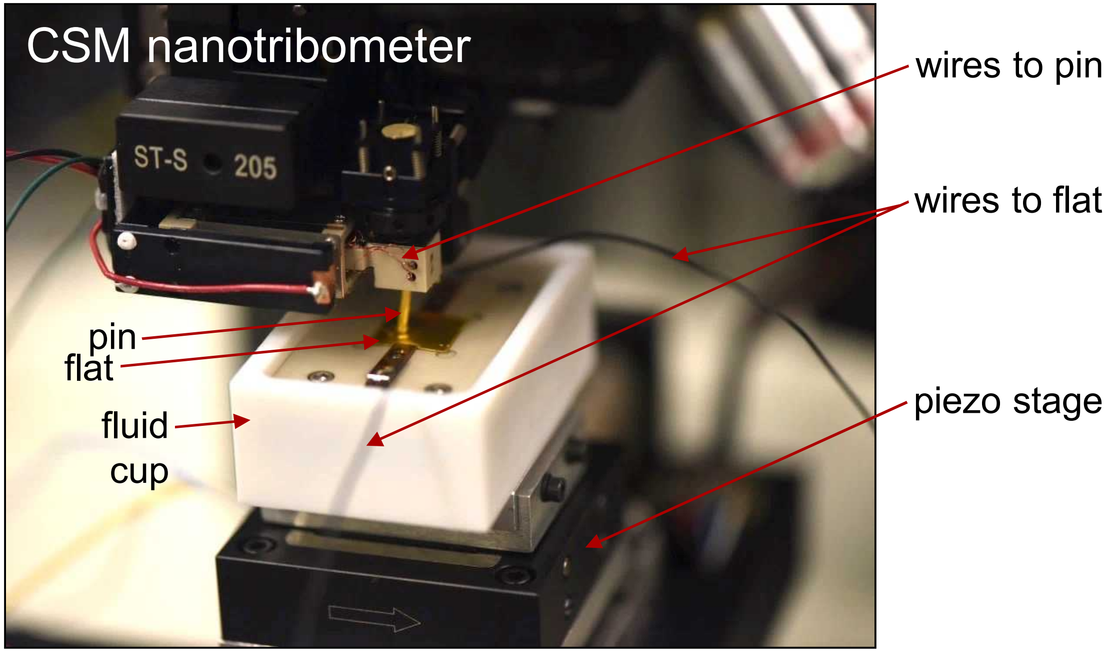


Ni-W shows a potential for relatively stable NC structures with tunable grain sizes and mechanical properties!

Additionally, the exceptionally low wear rates under sliding make these metals ideal for applications requiring ultrahigh hardness, strength, and wear resistance.



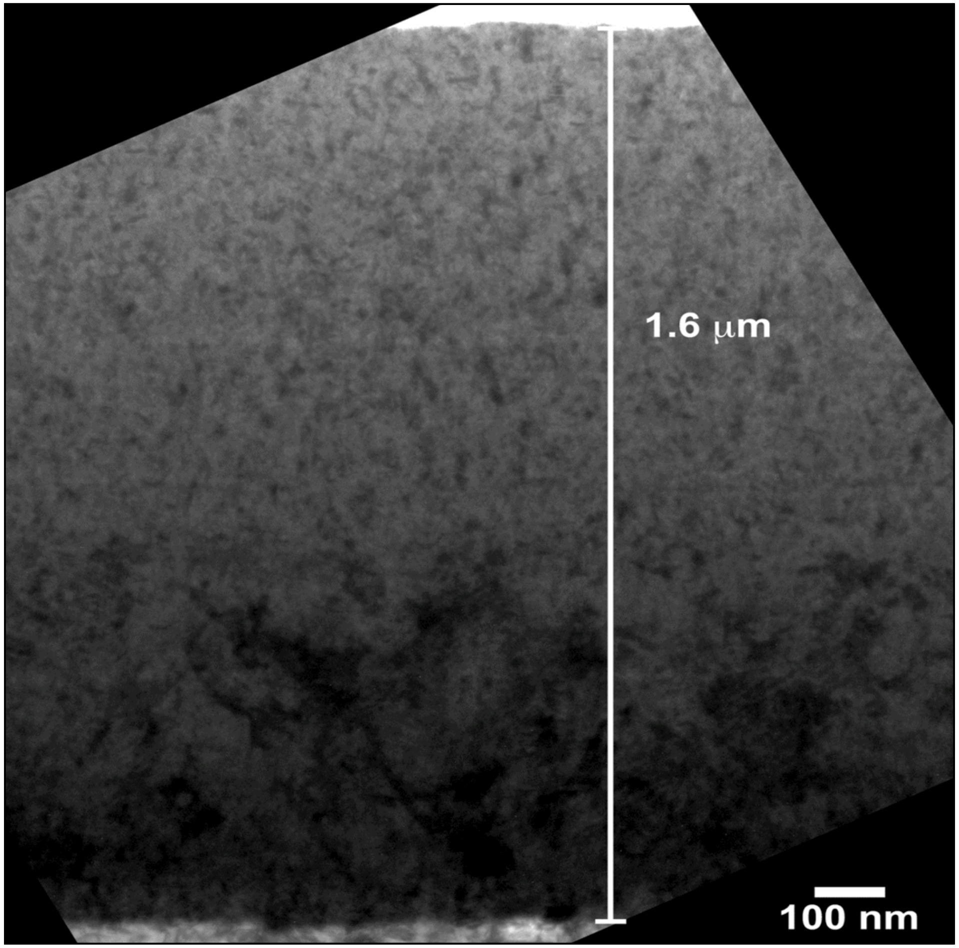
Sliding experiments were conducted to assess the ***mechanical*** stability and corresponding ***friction*** response in NC Ni-W



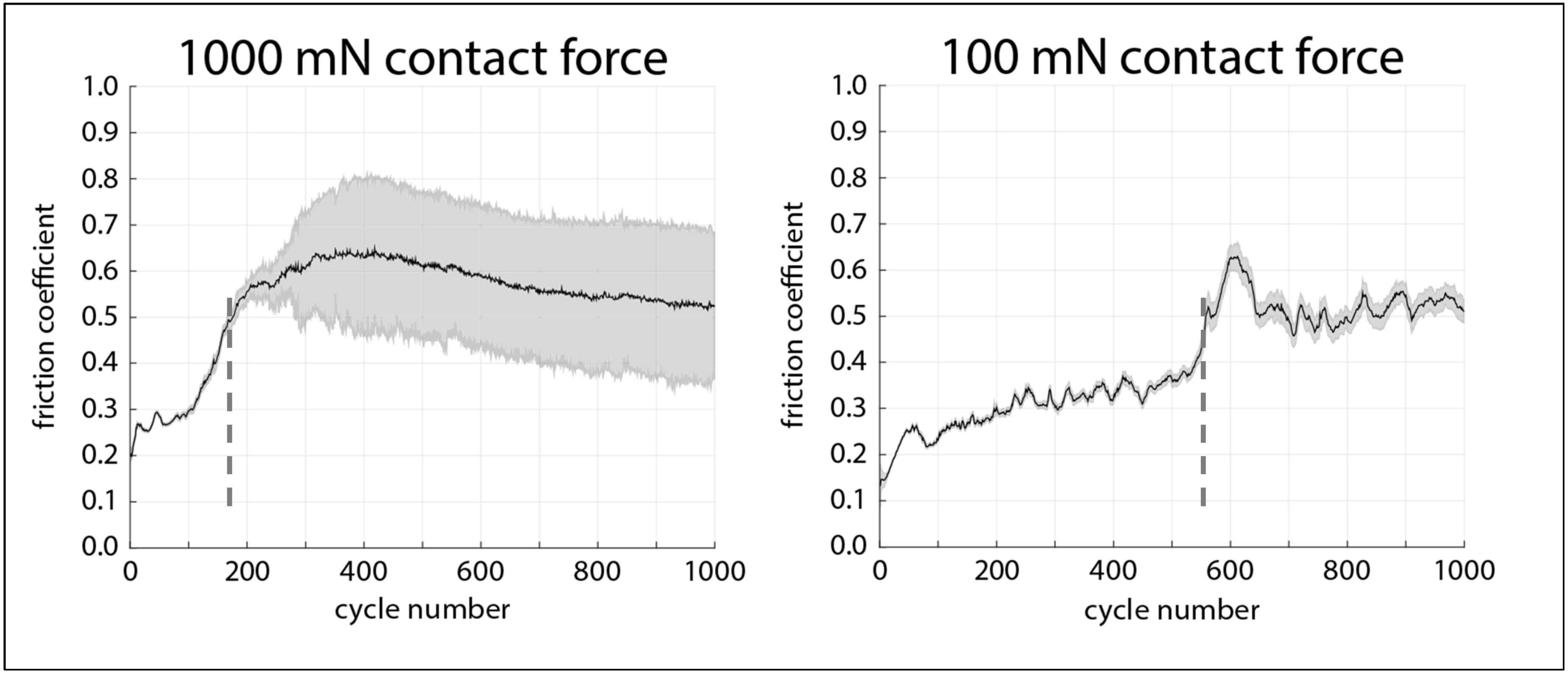
- Test parameters:
  - 1 mm/s sliding speed
  - Bidirectional sliding (to/from = 1 cycle)
  - 1.6 mm sapphire ball (chosen to match H=9GPa)
  - 2 mm track length
  - In air (10% humidity)
- Three contact forces:
  - 1 mN, 100 mN, 1000 mN

In this study, 5nm grain sized Ni-40wt%W was used as a representative NC material

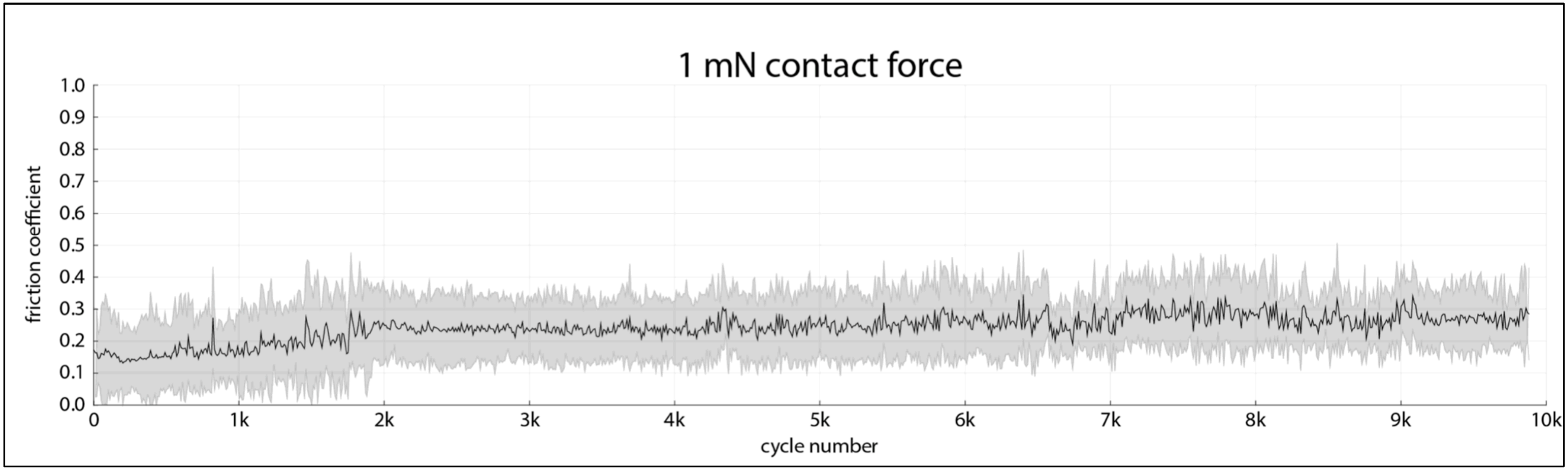
- Ni-40wt%W deposited on a brass substrate
- 1.6 µm thick coating
- 5.2 ± 0.2 nm grain size (via XRD)
- Demonstrated NC stability under annealing for 24 hours up to 500 ° C



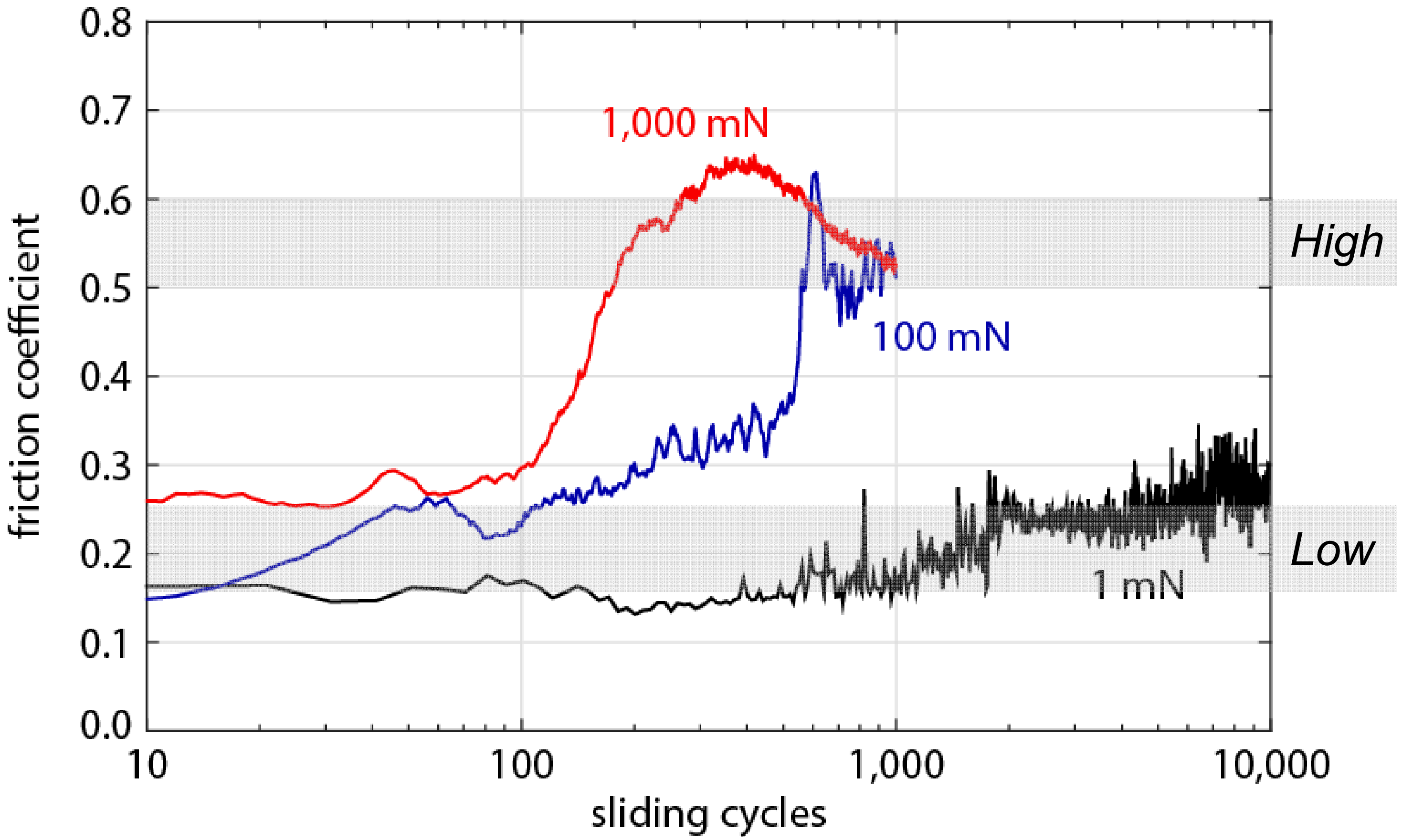
In the higher contact force cases, a transition is observed from initially low friction (COF ~0.15-0.25) to high friction (COF ~0.5-0.6) within hundreds of cycles



But, when the contact force is sufficiently low, e.g., 1mN, persistently low friction is observed (beyond 10k cycles)!

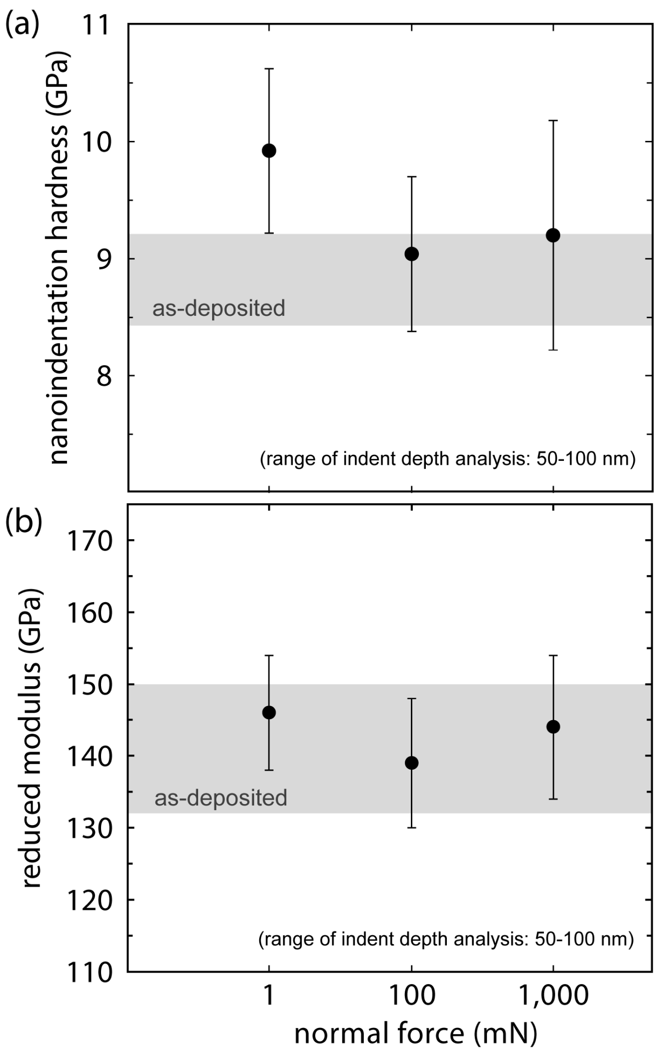


Friction response as a function of contact force:



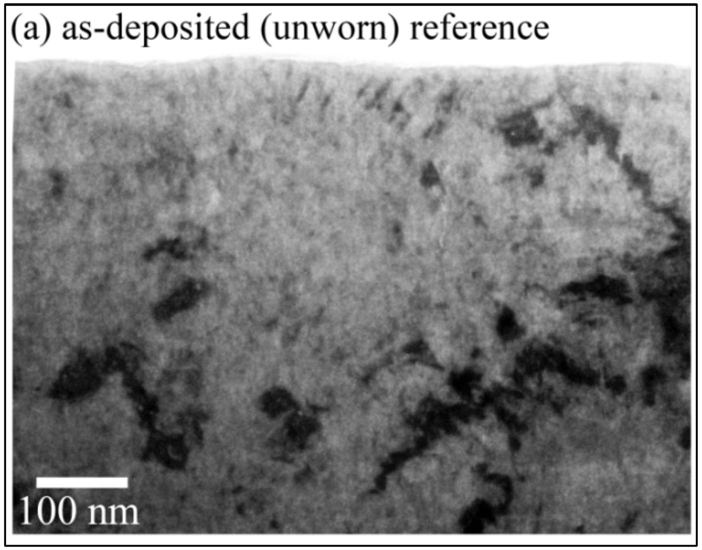
- Friction coefficient is initially low (0.15-0.25) for all cases for the first ~100 cycles
- In higher force cases, friction ultimately transitions to the same COF
- No transition in the low force case

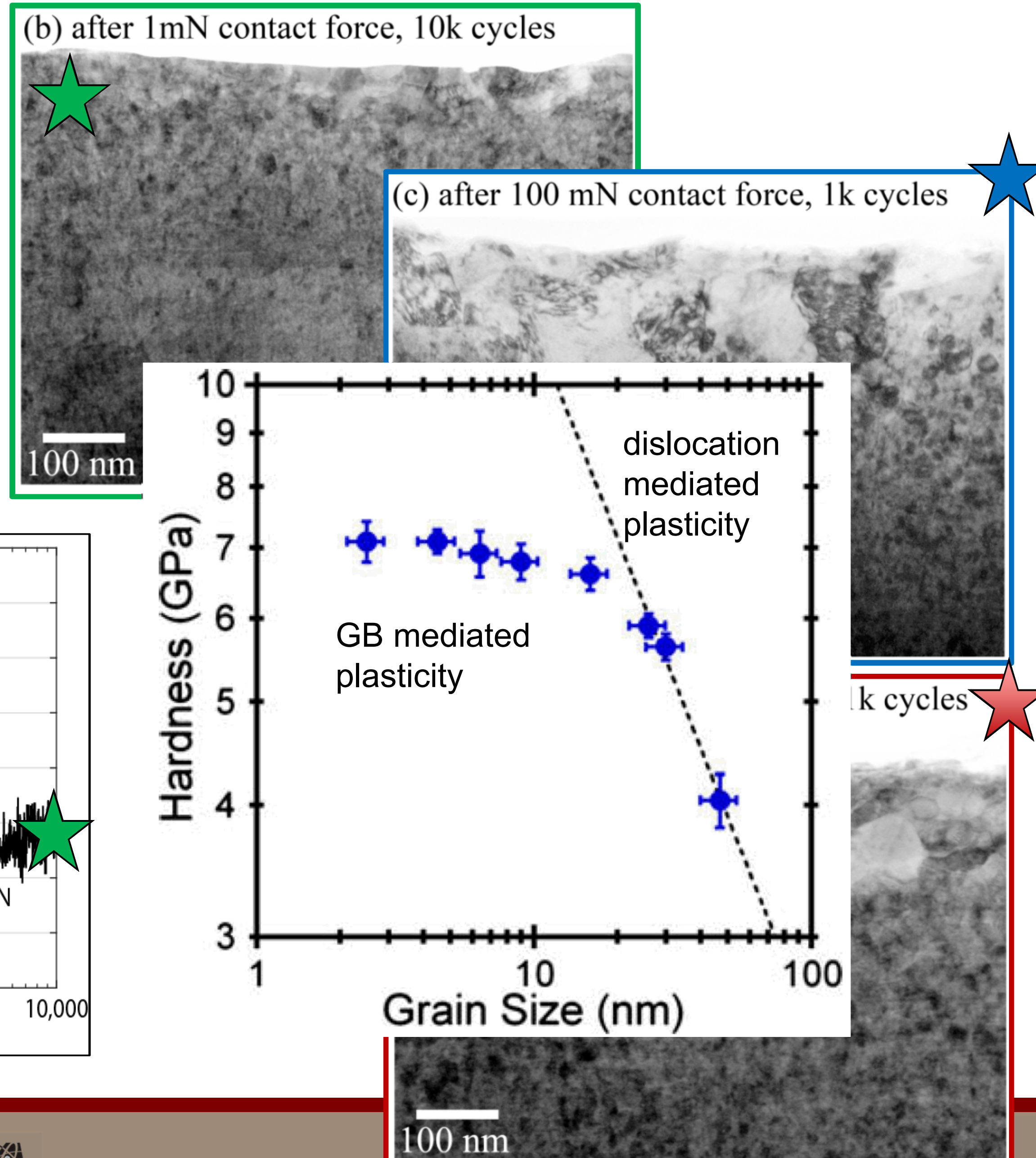
Are the friction transitions due to changes in hardness?

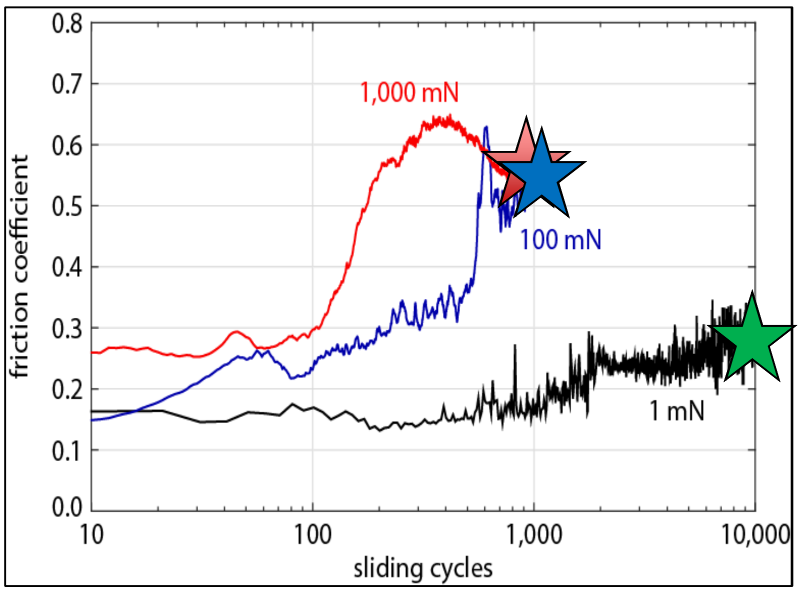


- Slight increase (~13%) in hardness found in the 1mN wear track compared to original hardness
- 100mN and 1000mN tracks surface grains showed comparable hardness to as-deposited hardness
- Changes in hardness alone do not substantiate the friction transitions

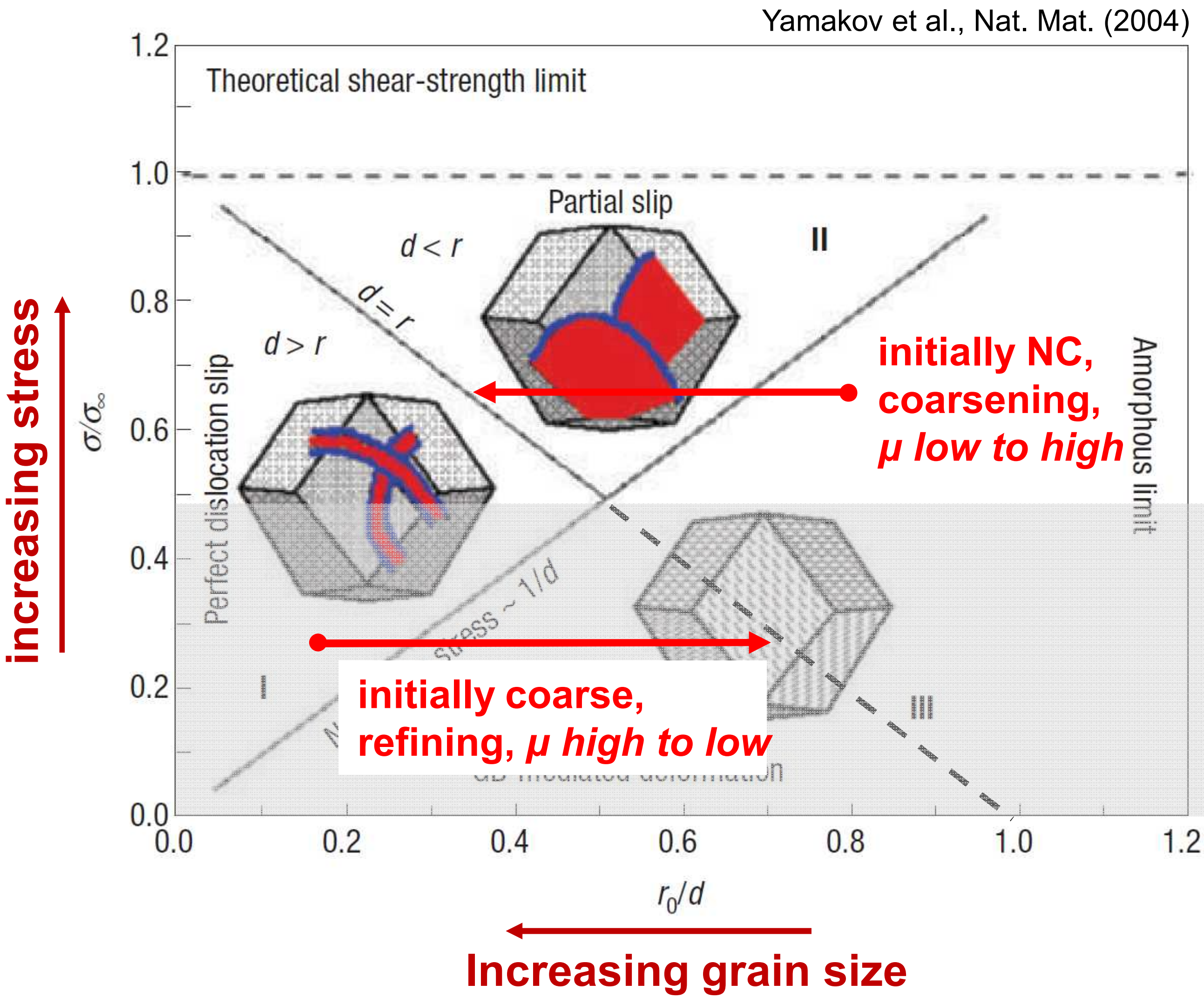
What do the microstructures look like under the wear tracks?





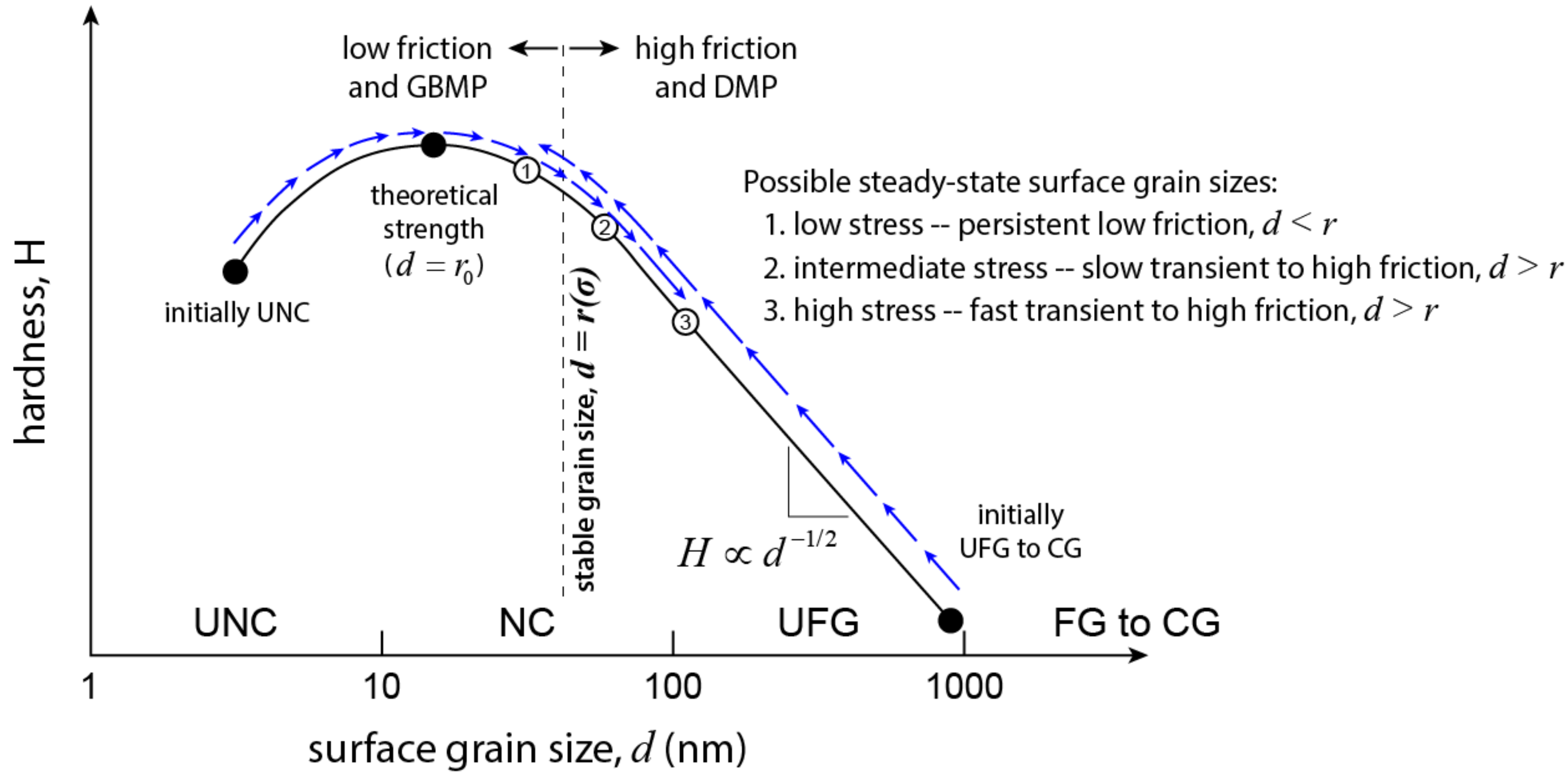


Deformation map (Yamakov et al.) for dominant deformation mechanisms vs. stress and grain size



Low friction response would be expected for stresses in this grain boundary-mediated plasticity range

What does this mean for microstructural evolution and friction transitions during sliding?



We hypothesize that the evolved microstructure is highly dependent on the contact force (i.e., surface stress), and that maintaining a microstructure that is predominantly dominated by GB-mediated plasticity is the key for persistently low friction.

Summary

- Microstructural stability of Ni-W was evaluated under sliding conditions over a range of contact forces
  - Significant grain coarsening observed for 100 and 1000 mN, corresponding to a transition from low-to-high friction within hundreds of cycles
  - Minimal grain coarsening observed for 1 mN case → persistently low friction found for beyond 10k cycles
- No dramatic change in hardness in any case; however, hardness measurements indicate a breakdown in the H-P relationship in 1 mN case, indicative of GB-mediated plasticity
- We hypothesize that a stress limit exists, below which the stress-induced evolved microstructure is still dominated by GB-mediated plasticity – remaining below this limit is likely the key to achieving persistently low friction in NC metals
- Additional work is currently underway to couple experimental results to MD simulations for detailed understanding of the relationship between dominant deformation mechanisms and the friction response