The primary goals of the project are:

(1) To perform the experimental setup and protocol for nanoindentation of polycrystalline Al and Cu thin films under in-plane stress providing fundamental insights into the basic dynamical properties of dislocation plasticity in FCC crystals: microplastic discrete plastic event statistics, microplasticity yield and abruptness dependence on grain orientation, size and strain-rate effects, tension/compression asymmetry, spatial and temporal correlation effects in polycrystal plasticity. Success will be gauged by internal consistency, simplicity, and coherence of the approach, its explanatory power, and the simplicity and clarity with which its predictions are extracted.

The main hypotheses of the project are that:

A. Nanoindentation of grains that are micron-sized and are near in-plane plastic yielding should develop a signature on the absence of the nanoindentation pop-in event. Namely, a small enough grain that is about to plastically yield should not display a plastic “pop-in” event when nano-indented. Since the pop-in event is intrinsically a stochastic event, our investigation is statistical in nature. We aim to show that nanoindentation of micron-sized grains has micropillar-like stochastic features: power-law plastic strain jumps at stresses above the macroscale yield strength, displaying strong size and rate effects.

B. The statistical distribution of pop-in events in micron-sized grains of FCC crystals should show a gradual dependence on in-plane stress, as the crystal approaches the tensile yield point. Our results should be in agreement with the Schmid Rule for FCC metals.

In order for our approach to be accepted by other research groups, we aim to demonstrate the similarity of our results in drastically different FCC metals Cu and Al. We will also report the degree to which our ideas are being accepted and utilized in the plasticity community, by reporting citations and invited talks from experimental and theoretical groups within the fields of mechanics, condensed matter physics and materials science and engineering.

(2) To develop and extend multiscale modeling approaches for our experimental setup, with successful experimental/simulation comparisons, and to facilitate and inspire new simulation tests by others. Discrete Dislocation Plasticity (DDP) simulations aim to provide a wealth of evidence on the ubiquitous nature of abrupt slip events and the patterning features they induce during nanoindentation. We aim to make concrete efforts to characterize the microstructure through the study of misorientation distributions and orientational correlation function that will make contact possible with the real-space features of our experiments.

On the theory side, our success is gauged by the level of generality (in terms of grain orientation and stress levels) with which our Hypotheses A, B will be confirmed or refuted. The possible generality of our studies and strength of our data should be proportional to the number and specificity of predictions we make each year for experiments and microscopic simulations, and the number of experimental and computational colleagues and collaborators we inspire to test our ideas and cite our work.

Our Hypotheses A, B are clearly at the frontier of research in the field of understanding microplastic dynamic phenomena in FCC metals. Proving or refuting either of the two hypotheses should lead to major leaps in the modern understanding of crystal plasticity at the microscale. For example, failure to identify a power-law plastic event regime in nanoindentation (Hypothesis A) should provide new interpretations on micropillar experiments (for example, the surface may ultimately be fully responsible even for power-law distributed plastic events).

(3) To engage talented researchers with interests in solid mechanics, stochastic processes, statistical mechanics and industrial applications. The most tangible measure of success here will be the quality and success of the graduate students and post-doctoral fellows we attract to work in the project, and we will naturally report on this each year.

2. What was accomplished under these goals?

(For the grant period describe: 1) major activities; 2) specific objectives; 3) significant results, including major findings, developments, or conclusions (both positive and negative); and 4) key outcomes or other achievements. Include a discussion of stated goals not met. As the project progresses, the emphasis in reporting in this section should shift from reporting activities to reporting accomplishments.)

During the DOE project (Aug.2015-July.2019), 11 peer-reviewed publications were produced, 6 research members were funded by the project (graduate students, postdocs, faculty), a data library and associated software were produced, and finally, co-PI (prior PI) Papanikolaou accepted an assistant professor position at the West Virginia University (WVU), Mechanical & Aerospace Engineering and officially joined in August 2016. The co-PI Papanikolaou also held an adjunct professor position at JHU-ME during part of the grant period.

During this grant there have been the following major activities:

a. The PI hired three postdoctoral associates during the grant period, Rongguang Xu, Hengxu Song and Hakan Yavas, that have been working on the theory and experimental aspects of the project. Rongguang Xu was employed for 6 months to produce molecular simulations of nanoindentation in 2018. Hengxu Song performed discrete dislocation dynamics simulations throughout the 2 years he was funded by the project. Hakan Yavas worked on the experimental side of the project, preparing samples and producing nanoindentation data in a variety of FCC metals (Ni, Cu, Al, single and poly crystals).

b. The PI recruited one talented Masters WVU graduate student, Ryder Bolin, that intensely worked on this project, since August 2016. Bolin successfully graduated with a WVU Masters degree in July 2018.

c. The PI held monthly visits and conference calls with JHU to connect with his co-PI, postdocs and graduate students throughout the grant period.

c. The co-PI used a large part of his startup fund to acquire a dedicated nanoindentation device, iNano, from Nanomechanics, http://nanomechanicsinc.com/, which was focused solely on this project.

d. The co-PI Papanikolaou had a JHU-Sandia DOE partnership with David

Adams, dpadams@sandia.gov, and Deidre Hirschfeld, dhirsch@sandia.gov at Sandia National Laboratories. David Adams fabricated thin films with characteristic granular microstructure, together with Electron BackScatter Diffraction Maps, that the PI plans to use towards grain orientation mapping and correlation with nanoindentation data. The delivery of samples was done in 2018 and data is still under analysis.

e. The co-PI Papanikolaou had a fruitful collaboration with J. Greer at Caltech, and W. Cai at Stanford U, which delivered two high-impact publications.

f. The co-PI Papanikolaou established a collaboration with I. Groma and P. Ispanovity in Budapest, Hungary, in an effort to cross-validate experimental results.

The primary goals of the project had the following results:

1. The first primary goal was successfully accomplished by manufacturing 2 4-pt bending fixtures that were used to perform in-situ under-tension nanoindentations on a large variety of samples, single and poly crystalline Ni, Cu, Al. Stochastic nanoindentation noise was studied in all FCC materials under study and several dependences, in connection to theoretical discrete dislocation investigations, were identified. Even though 11 publications have been already produced, the correlation of grain type (Rodrigues vectors of incident grain-boundaries) with nanoindentation statistics near associated grain boundaries are still under way and have not yet been completed.

2. The second primary goal has been successful. A minimal model has been developed that consistently predicts in both two and three dimensions the occurence and statistics of pop-in events in FCC metals. The model has been discussed in numerous publications and it has been the focus of the project.

3. The third primary goal has been successful. 1 graduate student, 4 undergraduate students and 3 postdoctoral associates have been trained throughout the project. Collaboration with a DOE-funded national lab (Sandia) and several major researchers has been pursued throughout the project.

During the period there have been the following specific objectives:

a. To build a 4-pt bending fixture that fits the dimensions of the specific nanoindenter device of interest (iNano), which exists now in both JHU and WVU sites.

b. To acquire or/and fabricate high quality polycrystalline thin-film and bulk samples of Cu, Al and other FCC metals (Ni, Pt) with various stacking fault energies.

c. To perform large arrays (~100,000 nanoindentations) on polycrystalline FCC samples of Cu and Al that are under simultaneous bending stresses.

d. To perform Discrete Dislocation Dynamics (DDD) and continuum simulations of indentation and 4-pt bending.

e. To develop an open-source software for analyzing Large Data from nanoindentation measurements.

f. To acquire correlated grain orientation/size and nanoindentation measurements on thin-film and bulk samples of Cu and Al.

g. To acquire a number (6) of computer cluster nodes (=~240 threads), for facilitating DDD simulations.

During the grant period there have been the following significant results:

a. Through a combined simulation and testing study, the PI and his postdocs developed 2 4-pt bending fixtures at two different scales, made of stainless steel, that fit the iNano nanoindenter and can be used to perform in-plane stresses during nanoindentation. One of the devices is large, that can be used to study plasticity in thick (>5mm) samples, while the other one is scaled down and can be only used for thin (<1mm) samples.

b. The PI, H. Yavas, and R. Bolin, installed and calibrated the iNano device at the WVU site in a noise-insulated room, that can now produce high quality and long-time nanoindentation measurements.

c. The PI and H. Song performed intensive two and three dimensional Discrete Dislocation Dynamics simulations that have been used to interpret experimental data.

d. H. Yavas, R. Bolin and the PI performed approximately 1,000,000 nanoindentations to date in various samples of Cu, Al and Ni, of various thicknesses using Berkovich diamond tips. The data have been stored and will become available to other researchers for sharing and analysis purposes some time during the next grant period.

e. The PIs developed an open-source and efficient Python-based software for analyzing experimental nanoindentation data, pop-in events, hardness and stiffness, as function of surface location. The software will become available to other researchers some time during the next grant period.

f. The PIs invented an approach to derive microstructural random yield point distributions from nanoindentation and other avalanche timeseries, using Principal Component Analysis, that was published in npj Computational Materials in 2018.

g. H. Yavas, the PI, H. Song and K. Hemker (co-PI) discovered a novel hardness size effect in simulations and experiments (Al) that takes place under 20nm indentation depth, and distinguished in-plane elastic from plastic behavior. If we and other groups confirm the existence of this transition, it should lead to a novel mechanical spectroscopy tool using nanoindentation. This result is under submission status to Scripta Materialia. We currently investigate also Cu and Ni samples in order to confirm the existence of the transition.

h. H. Song, the PI, H. Yavas, and E. Van der Giessen investigated in detail, using load control and displacement control, the collective aspects of nanoindentation in 2D-DDD simulations. We discovered the aforementioned hardness transition as function of in-plane applied stress and have also characterized the aspects of the crackling noise that is prevalent in nanoindentation loading. This manuscript is being submitted to Journal of Mechanics and Physics of Solids. We currently investigate how our results generalize in 3D-DDD, using the open-source code of N. Ghoniem at UCLA.

i. The co-PI Papanikolaou lead-authored a review on avalanches and flow in crystal plasticity. The co-authors are Y. Cui and N. Ghoniem. The manuscript was published in MSMSE in 2018.

j. The PI co-authored with X. Ni and J. Greer (Caltech) a publication in Physical Review Letters that can help experimenters to detect plastic events that lie beneath the machine noise.

k. The PI co-developed with W. Cai (Stanford) a coarse-grained DDD approach,

labeled as Geometrically Projected Discrete Dislocation Dynamics, which is at least 1000 times faster than typical DDD approaches. The manuscript was published in MSMSE in 2018.

In total, the following 11 publications are results of the project, in major, peer-reviewed journals:

1. M. Tzimas, J. Michopoulos, G. Po, A. Reid, S. Papanikolaou, Inference and Prediction of Nanoindentation Response in FCC crystals: Methods and Discrete Dislocation Simulation Examples (to appear)
2. H. Song, D. M. Dimiduk, S. Papanikolaou, Universality Class of Nanocrystal Plasticity: Localization and Self-Organization in Discrete Dislocation Dynamics, Phys. Rev. Letters, 122, 178001 (2019), arXiv:1810.11964
3. P. Ispanovity, S. Papanikolaou, I. Groma, The emergence of Dipolar Dislocation Walls in Discrete and Continuum Theory Formulations, to appear in Phys.Rev.E (2019)), arxiv1711.0818
4. H. Yavas, H. Song, K. J. Hemker, S. Papanikolaou, Detecting in-plane tension induced crystal plasticity transition withnanoindentation, (to appear Crystals (2019)),arXiv:1704.0818
5. H. Song, H. Yavas, E. van der Giessen, S. Papanikolaou, Discrete Dislocation Dynamics Simulations of Nanoindentation withPre-stress: Hardness and Statistics of Abrupt Plastic Events, J. Mech. Phys. Solids,123, 332 (2019), arXiv:1707.03915
6. Sh. Akhondzadeh, R. B. Sills, S. Papanikolaou, E. Van der Giessen, and W. Cai, Geometrically projected discrete dislocation dynamics, Modelling Simul. Mater. Sci. Eng. 26 065011 (2018), arXiv:1804.0818
7. S. Papanikolaou, Learning local, quenched disorder distributions in plasticity and other crackling noise phenomena, NPJ Computational Materials 4, 1-7, (2018), arXiv:1806.0818
8. H. Swan, W. Choi, S. Papanikolaou, M. Bierbaum, Y. S. Chen, J. P. Sethna, "Irregularization" of Systems of Conservation Laws, Materials Theory 2, 5 (2018), arXiv: 1506.05743
9. S. Papanikolaou, Y. Cui, N. Ghoniem, Avalanches and Plastic Flow in Crystal Plasticity: An Overview, Modelling and Simulation in Materials Science and Engineering 26, no. 1 (2017): 013001, arXiv:1710.0818
10. X. Ni, S. Papanikolaou, G. Vajente, R. X Adhikari, and J. R Greer, Probing microplasticity in small-scale fcc crystals via dynamic mechanical analysis, Physical reviewletters 118, no. 15 (2017): 155501, arXiv:1612.09011
11. S. Papanikolaou, H. Song, E. Van der Giessen, Obstacles and sources in dislocation dynamics: Strengthening andstatistics of abrupt plastic events in nanopillar compression, Journal of the Mechanics andPhysics of Solids 102 (2017): 17-29, arXiv:1511.04613

During the grant period there have been the following key outcomes and other accomplishments:

During the grant period there was a stated goal of performing grain orientation

measurements and correlate them with nanoindentation measurements. This goal was not met in the grant period, besides the intense efforts of the PI towards establishing collaborations with experts in large scale EBSD measurements. We expect that this goal will be met in the next grant period. Furthermore, the goal of acquiring computer nodes has not yet met, since the PI moved from JHU to WVU. The PI established a sub-contract to WVU, effective May 1st 2017, which should provide him the capability to acquire 3 multi-threaded workstations (~230 threads) that will facilitate the efficient identification of 3D dislocation mechanisms during nanoindentation under external in-plane stress. It will also provide him the capacity to fund the Masters of the graduate student R. Bolin.

There are several efforts that facilitated the accomplishment of our goals and objectives in the next grant period:

a. The PIs collaborated and co-authored a publication with P. Ispanovity and I. Groma on a constitutive formulation of dipolar dislocation walls that emerge during fatigue in metals.

b. The PIs developed ongoing collaborations in a sequence of related efforts, in deep relation to this project, with a number of esteemed colleagues: D. Dimiduk, C. F. Woodward, N. Ghoniem, I. Groma, J. Greer, W. Cai, E. Van der Giessen and F. Roters.

c. The PIs pursued heavily the identification of a novel-identified hardness transition for other FCC metals, such as Ni and Cu, and using various hardness measurement approaches. The PIs performed 2D-DDD and 3D-DDD simulations, in order to understand in detail the fundamental origin of the transition and whether it can be utilized for technological purposes.

d. David Adams at Sandia National Labs, produced high quality thin films with EBSD grain orientation maps, for polycrystalline Ni, Al and Cu, for the project. The samples have been tested and there are more works underway, with correlations between grain orientation and grain size with nanoindentation hardness and pop-in events as function of in-plane stresses. The completion of these experiments and data analysis is projected in 2020.

e. The co-PI Papanikolaou acquired 4 multi-core workstations at WVU, in order to facilitate code development and high-throughput data analysis using 2D-DDD, 3D-DDD simulations and experimental data.

f. The PIs developed an Open-Source software and experimental data library, and made it available online to the research community.

g. The PIs applied novel Machine Learning (ML) approaches into nanoindentation pop-in timeseries data in order to extract the statistical dislocation microstructure of Frank Read sources.

Report only the major publication(s) resulting from the work under this award. There is no restriction on the number. However, agencies are interested in only those publications that most reflect the work under this award in the following categories:
Journal publications. List peer-reviewed articles or papers appearing in scientific, technical, or professional journals. Include any peer-reviewed publication in the periodically published proceedings of a scientific society, a conference, or the like. A publication in the proceedings of a one-time conference, not part of a series, should be reported under "Books or other non-periodical, one-time publications." Identify for each publication: Author(s); title; journal; volume: year; page numbers; status of publication (published; accepted, awaiting publication; submitted, under review; other); acknowledgement of federal support (yes/no).

Main Journal Publications:

1. M. Tzimas, J. Michopoulos, G. Po, A. Reid, S. Papanikolaou, Inference and Prediction of Nanoindentation Response in FCC crystals: Methods and Discrete Dislocation Simulation Examples (to appear)
2. H. Song, D. M. Dimiduk, S. Papanikolaou, Universality Class of Nanocrystal Plasticity: Localization and Self-Organization in Discrete Dislocation Dynamics, Phys. Rev. Letters, 122, 178001 (2019), arXiv:1810.11964
3. H. Yavas, H. Song, K. J. Hemker, S. Papanikolaou, Detecting in-plane tension induced crystal plasticity transition withnanoindentation, (to appear Crystals (2019)),arXiv:1704.0818
4. H. Song, H. Yavas, E. van der Giessen, S. Papanikolaou, Discrete Dislocation Dynamics Simulations of Nanoindentation withPre-stress: Hardness and Statistics of Abrupt Plastic Events, J. Mech. Phys. Solids,123, 332 (2019), arXiv:1707.03915
5. S. Papanikolaou, Learning local, quenched disorder distributions in plasticity and other crackling noise phenomena, NPJ Computational Materials 4, 1-7, (2018), arXiv:1806.0818
6. H. Swan, W. Choi, S. Papanikolaou, M. Bierbaum, Y. S. Chen, J. P. Sethna, "Irregularization" of Systems of Conservation Laws, Materials Theory 2, 5 (2018), arXiv: 1506.05743
7. S. Papanikolaou, Y. Cui, N. Ghoniem, Avalanches and Plastic Flow in Crystal Plasticity: An Overview, Modelling and Simulation in Materials Science and Engineering 26, no. 1 (2017): 013001, arXiv:1710.0818

Other publications, conference papers and presentations:
Identify any other publications, conference papers and/or presentations not reported above. Specify the status of the publication as noted above:

1. Xiaoyue Ni, Stefanos Papanikolaou, Gabriele Vajente, Rana X Adhikari, and Julia R. Greer, Probing Microplasticity in Small-Scale FCC Crystals via Dynamic Mechanical Analysis, Phys. Rev. Lett. 118, 155501 (2017) acknowledgement of federal support (yes)
2. Papanikolaou, S., Song, H. and Van der Giessen, E., 2017. Obstacles and sources in dislocation dynamics: Strengthening and statistics of abrupt plastic events in nanopillar compression. Journal of the Mechanics and Physics of Solids, 102, pp.17-29. acknowledgement of federal support (yes)
3. P. Ispanovity, S. Papanikolaou, I. Groma, Dipolar Dislocation Walls in Continuum Plasticity, to be submitted to Physical Review Letters.
4. Sh. Akhondzadeh, R. B. Sills, S. Papanikolaou, E. Van der Giessen, and W. Cai, Geometrically projected discrete dislocation dynamics, Modelling Simul. Mater. Sci. Eng. 26 065011 (2018), arXiv:1804.0818

Other significant products that have been developed under this project:

1. NanoIndentAnalyze Python Library for Data Analysis of experimental Indentation Data. Open-Source, shared through GitHub.
2. Nanoindentation Database of raw Load Depth Indentation and Imaging Data. Open-source, shared through Globus.

3. What opportunities for training and professional development has the project

provided?

(Describe opportunities for training and professional development provided to anyone who worked on the project or anyone who was involved in the activities supported by the project. .“Training” activities are those in which individuals with advanced professional skills and experience assist others in attaining greater proficiency. Training activities may include, for example, courses or one-on-one work with a mentor. “Professional development” activities result in increased knowledge or skill in one’s area of expertise and may include workshops, conferences, seminars, study groups, and individual study. Include participation in conferences, workshops, and seminars not listed under major activities.)

During the grant period, there have been employed by the PI four young researchers, the graduate student R. Bolin at WVU (MS, 2018), as well as postdocs H. Yavas and H. Song, R. Xu. The following opportunities have been provided by the project during the grant period:

1. The PI organized a symposium on “Stochastic Aspects in Crystal Plasticity and Soft Matter” in the International Plasticity Conference at Puerto de Vallarta, Mexico, in January of 2017. The symposium attracted 15 internationally known researchers that helped the professional development of the PI.
2. The PI was an invited speaker in the Science & Engineering Society Conference in Bethesda, MD, in September 2016.
3. The PI was an invited speaker in a dedicated workshop on “Dislocation Plasticity Challenges” in Lugano, Switzerland, in February 2017.
4. The student R. Bolin was mentored by the PI, and has become proficient in the use of the nanoindentation equipment and scanning electron microscopy, as well as in the use of Python and general programming.
5. The postdoctoral associate Hakan Yavas participated in the American Physical Society March Meeting in New Orleans, Louisiana and also in the Materials Research Society Spring Meeting in Phoenix, Arizona in April 2017, giving contributed talks.
6. The PI and the postdoctoral associate Hakan Yavas have been pursuing the publication of a book on Nanoindentation Use for Mechanical Spectroscopy.
7. The postdoctoral associate Hakan Yavas has been mentored by the PI in using programming languages and Python for performing Data Science in nanoindentation measurements. He has also been mentored by the co-PI Hemker in general experimental techniques.
8. The postdoctoral associate Hengxu Song participated in the Materials Research Society Spring Meeting in Phoenix, Arizona in April 2017, giving a contributed talk.
9. The postdoctoral associate Hengxu Song and the PI visited UCLA for 10 days and were mentored by N. Ghoniem in using his open-source 3D-DDD software, and modifying the code (written in C++).

10.In the years 2016-2019, co-PI Papanikolaou gave a number of presentations on this project:

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16. X Brazilian Meeting on Simulational Physics, Ouro Preto, Brazil, July 2019
Complexity, Topology and Elastic Instabilities in Dislocation Ensembles
15. Eotvos University, Budapest, Hungary, June 2018
From Micropillars to Macroscale Plasticity: What can we learn from the noise?

14. D'Alembert Institute, Paris, France, June, 2018
From Micropillars to Macroscale Plasticity: What can we learn from the noise?
13. ICACM Workshop, Paris, France, June, 2018
From Micropillars to Macroscale Plasticity Studies.
12. Norditta Workshop on Materials, Stockholm, Sweden, May, 2018
Avalanche Oscillators and Micropillar Compression Experiments.
11. MRS Conference, Phoenix, AZ, April, 2018
Inferring quenched disorder plasticity distributions.
10. George Washington University, Department of Mechanical Engineer- ing, Nov. 2017
From nanoindentation to microcrystal plasticity.
9. University of Grenoble, Grenoble, France, June 2017
Detecting the crystal plasticity transition using nanoindentation probes.
8. ICF14, Rhodes, Greece, June 2017
Competition of length scales in notch-initiated fracture for metals with structural disorder
7. Dislocations Challenges Workshop, Lugano, Switzerland, Feb.2017
The Crystal Plasticity Transition: From Dislocation Dynamics to Continuum Modeling
6. SES 2016, Bethesda, MD, 2016
Multiscale Modeling and vibrational character of maximally dense frictional disks under shear
5. ECCOMAS 2016, Crete, Greece, June 2016
Size effects and stochastic plastic flow in uniaxial crystal compression: a minimal discrete dislocation model
4. University of Kentucky, Department of Mechanical Engineering, William Maxwell Reed Seminar, Feb. 2016
Size effects and stochastic plastic events in uniaxial crystal compression: a minimal discrete dislocation model
3. University of Illinois, Department of Mechanical Science and Engineering, Feb. 2016
Size effects and stochastic plastic events in uniaxial crystal compression: a minimal discrete dislocation model
2. George Mason University, Department of Computational and Data Sciences, Jan. 2016
Size effects and stochastic plastic events in uniaxial crystal compression: a minimal discrete dislocation model
1. International Plasticity Conference, Kona, HI, Jan.2016
Size effects and stochastic plastic events in uniaxial crystal compression: a minimal discrete dislocation model

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11. In addition, the following symposia were co-organized by the co-PI Papanikolaou on the topic of the grant:

A. WCCM, NY, 2018, 12 speakers.

B. MMM, Osaka, Japan, 2018, 16 speakers.

C. APS March Meeting Focus Session, Los Angeles, CA, 2018, 11 speakers.

D. IJP Plasticity Conference, Mexico, 2017, 13 speakers.

4. How have the results been disseminated to communities of interest?

(Describe how the results have been disseminated to communities of interest. Include any outreach activities that have been undertaken to reach members of communities who are not usually aware of these research activities, for the purpose of enhancing public understanding and increasing interest in learning and careers in science, technology, and the humanities.)

1. An open-source Python-based software has become available to experimenters in order to analyze experimental nanoindentation data, as well as other mechanical engineering experimental data.
2. A library of nanoindentation experimental and simulation raw data has become become available through Globus.

In addition, data and related information is included in the main journal publications:
1. M. Tzimas, J. Michopoulos, G. Po, A. Reid, S. Papanikolaou, Inference and Prediction of Nanoindentation Response in FCC crystals: Methods and Discrete Dislocation Simulation Examples (to appear)
2. H. Song, D. M. Dimiduk, S. Papanikolaou, Universality Class of Nanocrystal Plasticity: Localization and Self-Organization in Discrete Dislocation Dynamics, Phys. Rev. Letters, 122, 178001 (2019), arXiv:1810.11964
3. H. Yavas, H. Song, K. J. Hemker, S. Papanikolaou, Detecting in-plane tension induced crystal plasticity transition withnanoindentation, (to appear Crystals (2019)),arXiv:1704.0818
4. H. Song, H. Yavas, E. van der Giessen, S. Papanikolaou, Discrete Dislocation Dynamics Simulations of Nanoindentation withPre-stress: Hardness and Statistics of Abrupt Plastic Events, J. Mech. Phys. Solids,123, 332 (2019), arXiv:1707.03915
5. S. Papanikolaou, Learning local, quenched disorder distributions in plasticity and other crackling noise phenomena, NPJ Computational Materials 4, 1-7, (2018), arXiv:1806.0818
6. H. Swan, W. Choi, S. Papanikolaou, M. Bierbaum, Y. S. Chen, J. P. Sethna, "Irregularization" of Systems of Conservation Laws, Materials Theory 2, 5 (2018), arXiv: 1506.05743
7. S. Papanikolaou, Y. Cui, N. Ghoniem, Avalanches and Plastic Flow in Crystal Plasticity: An Overview, Modelling and Simulation in Materials Science and Engineering 26, no. 1 (2017): 013001, arXiv:1710.0818

5. What do you plan to do during the next grant period to accomplish the goals?

(Describe briefly what you plan to do during the next grant period to accomplish the goals and objectives.)

N/A -- Current Final Report.

3. Technologies or Techniques

Identify technologies or techniques that have resulted from the research activities. Describe the technologies or techniques and how they are being shared.

IV. Participants & Other Collaborations: Mandatory

During this reporting 2016-2019 period, the individuals that have worked on the project

are:
1) Name: Rongguang Xu
2) Project Role: Postdoctoral associate
3) Nearest person month worked: 6
4) Contribution to Project: Dr. Xu has performed work in the area of molecular dynamics simulations for nanoindentation and crystal plasticity.
6) Collaborated with individual in foreign country: No
7) Country(ies) of foreign collaborator: N/A
8) Travelled to foreign country: No

1) Name: Hengxu Song
2) Project Role: Postdoctoral associate
3) Nearest person month worked: 24
4) Contribution to Project: Dr. Song has performed work in the area of dislocation dynamics simulations and crystal plasticity theory.
6) Collaborated with individual in foreign country: Yes
7) Country(ies) of foreign collaborator: Netherlands
8) Travelled to foreign country: No

1) Name: Hakan Yavas
2) Project Role: Postdoctoral Associate
3) Nearest person month worked: 10
4) Contribution to Project: Mr. Yavas has performed work in the area of experimental nanoindentation and data analysis.
6) Collaborated with individual in foreign country: No
8) Travelled to foreign country: No

1) Name: Ryder Bolin
2) Project Role: WVU Graduate with Masters in Mechanical Engineering
3) Nearest person month worked: 20
4) Contribution to Project: Mr. Bolin performed work in the area of experimental nanoindentation and data analysis.
5) Funding Support: WVU Start-Up fund for PI Papanikolaou.
6) Collaborated with individual in foreign country: No.
8) Travelled to foreign country: No

1) Name: Stefanos Papanikolaou
2) Project Role: co-Principal Investigator
3) Nearest person month worked: 2
4) Contribution to Project: Mr. Papanikolaou has performed work in the area of theory and experiments on nanoindentation.
5) Funding Support: WVU Start-Up fund.
6) Collaborated with individual in foreign country: Yes
7) Country(ies) of foreign collaborator: Hungary, Netherlands, Germany
8) Travelled to foreign country: Yes
9) If traveled to foreign country(ies), duration of stay: 1 months

1) Name: Kevin Hemker
2) Project Role: Principal Investigator
3) Nearest person month worked: 0.5
4) Contribution to Project: Dr. Hemker has provided overall advice and suggestions to the other members of the project.
6) Collaborated with individual in foreign country: No

2. Partners:
What other organizations have been involved as partners?
(Describe partner organizations – academic institutions, other nonprofits, industrial or commercial firms, state or local governments, schools or school systems, or other organizations (foreign or domestic) – that have been involved with the project. Partner organizations may provide financial or in-kind support, supply facilities or equipment, collaborate in the research, exchange personnel, or otherwise contribute. Provide the following information for each partnership:

1) Organization Name: Sandia National Laboratory
2) Location of Organization: Albucquerque, NM
3) Develop thin films and perform EBSD measurements.
7) Collaborative research: David Adams collaborates with Papanikolaou
9) More detail on partner and contribution: Materials Science for developing indentation-specific granular microstructure in FCC metals, for efficient statistical sampling.

1) Organization Name: Ames National Lab
2) Location of Organization: Ames, Iowa
3) Develop thin films and perform EBSD measurements.
7) Collaborative research: Matt Besser collaborates with Papanikolaou
9) More detail on partner and contribution: Materials Science for developing indentation-specific granular microstructure in FCC metals, for efficient statistical sampling.

1) Organization Name: Carnegie Mellon University
2) Location of Organization: Pittsburgh, PA
3) Perform EBSD measurements.
7) Collaborative research: Yoosuf Picard collaborates with Papanikolaou
9) More detail on partner and contribution: Materials Science for developing indentation-specific granular microstructure in FCC metals and EBSD grain orientation mapping, for efficient statistical sampling and correlation between indentation and grain orientation measurements.

3. Other Collaborators:
Have other collaborators or contacts been involved?
(Some significant collaborators or contacts within the recipient's organization may not be covered by "What people have worked on the project?" Likewise, some significant collaborators or contacts outside the recipient's organization may not be covered under "What other organizations have been involved as partners?" For example, describe any significant: collaborations with others within the recipient's organization; especially interdepartmental or interdisciplinary collaborations; collaborations or contact with others outside the organization; and collaborations or contacts with others outside the United States or with an international organization, country(ies) of collaborations or contacts. It is likely that many recipients will have no other collaborators or contacts to report.)

1. Erik Van der Giessen, University of Groningen, Netherlands
2. Peter Ispanovity and Istvan Groma, Eotvos University, Hungary
3. Wei Cai, Stanford University, USA
4. Julia Greer, California Institute of Technology, USA
5. Nasr Ghoniem, University of California, Los Angeles, USA
6. Giacomo Po, University of Miami, Florida, USA

V. IMPACT: Optional (but strongly encouraged)
What is the impact of the project? How has it contributed?

The impact of the project can be summarized in three main domains:

1. First, on the basic materials science of pop-in events, nanoindentation noise in FCC metals at small indentation depths less than 200nm: Through this project, it has become clear that the noisy nanoindentation response at the ultra-nano regime is characteristic of the crystalline structure and follows a statistical distribution that has significant dependence on grain orientation and applied tensile stress. For the first time, analogies of nanoindentation and uniaxial micropillar compression size effects have been drawn in the context of an explicit minimal discrete dislocation dynamics model, demonstrating cross-slip relaxation and dislocation-drag effects into the statistical behavior of pop-in events. The ideas and perspectives developed in the project will have a strong, long-lasting influence in the materials science and mechanics communities.

2. Second, on the use of in-situ loads to manipulate and control nanoindentation response at submicron indentation depths: Through this project, the character of the ultra-nano-mechanical indentation response has been elucidated at levels never studied in the past. In particular, the application of tensile stress has shown that the nanoindentation response at ultra-small depths strongly depends on the applied stress in a way that was described by constitutive models of geometrically necessary dislocation densities, that were benchmarked by discrete dislocation modeling.

3. Third, on the data sharing and analysis in micromechanics: Through this project, the first library of raw nanoindentation data for copper, nickel and aluminum samples has been created. The library contains analysis files and tutorials, for the purpose of exploring datasets using personal computing facilities.

1. What is the impact on the development of the principal discipline(s) of the project?
(Describe how findings, results, and techniques that were developed or extended, or other products from the project made an impact or are likely to make an impact on the base of knowledge, theory, and research and/or pedagogical methods in the principal disciplinary field(s) of the project. Summarize using language that an intelligent lay audience can understand (Scientific American style). How the field or discipline is defined is not as important as covering the impact the work has had on knowledge and technique. Make the best distinction possible, for example, by using a "field" or "discipline", if appropriate, that corresponds with a single academic department (i.e., physics rather than nuclear physics).)

The principal discipline of the project is that of materials science. The impact on the

development of materials science has been significant, given that the basic materials science of pop-in events in FCC metals has been unveiled. It has become clear that the noisy nanoindentation response at the ultra-nano regime is characteristic of the crystalline structure and follows a statistical distribution that has significant dependence on grain orientation and applied tensile stress. For the first time, analogies of nanoindentation and uniaxial micropillar compression size effects have been drawn in the context of an explicit minimal discrete dislocation dynamics model. The ideas and perspectives developed in the project will have a strong, long-lasting influence in the materials science and mechanics communities.

2. What is the impact on other disciplines?

(Describe how the findings, results, or techniques that were developed or improved, or other products from the project made an impact or are likely to make an impact on other disciplines.)

Associated disciplines of the project are those of micromechanics, physics and data science.

The impact on micromechanics has been significant given that the use of in-situ loads to manipulate and control nanoindentation response at submicron indentation depths. the character of the ultra-nano-mechanical indentation response has been elucidated at levels never studied in the past. In particular, the application of tensile stress has shown that the nanoindentation response at ultra-small depths strongly depends on the applied stress in a way that was described by constitutive models of geometrically necessary dislocation densities, that were benchmarked by discrete dislocation modeling.

The impact on physics has been significant given the basic materials science of pop-in events, nanoindentation noise in FCC metals at small indentation depths less than 200nm. It has become clear that the noisy nanoindentation response at the ultra-nano regime is characteristic of the crystalline structure and follows a statistical distribution that has significant dependence on grain orientation and applied tensile stress. For the first time, analogies of nanoindentation and uniaxial micropillar compression size effects have been drawn in the context of an explicit minimal discrete dislocation dynamics model. The ideas and perspectives developed in the project will have a strong, long-lasting influence in the materials science and mechanics communities.

The impact on data science has been significant given that the data sharing and analysis in micromechanics. The first library of raw nanoindentation data for copper, nickel and aluminum samples has been created. The library contains analysis files and tutorials, for the purpose of exploring datasets using personal computing facilities.

3. What is the impact on the development of human resources?

(Describe how the project made an impact or is likely to make an impact on human resource development in science, engineering, and technology. For example, how has the project: provided opportunities for research and teaching in the relevant fields; improved the performance, skills, or attitudes of members of underrepresented groups that will improve their access to or retention in research, teaching, or other related professions; developed and disseminated new educational materials or provided scholarships; or provided exposure to science and technology for practitioners, teachers, young people, or other members of the public?)

The project employed three postdoctoral associated that have successfully landed jobs in academic jobs and the materials engineering industry. In addition, the innovational

approaches of the project have attracted the interest of undergraduate students in the Appalachian region of West Virginia towards materials science and research.

VI. CHANGES/PROBLEMS: Optional (but strongly encouraged); Carryover Amount Mandatory

(The PI is reminded that the grantee is required to obtain prior written approval from the Contracting Officer whenever there are significant changes in the project or its direction. Requests for prior written approval must be submitted to the Contracting Officer (submission via Fedconnect is acceptable). If not previously reported in writing, provide the following additional information, if applicable: Changes in approach and reasons for change; Actual or anticipated problems or delays and actions or plans to resolve them; Changes that have a significant impact on expenditures; Significant changes in use or care of animals, human subjects, and/or biohazards.)

1. Changes in approach and reasons for change

(Describe any changes in approach during the grant period and reasons for these changes. Remember that significant changes in objectives and scope require prior approval of the agency.)

During the grant period, the PI Papanikolaou accepted an assistant professor position at The West Virginia University, Mechanical and Aerospace Engineering and Physics Departments. Furthermore, last grant period, no postdoctoral associate was hired. For this purpose, it was decided that two talented postdoctoral associates were hired during the grant period, as well as a graduate student. This is a change of approach (only one postdoctoral associate was originally budgeted), which nevertheless facilitated greatly the smooth transition of the PI without significantly influencing the performance of the project.

2. Actual or anticipated problems or delays and actions or plans to resolve them

(Describe problems or delays encountered during the grant period and actions or plans to resolve them.)

During the grant period, there has been an ongoing hurdle of the PIs to get access to high quality samples and EBSD grain orientation maps. The PIs decided to partner with experts in DOE national labs (Sandia), with the hope of long-standing partnerships in the years to come. These partnerships delivered during the grant period. Furthermore, data sharing is largely absent in the nanoindentation and nanomechanics community, which makes reproducibility of experimental data very rare. A fully online library and associated software to promote raw data sharing in the community is being developed.

3. Changes that have a significant impact on expenditures

(Describe changes during the grant period that may have a significant impact on expenditures, for example, delays in hiring staff or favorable developments that enable meeting objectives at less cost than anticipated.)

The move of Papanikolaou from JHU to WVU have caused various changes in expenditures:

1. The postdoctoral associate hire was delayed to the grant period.
2. Two postdoctoral associates were hired instead of one.
3. The co-PI Papanikolaou used a significant amount of start-up funds at his new position for travel and experimental equipment and samples, since the contract had remained at JHU during the grant period.

5. Change of primary performance site location from that originally proposed

(Identify any change to the primary performance site location identified in the proposal, as originally submitted.)

The primary performance site location changed from JHU to WVU, effective on July 1st 2017. A subcontract, in agreement with the Contracting Officer, facilitated the change of the primary performance site location.

6. Carryover amount

(Provide an estimate of the carryover amount expected at the grant period end date.)

N/A

VII. DEMOGRAPHIC INFORMATION: Mandatory (providing email addresses)

Provide email addresses for each participant listed in the participant section of this report. Once you submit this report, PAMS will send the participants not registered in PAMS an email inviting them to register and complete their PAMS person profiles so that any demographic information provided can be collected. Entering demographic information is optional for participants. Demographics are collected for reporting purposes.

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