

# Deformation and Damage in Structurally Graded Nano-Crystalline Aluminum Alloys

NARI

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# Overview of Presentation

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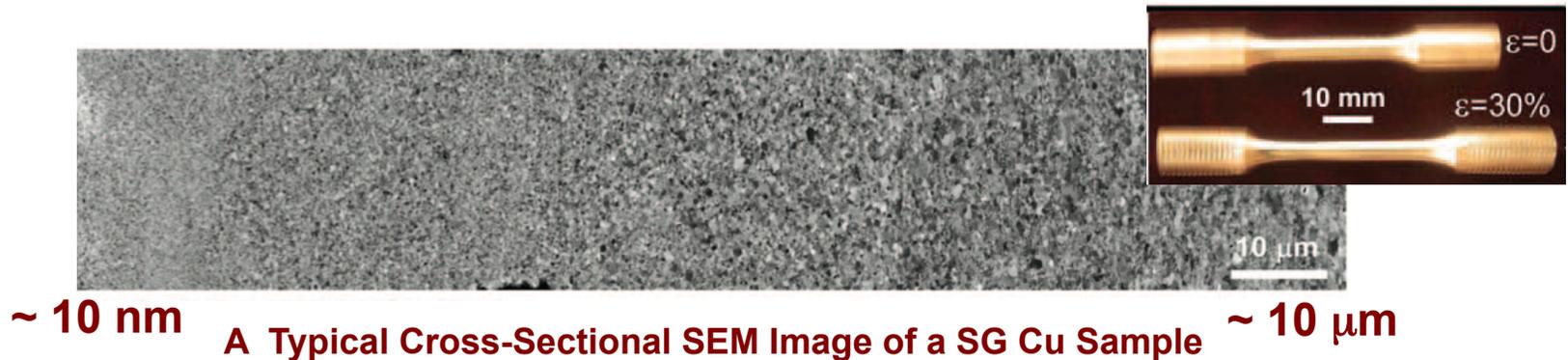
- **Structurally-Graded Materials – Innovation & Impact**
- **Overarching Methodology – Damage Science**
- **Molecular Dynamics Simulation for Smaller Grains**
  - ⊠ **Methodology**
  - ⊠ **Microstructures of Interest**
  - ⊠ **Deformation and Damage Mechanisms**
- **Multiscale Modeling for Larger Grains**
  - ⊠ **Methodology (we had to develop one)**
    - ⊠ **Discrete Dislocation Plasticity & Continuum Crystal Plasticity**
    - ⊠ **Inverse Method for Continuum Parameterization**
  - ⊠ **Microstructures of Interest**
  - ⊠ **Deformation and Damage Mechanisms**
- **Publications/Presentations**
- **Milestones & Plans**
- **Materials Genome Initiative**
- **Concluding Remarks**



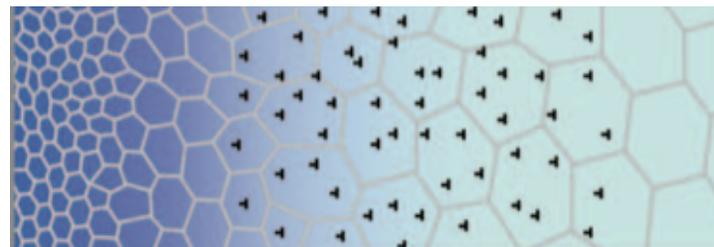
# Structurally-Graded Materials\*

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- Structurally-graded metallic materials consist of regions in which the grain size varies from relatively fine (10nm-100nm) to relatively coarse (1.0 $\mu$ m - 10.0 $\mu$ m)
- Finer grains contribute much of the overall material strength while the coarser grains contribute much of the ductility and toughness
- Primary mechanism is attributed to the reduction of strain localization and necking that immediately follows yielding in fine grained materials



A Typical Cross-Sectional SEM Image of a SG Cu Sample



Schematic of Microstructure from SEM Image

\*Fang, Science, 2010

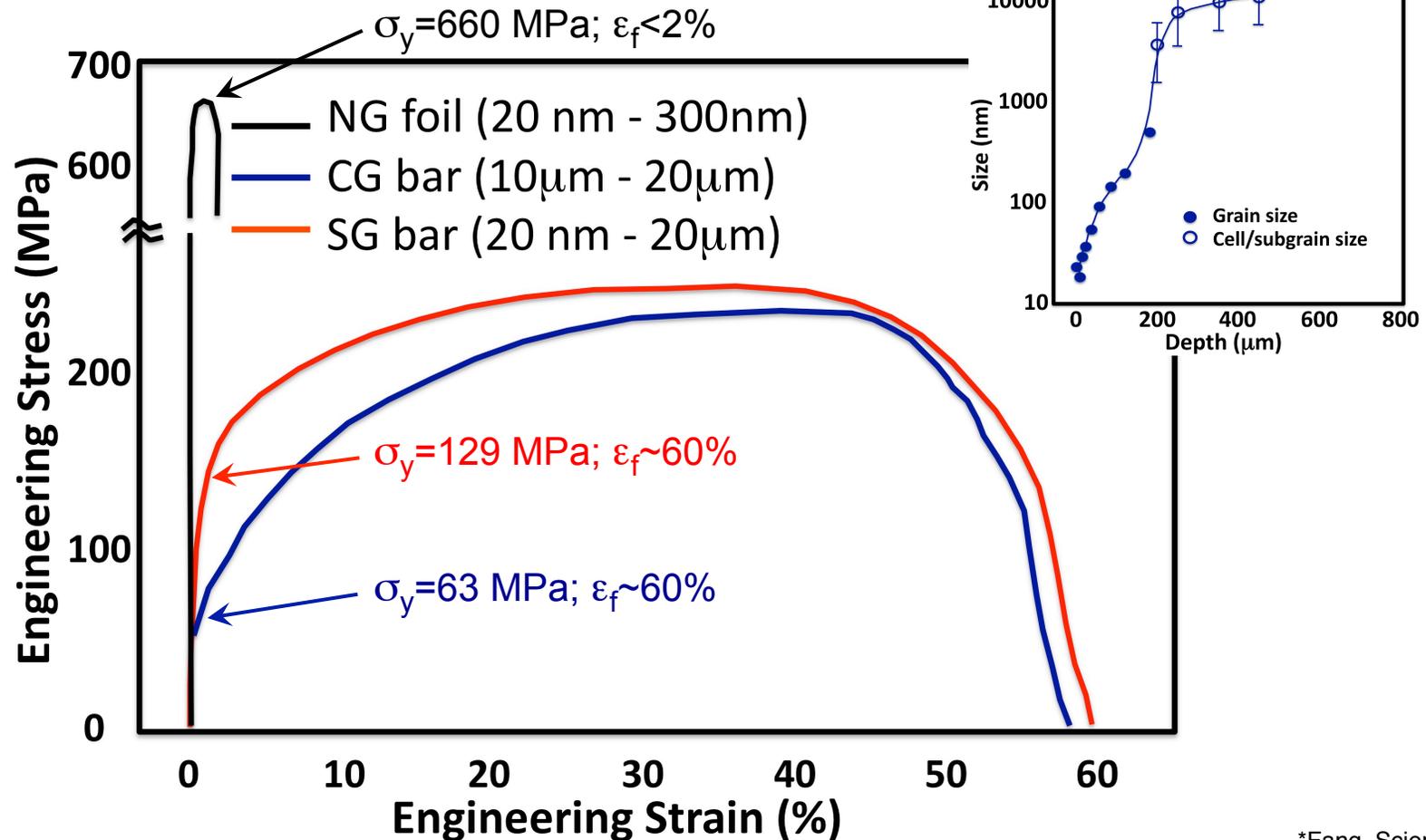


# Structurally-Graded Materials: Performance of SG Copper\*

Impact

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- Combining nano-grained (NG) and coarse-grained (CG) regions into a structurally graded (SG) material provides a significant increase in yield stress while maintaining ductility (and toughness)

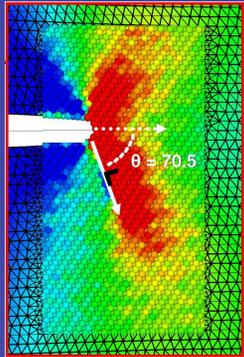




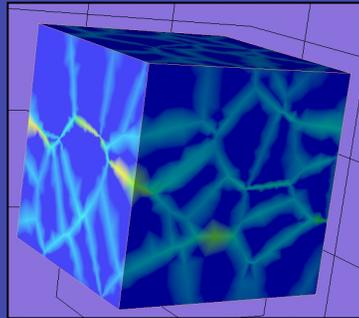
# Integrated Computational Materials Science and Engineering

Approach

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Modeling Plasticity at a Crack Tip



Simulation of Crack Growth in a Material Microstructure

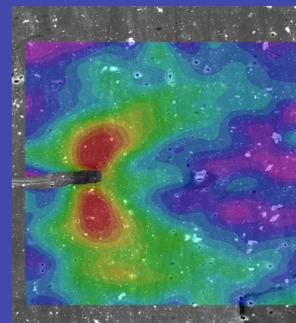
## Simulate the Physics of Damage via Multiscale Modeling

- Simulate critical damage processes
- Quantify effect of microstructure on damage rates
- Design materials to extend structural life
- Model & optimize processing methods
- Incorporate multi-physics approaches for design of multifunctional materials

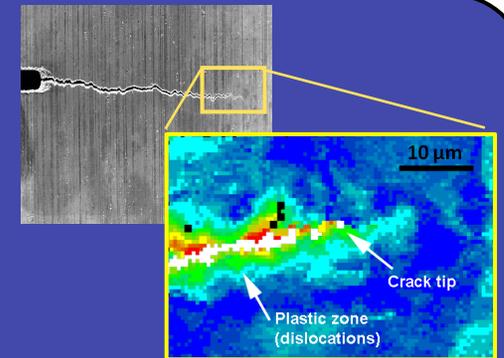
Physics-Based Material Design & Development Requires Close Collaboration Between Analysis and Experimentation

## Characterize the Physics of Damage via Experimental Evaluation

- Characterize damage at micro/nano-scale
- Quantify effects of operating environments
- Validate predicted damage models
- Fabricate and evaluate candidate materials
  - Optimized microstructures
  - Multifunctional materials
  - Nanoengineered materials



Measure Deformation at Crack Tip



Characterize Damage Evolution



# Characteristic Scaling Lengths and Associated Simulation Methods

Approach

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Representation of Physical Mechanisms

Structural Mechanics

Continuum  
Plasticity

Microstructure  
Mechanics

Crystal Plasticity

Gradient Plasticity

Dislocation  
Dynamics

Molecular  
Dynamics

Ab initio MD



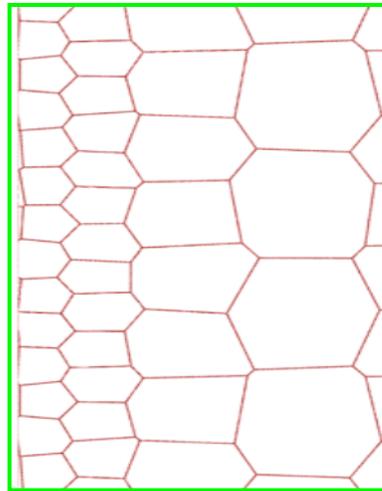
Characteristic Structure / Dimension (m)

NASA Aeronautics Mission Directorate FY11 Seedling Phase I Seminar

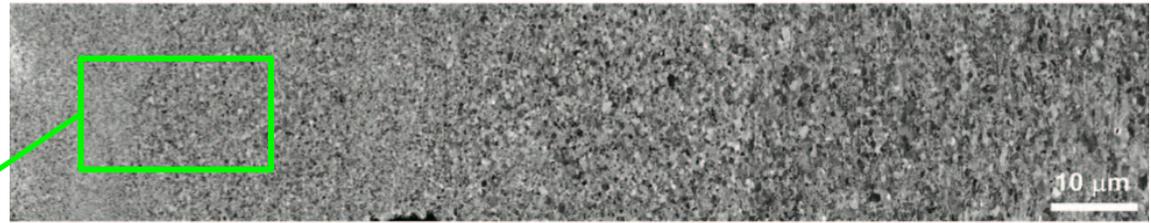


# Methodology for SG Microstructure Modeled by MD

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Graded Microstructure<sup>†</sup>  
(Grain sizes: 32 – 90 nm)



~ 10 nm

Structurally-Graded Microstructure\*

~ 10 μm

- Molecular Dynamics (MD) simulations<sup>†</sup>
  - EAM Aluminum potential<sup>§</sup> at T=300K
  - Nano-crystalline samples by Voronoi tessellation
  - Grain sizes of between 32 nm and 90 nm
  - Three crystallographic axes: [110], [111] and [211]
  - Domains of about 900 nm x 350 nm x 2 nm
  - $40 \times 10^6$  to  $50 \times 10^6$  atoms
  - Strain rate  $5 \times 10^6$  to  $10^7 \text{ s}^{-1}$ : times of  $> 20 \text{ ns}$

\*Fang, Science, 2010

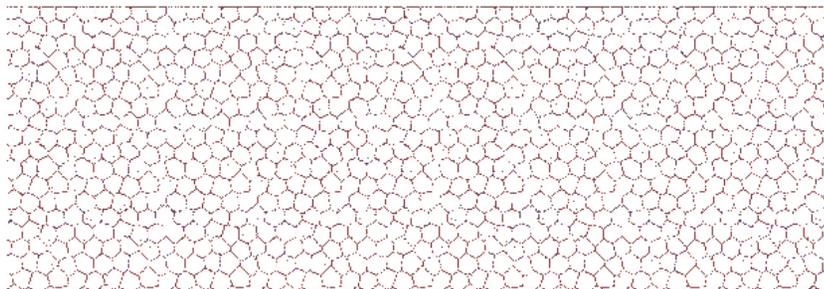
†Mishin, unpublished, 2012

§Mishin, Phys. Rev. B, 1999

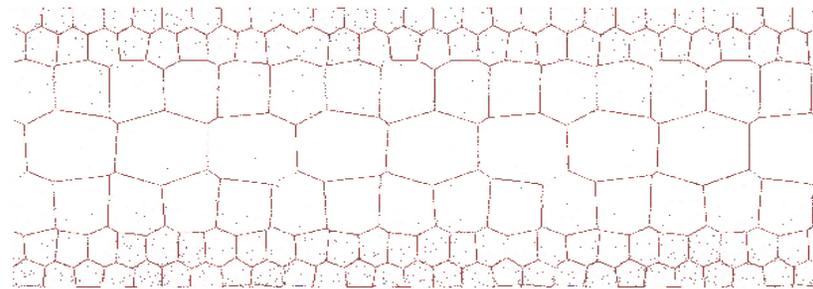


# Microstructural Models for MD Simulation

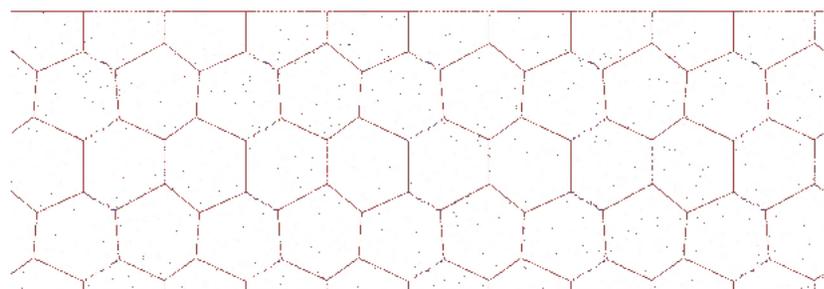
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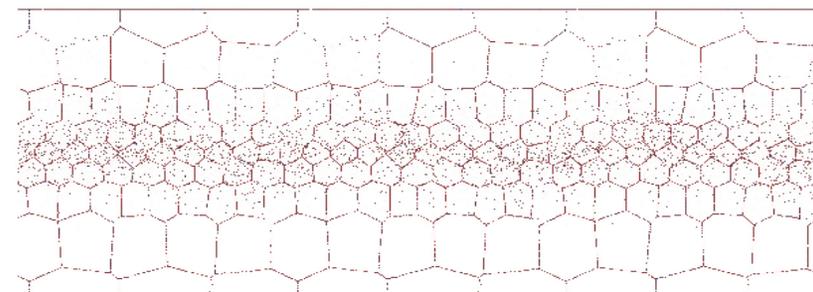
**Nano-crystalline Al, grain size 19 nm**



**Nano-graded Al, grain size 30 to 94 nm**



**Nano-crystalline Al, grain size 94 nm**



**Nano-graded Al, grain size 94 to 30 nm**

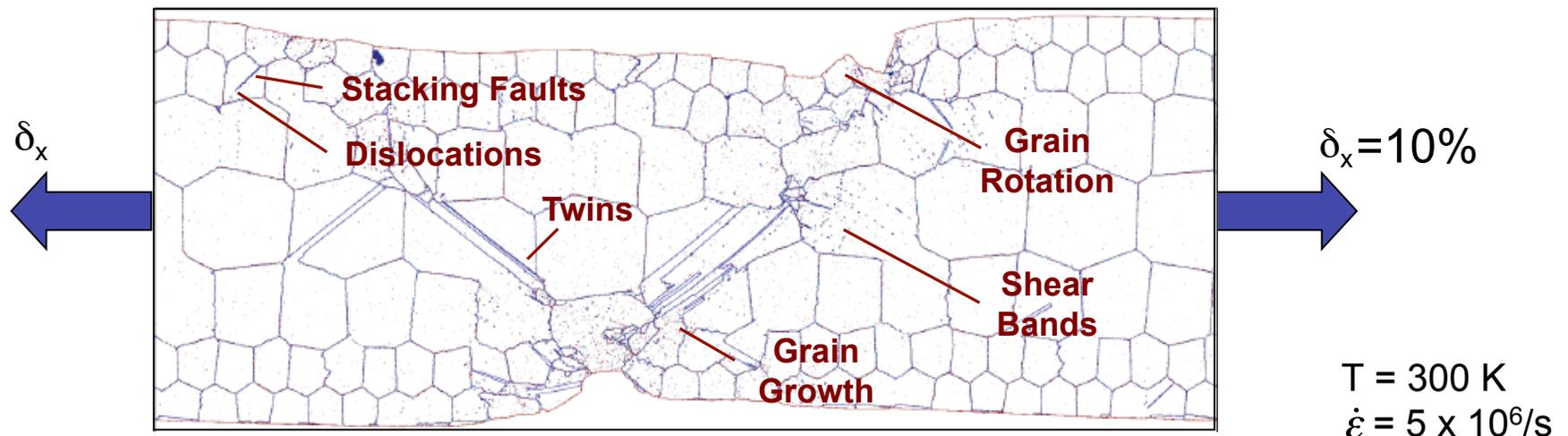


# SG Microstructure: Mechanisms & Deformation from MD

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- Deformation is primarily caused by dislocation slip and GB rotation
- Simulates complex mechanisms of dislocation nucleation and interactions, shear bands, GB structure, and rotation of small grains at atomic resolution
- Preferred method for simulation of small volumes

Grain sizes: 32 nm, 38 nm, 65 nm, 90 nm (147 total)  
Dim: 900.0 nm x 367.5 nm x 2.0 nm (39.5 M atoms)

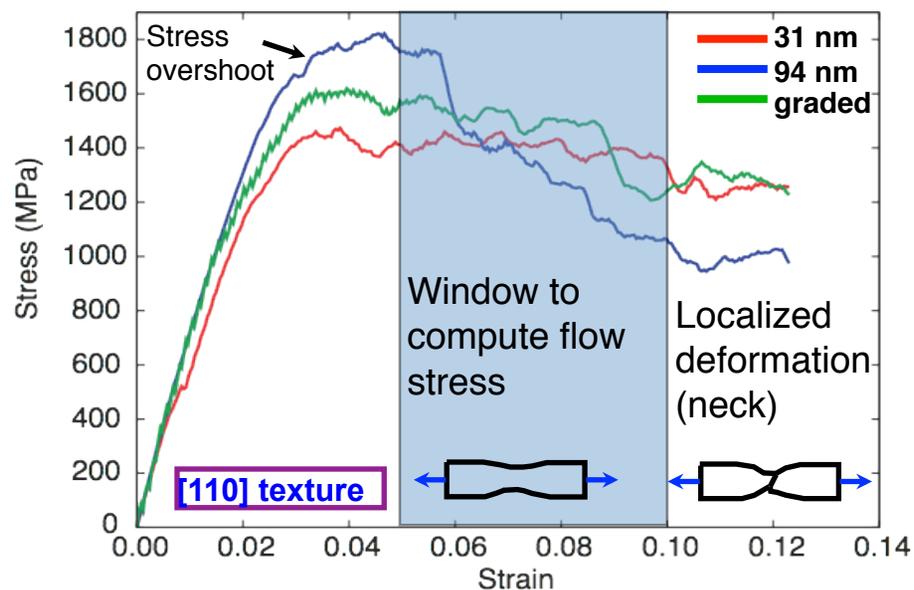


**Predicted Deformation in SG Material**

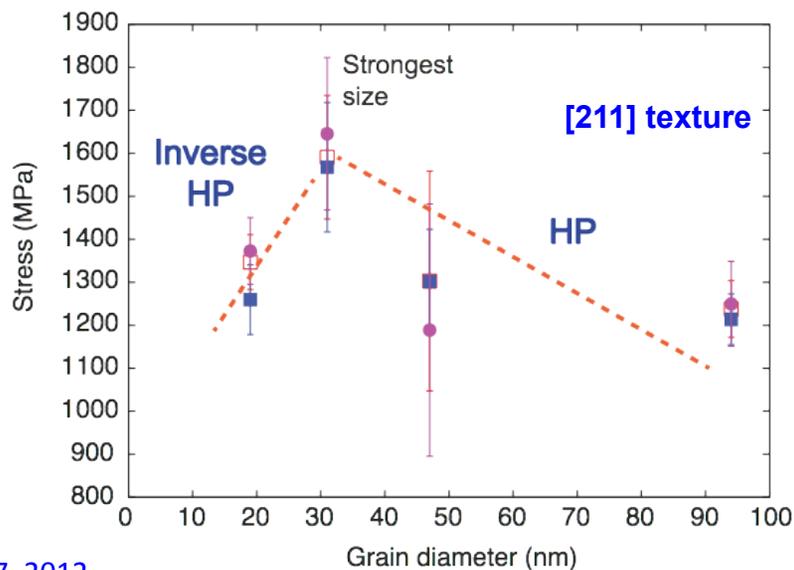


# Overall Material Response

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- Stress peak for relatively large grain sizes (“stress overshoot”) due to delayed nucleation of dislocations
- Strong localization of strain after ~10%. Formation of shear bands and (later) a neck
- The large-grained material is relatively soft at large deformations
- The graded structure shows promising strength



- The flow stress reaches a maximum at the grain size of about 30 nm, decreases at larger and smaller sizes
- The simulations reproduce both the direct and inverse Hall-Petch effect



# Summary of Phase I MD Investigation

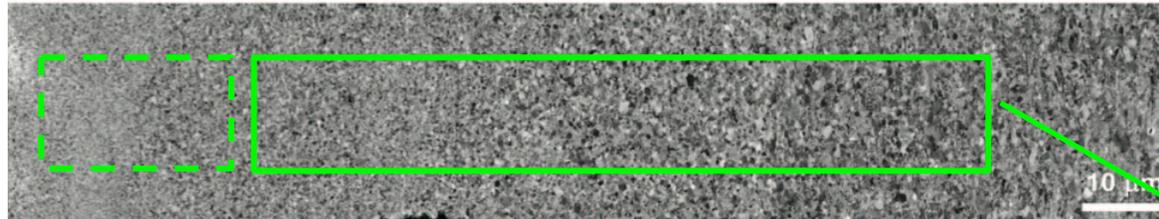
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- MD simulations tensile deformation have been performed for a series of nano-structured Al samples with different sizes, including several nano-graded structures.
- The simulations were designed to include the surface effect on deformation and to allow the material to develop strain localization. This conditions reflect the fact that nano-graded structures are experimentally created in near-surface layers and are expected to improve the ductility and stability of plastic flow against strain localization.
- The materials tested had a columnar structures with three crystal orientations of the grains: [211], [111] and [110], featuring different slip systems and twinnability.
- The nano-graded structures tested in this work showed a larger strength than typical coarse-grained Al structures. Furthermore, they deformed by developing relatively wide neck areas as opposed to uniform nano-grained structures which formed highly localized slip bands already at early stages of deformation.
- Thus the MD simulations performed so far indicate that nano-graded structures created in surface layers hold a promise for increasing the mechanical strength and improving flow stability in comparison with uniform nano-grained materials.
- Based on the slip-vector method, an efficient parallel computer code has been developed for visualization of multi-million atom structures produced by massive parallel MD simulations.
- Mechanisms of deformation processes in uniform and nano-graded structures have been studied in detail, including the dislocation nucleation mechanisms and their interaction with GBs.
- The results of the MD simulations can provide a mechanistic understanding and input data for simulations of deformation processes on larger length scales using DD and continuum methods.



# SG Microstructure Modeled by DD and CP

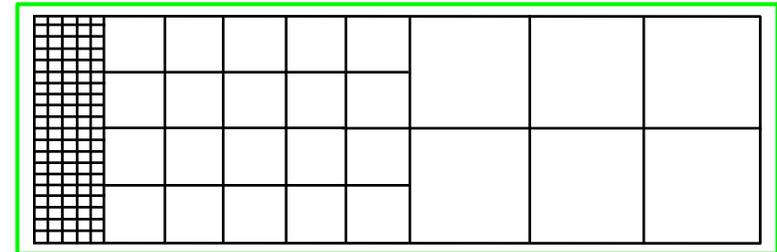
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~ 10 nm

Structurally-Graded Microstructure\*

~ 10 μm



Graded Microstructure  
(Grain sizes: 100 nm – 2 μm)

- Multiscale simulations
  - Aluminum
  - Grain sizes of between 100 nm and 2 μm
  - Arbitrarily large domains
- Dislocation Dynamics (DD) to capture essential physics
- Crystal Plasticity (CP) to enable modeling of large domains and parameter studies
- Inverse method for continuum parameterization

\*Fang, Science, 2010



# Parameters for DD Simulations

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- DD enables analyses of microstructures at larger length scales than MD by representing
  - Atomic assemblages as discrete objects (dislocations, obstacles, sources)
  - Long-range effects (lattice distortions) by analytical stress and strain fields
- Resolution of deformation processes greater than that of continuum plasticity
- Initial state consists of assumed distribution of
  - Initial dislocations, sources and obstacles
  - Orientation and spacing of independent slip planes

## Input Parameters for Al\*

Time Step	$\Delta t$	0.25 ns
Shear Modulus	$\mu$	25.3 GPa
Poisson's Ratio	$\nu$	0.341
Burger's Vector	$B$	0.285 nm
Source Strength	$\tau_s$	0.027 GPa
Obstacle Strength	$\tau_o$	0.08 GPa
Source Density	$\rho_s$	4.5e13/m <sup>2</sup>
Obstacle Density	$\rho_o$	1.5e13/m <sup>2</sup>
Standard Dev.	$Sd$	0.2
Nucleation Time	$t_{nuc}$	10.0 ns
Core Diameter	$c$	6b nm
Capture Distance	$l_{cd}$	6b nm
Slip Plane Separation	$l_{slp}$	100 b
Mobility Factor	$B$	1.0e-4 Pa s

## Some dislocation mechanisms approximated by DD:

- Annihilation
- Nucleation
- Pinning
- Pile-ups
- Junction formation
- Dynamic source generation

\*Segurado, MSMSE, 2007

\*Bezerga, MSMSE, 2004

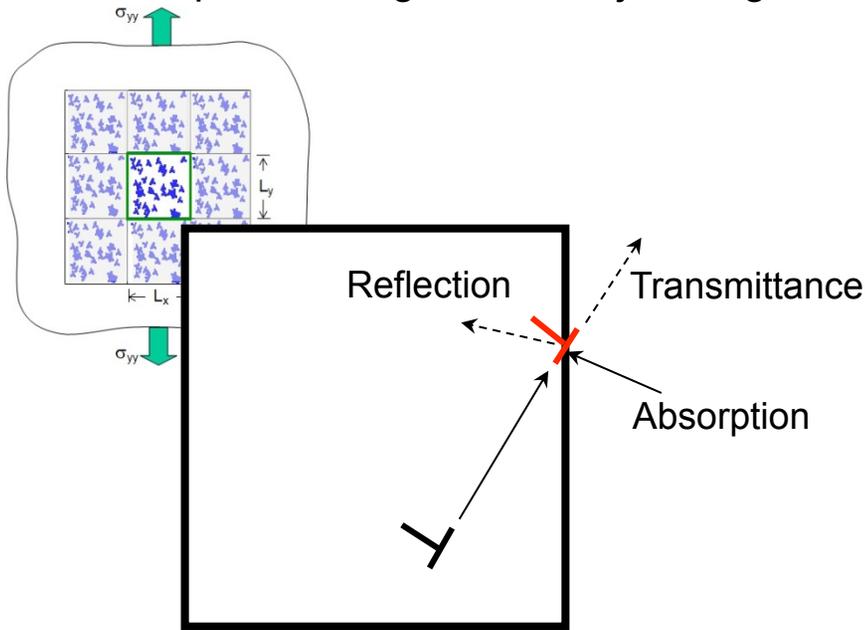
\*Van der Giessen and Needleman, MSMSE, 1995



# Dislocation-GB Interactions

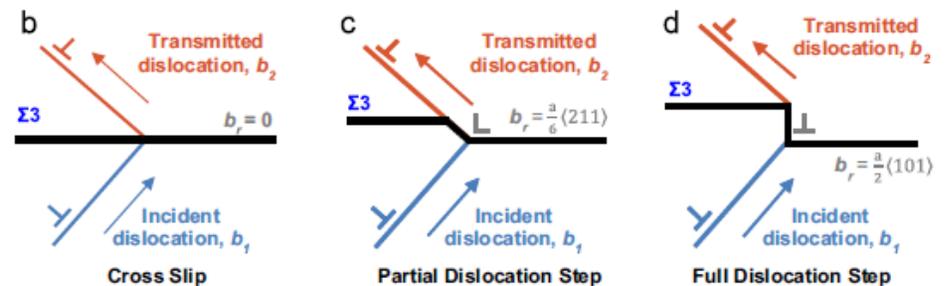
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- **Reflection**: simulated by preventing dislocation motion into a GB and allowing these dislocations to freely glide back into the grain interior.
- **Absorption**: simulated by pinning dislocations at the GB.
- **Transmittance**: simulated by allowing dislocations to either exit the model or pass through GB to adjacent grain.



## GB Representations

- GB-dislocation interactions are generally complex and have not been examined in detail for the present study.
- Only three simple mechanisms have been implemented to approximate GB influences on single- and poly-crystal behavior.
- For transmitted dislocations, the residual burgers vector retained at a GB is directly related to resistance to slip transmission, thereby influencing hardening behavior.\*



\*Abuzaid, JMPS, 2012

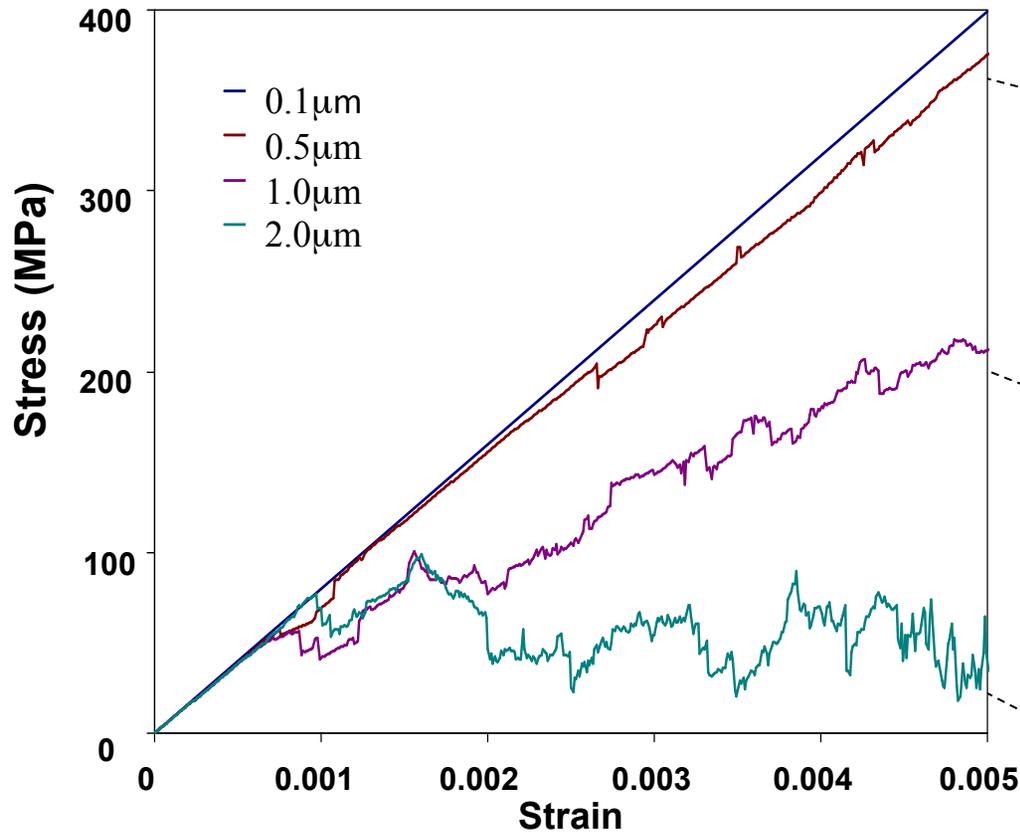
MD simulations can provide a mechanistic understanding and input data for multiscale simulations



# Effects of Grain Size on Stress-Strain Response\*

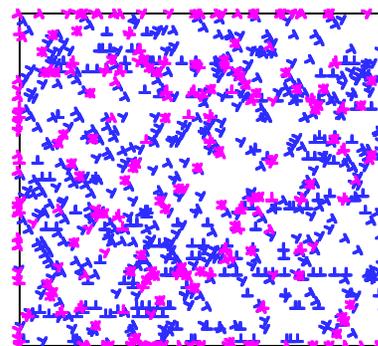
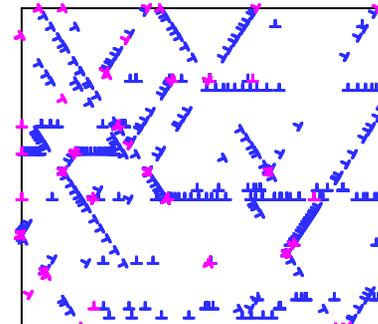
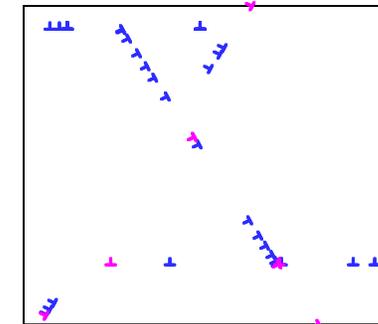
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DD Stress-strain response for 0.1 $\mu\text{m}$ , 0.5 $\mu\text{m}$ , 1.0 $\mu\text{m}$ , and 2.0 $\mu\text{m}$  grains



## Dislocation Profiles

Dislocation codes:  $\perp$  - mobile,  $\lrcorner$  - pinned



\* Assume reflective grain boundaries



# Crystal Plasticity Model and Key Parameters\*

Approach

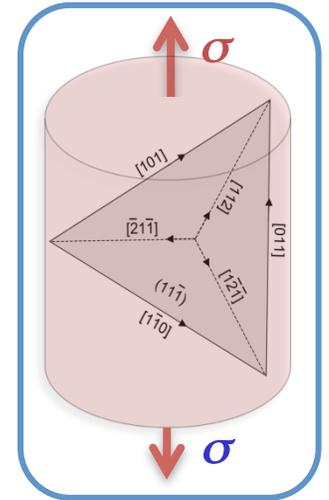
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- CP homogenizes dislocation slip within assumed slip system orientations
- Various models with different assumptions have been developed to combine slip on various planes into a consistent measure of continuum plasticity

• Multiplicative decomposition of deformation gradient....  $\mathbf{F} = \mathbf{e} \mathbf{F} \mathbf{p} \mathbf{F}$

• Slip rate on slip system  $\alpha$ .....  $\dot{\gamma}^\alpha = \dot{\gamma}_o \frac{\tau^\alpha}{g^\alpha} \left| \frac{\tau^\alpha}{g^\alpha} \right|^{\frac{1}{m}-1}$  Slip when  $\frac{\tau^\alpha}{g^\alpha} > 1$

• Hardness evolution (Voce-Kocks).....  $\dot{g} = G_o \left( \frac{g_s - g}{g_s - g_o} \right) \dot{\gamma}$  Latent hardening=self hardening



## Key Parameters

$\alpha$  = the slip system

$\dot{\gamma}^\alpha$  = the time rate of slip

$\dot{\gamma}_o$  = the reference slip rate

$\tau^\alpha$  = the resolved shear stress on system  $\alpha$

$g^\alpha$  = the current hardness on system  $\alpha$

$m$  = a rate sensitivity parameter

$G_o$  = hardening coefficient

$g_o$  = initial hardness

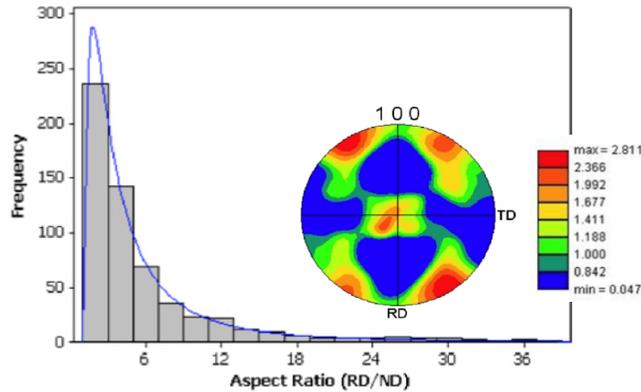
$g_s$  = the saturation value of the hardness

\*Mantous and Maniatty, IJNME, 2004

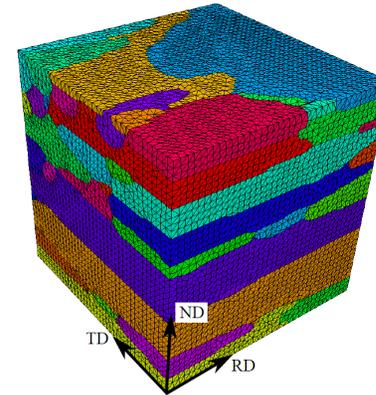


# Typical Calibration of CP Parameters

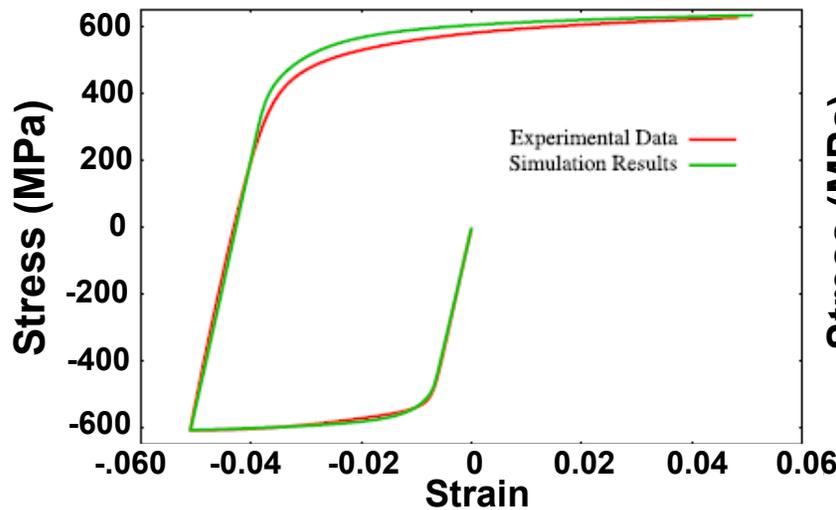
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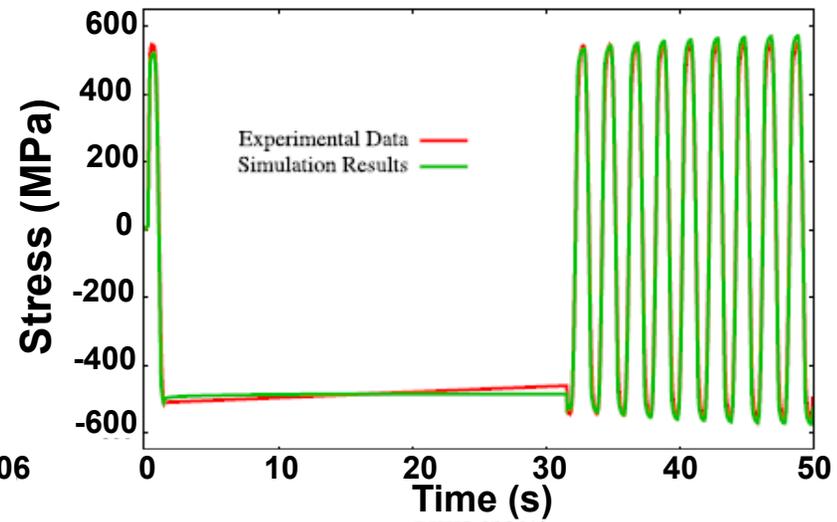
Characterize Microstructure Morphology\*



Generate a Digital Polycrystal



Fit to a Single Loading Cycle†



Fit to Several Loading Cycles§

\*Veilleux et al., 2012, MSMSE, in process †Horstemeyer et al., unpublished §Papazian et al., unpublished

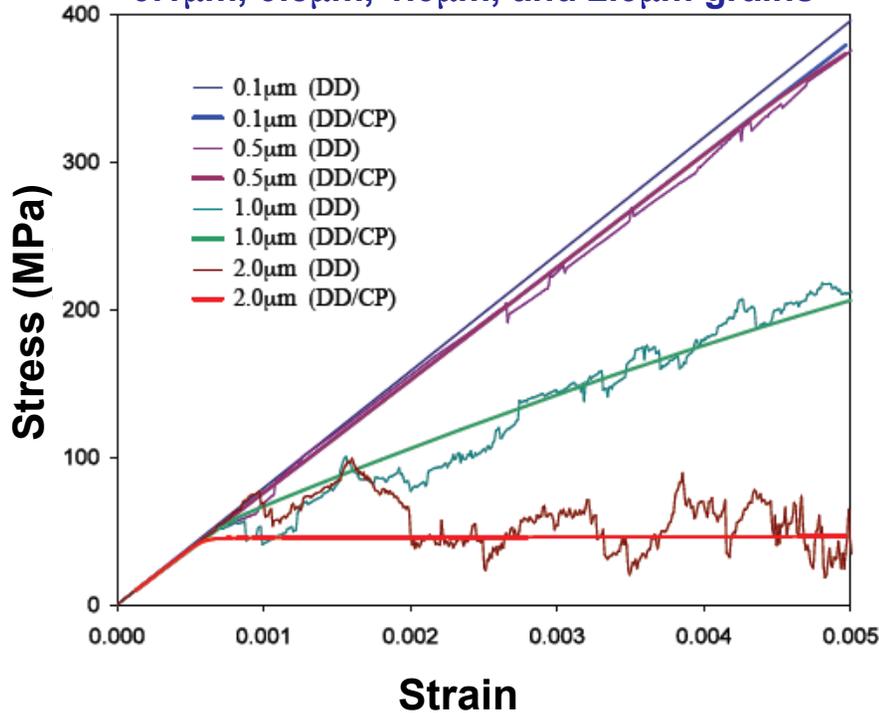


# Multiscale Linking of DD and CP Simulations

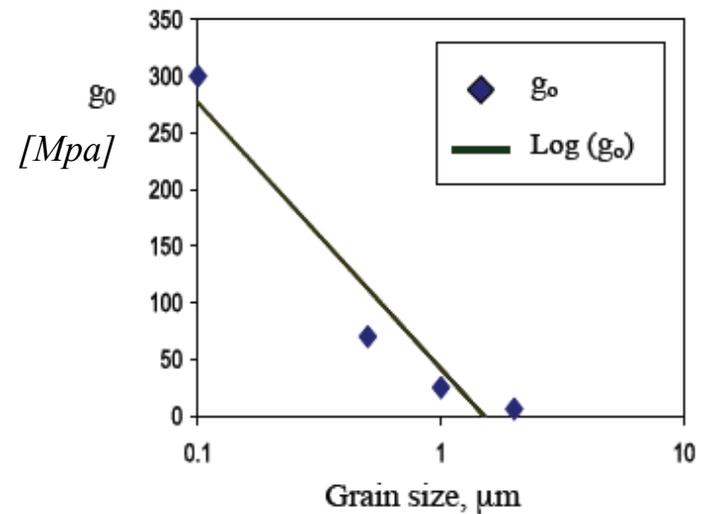
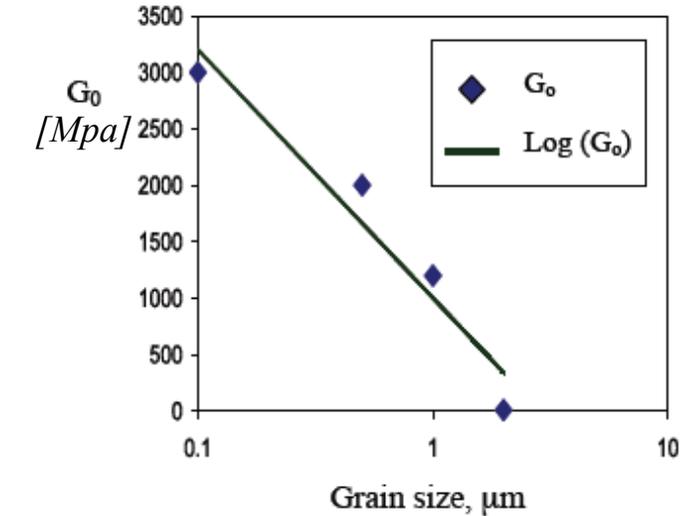
Approach

NARI

Results for  
0.1 $\mu\text{m}$ , 0.5 $\mu\text{m}$ , 1.0 $\mu\text{m}$ , and 2.0 $\mu\text{m}$  grains



- Calibrate CP simulation to DD predictions
- Log fit of optimized parameters is  $\sim$ linear
  - Information that may be used in a size-dependent CP formulation



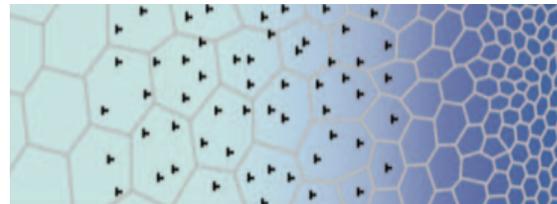


# Structurally-Graded Polycrystal Models

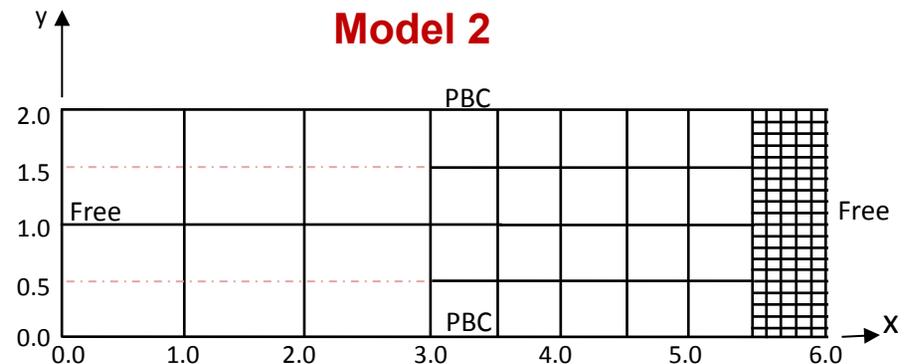
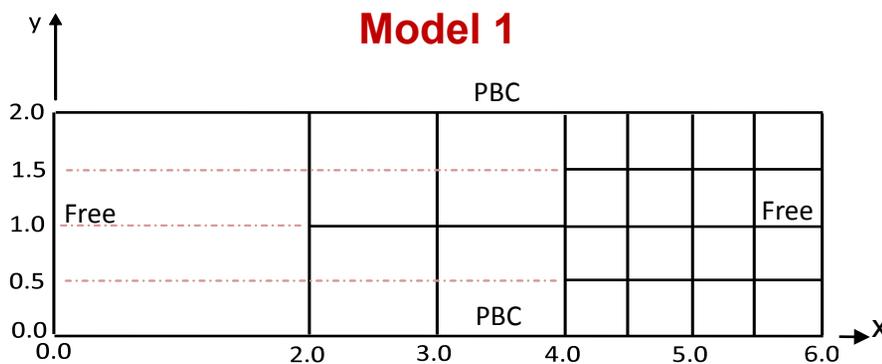
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- Structurally-graded polycrystal models developed using square grains
  - Model 1 composition: 33% 2.0 $\mu\text{m}$ , 33% 1.0 $\mu\text{m}$ , and 33% 0.5 $\mu\text{m}$  grains
  - Model 2 composition: 50% 1.0 $\mu\text{m}$ , 41.7% 0.5 $\mu\text{m}$ , and 8.3% 0.1 $\mu\text{m}$  grains
- Boundary conditions applied to model faces are identified as Free or PBC
- GB-dislocation interactions assumed as 'reflective' in which dislocations are prevented from crossing GB and are free to glide back into the interior

## Graded Microstructures



(Idealization from Fang, 2010)

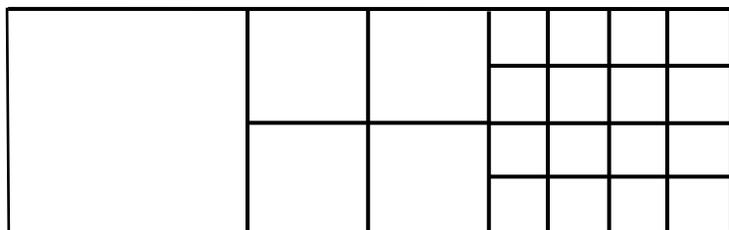




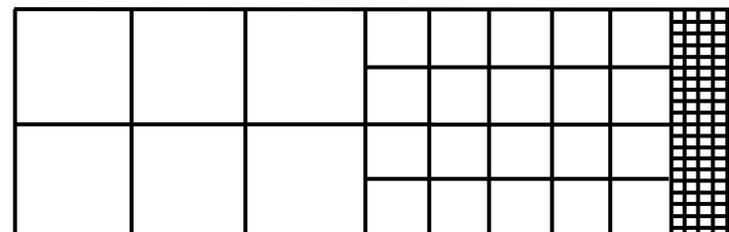
# Response of Structurally-Graded Polycrystal Models

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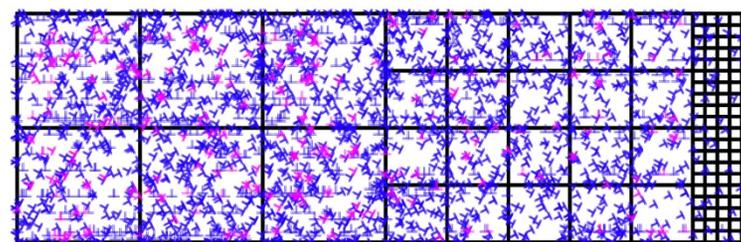
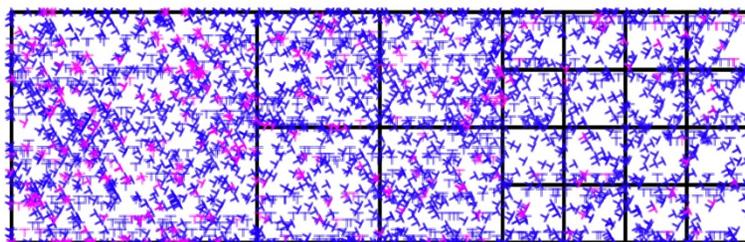
Model 1



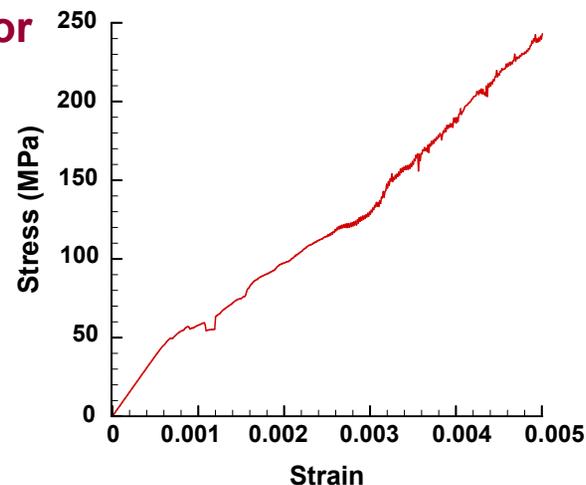
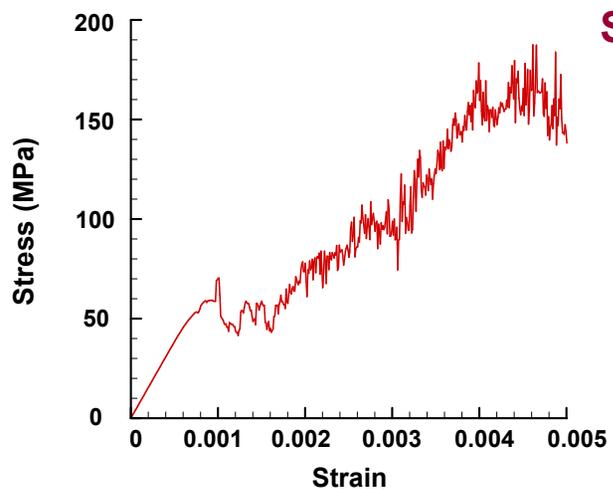
Model 2



Dislocation Profiles at 0.5% Strain



Stress-Strain Behavior

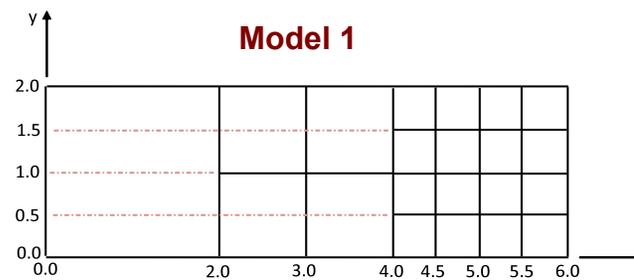
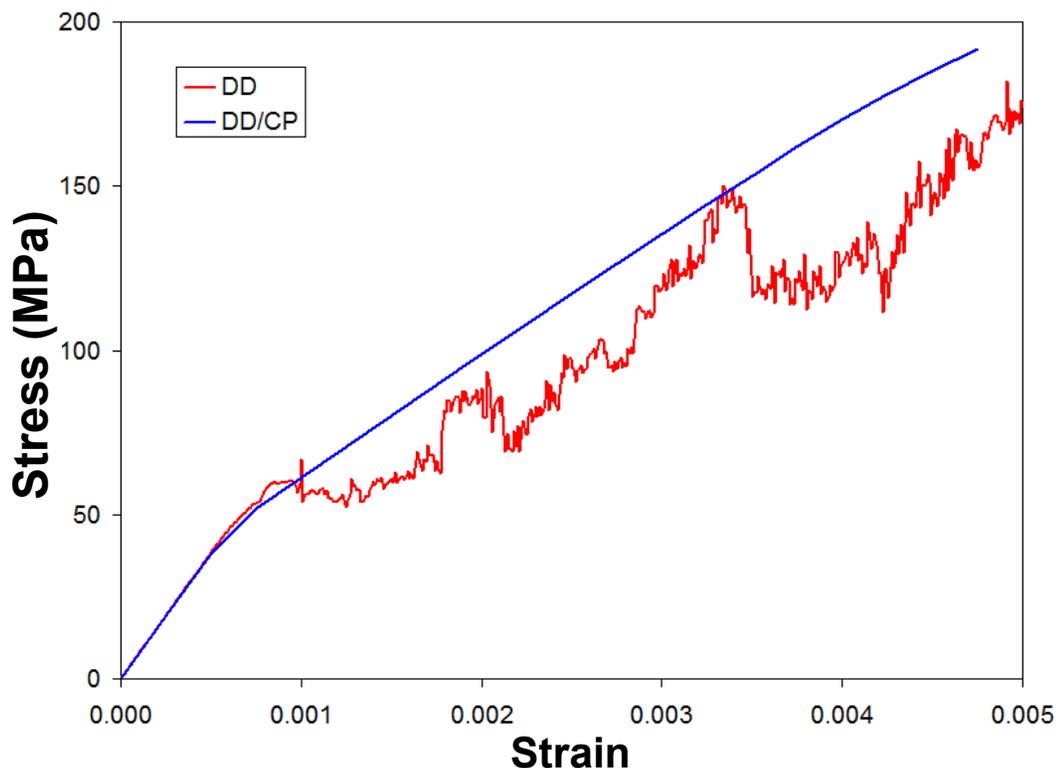




# DD and DD/CP Model Predictions: Model 1

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Comparison of DD- and DD/CP-predicted stress-strain behavior in graded polycrystal Model 1



## Observations

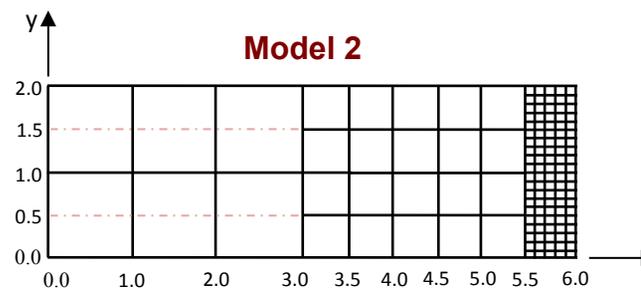
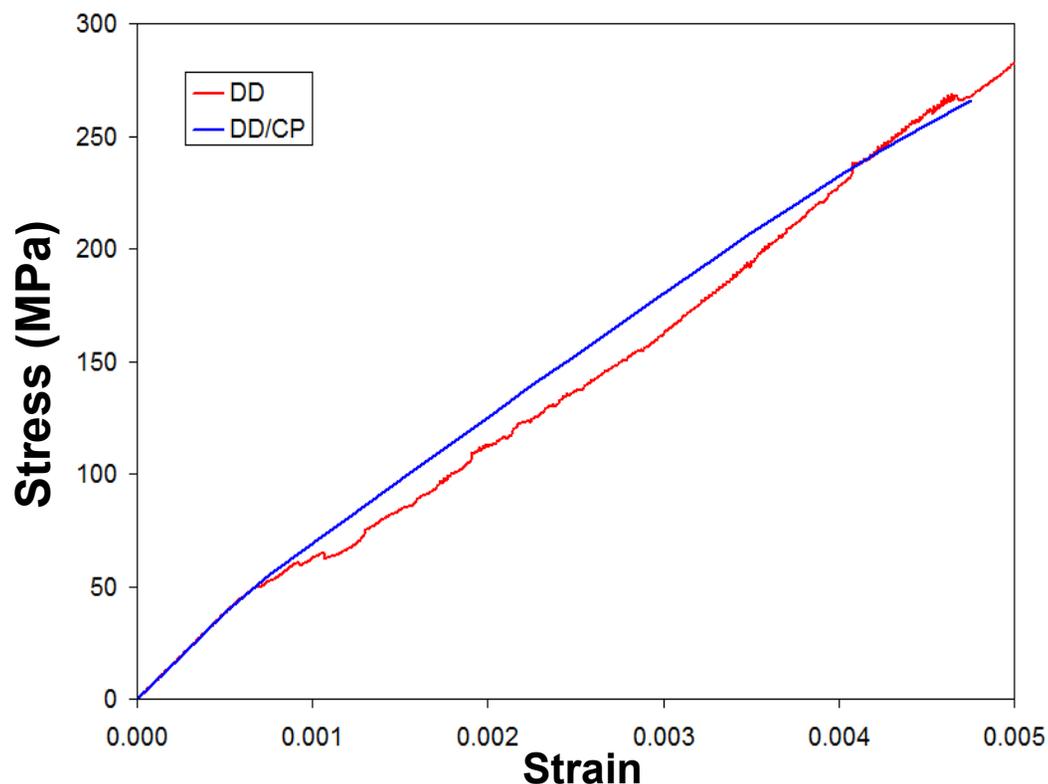
- DD/CP model duplicates yield stress and strain hardening slope
- DD stress relaxation not captured by DD/CP model due to assumed hardening law
- DD may be exhibiting a dynamic overshoot due to a strain-rate effect



# DD and DD/CP Model Predictions: Model 2

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Comparison of DD- and DD/CP-predicted stress-strain behavior in graded polycrystal Model 2



## Observations

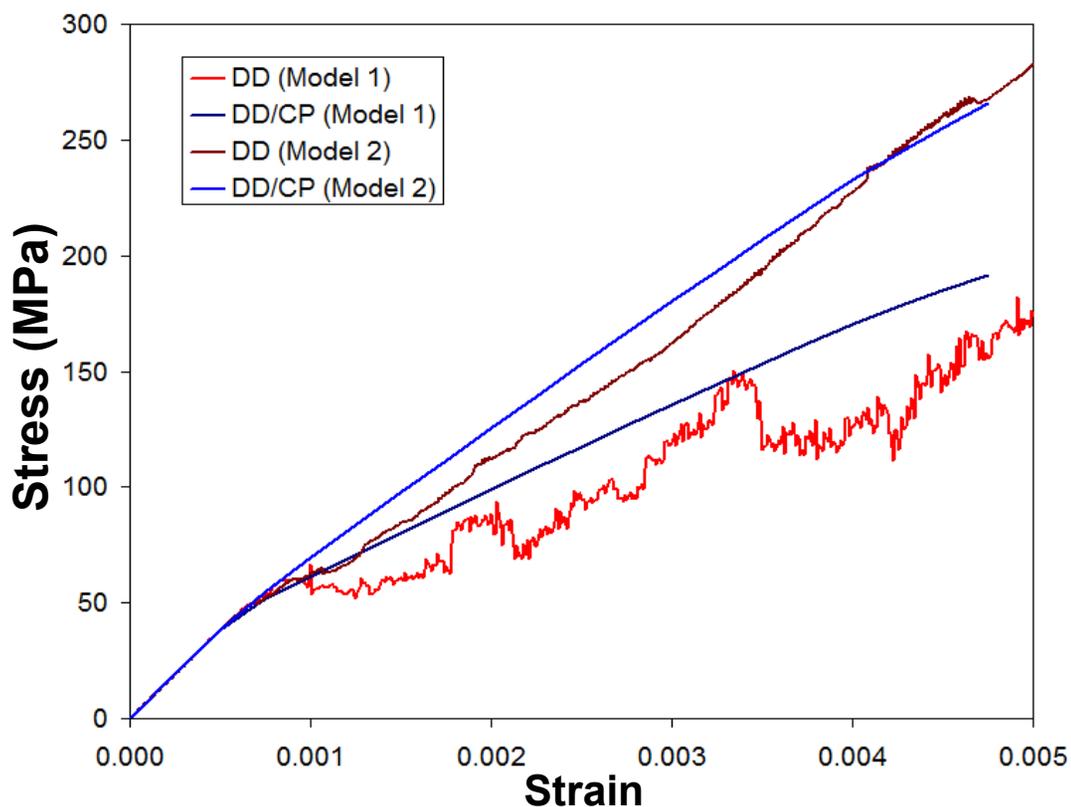
- Model 2 exhibits a stiffer response than Model 1 due to smaller grain sizes.
- Good agreement between DD and DD/CP predictions for yield stress, slope of strain hardening slope, and final stress level at 0.5% strain.
- The reduced nonlinearity appears to mitigate any strain rate effects after yield.



# DD and DD/CP Model Predictions: Comparison

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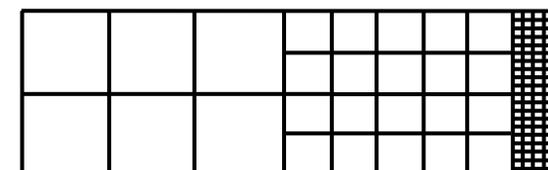
Comparison of DD- and DD/CP-predicted stress-strain behavior for the structurally-graded polycrystal models



Model 1



Model 2



## Observations

- The smaller grains (on average) in Model 2 result in a stiffer response than seen in Model 1
- The magnitude of fluctuation in stress-strain response appears to increase with grain size
- Increasing GB-dislocation interactions cause increased hardening (Model 1)



# Summary of Phase I DD/CP Investigation

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- Dislocation dynamics (DD) simulations are being developed to model deformation of SG materials with grain sizes of between about 0.1  $\mu\text{m}$  and 2.0  $\mu\text{m}$
- For the specific parameters considered, a significant grain size effect was demonstrated
  - Grains of 0.1  $\mu\text{m}$  were nearly linear elastic
  - Grains of 2.0  $\mu\text{m}$  were nearly elastic-perfectly plastic
- A multiscale analysis was developed that used an inverse procedure to calibrate hardening parameters for a crystal plasticity (CP) model using the DD results
- The calibrated DD/CP model was used to determine the stress-strain behavior of idealized SG aluminum configurations



# Publications/Presentations

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E. Saether, J.D. Hochhalter, and E. Glaessgen, “Multiscale Modeling of Structurally-Graded Materials Using Discrete Dislocation Plasticity Models and Continuum Crystal Plasticity Models,” 53<sup>rd</sup> AIAA/ASME/ASCE/ AHS/ASC Structures, Structural Dynamics and Materials Conference and Exhibit, Honolulu, HI, April 23-26, 2012.

G.P. Puja Pun and Y. Mishin: Size effect on plastic deformation and strain localization in nano-crystalline aluminum: a molecular dynamics study, Scripta Materialia, in progress.

G.P. Puja Pun and Y. Mishin: Molecular dynamics simulation of deformation and fracture of graded nano-crystalline Al, Acta Materialia, in progress.



# Phase I Milestone Status

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## 6 months:

- Develop computational models of nano-structured Al with a grain size gradient  
**Achieved**
- Determine role of grain size and gradient on strength, ductility and damage mechanisms  
**Achieved**

## 12 months:

- Continue to investigate mechanical properties and damage mechanisms  
**Achieved** (will be continued in Phase II)
- Conduct similar studies on uniform nanocrystalline samples as a baseline  
**Achieved**
- Summarize the simulation results and rank candidate nano-structures by strength and ductility  
**In progress**
- Evaluate possible processing methods including plasma spray and e-beam free-form fabrication  
**Friction stir welding and surface plastic deformation will be used in Phase II**  
**Plasma spray and e-beam free-form fabrication may be more suitable for making large quantities of material during a production phase**
- Determine a test matrix for Phase II experimental evaluation  
**Achieved**



## Phase II Milestones

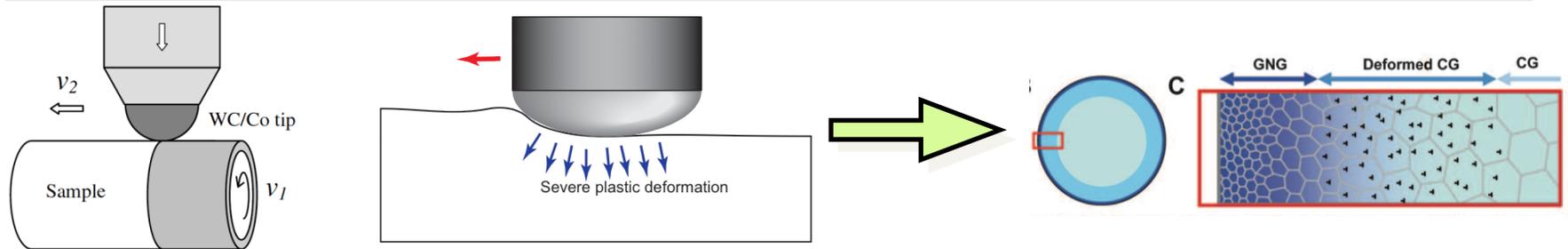
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- Evaluate stress-strain response of SGNC microstructures under loadings up to failure  
**12 months** – catalogue of stress-strain curves for a variety of microstructures (<100 nm grains)
- Extend DD/CP multiscale modeling capabilities to include GB characterization from MD simulations – apply analyses to evaluate microstructures with grain sizes from about 100 nm to several microns.  
**18 months** – catalogue of stress-strain curves for a variety of microstructures (>100 nm grains)
- Evaluate friction stir welding and surface plastic deformation as candidate processing methods for SGNC materials. Both methods will be evaluated, with the more promising method being selected to produce specimens for characterization.  
**9 months** to down-select, **12 months** to produce specimens
- Characterize material microstructures, including quantitative assessment of their deformation.  
**15 months** – deformation quantified
- Compare results of experimental tests and computational analyses.  
**18 months** – comparison of test and analysis of SGNC microstructures
- Determination of SGNC microstructures suitable for production.  
**18 months** – down select of 3 candidate SGNC microstructures for further development

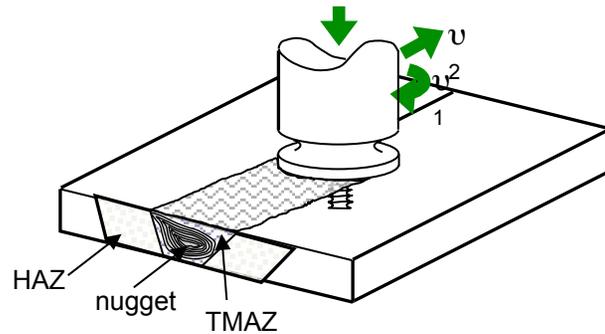


# Processing of SGNC Materials

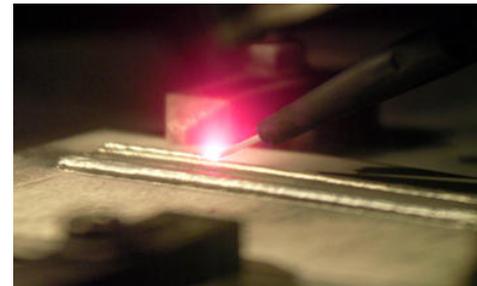
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### Surface Mechanical Grinding Method (SMGT)



### Friction Stir Welding (FSW)



### Additive Manufacturing Electron Beam Free Form Fabrication (EBF3)

Severe plastic deformation of the material results in formation of fine deformed cells. The sample is cooled to cryogenic temperatures to prevent grain growth. Several passes are made to grain sizes or graded structure with 20-40 nm grains at the surface.

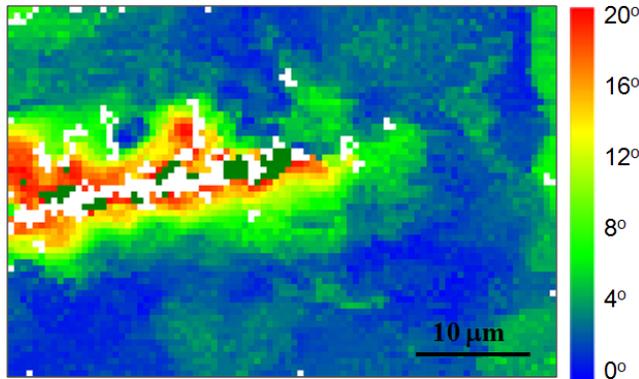
Grain structure for additive manufacturing processes can be controlled by processing parameters, structure of feed stock and cooling rates. Additive manufacturing can be applied to develop nano-crystalline structures for complex structural configurations.



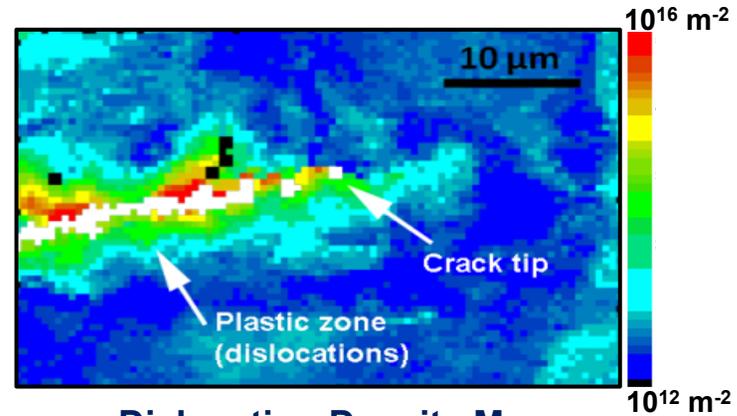
# Experimental Characterization of Microstructural Effects

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## Local Plastic Deformation and Microstructure Evolution

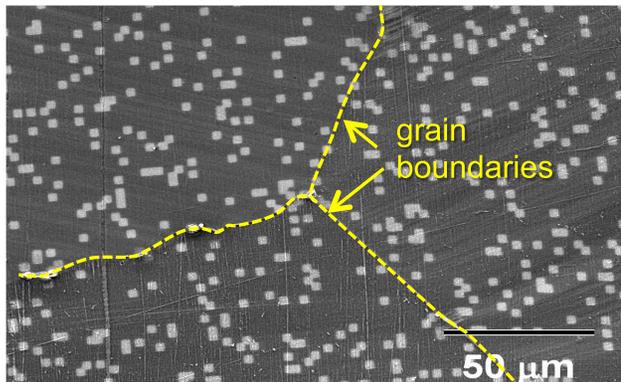


Local Crystallographic Rotation



Dislocation Density Map

## Image Correlation for Microstructural Effects on Deformation



E-beam Lithography/Microstructure

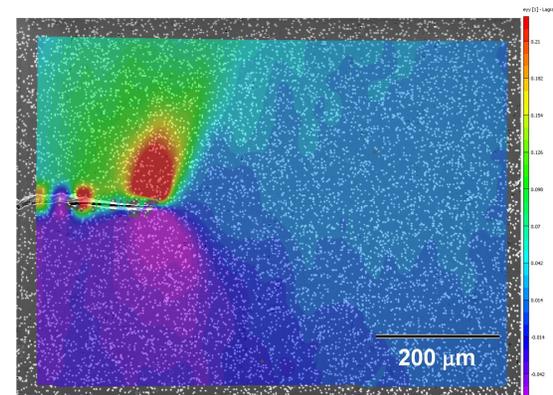
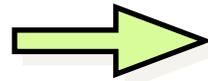


Image Correlation Near a Crack Tip



# Materials Genome Initiative

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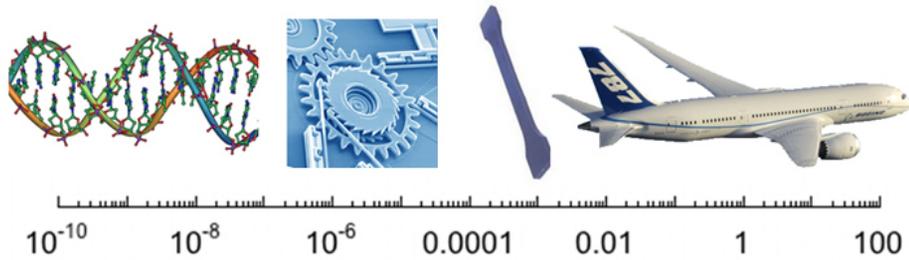


- MGI is organized by OSTP “to explore the vision and challenges to be overcome in harnessing the power of computing and communications technologies for rapid development and use of advanced materials.”
- MGI’s aim is to revitalize the materials innovation infrastructure within the U.S.
- Reduce cost and time for development/insertion of new materials by ½ (5-10 years vs. 15-20 years)
- MGI is a collaboration of DoD, DoE, NSF, NIST, over 60 U.S. companies and numerous universities
- MGI presents a unique opportunity for NASA to make significant advances in its own critical materials technology areas

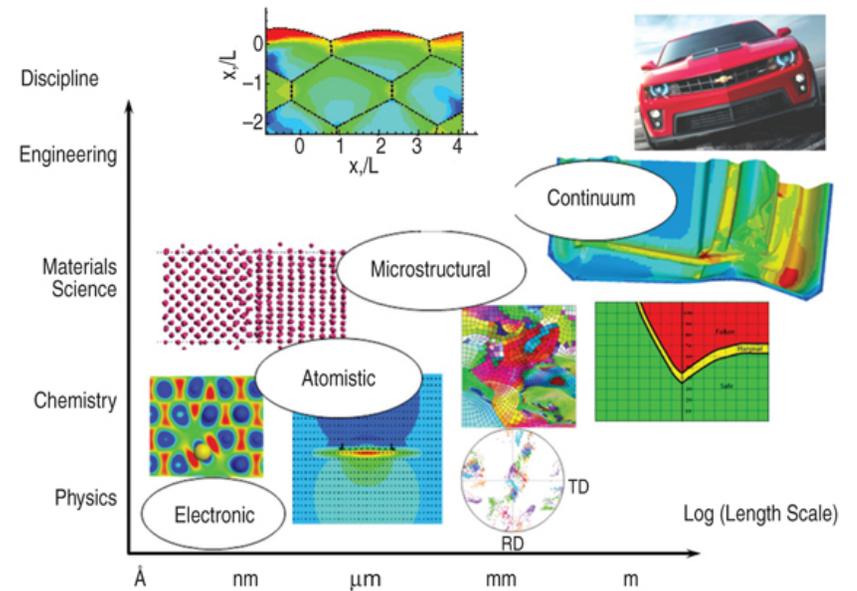


# Atoms to...Everything

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...Airplanes (AFRL, Boeing, et al.)



...Autos (Automakers, Brown, MSU, et al.)



# Concluding Remarks

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- Structurally-graded (SG) metallic materials offer the promise of combining the strength of nanocrystalline materials with the ductility and toughness of coarse grained materials
- Molecular dynamics simulations are being developed to model deformation of SG materials with grain sizes less than about 100 nm
- DD/CP multiscale simulations are being developed to model deformation of SG materials with grain sizes of between about 100 nm and 2.0  $\mu\text{m}$  (or larger)
- Deformation response and damage mechanisms are being catalogued, microstructures are being ranked and lessons learned are being collected
- Phase II Milestones and Plan have been developed, focused on
  - Processing and characterization of SG materials
  - Continuation of MD simulations to fully evaluate failure
  - Incorporation of MD simulation results within DD/CP multiscale simulation
- This activity fits within the mainstream of OSTP's Materials Genome Initiative