DOE award number: DE-FG02-10ER46398

Purdue University

Project title: Plastic Strain Recovery in Nanocrystalline Materials

PI: Marisol Koslowski

Date of the report: 4/14/15

Period: 4/15/11 to 4/14/15

Program Scope

Understanding the mechanisms of deformation of nanocrystalline (nc) materials is critical to the design of micro and nano devices and to develop materials with superior fracture strength and wear resistance for applications in new energy technologies. In this project we focused on understanding the following plastic deformation processes described in detail in the following sections:

1. Plastic strain recovery (Section 1).
2. Effect of microstructural variability on the yield stress of nc metals (Section 2).
3. The role of partial and extended full dislocations in plastic deformation of nc metals (Section 3).

1. Plastic strain recovery

When nc samples are loaded beyond their yield stress and then unloaded part of the plastic strain recovers over time. This process was observed by Spolenak (Spolenak,2001) in ultrafine grained copper thin films and was termed "reverse stress relaxation" and was later named "*plastic strain recovery*" in the work of Rajagopalan (Rajagopalan,2006). Experiments in nc aluminum and gold thin films (Rajagopalan,2006) and more recently in copper thin films (Wei,2011) show recovery of plastic strain ranging from 50% to 100%. This phenomenon was also observed in bulk nc and ultra fine crystalline (ufc) aluminum (Lonardelli,2009). That the amount of plastic strain recovered varies in different experiments shows that this process depends on the microstructure, the grain size and the loading history.

Several models suggest that the inhomogeneous stress field is responsible for this process, but the sources of the stress and the carriers of plastic strain differ among approaches. The theories developed by Spolenak (Spolenak,2001), Rajagopalan (Rajagopalan,2006) and Koslowski (Koslowski,2010) assume that plastic strain recovery occurs as a consequence of creep deformation due to residual stresses resulting from grain size heterogeneity and/or texture. Grains with different size have different yield stress due to the Hall-Petch effect with larger grains yielding at lower stress. Similarly,

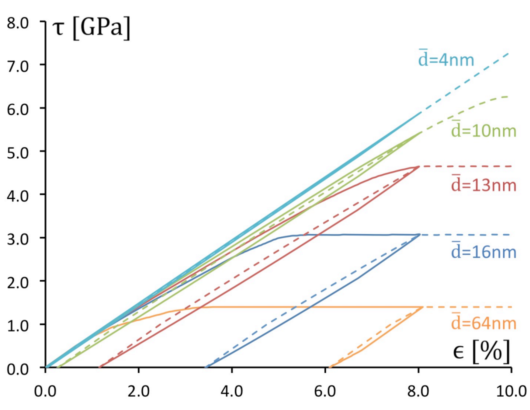
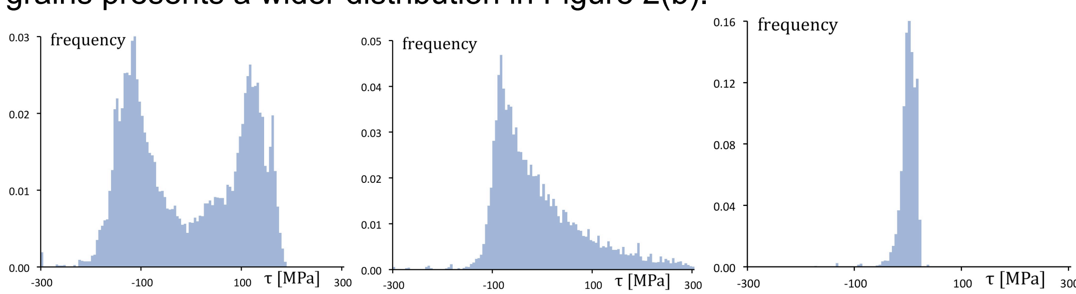


Figure 1: Simulated stress-strain curves for microstructures with different average grain size.

grains with favorable orientation have larger plastic deformation due to a larger Schmid's factor. Upon unloading, grains with larger plastic activity are in compression while some grains remain in tension. This stress difference drives recovery of plastic strain until the stress is relaxed. Other approaches suggest that plastic strain recovery is driven by grain boundary sliding (Wei,2008) and a combination of dislocation processes in samples with grains ranging from 10 nm to 30nm (Li,2009).

To understand the effect of residual stresses due to microstructure inhomogeneity and dislocation interactions during plastic strain recovery, we perform simulations using a phase field dislocation dynamics (PFDD) approach in microstructures composed of two types of grains, small grains with size 4nm and large grains with size 16nm. The volume fraction of large grains is indicated by the quantity v_l. Figure 1 shows the stress versus strain and plastic strain during cyclic loading for different microstructures with a maximum applied strain 8%. The Hall-Petch effect is evident and arises from the confinement of dislocations in the grains, with a higher yield stress in the samples with smaller average grain size independently of the grain size distribution.

To quantify the residual stress upon unloading we calculate the stress distribution on different microstructures. Figure 2 shows these residual stress distributions after applying a strain ε_{max}=8%. The residual stress for the structure with v_l =0.5 is shown in Figure 2(a), v_l =0.0 in Figure 2(b), and v_l =1.0 in Figure 2(c). During loading large grains deform plastically while small grains are still in the elastic regime. Upon unloading the small grains are in tension and the large grains are in compression. This can be seen in Figure 2(a) where the stress distribution shows two peaks corresponding to the small (positive) and large (negative) grains. Figures 2(b) and 2(c) are the residual stress distributions in uniform grain size structures and therefore, present only one peak. In this case, the heterogeneity of the stress field is a consequence the dislocation structures that develop close to grain boundaries and therefore, the microstructure with smaller grains presents a wider distribution in Figure 2(b).



(a) (b) (c)

Figure 2: Distribution of residual stresses upon unloading for microstructures with (a) v_l=0.5, (b) v_l= 0 (c) v_l=1.

After unloading the simulated dislocation ensemble evolves with a kinetic Monte Carlo (KMC) algorithm in which the dislocation-dislocation interactions, the interactions with grain boundaries and residual stresses are built into the energy of the PFDD. The KMC method provides a general approach to simulate the temporal evolution of complex systems exploring sequences of transitions between different states in the system and accounting for thermally activated mechanisms linking long time scale stress relaxation to dislocation mechanisms.

Figure 3, shows the plastic strain recovered over time, for the different grain structures after the system is loaded up to ε_{max}=8% and then unloaded. The maximum extent of plastic strain recovery occurs for larger grain sizes due to extensive dislocation activity as shown in Figure 3(a). However, the maximum of the ratio between the plastic strain recovery and the value of plastic strain upon unloading, shown in Figure 3(b), occurs for v_l =0.50. Even for uniform grain size our simulations render plastic strain recovery in contrast to previous models (Rajagopalan:2006, Koslowski:2010) that do not consider individual dislocations.

In summary, the simulations indicate that the inhomogeneous stress fields due to the Hall-Petch effect in microstructures with different grain sizes have a strong effect on plastic strain recovery. Microstructures with the largest distribution of grain sizes, v_l = 0.5, acchieve 40% of plastic strain recovery while in the other structures the recovery is below 15%. But contrary to the predictions in previous models, we observe plastic strain recovery in samples with uniform grain size. This is explained by the formation of dislocation structures that create a residual stress field, Figure 2, that drives the evolution of dislocations.

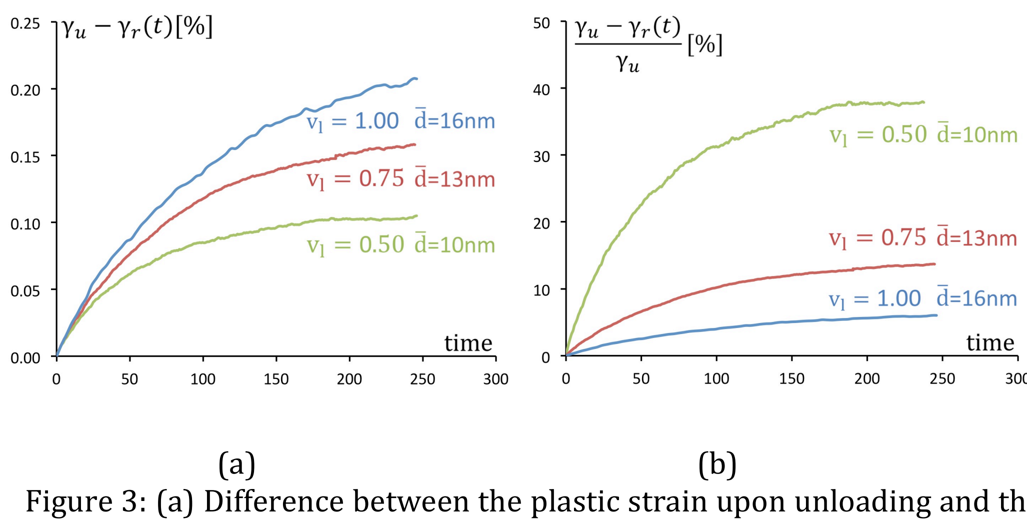


Figure 3: (a) Difference between the plastic strain upon unloading and the recovered plastic strain. (b) Ratio between the plastic strain recovery and the value of plastic strain upon unloading.

1.1 DOE sponsored research publications in this area

- *Marisol Koslowski,* Effect of grain size distribution on plastic strain recovery, Physical Review B **82**, 054110, 2010.
- Yuesong Xie and Marisol Koslowski, Inelastic recovery in nano and ultra fine grained materials, *Journal of the Mechanics and Physics of Solids,* submitted, 2015*.*

2 Effect of microstructural variability on the yield stress of nc metals

Numerical simulations can be exploited to understand the sensitivity of the mechanical properties of materials to the microstructure variability and hence improve their performance and reliability. We investigate the effect of the initial microstructure of nc nickel, including: grain size, grain size distribution and initial dislocation density, on the yield stress through numerical simulations with the PFDD model. The results reveal that the grain size distribution has a significant influence on the yield stress for grain sizes under 32 nm and that the initial dislocation density is of key importance to determine the yield stress. Simulations with no initial dislocation density exhibit almost size independent stress-strain behavior, while Hall-Petch effect is observed in simulations with initial dislocation structures.

In Figure 4 the simulated stress-strain curves for polycrystals with various grain sizes, and for initial dislocation density $\rho = 0$, $\rho = 2.5\times10^{16}\,\mathrm{m}^{-2}$ and $\rho = 5\times10^{16}\,\mathrm{m}^{-2}$ are shown. When the initial dislocation density is set to zero no size dependency is observed. The onset of plastic deformation in this case, is dominated by the nucleation of dislocations, which is a size independent process. In contrast, when the initial dislocation density is higher, dislocation gliding starts at lower applied stress resulting in a marked reduction of the yield stress.

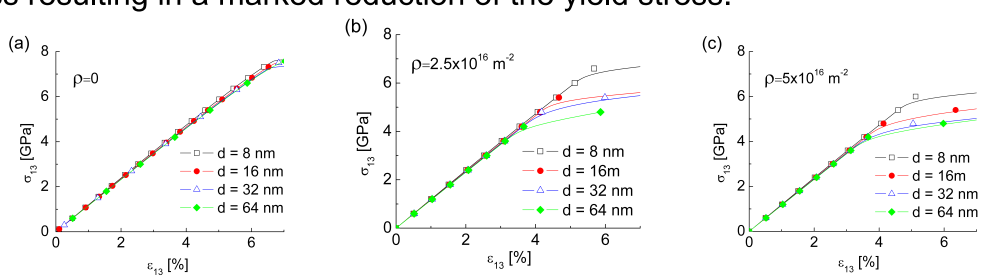


Figure 4: Stress-strain curves for various grain sizes with initial dislocation density (a) $\rho = 0$, (b) $\rho = 2.5\times10^{16}\,\mathrm{m}^{-2}$, (c) $\rho = 5\times10^{16}\,\mathrm{m}^{-2}$.

With these results we build a response surface function of the yield stress as a function of the grain size and the initial dislocation shown in Figure 5. The yield stress has a strong dependency on the microstructure variability and therefore, deterministic simulations using the mean yield stress can lead to large prediction errors. The goal is to build a probability density function (pdf) that can be used to predict a range of yield stress due to uncertainties in the microstructure.

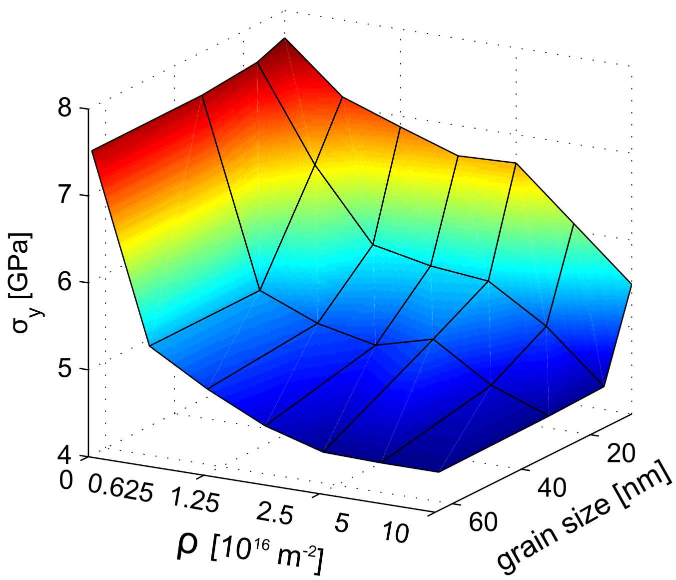


Figure 5: Response surface of the yield stress as a function of the average grain size and the initial dislocation density for uniform grain size.

The pdf of the yield stress for samples with average grain size 8nm, 32 nm and 64nm is shown in Figure 6. We assume that the average grain size is known but the grain size distribution is not given. Therefore for a given grain size the pdf of the yield stress is a uniform distribution. To include the effect of the uncertainty of the initial dislocation density we use a normal distribution with mean $\rho = 2.5\times10^{16}\ \mathrm{m}^{-2}$ and standard deviation $0.1\times10^{16}\ \mathrm{m}^{-2}$. It can be seen that when the average grain size increases the mean value of the yield stress decreases. On the other hand, the dispersion on the predicted yield stress due to the initial dislocation density is reduced with increasing grain size due to the strong dependency of the yield stress on the initial microstructure for small grain size samples.

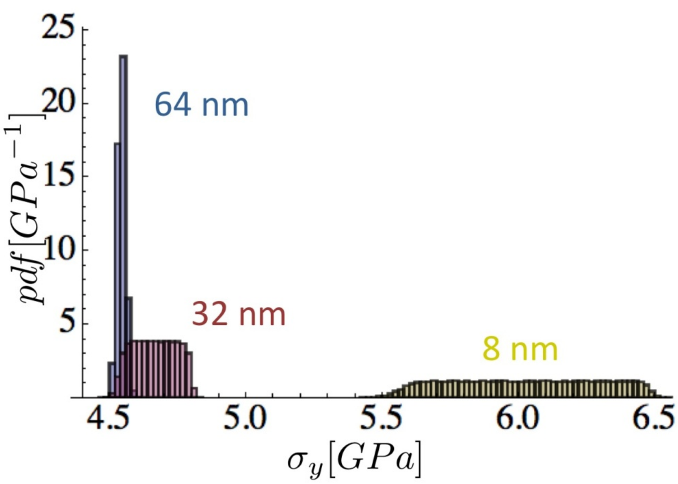


Fig. 7. Predicted PDF of the yield stress for average grain sizes d=8nm, 32nm and 64 nm.

2.1 DOE sponsored research publications in this area

- Lei Cao and Marisol Koslowski, Effect of microstructural uncertainty on the yield stress of nanocrystalline nickel, *Acta Materialia*, 61 1413-1420, 2013.

3. The role of partial and extended full dislocations in plastic deformation of nc metals

Numerical simulations at the nanometer scale have identified several mechanisms of plastic deformation. However, high strain rate regimes are required to resolve nanometer length scales. Extrapolating numerical predictions at high strain rates to experimental conditions remains an unresolved challenge. We perform 3D simulations of the evolution of dislocations using a phase field dislocation dynamics approach in which the material gamma surface is incorporated to account for dislocations dissociating into partials in Al and Ni. The simulations are carried out in nc materials with grain sizes in the range 5-50 nm in a 3D cell with periodic boundary conditions.

The details of the dislocation nucleation process in Al in response to an applied strain $\varepsilon_{13} = 0.04$ and in Ni at $\varepsilon_{13} = 0.02$ are shown in Figure 8. In both materials a leading partial is nucleated from the grain boundary, the yellow area is the stacking fault left behind by the leading partial. In Figures 8(b), and 8(c) the trailing partials have nucleated and remove part of the stacking fault. Afterwards the two partials form extended full dislocations that glide as a pair.

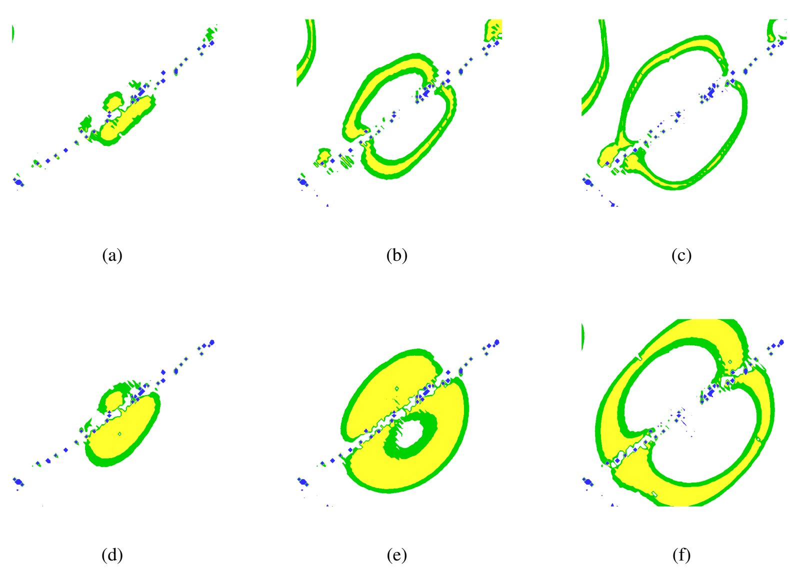
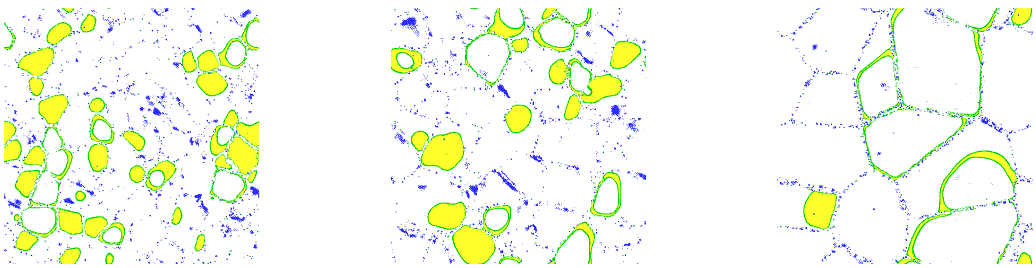


Figure 8: Dislocation nucleation at a grain boundary (a)-(c) in Al and (d)-(f) in Ni

Figure 9 shows dislocation structures in one plane of the simulation domain for an applied strain ε_{13} = 0.024 for Ni in grain structures with grain sizes *d*=10, 15, and 30 nm. The dislocation activity in smaller grain size structures occurs only in a limited number of grains. The 30 nm and 40 nm grain size structures have a larger amount of extended full dislocations.



(a) d = 10 nm (b) d = 15 nm (c) d = 30 nm

Figure 9: Dislocation structures in one plane of the simulation domain. Blue regions are grain boundaries, yellow areas are stacking faults and green lines are dislocations.

The effect of strain rate on the deformation process is studied in a nc Ni sample with an average grain size of 15 nm. The impact on the stress-strain response and the evolution of partials and extended full dislocations is investigated. Figure 10 shows the simulated stress-strain curves, with strain rates in the range $10^6 s^{-1}$-$10^9 s^{-1}$. A significant growth of the stress with increasing strain rate and an overshoot can be observed. The stress overshoot is reduced with decreasing strain rate, as the dislocations have enough time to glide and reduce the local stress between strain increments. Another feature of Figure 10 is the jerky character of the stress-strain curves at lower strain rates, $1 \times 10^6 s^{-1}$ and $1 \times 10^7 s^{-1}$.

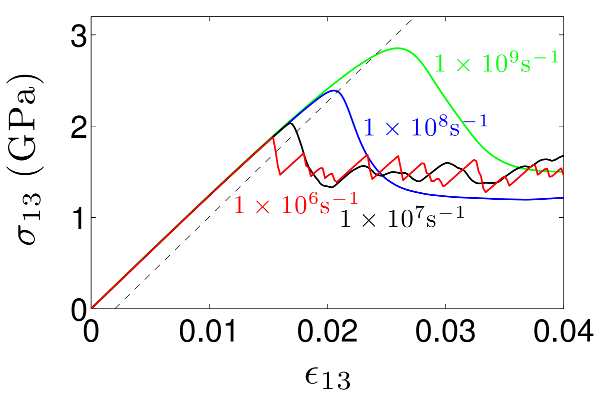


Figure 10: Stress-strain response for nc Ni at different strain rates.

To examine the relative contribution of partial and extended full dislocations to plastic strain at different strain rates the area slipped by partial and extended full dislocations is measured (Vo, 2008). Figure 11 shows A_p, the stacking fault area, and A_f , the area swept by extended full dislocations, as a function of the applied strain at different strain rates. At strain rates $10^8 s^{-1}$ and $10^9 s^{-1}$, the activity of partial dislocations reaches a maximum and then decreases when trailing dislocations start to glide to form an extended full dislocation. In contrast, A_f increases monotonically with the applied strain in all the cases.

Even though the onset of dislocation gliding occurs at the same applied strain for different strain rates, at lower strain rates partial dislocations can glide larger distances and trailing dislocations become active to form extended full dislocations during one strain increment in the simulation. At larger strain rates, the area glided by partial dislocations is limited during each strain increment bounding its contribution to the total slip. This leads to an effective delay in plastic strain illustrated in Figure 11. This effective strain delay is responsible for the increase in yield stress as the strain rate is larger (Brandl, 2009).

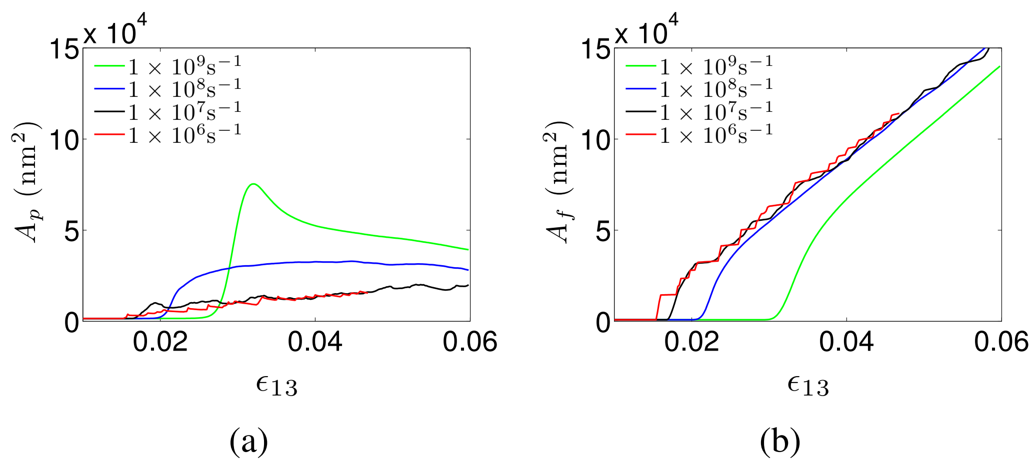
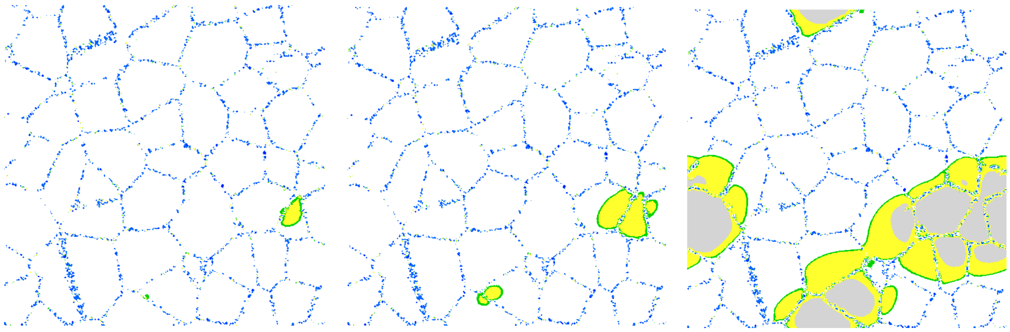


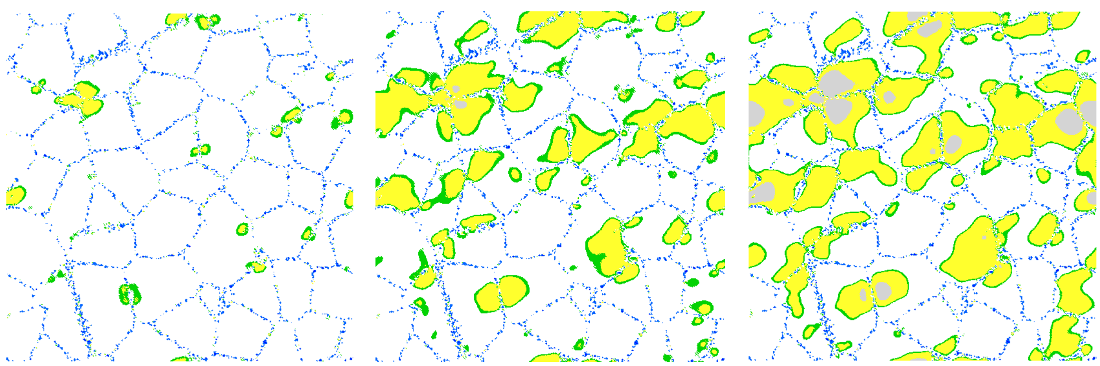
Figure 11: Activity of partial dislocations in (a) and extended full dislocations in (b).

The dislocation microstructures that form at different strain rates also have striking differences that are exhibited in Figures 12 and 13. At lower strain rate, the initial dislocation activity is limited to a few GBs and glide events with large areas slipped by extended full dislocations are observed. In contrast, dislocation activity is observed simultaneously at several GBs across the entire sample at high strain rates but the activity is limited to only leading partial dislocations with small areas slipped reducing the plastic strain.



(a) $\bar{\epsilon} = 0.0164$ (b) $\bar{\epsilon} = 0.0166$ (c) $\bar{\epsilon} = 0.0170$

Figure 12: Dislocation glide at strain rate of 1 × $10^7 s^{-1}$. The area slipped by a leading partial dislocation is in yellow; the area slipped by an extended full dislocation is in gray.



(a) $\bar{\epsilon} = 0.0272$ (b) $\bar{\epsilon} = 0.0296$ (c) $\bar{\epsilon} = 0.0316$

Figure 13: Dislocation glide at strain rate of 1 × $10^9 s^{-1}$. The area slipped by a leading partial dislocation is in yellow; the area slipped by an extended full dislocation is in gray.

3.1 DOE sponsored research publications in this area

- *DongWook Lee, Hojin Kim, Alejandro Strachan and Marisol Koslowski, Effect of core energy on mobility in a continuum dislocation model, Physical Review B,* ***83*** *104101, 2011.*
- *Hunter, A., Beyerlein, I., Germann, T. and Koslowski, M. Influence of the stacking fault energy surface on extended partials with a 3D Phase Field Dislocations Model, Physical Review B*, **84** 144108, 2011.

- Hunter, Abigail; Zhang, Ruifeng; Beyerlein, Irene; Germann, Timothy; Koslowski, Marisol, Dependence of equilibrium stacking fault width in fcc metals on the γ-surface, *Modeling and Simulations in Materials Science and Engineering*, 21 025015-025034, 2013.
- Lei Cao, Abigail Hunter, Irene Beyerlein and Marisol Koslowski, The role of partial mediated slip during quasistatic deformation of nanocrystalline nickel, *Journal of the Mechanics and Physics of Solids,* **78** 415-426, 2015.
- Lei Cao and Marisol Koslowski, Rate limited plastic deformation in nanocrystalline nickel, *Journal of Applied Physics*, submitted, 2015.

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Rajagopalan, 2006. J. Rajagopalan, J. H. Han, and T. A. Saif, Science 315, 427, 2006.

Koslowski, 2010. *Marisol Koslowski,* Effect of grain size distribution on plastic strain recovery, Physical Review B **82**, 054110, 2010.

Wei, 2011. Wei, X., And Kysar, J. W. Residual plastic strain recovery driven by grain boundary diffusion in nanocrystalline thin films. *Acta Materialia 59*, 10 3937–3945, 2011.

Lonardelli, 2009. Lonardelli, I., Almer, J., Ischia, G., Menapace, C., And Molinari, A. Defor- mation behavior in bulk nanocrystalline-ultrafine aluminum: in situ evidence of plastic strain recovery. *Scripta Materialia 60*, 520–523, 2009.

Wei, 2008. Wei, Y., Bower, A., And Gao, H. Recoverable creep deformation and transient local stress concentration due to heterogeneous grain-boundary diffusion and sliding in polycrys- talline solids. *Journal of the Mechanics and Physics of Solids 56*, 4, 1460–1483, 2008.

Li, 2009. Li, X., Wei, Y., Yang, W., And Gao, H. Competing grain-boundary-and dislocation- mediated mechanisms in plastic strain recovery in nanocrystalline aluminum. *Proceedings of the National Academy of Sciences of the United States of America 106*, 38 16108, 2009.

Budrovic, 2004. Z. Budrovic, H. Van Swygenhoven, P. M. Derlet, S. Van Petegem, and B. Schmitt, *Science* **304**, 273, 2004.

Brandl, 2009. Christian Brandl, Peter M. Derlet, and Helena Van Swygenhoven. Strain rates in molecular dynamics simulations of nanocrystalline metals. *Philosophical Magazine*, 89(34-36):3465–3475, 2009.

Vo, 2008. N. Q. Vo, R. S. Averback, P. Bellon, S. Odunuga, and A. Caro. Quantitative description of plastic deformation in nanocrystalline cu: Dislocation glide versus grain boundary sliding. *Phys. Rev. B*, 77:134108, Apr 2008.

DOE sponsored research publications

Journal Publications (1-7 published during current period, 8-9 submitted during current period)

1. *DongWook Lee, Hojin Kim, Alejandro Strachan and Marisol Koslowski, Effect of core energy on mobility in a continuum dislocation model, Physical Review B,* ***83*** *104101, 2011.*
2. *Marisol Koslowski, DongWook Lee and Lei Lei, Role of the grain boundary energetics on the maximum strength of nanocrystalline Nickel, Journal of the Mechanics and Physics of Solids,* **59** 1427-1436, 2011.
3. *Hunter, A., Beyerlein, I., Germann, T. and Koslowski, M. Influence of the stacking fault energy surface on extended partials with a 3D Phase Field Dislocations Model, Physical Review B*, **84** 144108, 2011.
4. Lei Cao and Marisol Koslowski, Effect of microstructural uncertainty on the yield stress of nanocrystalline nickel, Acta Materialia, 61 1413-1420, 2013.
5. Lei Lei, J. L. Marin and M. Koslowski, Phase field modeling of defect initiation and propagation, *Modeling and Simulations in Materials Science and Engineering*, 21 025009, 2013.
6. Hunter, Abigail; Zhang, Ruifeng; Beyerlein, Irene; Germann, Timothy; Koslowski, Marisol, Dependence of equilibrium stacking fault width in fcc metals on the γ-surface, *Modeling and Simulations in Materials Science and Engineering*, 21 025015-025034, 2013.
7. Lei Cao, Abigail Hunter, Irene Beyerlein and Marisol Koslowski, The role of partial mediated slip during quasistatic deformation of nanocrystalline nickel, *Journal of the Mechanics and Physics of Solids,* **78** 415-426, 2015.
8. Yuesong Xie and Marisol Koslowski, Inelastic recovery in nano and ultra fine grained materials, *Journal of the Mechanics and Physics of Solids,* submitted, 2015.
9. Lei Cao and Marisol Koslowski, Rate limited plastic deformation in nanocrystalline nickel, *Journal of Applied Physics*, submitted, 2015.

Presentations

Invited:

1. Marisol Koslowski, Deformation mechanisms in nanocrystalline Ni for MEMS applications, Physical Metallurgy *Gordon Research Conference*, Stonehill College Easton, MA, July 31 - August 5 2011.
2. Strengthening of metals by microstructural constraints, Workshop on Complex dynamics of dislocations, defects and interfaces. Los Alamos National Laboratory, Los Alamos, NM, November 2011.
3. Marisol Koslowski, Strengthening of metals by microstructural constraints, *Plasticity 2012*, San Juan, Puerto Rico, January 3-8 2012.

4. Effect of grain size distribution on the mechanical response of nanocrystalline Ni for MEMS applications, Livermore National Laboratory, Livermore, CA, February 2012.
5. Effect of microstructural uncertainties on the behavior of nanocrystalline metals, Institute of Pure and Applied Mathematics, UCLA, CA, October 2012.
6. Marisol Koslowski, Deformation mechanisms in nano and ultrafine crystalline Nickel, *The Minerals, Metals and Materials Society Annual Meeting*, Lake Buena Vista, FL, March, 2012.
7. Lei Cao and Marisol Koslowski, Uncertainty quantification of yield stress prediction in nanocrystalline Nickel, *The Minerals, Metals and Materials Society Annual Meeting*, Lake Buena Vista, FL, March, 2012.
8. Marisol Koslowski, Adaptive continuum-atomisitc modeling of plasticity, Society of Engineering Science, Atlanta, GA, October 2012.
9. Marisol Koslowski, International Workshop on the Mechanical Behavior of Nanoscale Multilayers, IMDEA Materials Institute in Madrid, Spain, October 1-4, 2013.
10. Marisol Koslowski, (keynote) Materials Research Society, Fall Meeting, Boston, MA, December 1-6, 2013.
11. Marisol Koslowski, International Conference on Processing and Manufacturing of Advances Materials, Las Vegas, NV, Dec 2-6 2013.
12. Effect of microstructural uncertainties on the behavior of nanocrystalline metals, CMCSN Symposium on Microstructure evolution in driven materials systems, Purdue University, West Lafayette, IN, April 2013.
13. Defects in crystalline solids, Physics Seminar, Physics, Purdue University, March 2014.
14. Quantifying the effect of microstructure on the deformation of nanocrystalline metals, ONERA, France. July 2014
15. Rate-limited deformation mechanisms in deformation simulations of nanocrystalline metals, Aeronautics Graduate Seminar, University of Illinois at Urbana Champaign, December 2014.
16. Rate-limited deformation mechanisms in deformation simulations of nanocrystalline metals, Aeronautics Seminar, University of Illinois at Urbana Champaign, December 2014.
17. Rate-limited deformation mechanisms in deformation simulations of nanocrystalline metals, Materials Science Graduate Seminar, University of Illinois at Urbana Champaign, March 2015.

Contributed:

1. Marisol Koslowski, Lei Lei and Dong Wook Lee, Role of Grain Boundary energetics on the Maximum Strength of Nanocrystalline Nickel, *American Society of Mechanical Engineers Applied Mechanics and Materials Conference, McMAT-2011,* Chicago, IL, USA, May 30-June 1 2011.
2. Abigail Hunter, Irene Beyerlein, Tim Germann and Marisol Koslowski, Influence of Stacking Fault Energies on Equilibrium Stacking Fault Widths

Using 3D Phase Field Dislocation Dynamics (PFDD) Simulations, *11th US National Congress on Computational Mechanics*, Minneapolis, MN, July 25-29, 2011.

3. Marisol Koslowski, Lei Lei and DongWook Lee, Role of Grain Boundary and Stacking Fault Energies on the Maximum Strength of Nanocrystalline Nickel, *11th US National Congress on Computational Mechanics*, Minneapolis, MN, July 25-29, 2011.
4. Marisol Koslowski, Strengthening of metals by microstructural constraints, *Workshop on Complex dynamics of dislocations, defects and interfaces*, Los Alamos, NM, November 2011.
5. Lei Lei and Marisol Koslowski, Dislocations in confined volumes, *The Minerals, Metals and Materials Society Annual Meeting*, Lake Buena Vista, FL, March, 2012.
6. Marisol Koslowski and Yuesong Xie, Effects of grain size distribution on plastic strain recovery, *The Minerals, Metals and Materials Society Annual Meeting*, Lake Buena Vista, FL, March, 2012.
7. Yuesong Xie and Marisol Koslowski, A Kinetic Monte Carlo Simulation of Plastic Strain Recovery in Nanocrystalline Materials, *Society of Engineering Science 49th Annual Meeting*, Atlanta, GA, October, 2012.
8. Lei Cao, Hojin Kim, Alejandro Strachan and Marisol Koslowski, Phase-Field Dislocation Dynamics And Connection To Molecular Dynamics, MRS Fall Meeting, Boston, MA, November 2012.
9. Lei Lei, Yuesong Xie, and Marisol Koslowski, Effect of Microstructure on Plastic Strain Recovery, 2012 Materials Research Society Fall Meeting & Exhibit, Boston, MA, November, 2012.
10. Lei Cao, Hojin Kim, Alejandro Strachan and Marisol Koslowski, Atomistically informed dislocation dynamics, *The Minerals, Metals and Materials Society Annual Meeting*, San Antonio, TX, 2013.
11. Marisol Koslowski, Quantifying the effect of microstructure uncertainty on the deformation of nanocrystalline metals, World Congress of Computational Mechanics, Barcelona, Spain, July 2014.
12. Lei Cao and Marisol Koslowski, Achieving low strain rate simulations of nc metals, *Society of Engineering Science 50th Annual Meeting*, West Lafayette, IN, October, 2014.
13. Yuesong Xie and Marisol Koslowski, Local versus average field failure criteria in amorphous polymers, *Society of Engineering Science 50th Annual Meeting*, West Lafayette, IN, October, 2014.
14. Marisol Koslowski, Nano plasticity Laboratory, *Society of Engineering Science 50th Annual Meeting*, West Lafayette, IN, October, 2014.

People working on the project

Yuesong Xie, graduate student, 60% support
Lei Cao, graduate student, 20% support
Yifei Zheng, graduate student, 20% support
Marisol Koslowski, associate professor, 1 month summer salary.

Current and pending support

Current:

1. AFOSR. Real time dynamic measurement and characterization of mesoscale deformation and temperature fields in explosive materials. PI: W. Chen (Purdue), co-PI M. Koslowski, J. Roahds, M. Gonzales, S. Son. Award Amount: $1,327,427. 2014-2017.
2. Glaxo Smith Kline. Solid State amorphization of molecular crystals undergoing milling. PI: M. Koslowski, Award Amount: $51,474. 2015-2016.

Pending:

1. NSF. Controlling stress relaxation in thin films. PI: M. Koslowski, co-PI: C. Handwerker. Award Amount: $477,185
2. NSF. DMREF A materials innovation framework to accelerate the discovery of mismatched semiconductors. PI: M. Koslowski, co-PI: M. Manfra, O. Malis and A. Strachan. Award Amount: $1,470,630
3. DARPA. Value driven uncertainty quantification enabling the design of carbon fiber polymers through multi-physics/scale simulations. PI: I. Billionis (Purdue) Co-PI: M. Koslowski and others. Award Amount: $2,043,206.

Cost Status

The budget for the period 4/15/2011 to 4/15/2015 includes one graduate student for the entire period and 1 summer salary for the PI and travel to conferences. The expenses reach 100% of the budget for the period.