ArvinMed International

Journal of Nanomedicine, Nanoscience and Technology

JNNT

Research Article

Mitra M. J Nanom Nanos Tech : JNNT : 106

Grain Boundary and Dislocation Mediated Deformation Mechanisms in Nanocrvstalline Metals

Manu Mitra*

Alumnus of University of Bridgeport, Department of Electrical Engineering, US

***Corresponding author:** Manu Mitra, Alumnus of University of Bridgeport, Department of Electrical Engineering, US. Email: mmitra@my.bridgeport.edu

Citation: Mitra M (2019) Grain Boundary and Dislocation Mediated Deformation Mechanisms in Nanocrystalline Metals. J Nanom Nanos Tech: JNNT-106.

Received Date: 08 February, 2019; **Accepted Date:** 18 February, 2019; **Published Date:** 26 February, 2019

Abstract

Nanocrystalline metals performance of defects and mechanisms of plastic deformation and conventional polycrystalline are completely divergent in behavior and its performance.

This paper discusses about grain boundary and dislocation mediated deformation mechanisms in nanocrystalline metals. The plots are for burger vectors of single value, Gaussian and uniform characteristics considering various parameters such as elastic constants, plasticity, loading condition and uncertainty quantification.

Keyword Terms: Grain boundary, nanocrystalline metals, deformation, Burger vectors

Introduction

Grain boundary scattering and doping impurities escalates electrical resistivity of nanocrystalline materials [1]. In stress fields of grain boundary sources and concentrators, various mechanisms of plastic deformation work including generation of deformation twins, dislocation emission from grain boundary, transformation, decay and grain boundary migration [2]. Brittle and ductile process in nanocrystalline metallic materials are inclined by their structural features such as large amounts of grain boundaries and nanoscale sizes of grains. In specific, grain boundaries serve as preferable place because of nucleation and growth; atomic density is low and interatomic bonds are weak at grain boundaries in comparison to the grain interior [3].

Literature Review

One way to avoid overlapping grain problem is to define nanostructured metal foils by sputter deposition. The film thickness can be controlled in sputtering process. Alternatively, columnar grains can be attained, which can give some understanding in bulk deformation mechanisms [4].

Device Simulation

A simulation was performed for competing grain boundary and dislocation mediated deformation in nanocrystalline metals [5].

Grain Boundary and dislocation deformation in nanocrystalline metals with Burger Vector for Single Value

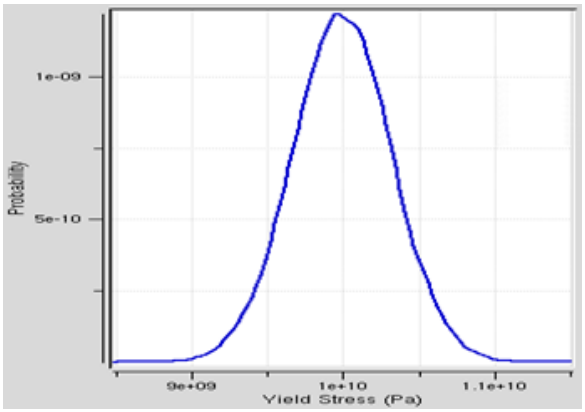

Figure 1: Illustrates Yield Stress (Pa) vs Probability for Burger vector single value.

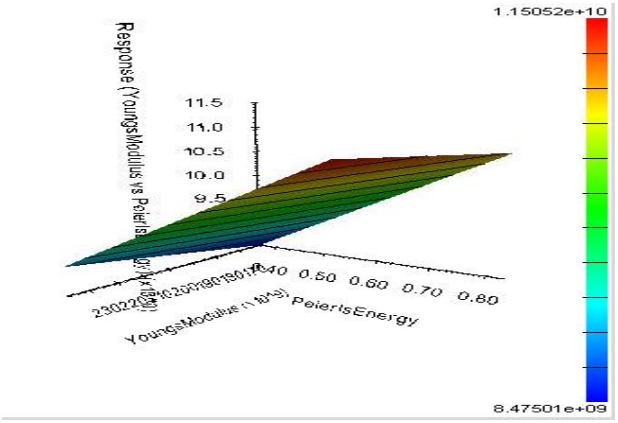

Figure 2: Illustrates Response (Young's Modulus vs Peierls Energy) for Burger vector single value

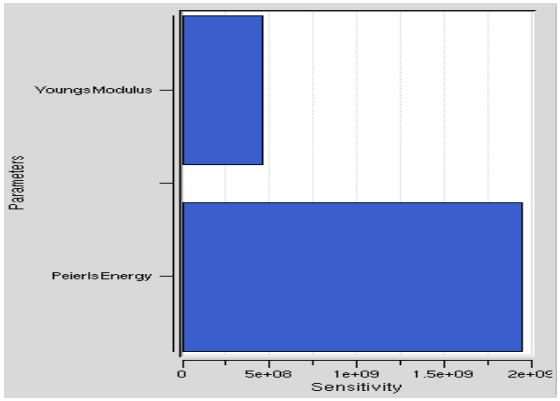

Figure 3: Illustrates Sensitivity (Sensitivity vs Parameters) for Burger vector single value

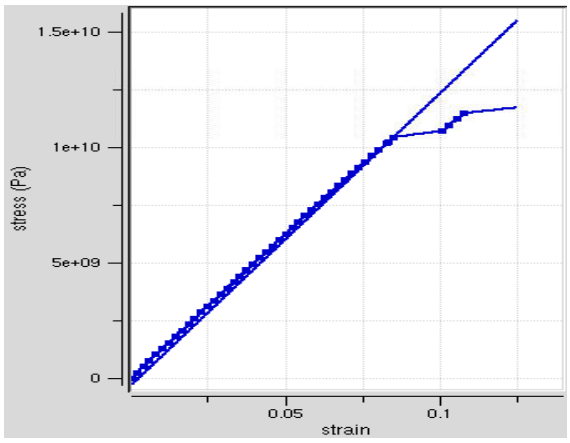

Figure 4: Illustrates Stress-strain curves for Burger vector single value.

TABLE 1
SIMULATION NOMENCLATURE FOR BURGER VECTOR AS SINGLE VALUE

Sl No:	Simulation Specifications	Value
1	Burger Vector	Single Value
2	Burger Vector	0.25nm
3	d1	32

TABLE 2
SIMULATION NOMENCLATURE FOR ELASTIC CONSTANTS FOR BURGER VALUE AS SINGLE VALUE

Sl No:	Simulation Specifications	Value
1	Source	Custom
2	Young's modulus	Gaussian
3	Deviation	10GPa
4	Poisson's ratio	Single Value
5	Poisson's ratio	0.3

TABLE 3
SIMULATION NOMENCLATURE FOR PLASTICITY FOR BURGER VALUE AS SINGLE VALUE

Sl No:	Plasticity	Value
1	Dislocation Glide: Peierl's Energy Barrier (J/m^2)	Gaussian
2	Mean	0.6
3	Deviation	0.06
4	Grain Boundary Sliding: Energy Barrier (J/m^2)	Single Value
5	Energy	0.5

TABLE 4
SIMULATION NOMENCLATURE FOR LOADING CONDITIONS FOR BURGER VALUE AS SINGLE VALUE

Sl No:	Loading Conditions	Value
1	Stress Scaling Factor	1.0
2	Maximum Strain	0.5

TABLE 5
SIMULATION NOMENCLATURE FOR UNCERTAINTY QUALIFICATION FOR BURGER VALUE AS SINGLE VALUE

Sl No:	Uncertainty Qualification	Value
1	Method	Smolyak+Polynomial Chaos with Legendre basis functions
2	Degree of polynomial expansion	1

Observations for Burger Vector as Single Value

- Maximum value for yield of stress is 1.23236e-09 @ 1.00113e+10Pa
- Response (Young's Modulus vs Peierls Energy) for Burger vector single value has been plotted
- Sensitivity is 4.58116e+08 @ Young's Modulus and 1.94019e+09 @ Peierls Energy
- Highest peak for stress-strain curves are 0.2% offset line 1.55115e+10Pa @0.124662 and interpolated 1.17234e+10Pa @ 0.124662

Grain Boundary and dislocation deformation in nanocrystalline metals with Burger Vector Gaussian

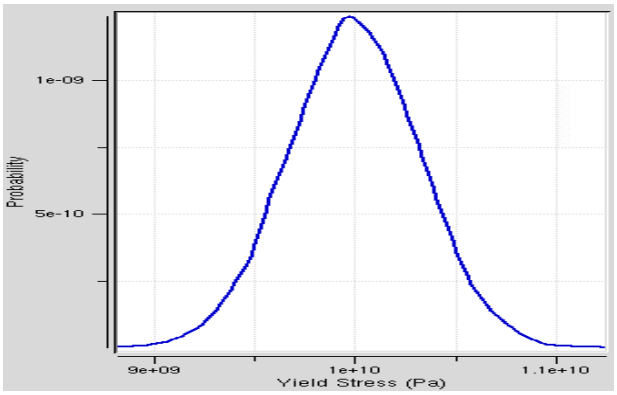

Figure 5: Illustrates Yield Stress (Pa) vs Probability for Burger vector as Gaussian.

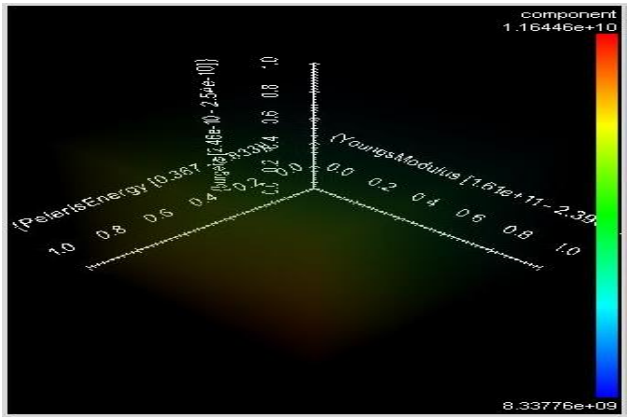

Figure 6: Illustrates Response (Young's Modulus vs Burgers vs Peierls Energy) for Burger vector Gaussian.

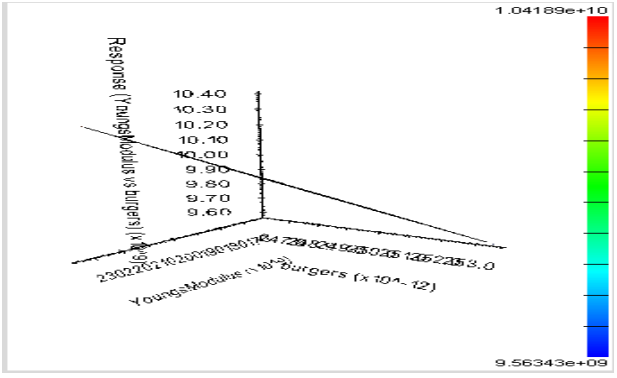

Figure 7: Illustrates Response (Young's Modulus vs burgers) for Burger vector Gaussian.

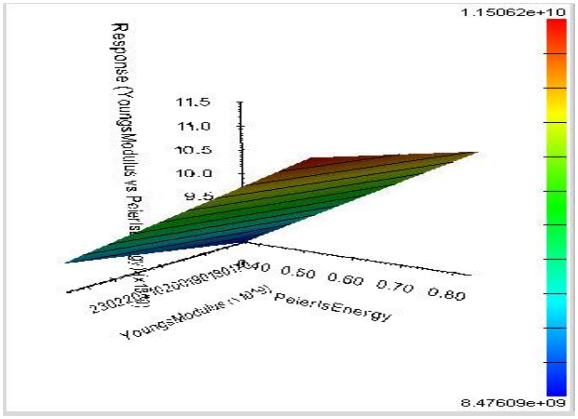

Figure 8: Illustrates Response (Young's Modulus vs Peierls Energy) for Burger vector Gaussian.

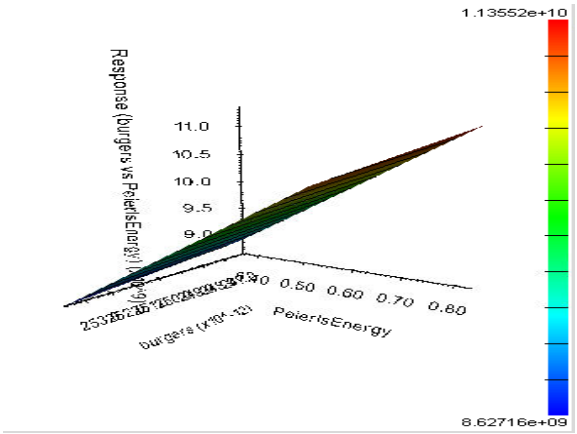

Figure 9: Illustrates Response (Burgers vs Peierls Energy) for Burger vector Gaussian

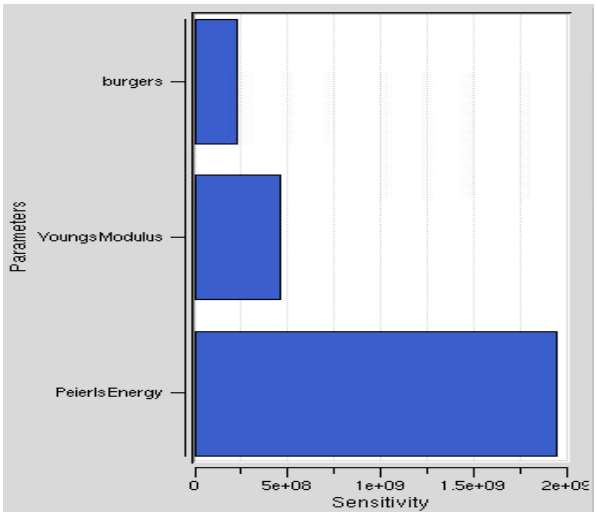

Figure 9: Illustrates Sensitivity (Sensitivity vs Parameters) for Burger vector Gaussian

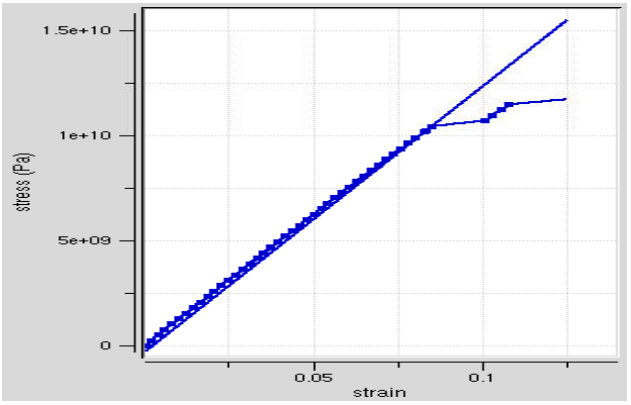

Figure 10: Illustrates Stress-Strain curves for Burger vector Gaussian

TABLE 6
SIMULATION NOMENCLATURE FOR BURGER VECTOR AS GAUSSIAN

Sl No:	Simulation Specifications	Value
1	Burger Vector	Gaussian
2	Mean	0.25nm
3	Deviation	0.001nm
4	d1	32

TABLE 7
SIMULATION NOMENCLATURE FOR ELASTIC CONSTANTS FOR BURGER VALUE AS GAUSSIAN

Sl No:	Simulation Specifications	Value
1	Source	Custom
2	Young's modulus	Gaussian
3	Mean	200GPa
4	Deviation	10GPa
5	Poisson's ratio	Single Value
6	Poisson's ratio	0.3

TABLE 8
SIMULATION NOMENCLATURE FOR PLASTICITY FOR BURGER VALUE AS GAUSSIAN

Sl No:	Plasticity	Value
1	Dislocation Glide: Peierl's Energy Barrier (J/m^2)	Gaussian
2	Mean	0.6
3	Deviation	0.06
4	Grain Boundary Sliding: Energy Barrier (J/m^2)	Single Value
5	Energy	0.15

TABLE 9
SIMULATION NOMENCLATURE FOR LOADING CONDITIONS FOR BURGER VALUE AS GAUSSIAN

Sl No:	Loading Conditions	Value
1	Stress Scaling Factor	1.0
2	Maximum Strain	0.5

TABLE 10
SIMULATION NOMENCLATURE FOR UNCERTAINTY QUALIFICATION FOR BURGER VALUE AS GAUSSIAN

Sl No:	Uncertainty Qualification	Value
1	Method	Smolyak+Polynomial Chaos with Legendre basis functions
2	Degree of polynomial expansion	1

Observations for Burger Vector as Gaussian

- Maximum value for yield of stress is 1.20046e-09 @ 1.00175e+10Pa
- Response of Young's Modulus vs Burgers vs Peierls Energy for Burger vector has value between 9.80 to 9.90
- Response of Young's Modulus vs Peierls Energy has been plotted
- Response of Burgers vs Peierls Energy has value of 9.5
- Sensitivity is 2.18971e+08 @ burgers, 4.58116e+08 @ Young's Modulus and 1.94019e+09 @ Peierls Energy
- Highest peak for stress-strain curves are 0.2% offset line 1.55115e+10Pa @ 0.124662 and interpolated 1.17234e+10Pa @ 0.124662

Grain Boundary and dislocation deformation in nanocrystalline metals with Burger Vector Uniform

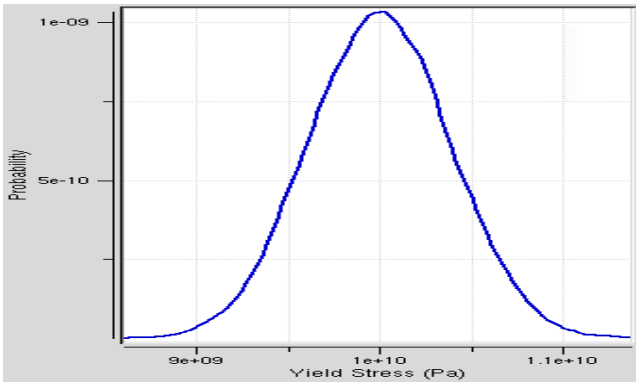

Figure 11: Illustrates Yield Stress (Pa) vs Probability for Burger vector uniform.

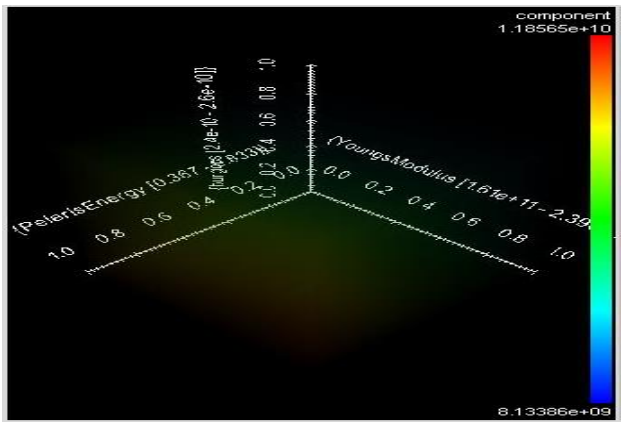

Figure 12: Illustrates Response (Young's Modulus vs Burgers vs Peierls Energy) for Burger Vector Uniform.

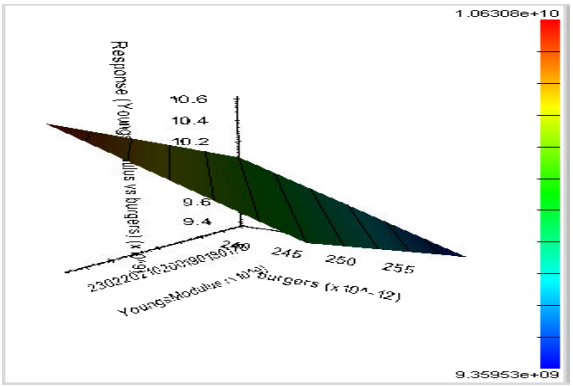

Figure 13: Illustrates Response (Young's Modulus vs burgers) for Burger Vector Uniform.

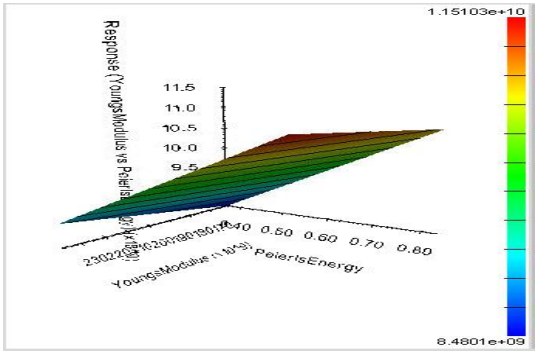

Figure 14: Illustrates Response (Young's Modulus vs Peierls Energy) for Burger Vector Uniform

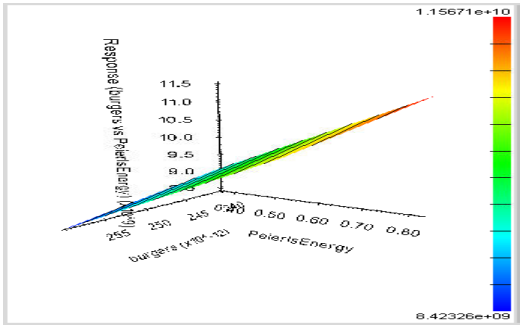

Figure 15: Illustrates Response (Burgers vs Peierls Energy) for Burger Vector Uniform.

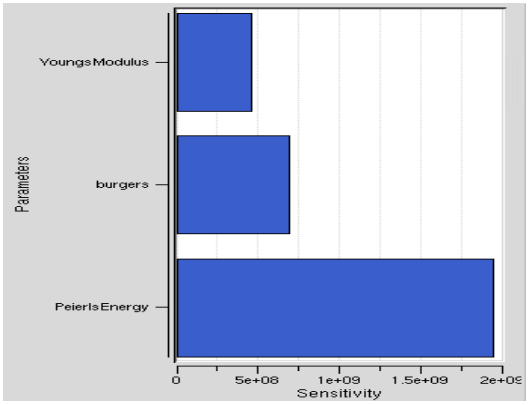

Figure 16: Illustrates Sensitivity (Sensitivity vs Parameters) for Burger Vector Uniform.

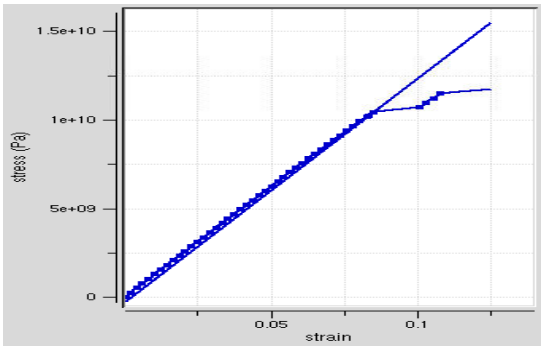

Figure 17: Illustrates Stress-Strain curves for Burger Vector Uniform.

TABLE 11
SIMULATION NOMENCLATURE FOR BURGER VECTOR AS UNIFORM

Sl No:	Simulation Specifications	Value
1	Burger Vector	Uniform
2	Min	0.24nm
3	Max	0.26nm
4	d1	32

TABLE 12
SIMULATION NOMENCLATURE FOR ELASTIC CONSTANTS FOR BURGER VALUE AS UNIFORM

Sl No:	Simulation Specifications	Value
1	Source	Custom
2	Young's modulus	Gaussian
3	Mean	200GPa
4	Deviation	10GPa
5	Poisson's ratio	Single Value
6	Poisson's ratio	0.3

TABLE 13
SIMULATION NOMENCLATURE FOR PLASTICITY FOR BURGER VALUE AS UNIFORM

Sl No:	Plasticity	Value
1	Dislocation Glide: Peierl's Energy Barrier (J/m^2)	Gaussian
2	Mean	0.6
3	Deviation	0.06
4	Grain Boundary Sliding: Energy Barrier (J/m^2)	Single Value
5	Energy	0.15

TABLE 14
SIMULATION NOMENCLATURE FOR LOADING CONDITIONS FOR BURGER VALUE AS UNIFORM

Sl No:	Loading Conditions	Value
1	Stress Scaling Factor	1.0
2	Maximum Strain	0.5

TABLE 15
SIMULATION NOMENCLATURE FOR UNCERTAINTY QUALIFICATION FOR BURGER VALUE AS GAUSSIAN

Sl No:	Uncertainty Qualification	Value
1	Method	Smolyak+Polynomial Chaos with Legendre basis functions
2	Degree of polynomial expansion	1

Observations for Burger Vector as Uniform

- Maximum value for yield stress is 1.02393e-09 @ 1.00066e+10Pa
- Response of Young's Modulus vs Burgers vs Peierls Energy has been plotted
- Response of Young's Modulus vs burgers is between 9.4 and 10.2
- Response of Young's Modulus vs Peierls Energy has value between 9.5 and 10.0
- Response of burgers vs Peierls Energy has value between 8.5 and 9.5
- Sensitivity is 4.58116e+08 @ Young's Modulus, 6.92486e+08 @ burgers, and 1.94019e+09 @ Peierls Energy
- Highest peak for stress-strain curves are 0.2% offset line 1.55115e+10Pa @ 0.124662 and interpolated 1.17234e+10Pa @ 0.124662

Results

Results for Burger Vector as Single Value

- Maximum value for yield of stress is 1.23236e-09 @ 1.00113e+10Pa
- Response (Young's Modulus vs Peierls Energy) for Burger vector single value has been plotted
- Sensitivity is 4.58116e+08 @ Young's Modulus and 1.94019e+09 @ Peierls Energy
- Highest peak for stress-strain curves are 0.2% offset line 1.55115e+10Pa @0.124662 and interpolated 1.17234e+10Pa @ 0.124662

Results for Burger Vector as Gaussian

- Maximum value for yield of stress is 1.20046e-09 @ 1.00175e+10Pa
- Response of Young's Modulus vs Burgers vs Peierls Energy for Burger vector has value between 9.80 to 9.90
- Response of Young's Modulus vs Peierls Energy has been plotted
- Response of Burgers vs Peierls Energy has value of 9.5
- Sensitivity is 2.18971e+08 @ burgers, 4.58116e+08 @ Young's Modulus and 1.94019e+09 @ Peierls Energy
- Highest peak for stress-strain curves are 0.2% offset line 1.55115e+10Pa @ 0.124662 and interpolated 1.17234e+10Pa @ 0.124662

Results for Burger Vector as Gaussian

- Maximum value for yield stress is 1.02393e-09 @ 1.00066e+10Pa
- Response of Young's Modulus vs Burgers vs Peierls Energy has been plotted
- Response of Young's Modulus vs burgers is between 9.4 and 10.2
- Response of Young's Modulus vs Peierls Energy has value between 9.5 and 10.0
- Response of burgers vs Peierls Energy has value between 8.5 and 9.5
- Sensitivity is 4.58116e+08 @ Young's Modulus, 6.92486e+08 @ burgers, and 1.94019e+09 @ Peierls Energy
- Highest peak for stress-strain curves are 0.2% offset line 1.55115e+10Pa @ 0.124662 and interpolated 1.17234e+10Pa @ 0.124662

Conclusion

One of the most important application is to predict mechanical behavior of materials ahead of experiments and provide sufficient information on the atomic scale [6]. Another example specifies that inhomogeneous deformation in a nanocryalline environment results in significant residual stresses in nanocrystals. This inner residual stress can cause strain regaining through inexpensive deformation mechanisms including dislocation reverse motion and grain boundary sliding [7].

This paper depicts visual representation of Burger Vectors for single, Gaussian and Uniform and graphs are plotted for yield stress, response of Young's Modulus vs Burgers vs Peierls Energy, response of Young's Modulus vs burgers, response of Young's Modulus vs Peierls Energy, response of burgers vs Peierls Energy, Sensitivity of Young's modulus, burgers and Peierls energy and stress-strain curves.

Acknowledgment

Author would like to thank Prof. Navarun Gupta, Prof. Hassan Bajwa, Prof. Linfeng Zhang and Prof. Hmurcik for their academic support. Author also thanks anonymous reviewers for their comments.

Conflicts of Interest

There are no conflict of interest as per Author's point of view.

References

1. Edelstein AS (2001) Nanomaterials. In Encyclopedia of Materials: Science and Technology (pp. 5916–5927). Elsevier. https://doi.org/10.1016/b0-08-043152-6/01031-7
2. Gutkin MY (2011) Elastic and plastic deformation in nanocrystalline metals. In Nanostructured Metals and Alloys (pp. 329–374). Elsevier. https://doi.org/10.1533/9780857091123.3.329
3. Ovid'ko IA (2011) Enhanced ductility and its mechanisms in nanocrystalline metallic materials. In Nanostructured Metals and Alloys (pp. 430–458). Elsevier. https://doi.org/10.1533/9780857091123.3.430
4. Milligan WW (2003) Mechanical Behavior of Bulk Nanocrystalline and Ultrafine-grain Metals. In Comprehensive Structural Integrity (pp. 529–550). Elsevier. https://doi.org/10.1016/b0-08-043749-4/08145-3
5. Martin Hunt; Lei Cao; Alejandro Strachan; Marisol Koslowski (2016), "NanoPlasticity Lab," https://nanohub.org/resources/nanoplasticity. (DOI: 10.4231/D3KD1QM6K)
6. Zhang L, Shibuta Y, Huang X, Lu C, Liu M (2019). Grain boundary induced deformation mechanisms in nanocrystalline Al by molecular dynamics simulation: From interatomic potential perspective. *Computational Materials Science*, *156*, 421-433. doi:10.1016/j.commatsci.2018.10.021
7. Li, Xiaoyan, Wei, Yujie & Yang, Wei & Gao, Huajian. (2009). 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. 16108-13. 10.1073/pnas.0901765106.