Deformation and Damage in Structurally Graded Nano-Crystalline Aluminum Alloys

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NASA Aeronautics Research Mission Directorate (ARMD)

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Overview

- Structurally-Graded Materials
- Multiscale Modeling of Polycrystals
- Molecular Dynamics Simulation of Atomistic Processes
- Dislocation Dynamics Simulation at Mesoscale Dimensions
- Parameterization of Continuum Crystal Plasticity
- Material Response of Macroscopic Graded Polycrystal Models
- Production of Nano-crystalline Aluminum Alloys
- Concluding Remarks

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Structurally-Graded Materials*

- **Motivation:** Historically, new materials have involved a trade-off between strength and ductility; structurally-graded materials offer the promise of increasing both simultaneously.
- Structurally-graded metallic materials consist of regions in which the grain size varies from relatively fine (10nm-100nm) to relatively coarse (1.0μm - 10.0μm).
- Finer grains contribute much of the overall material strength while the coarser grains contribute much of the ductility and toughness.

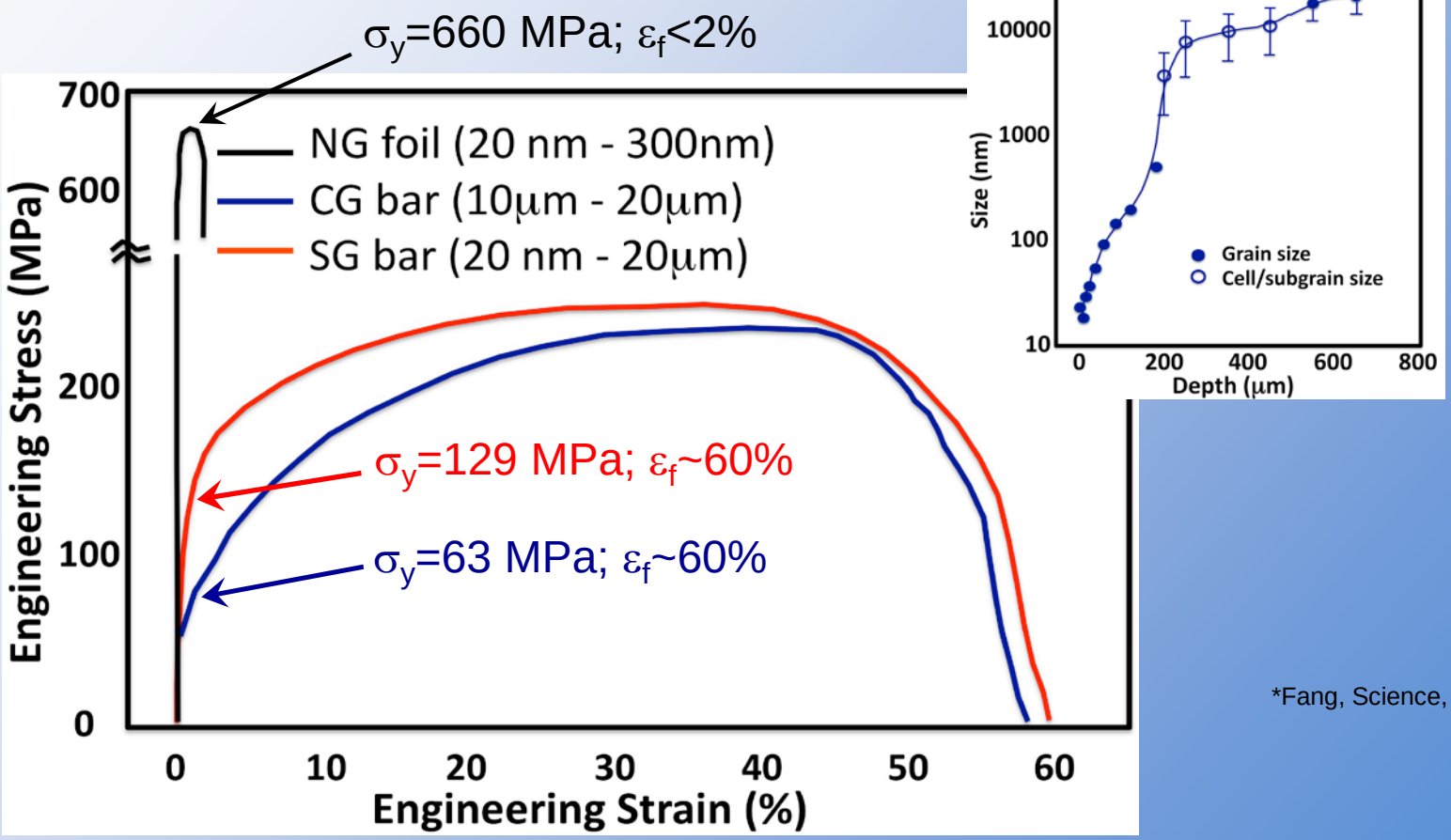
~ 10 nm **A Typical Cross-Sectional SEM Image of a SG Cu Sample** **~ 10 μm**

Schematic of Microstructure from SEM Image

*Fang, Science, 2011

Performance of Structurally-Graded Materials

- 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)*



*Fang, Science, 2011

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Multiscale Analysis Methodology

- Multiscale methods employ various computational models of the salient physics at different physical dimensions and link them across length and time scales.
- Simulations at the lowest scale represent fundamental material processes; analyses at higher scales simulate accumulations, homogenizations or complex secondary interactions over larger spatial domains and longer time periods.

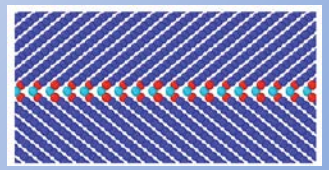
Computational methods

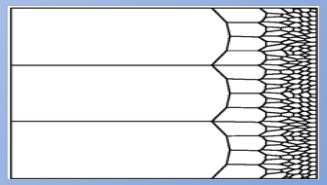
Molecular Dynamics (MD): Study the formation of dislocations, twins, stacking faults, grain growth and rotation, and grain boundary strengths leading to ultimate failure in microstructures at nanometer length scales.

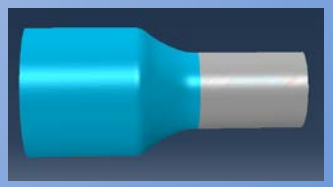
Dislocation Dynamics (DD): Analyze discrete dislocation interactions involved in yield, strain hardening, and load transfer in polycrystal assemblages at micron length scales. Various input material constants are determined from MD simulations.

Crystal Plasticity (CP): Calibrate CP parameters representing yield and strain hardening from DD predictions of stress-strain response. Use continuum finite element methods incorporating CP to analyze material domains of arbitrary size.

Typical models







Information flow

GB strength, dislocation mobility, failure mechanisms

Stress-strain behavior: yield stress, strain hardening

Predictions of macroscopic behavior of materials with complex microstructures

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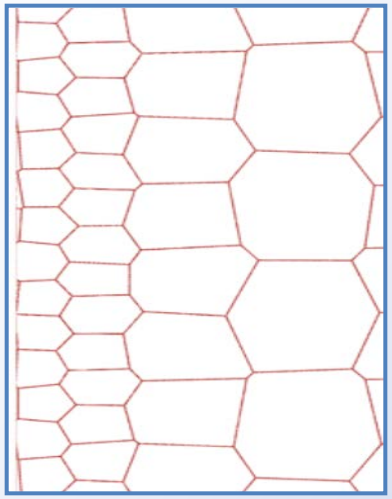
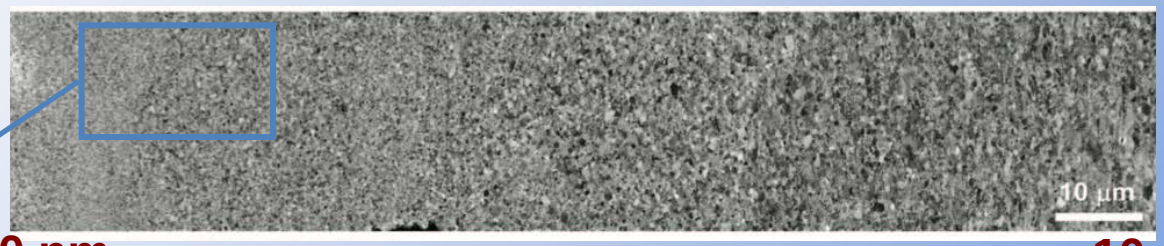
SG Microstructure Modeled by MD



Graded Microstructure†
(Grain sizes: 32 – 90 nm)



~ 10 nm

~ 10 µm

Structurally-Graded Microstructure*

- Molecular Dynamics (MD) simulations were developed for structurally-graded microstructures†
  - Aluminum
  - Grain sizes of between 19 nm and 90 nm
  - Domains of about 900 nm x 350 nm x 2 nm
  - 20 x 10^6 to 50 x 10^6 atoms
  - Evolution times of about 1 ns
  - Mishin-Farkas embedded atom method (EAM) potential §

*Fang, Science, 2011

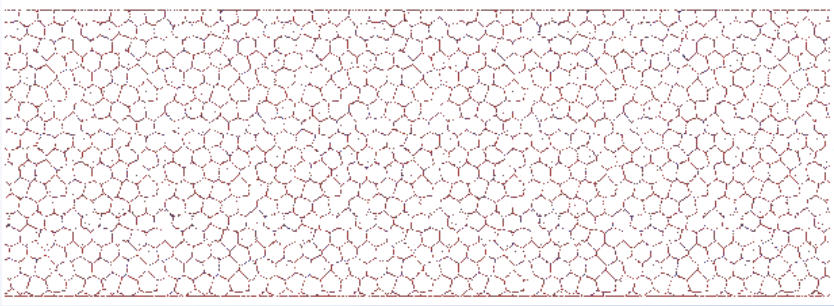
†Mishin, unpublished, 2012

§ Mishin, Phys. Rev. B, 1999

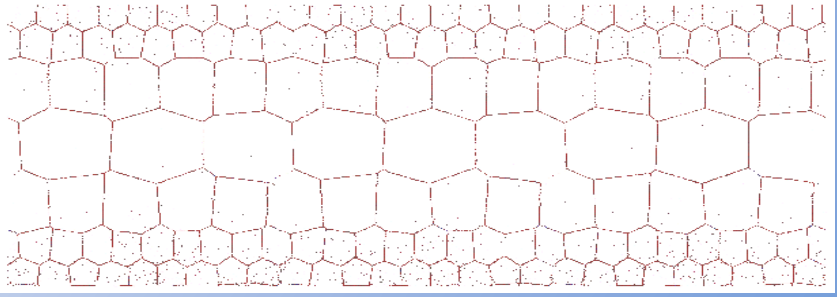
Microstructural Models for MD Simulation

Examples of initial structures for the particular case of [211] oriented grains

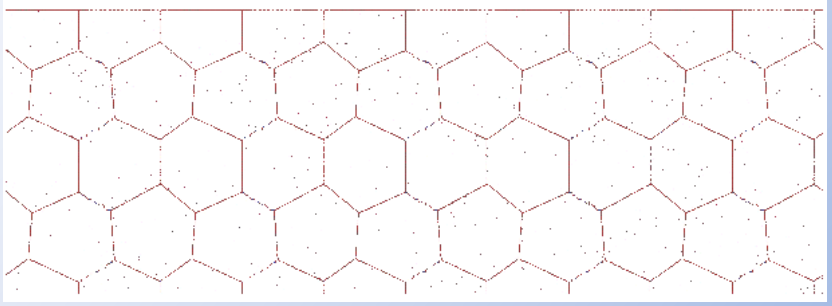
Nano-crystalline Al, grain size 19 nm



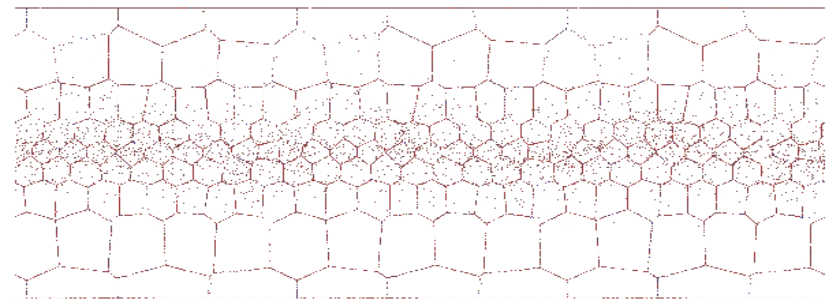
Nano-graded Al, grain size 30 to 94 nm



Nano-crystalline Al, grain size 94 nm

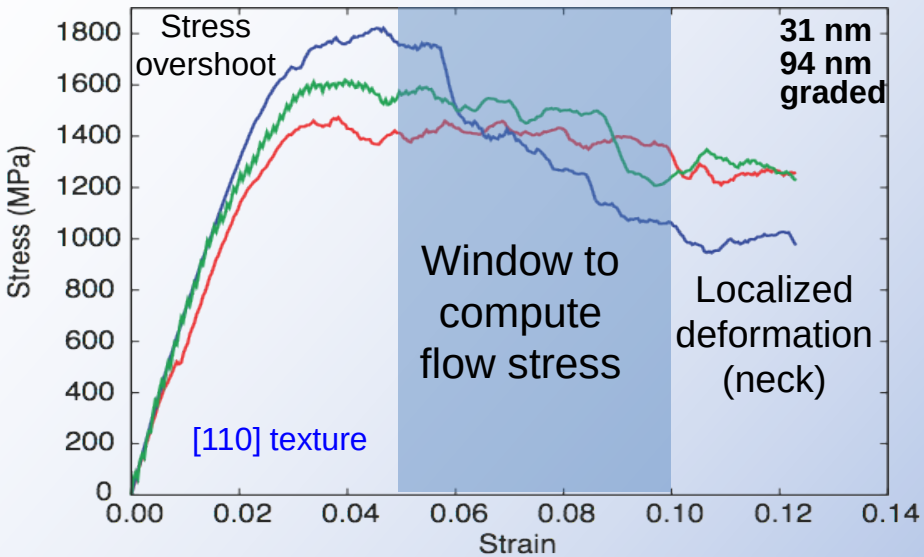


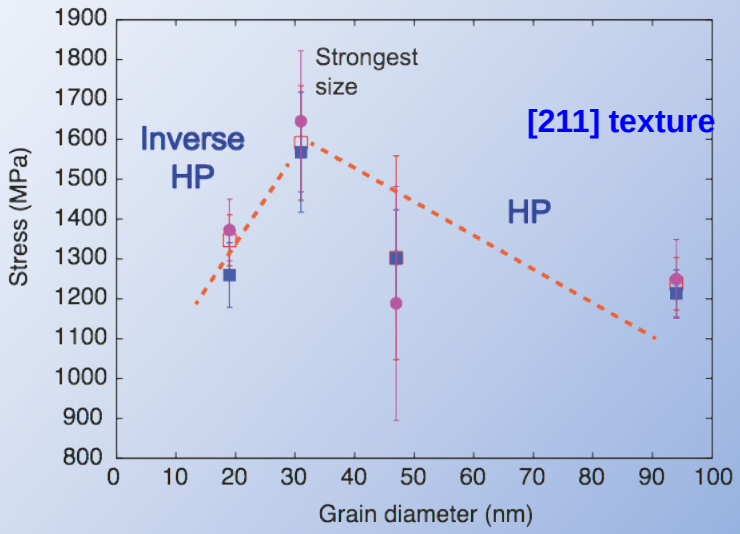
Nano-graded Al, grain size 94 to 30 nm



Graded models are similar to composite laminate layups in which layers of different grain sizes can be constructed to assess effect on strength and ductility.

Simulated Tensile Test Results





Observations

- Stress peak for relatively large grain sizes ("stress overshoot") due to delayed nucleation of dislocations
- The flow stress reaches a maximum at the grain size of about 30 nm, decreases at larger and smaller size
- The simulations reproduce both the direct and inverse Hall-Petch* (HP) effect
- The graded structure shows promising strength

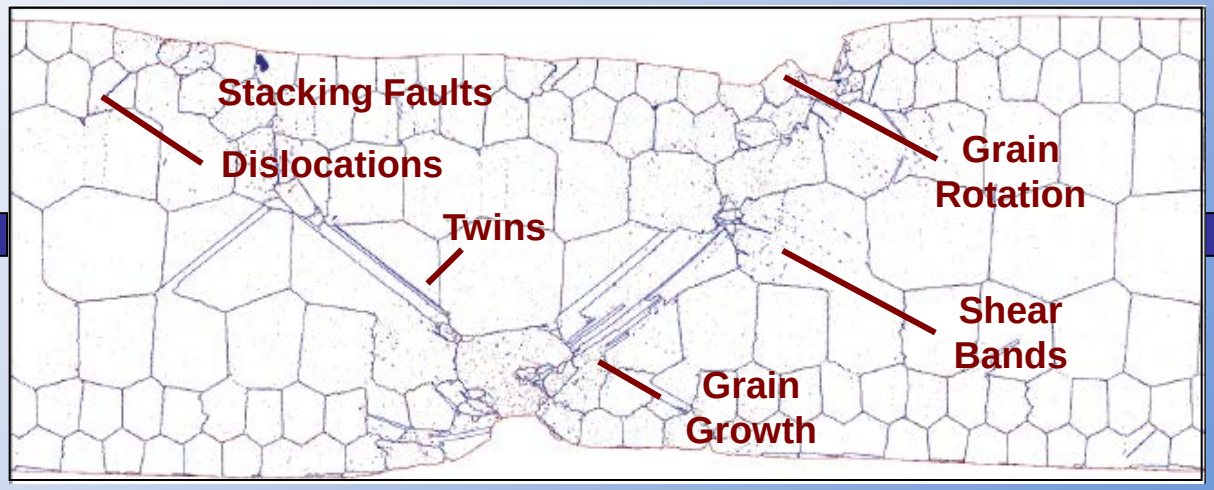
*Hall, *Proc. Phys. Soc.*,1951; Petch, *Iron and Steel Institute*, 1953

SG Microstructure: Mechanisms & Deformation from MD†

- Simulates complex mechanisms of dislocation nucleation and interactions, shear bands, stacking fault formation, and grain boundary (GB) migration at atomic resolution.
- Deformation is primarily caused by dislocation slip and grain boundary rotation.
- 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)

δ_x



δ_x =10%

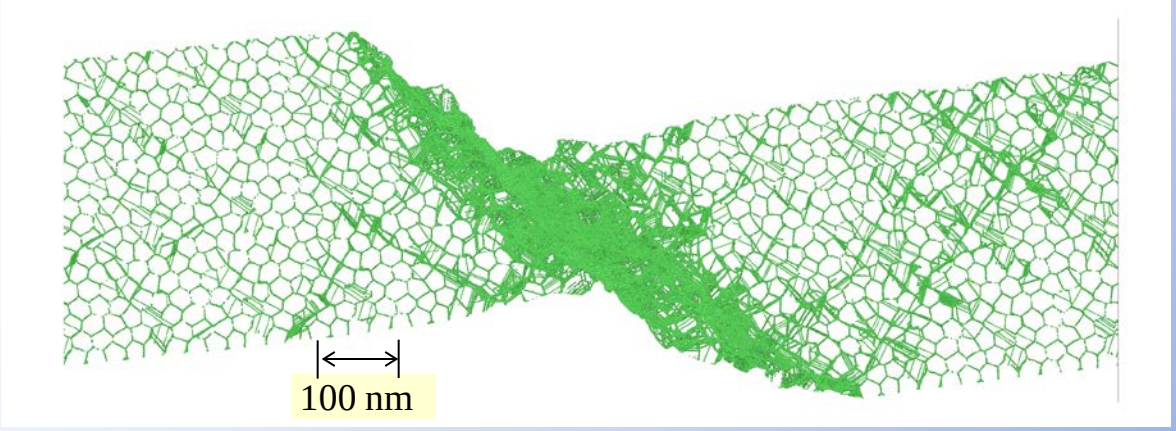
T = 300 K
$\dot{\varepsilon}$ = 5 x 10^6/s

Predicted Deformation Processes in SG Material

†Mishin, unpublished, 2012

Simulation of Deformation Near Final Failure

Typical deformation of a uniform nano-crystalline Al. Note strain localization in a shear band

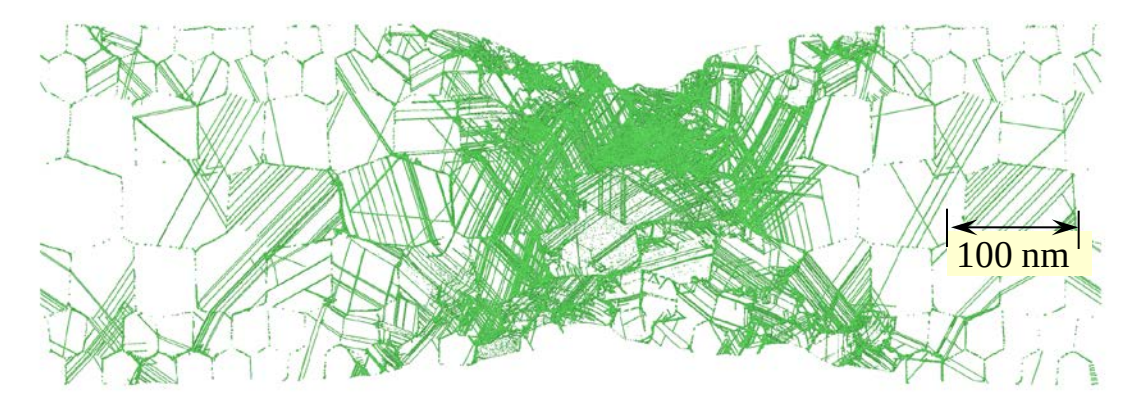


[211] texture

Grain size 20 nm
Strain 19%

Material is in the inverse HP regime with GB dominated deformation

Typical deformation of a graded nano-crystalline Al. Note the formation of a wide neck



[110] texture

Grain size varies from 30 to 90 nm
Strain 19%

Material is in the direct HP regime and exhibits ductile failure within grain

MD Model of Grain Boundaries

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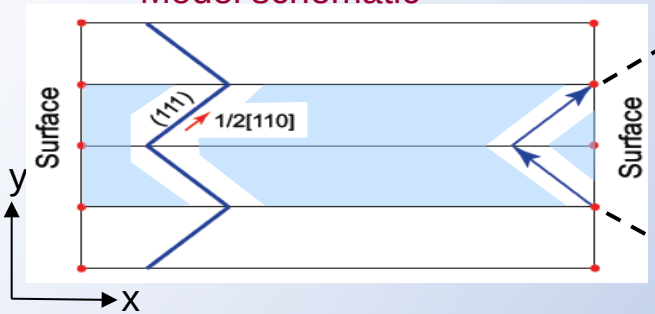
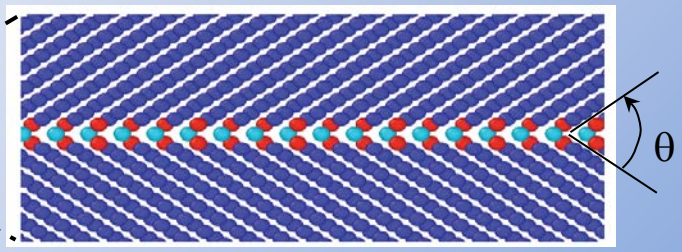
- 6-layer molecular dynamics model with symmetric tilt Σ5, Σ7, Σ25 boundaries analyzed.
- The triple junctions at the free edges served as initial dislocation sources

Model schematic

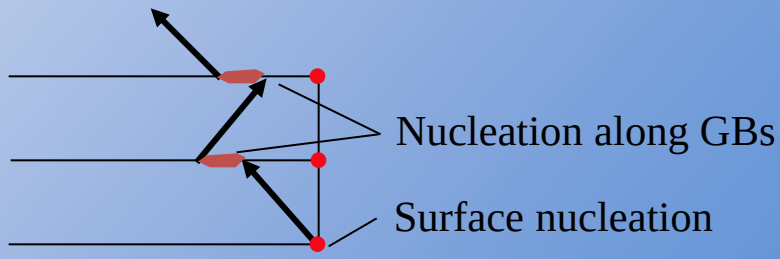


Σ5 GB configuration, θ = 78.46°



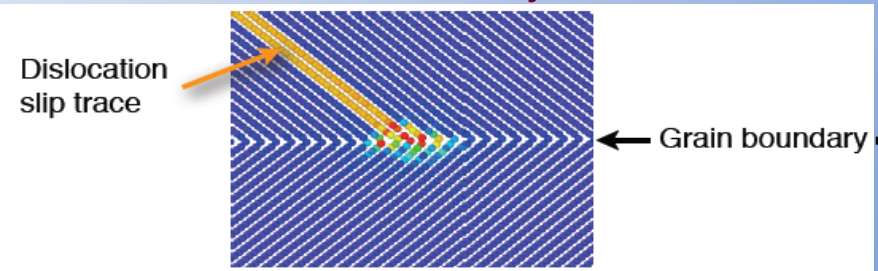
Dislocation nucleation

- Initial generation of dislocations from surface junctions
- Secondary generation of GB sources which nucleate additional dislocations

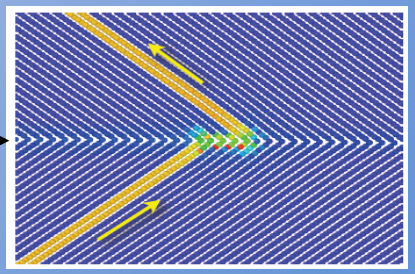


napshots of interaction mechanisms predicted by molecular dynamics simulation

Dislocation absorbed by a GB



Dislocation transmission with a shift

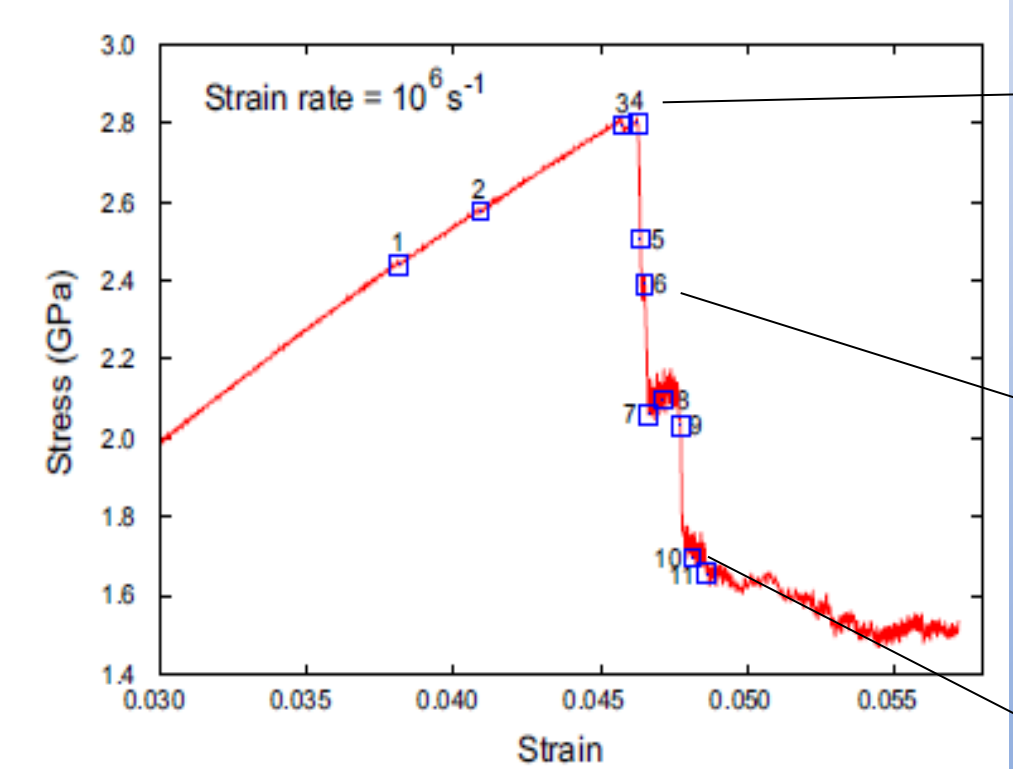


Progression of Early Stage Deformations

Stress-strain curve

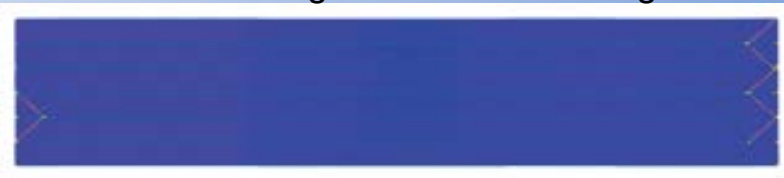
Σ5 [211](210), θ = 78.46°

T = 300 K, $\dot{e} = 10^6\ s^{-1}$

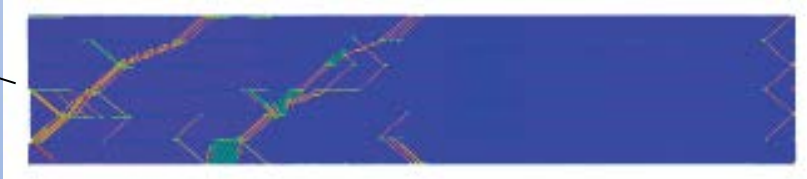


Dislocation formation

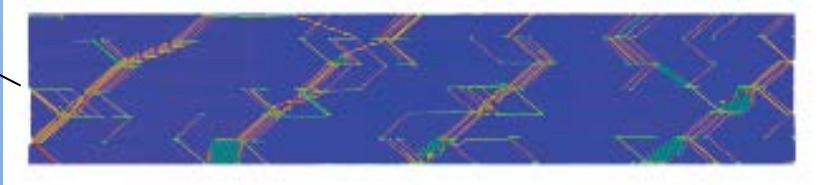
Snapshot #4. Peak stress reached. Dislocations begin to transmit through GB



Snapshot #6. Stress decreasing. Massive GB nucleation of dislocations.



Snapshot #10. Shear band formation.



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Dislocation Dynamics Simulation

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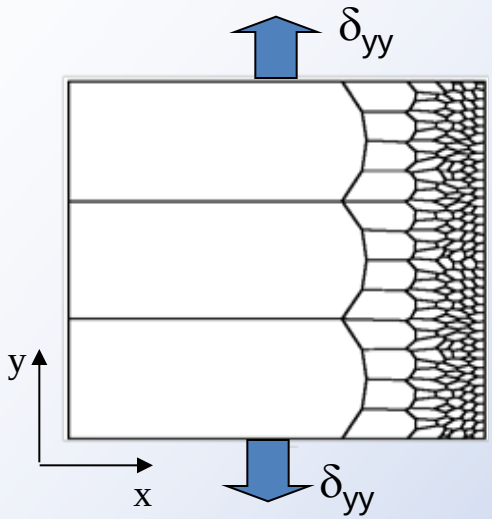
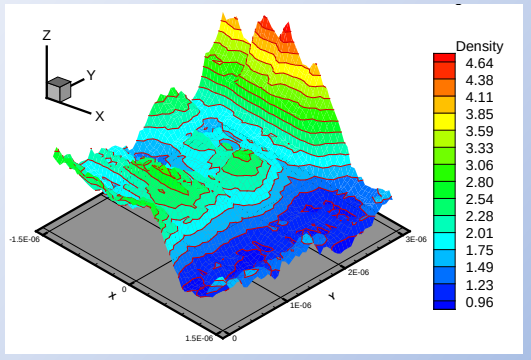
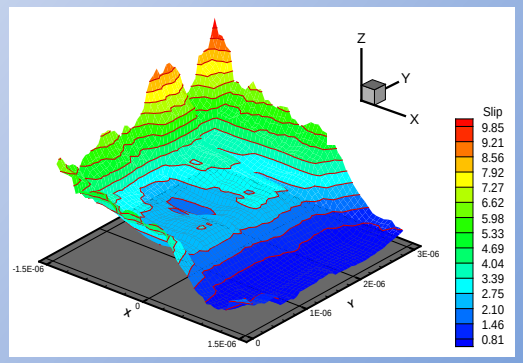
Polycrystal model for DD analysis

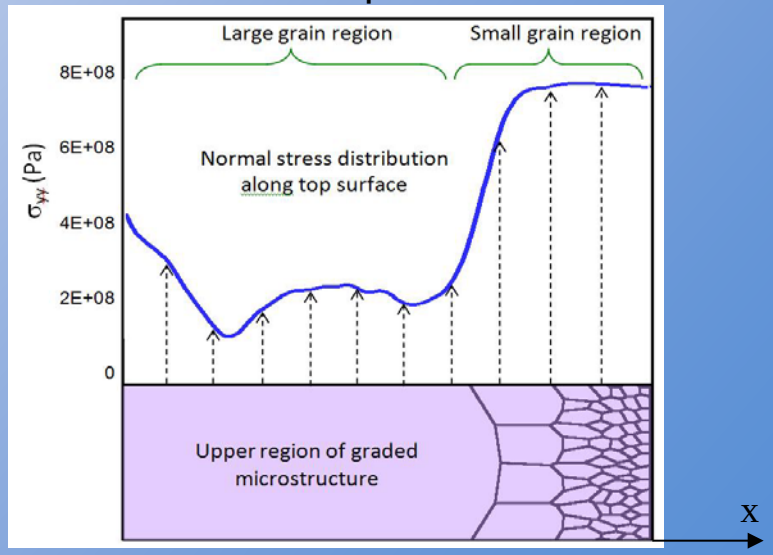


Dislocation density and slip distribution at 1% strain showing linear-elastic response in nanograin region





Stress profile



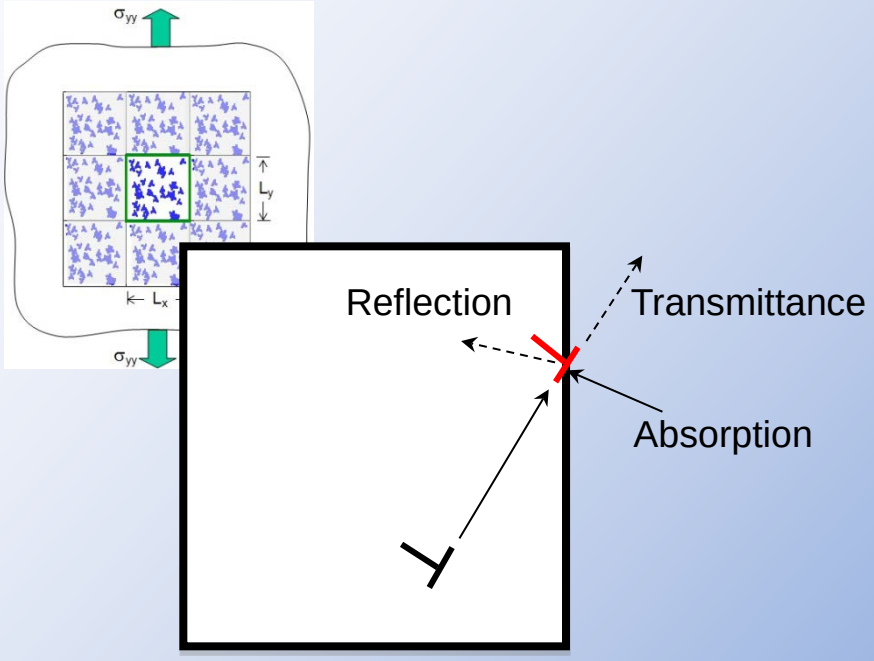
- **A graded polycrystal model based on Voronoi tesselation had grain diameters ranging from 0.7 μ to 15 nm.**
- **DD simulation shows the transfer of load to outer brittle layer with increasing applied strain.**
- **Ultimately strain levels initiate GB migration and strain localization extending into the outer region which precipitates final failure.**

Dislocation-GB Interactions

Reflection: Simulated by preventing dislocation motion into a GB and allowing these dislocations to freely glide back into the grain interior.

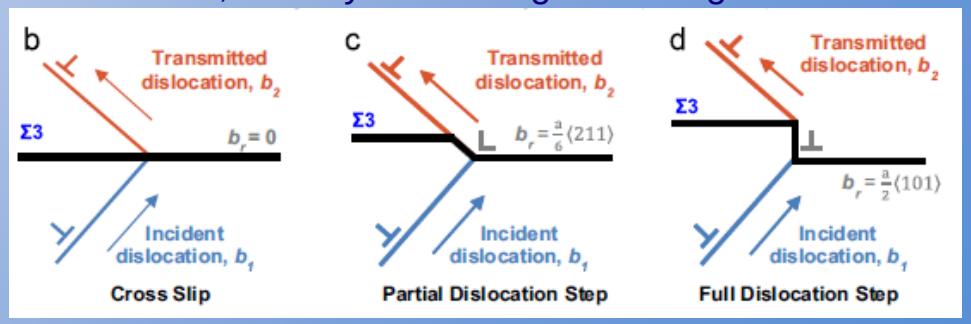
Absorption: Simulated by pinning dislocations at the GB.

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.*

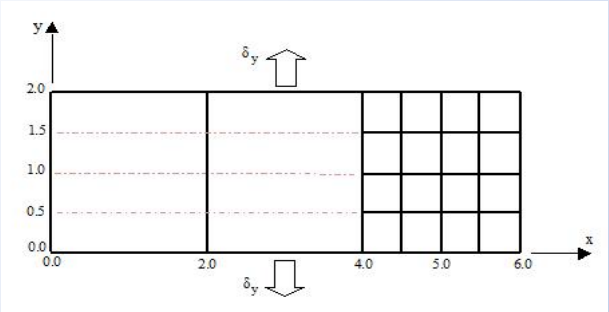


*Abuzaid, JMPS, 2012

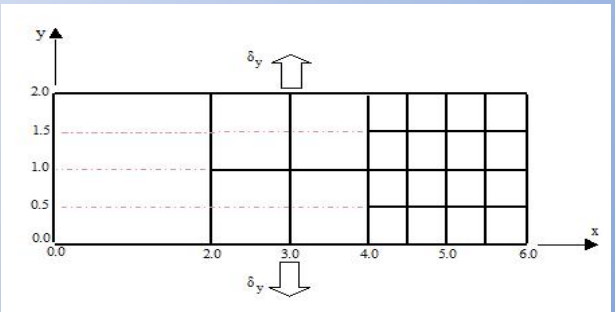
Dislocation Dynamics Simulation

- A series of graded polycrystal models composed of idealized grains were generated.
- Square grains were used to carefully control grain size in models. Actual shape of grains is immaterial in DD analysis.
- Transmissible GB behavior was assumed.
- Studies showed that 2μ grains are effectively perfectly plastic while 100 nm grains are essentially linear-elastic. The models represent microstructures within this range of grain sizes.

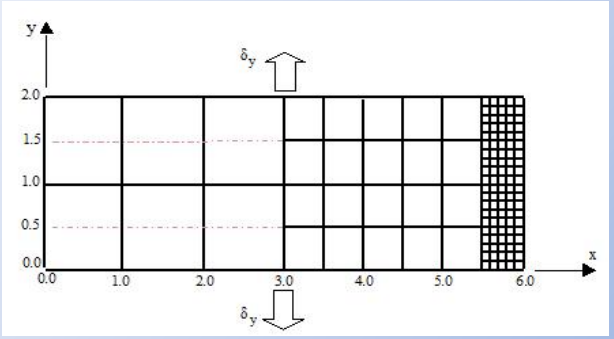
Model 1



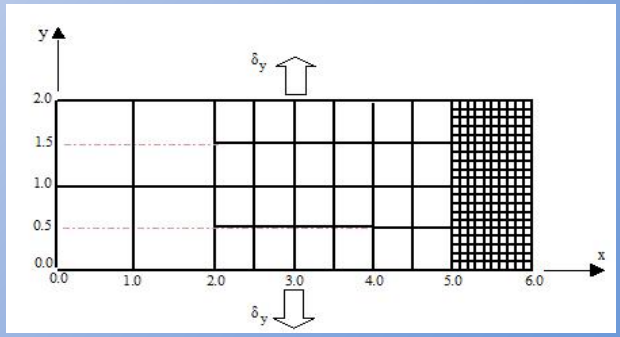
Model 2



Model 3



Model 4



Average Grain Size

Model 1: 0.8167μ

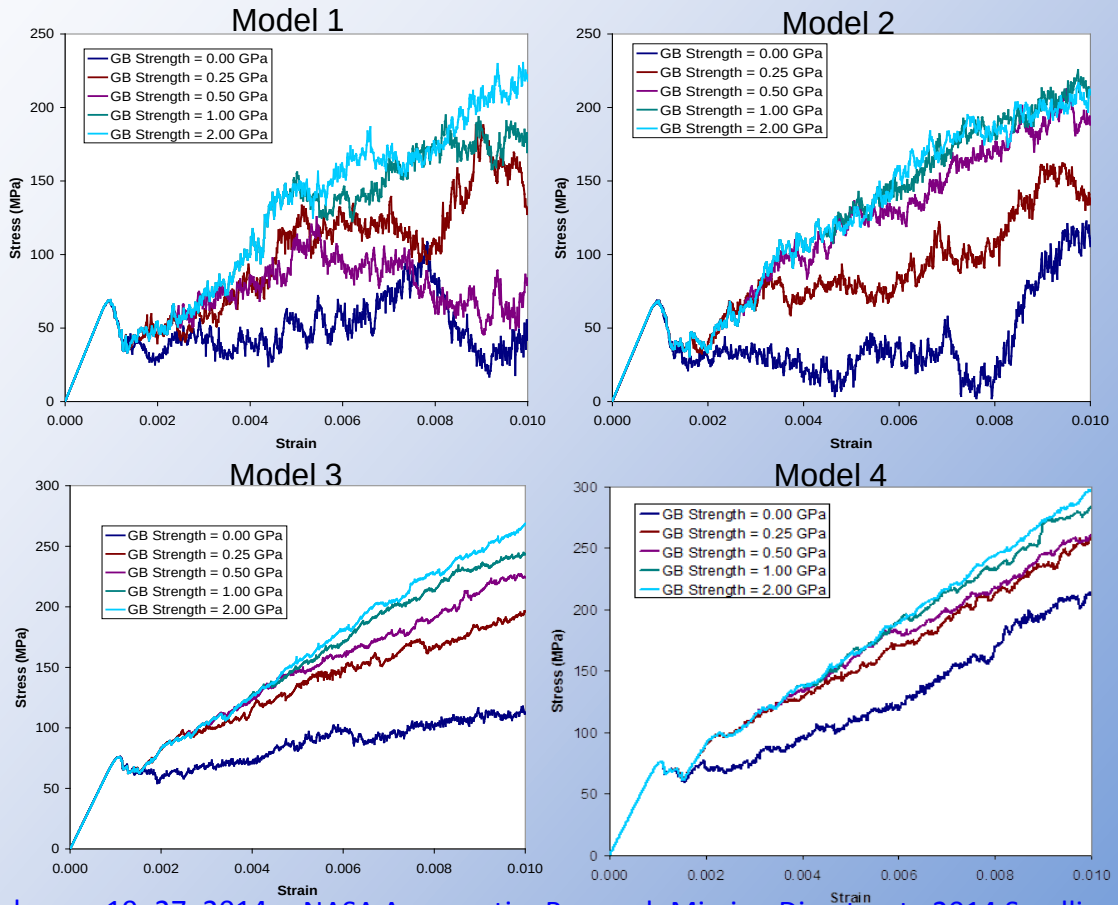
Model 2: 0.7559μ

Model 3: 0.3085μ

Model 4: 0.2293μ

Simulation of Stress-Strain Behavior

- Simulations used the graded DD models with varying GB strength for transmitting dislocations.
- While MD studies gave a 1.37 GPa strength for a Σ5 GB, DD results are obtained using 0.0 to 2.0 GPa to interpolate effective barrier strengths for other GB orientations.



Observations

- Families of stress-strain curves show increasingly brittle behavior with decreasing grain size.
- For each model, decreasing the barrier strength for dislocation transmission increases ductility.

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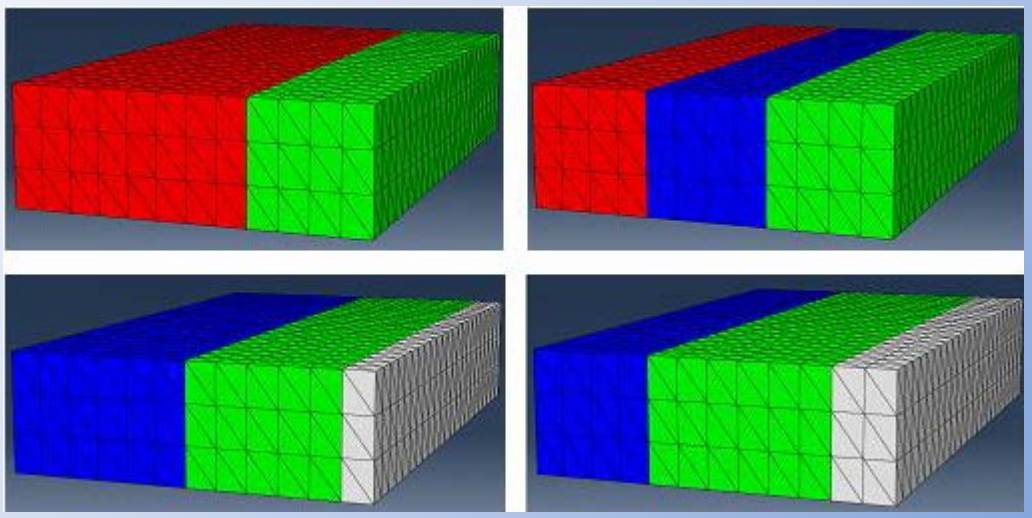
Calibration of Continuum Crystal Plasticity Parameters

- An Inverse method utilizing a formal minimization procedure maps DD stress-strain predictions into CP parameters.
- Earlier mappings of CP parameters were made to single crystal DD simulations using reflective GB behavior and periodic boundary conditions to approximate an infinite domain.
- Simulations model GBs as transmittable with an energy barrier that, when exceeded, will allow dislocations to glide into adjacent grains.
- A revision of original CP parameters using full polycrystal models with free boundary conditions was made to adjust parameters for transmittable GB behavior.

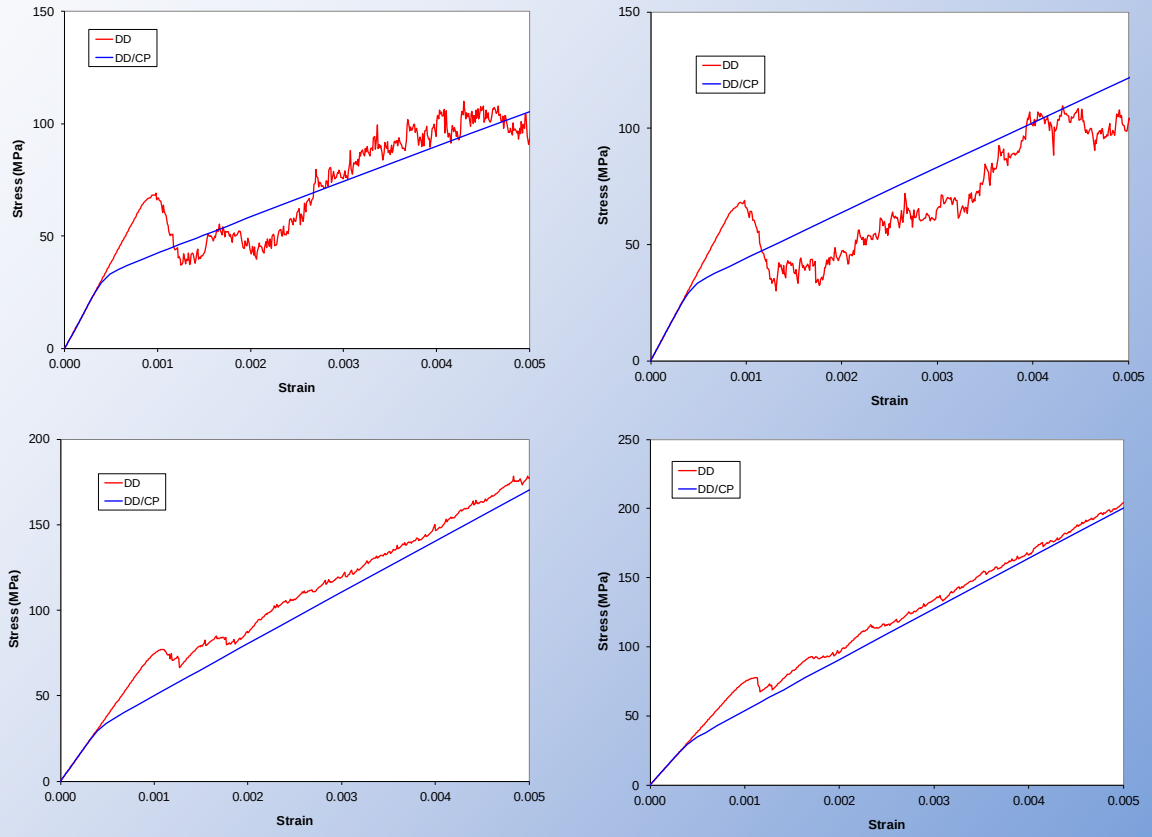


Designation of assumed grain sizes:

- = 2.0μ x 2.0μ
- = 1.0μ x 1.0μ
- = 0.5μ x 0.5μ
- = 0.1μ x 0.1μ

Comparing DD and CP Stress-Strain Predictions

- Stress-strain calculations were generated for each polycrystal model using DD and CP analyses.



Observations

- DD results exhibit an initial dynamic overshoot of yield stress which is neglected in CP calibration
- DD stresses show increased fluctuations for larger grains.
- The strain hardening slope increases with decreasing average grain size tending towards linear-elastic behavior
- Resulting stress-strain curves from DD and CP analyses compare reasonably well

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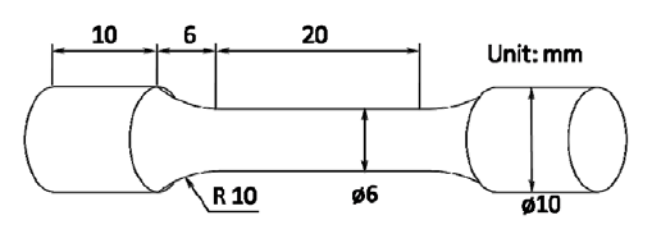
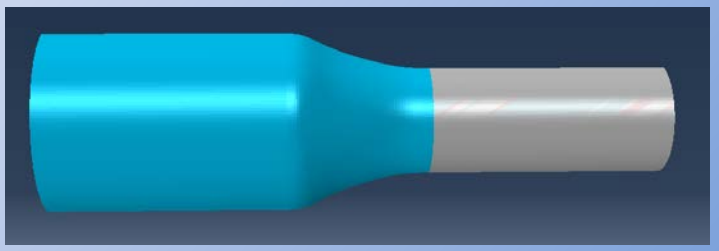
Concentric Layer Configuration for Graded Specimen

- A cylindrical dogbone model was simulated with several variations in radially graded microstructure.
- Multiscale analysis allowed the simulation of an experimentally accessible specimen geometry with a length of 52 mm and a diameter of 10 mm.

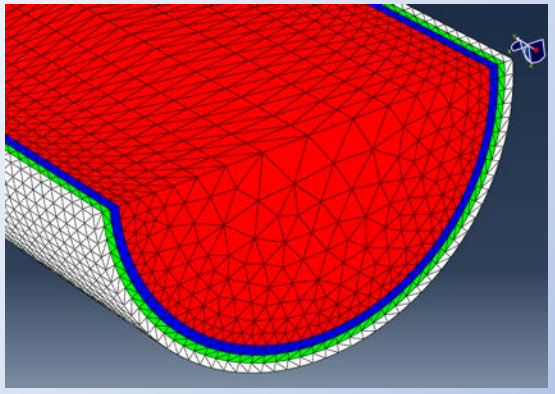
Tensile bar geometry



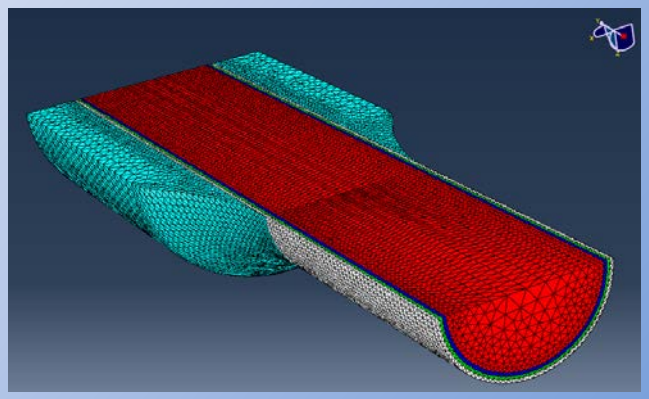
Axial profile of grip and test sections



Graded microstructure



FE model of dogbone specimen



Designation of assumed grain sizes:

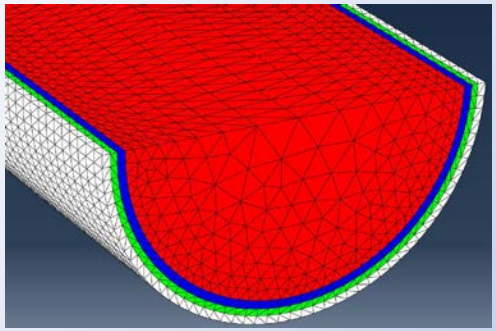
= 2.0μ x 2.0μ = 1.0μ x 1.0μ

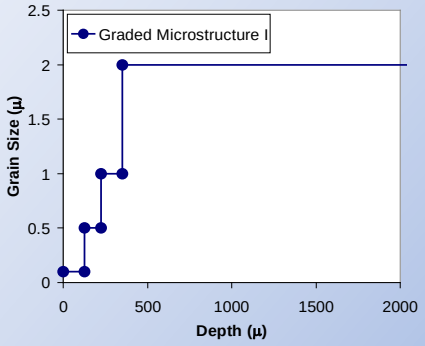
= 0.5μ x 0.5μ = 0.1μ x 0.1μ

Model Configurations for Graded Specimen

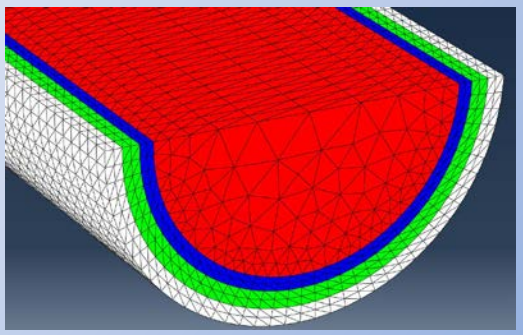
- Simulations were performed on cylindrical models composed of entirely nanoscale grains (d=100 nm), coarse grains (d=2 μ), and graded microstructures (d=100 nm - 2 μ).
- Simulations were limited to a small applied strain because the strain softening associated with grain rotation and grain boundary migration leading to final failure cannot be represented in a DD or CP framework.
- The results of these analyses provide guidance for further fabrication process developments.

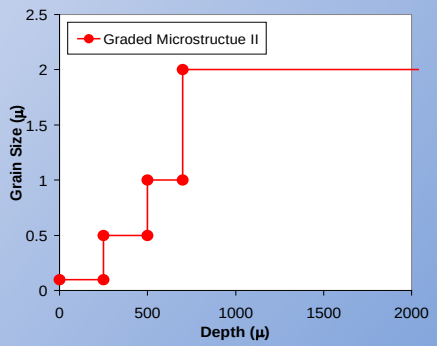
Microstructure I



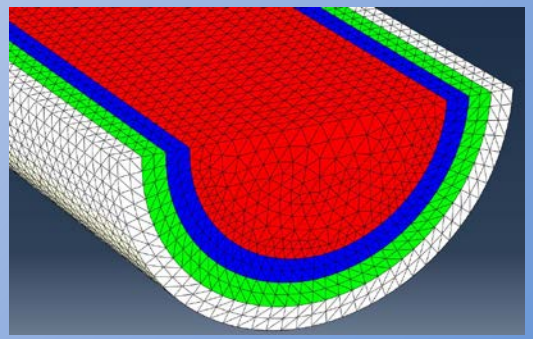


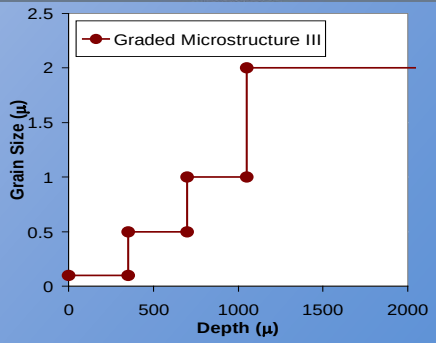
Microstructure II





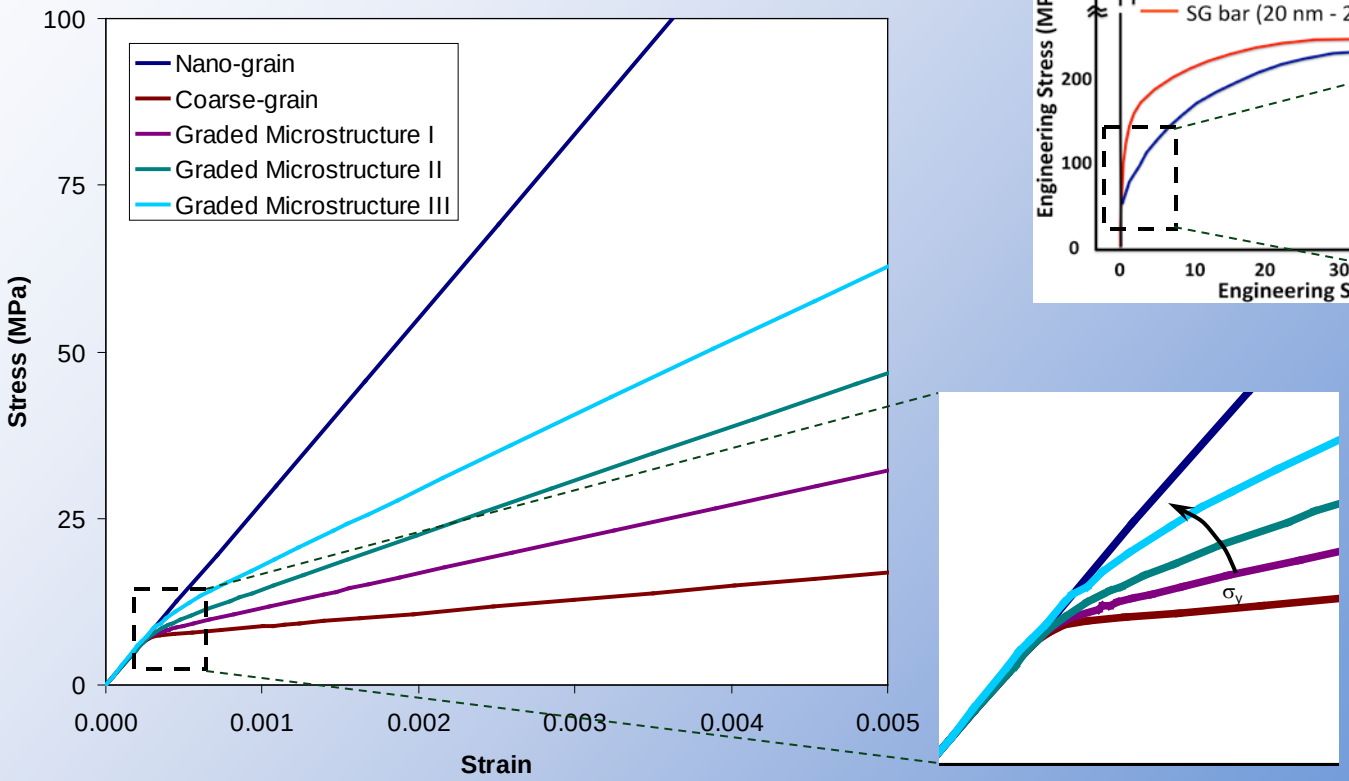
Microstructure III

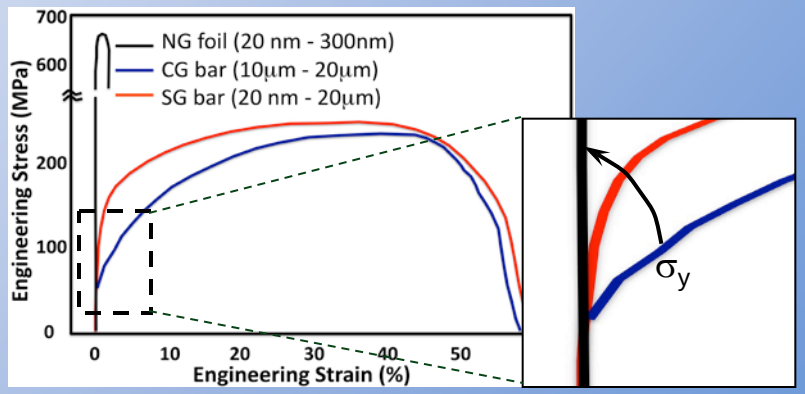




Analysis Results for Macroscopic Graded Specimen

Qualitative comparison between multiscale simulation of Al models show a similar trend in increased yield stress and preserved ductility with microstructural grading as shown by experiments with Cu specimens*





*Fang, Science, 2011

Overview

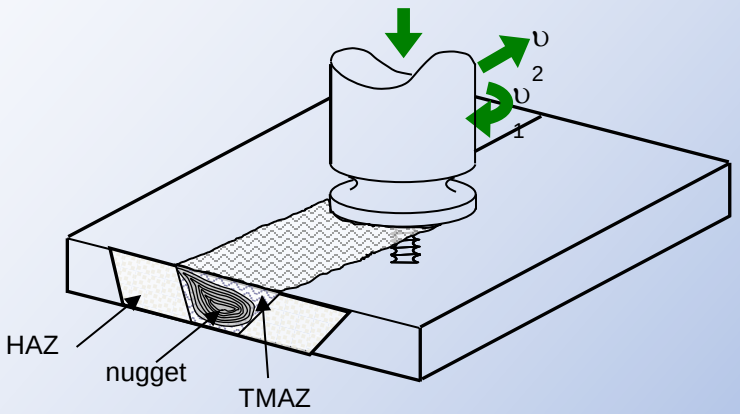
- Structurally-Graded Materials
- Multiscale Modeling of Polycrystals
- Molecular Dynamics Simulation of Atomistic Processes
- Dislocation Dynamics Simulation at Mesoscale Dimensions
- Parameterization of Continuum Crystal Plasticity
- Material Response of Macroscopic Graded Polycrystal Models
- **Production of Nano-crystalline Aluminum Alloys**
- Concluding Remarks

Production of Graded Fine-grain Material

- **Objective**: Produce material for mechanical testing for validation/verification of analytical results
- **Problem**: Pure-aluminum with grain sizes of interest to this study are not stable
- **Approach**: Use aluminum alloys with nano-scale (~20 nm) dispersoids
  - Consideration of multiple methods to produce fine-grain products
- Two broad classes of fine-grain production processes
  - Grain refinement by deformation processes (top-down)
  - Building up of material using fine powder

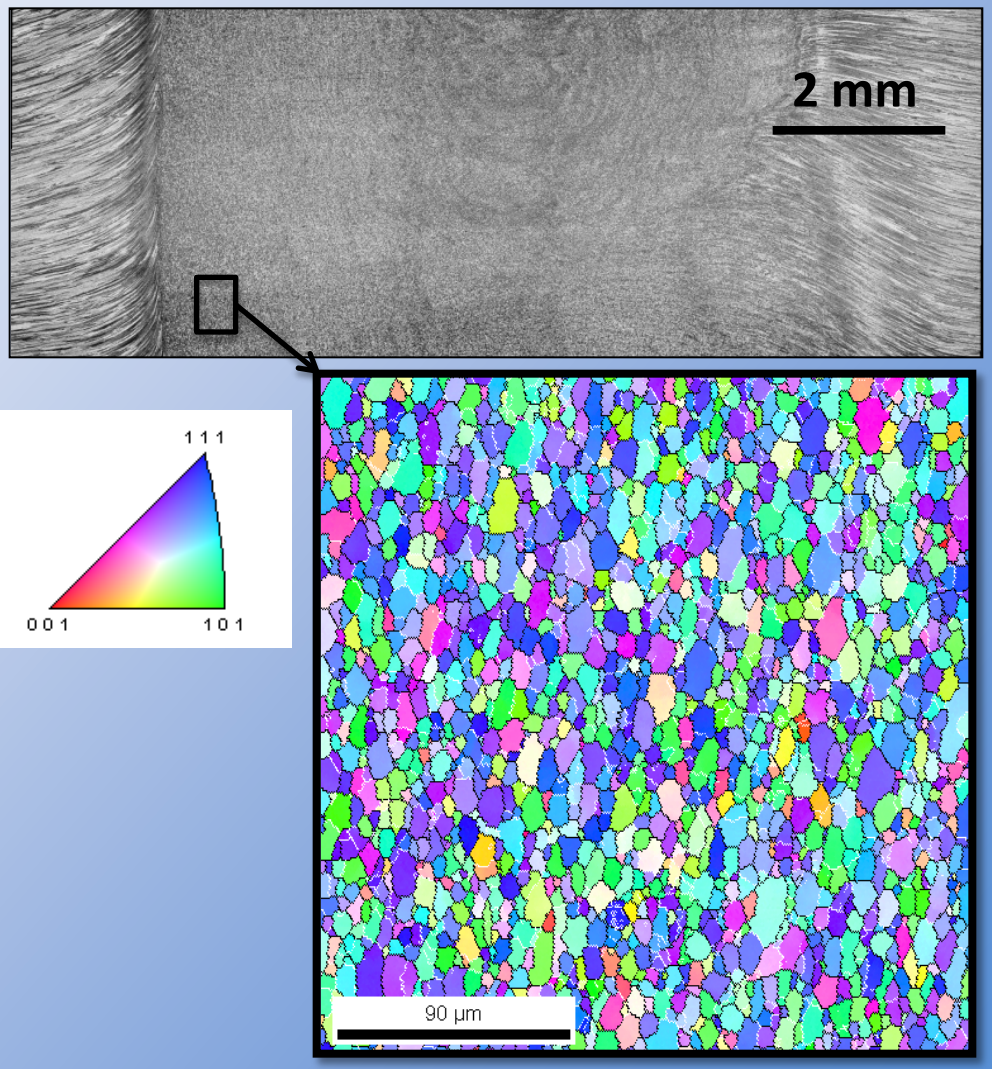
Grain Size Refinement (FSW)

- Friction Stir Welding results in grain refinement
  - Grain size reduction from ~100 μm to ~ 10 μm



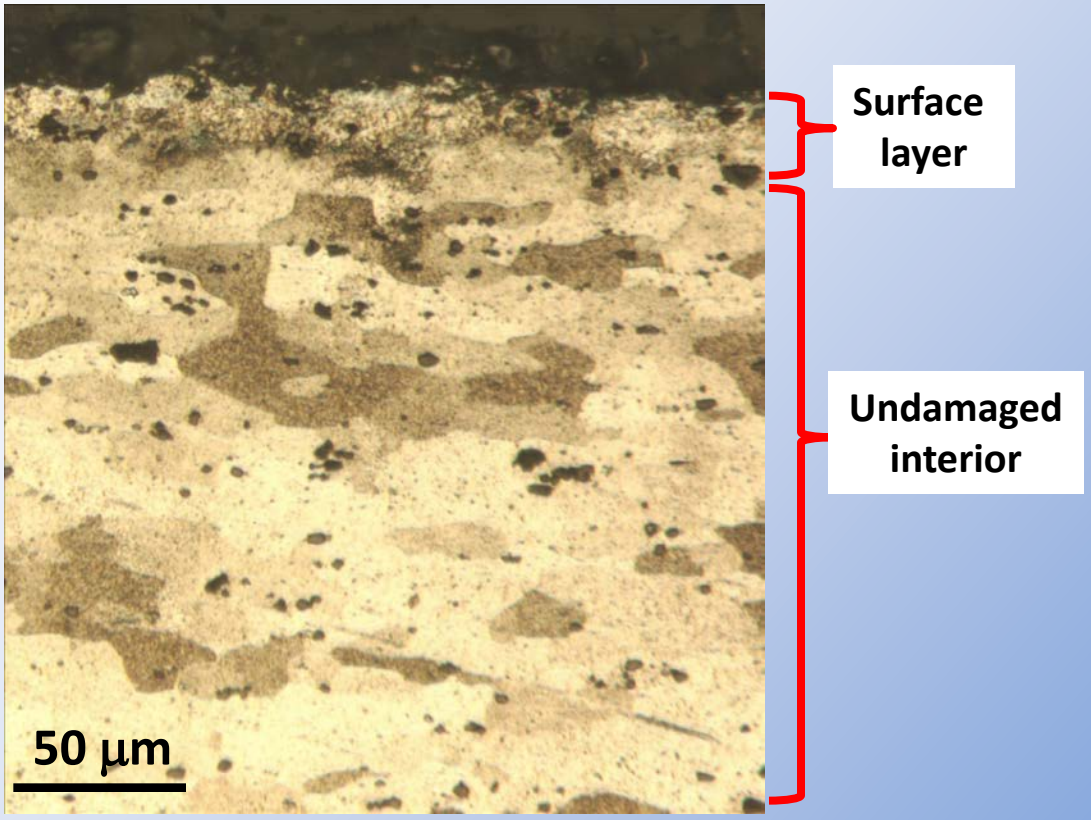
Friction Stir Welding (FSW)

HAZ – Heat affected zone
TMAZ – Thermo-mechanically affected zone



Grain Size Refinement (Surface Impact)

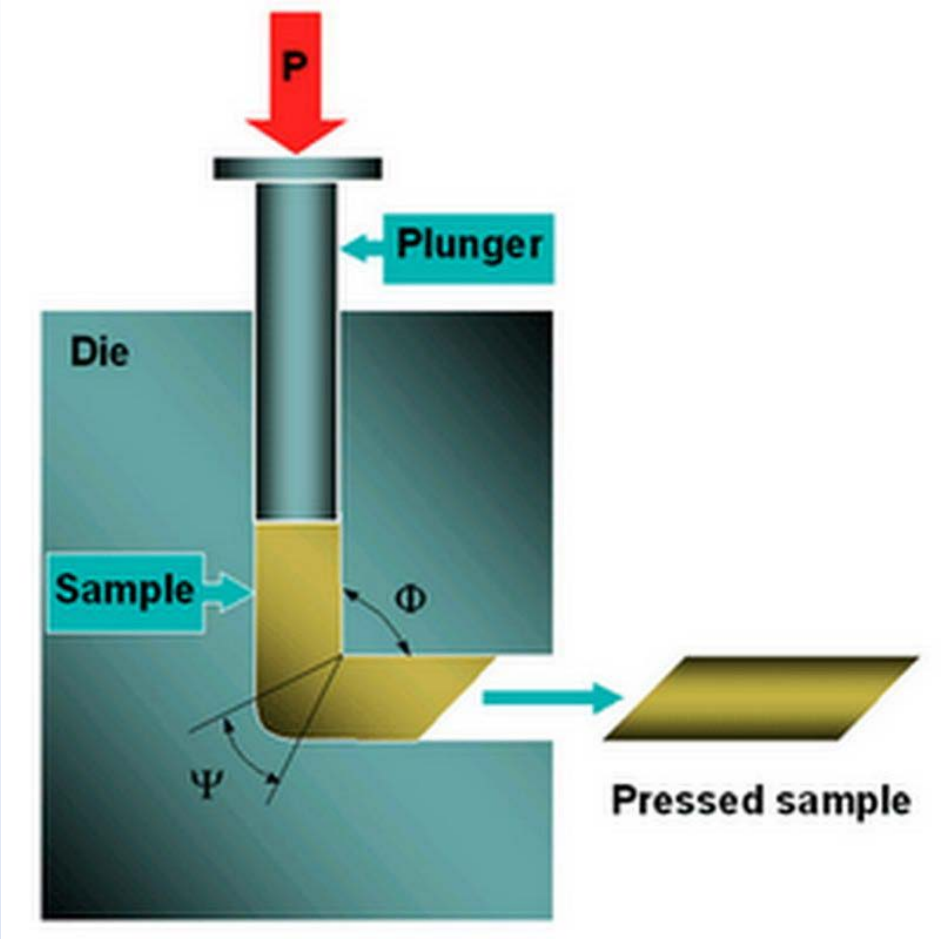
Cryogenic Bead Blasting



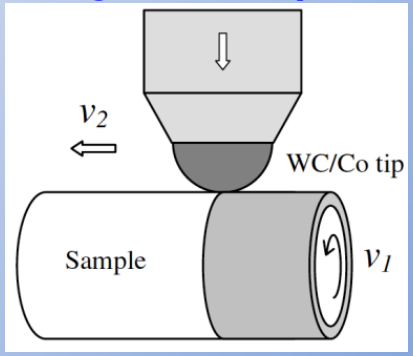
- Cooled material with liquid nitrogen
  - Aluminum 2024 sheet
  - Grain sizes ~100 μm
- Blasted surface with ceramic beads in an effort to damage near-surface material and refine grain size
  - Bead-blast affected layer <20 μm
  - Difficult to assess grain size

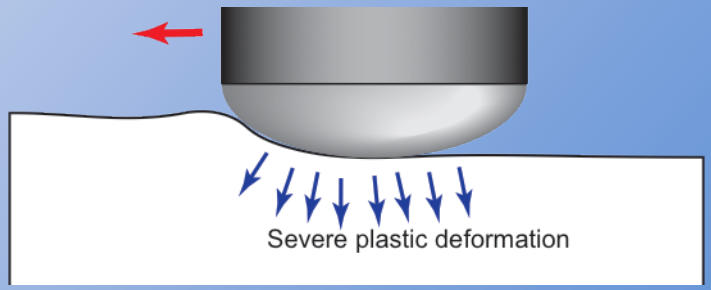
Other Grain Size Refinement Methods

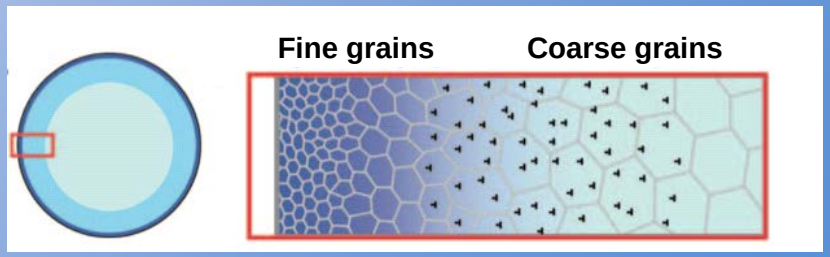
Equal Angle Channel Pressing (EACP)



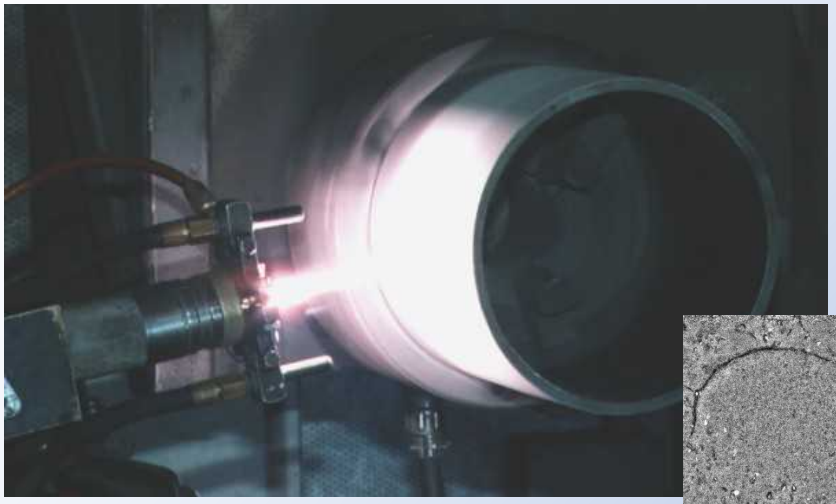
Surface Mechanical Grinding Method (SMGT)



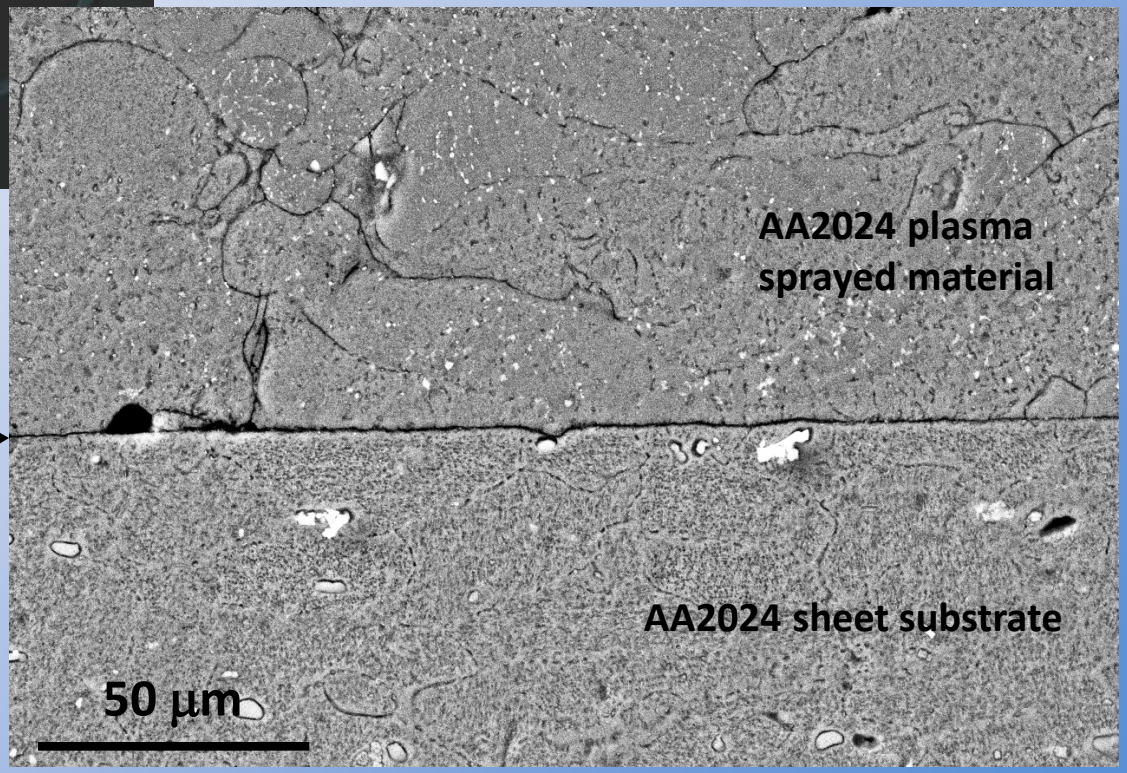




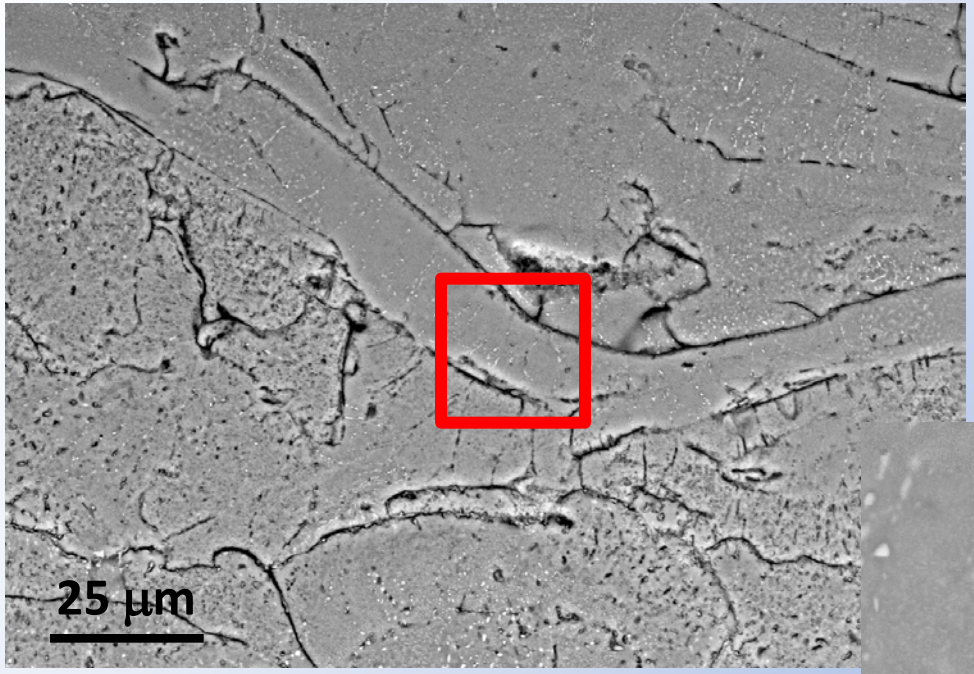
Powder Consolidation (Plasma Spray)



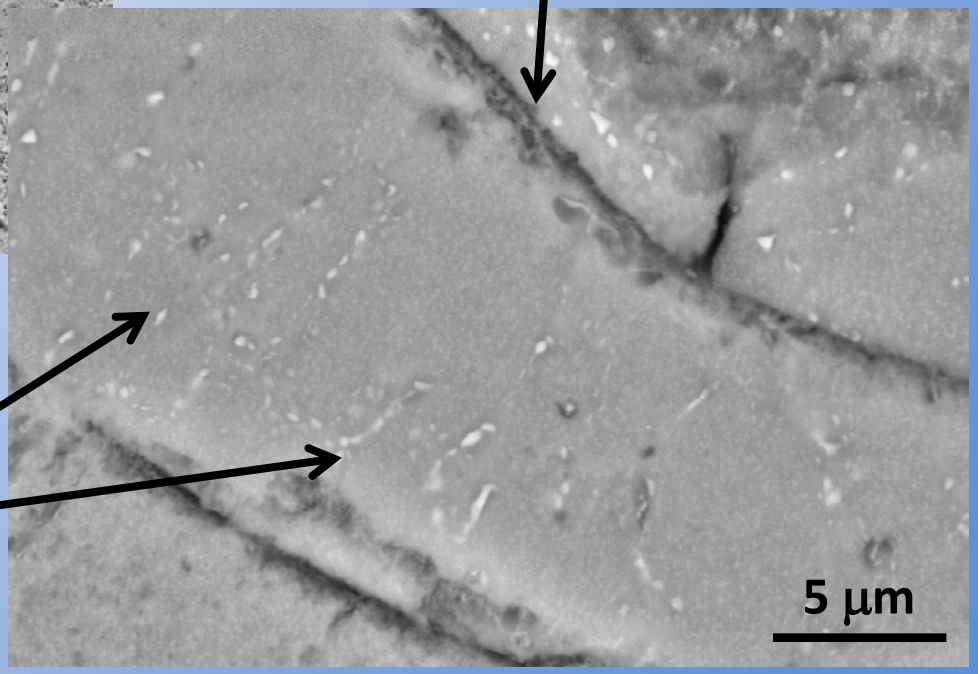
- Fine powder fed into plasma spray
  - Heated and collided with substrate
  - Cyro-ball-milled Aluminum 7075 powder on Aluminum 2024 sheet



Plasma Spray Microstructure

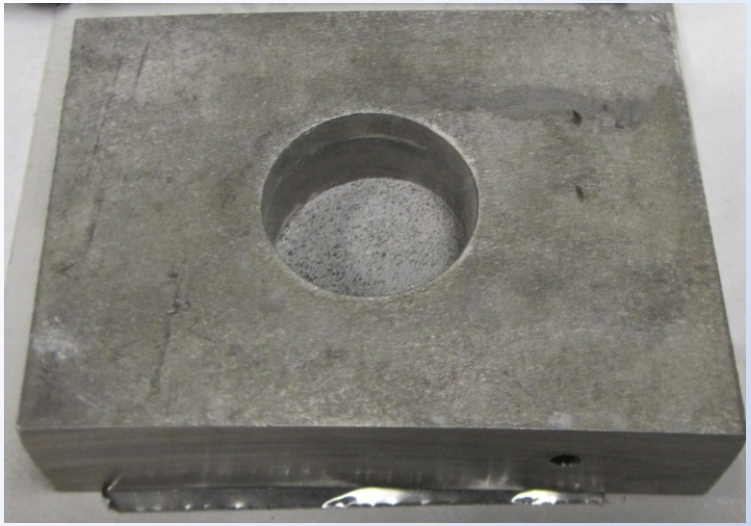


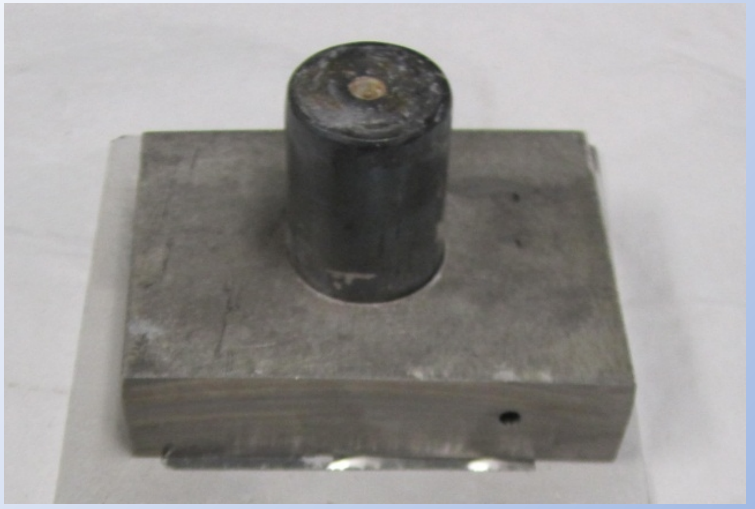
Plasma Spray Droplet Boundaries



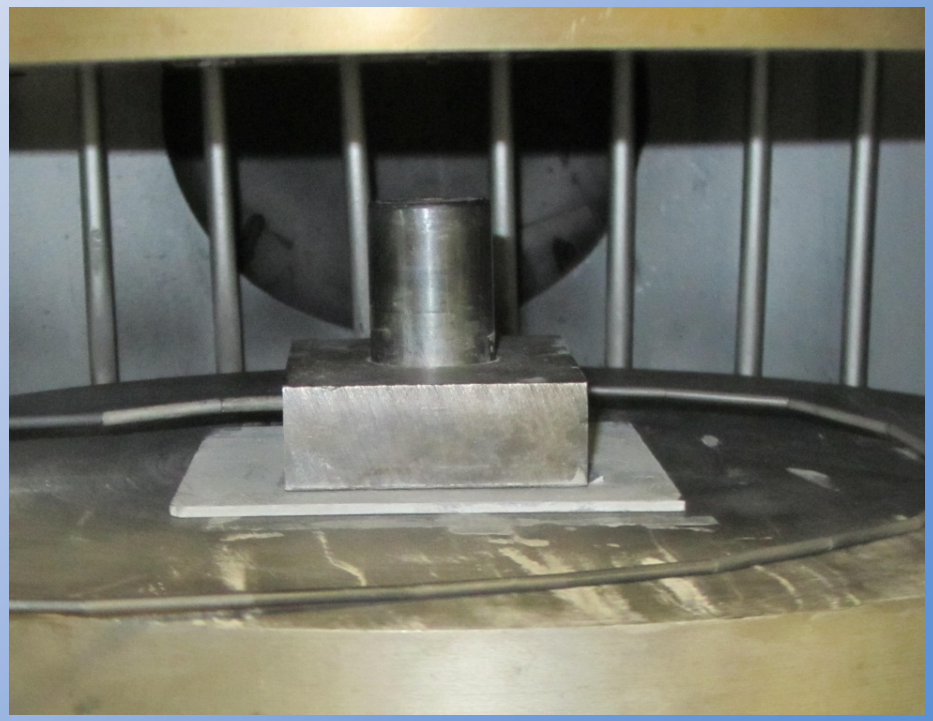
Small Al/Cu particles decorating GBs

Powder Consolidation (Vacuum Hot Press)

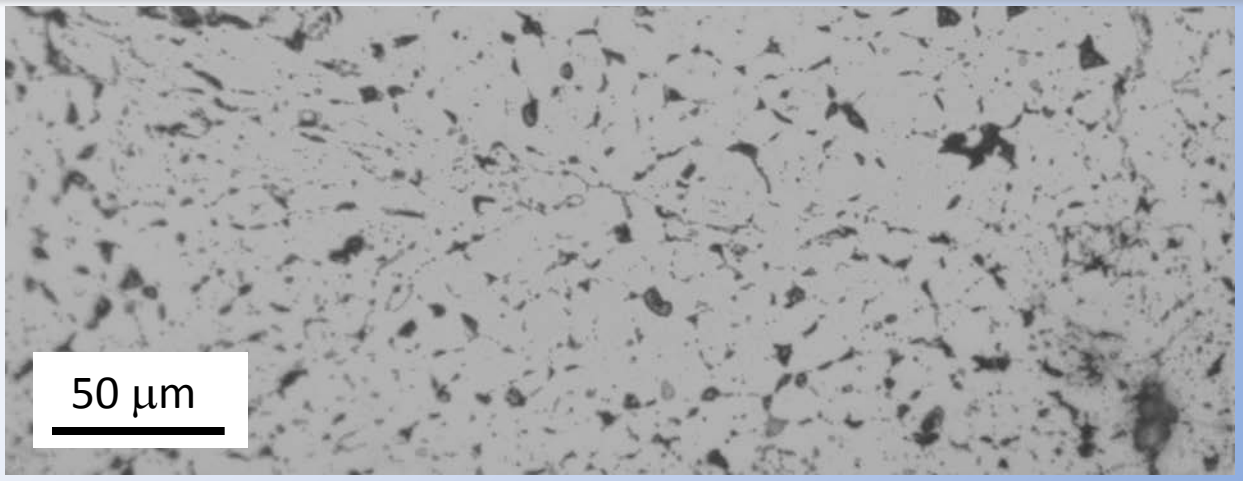




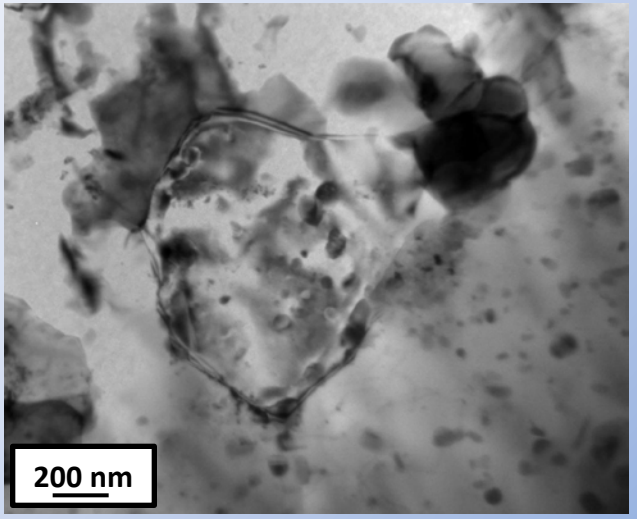
- Powder consolidation by vacuum hot press
  - Material placed in a die
  - Compressed at elevated temperature (typically 450-500°C, 100 MPa)



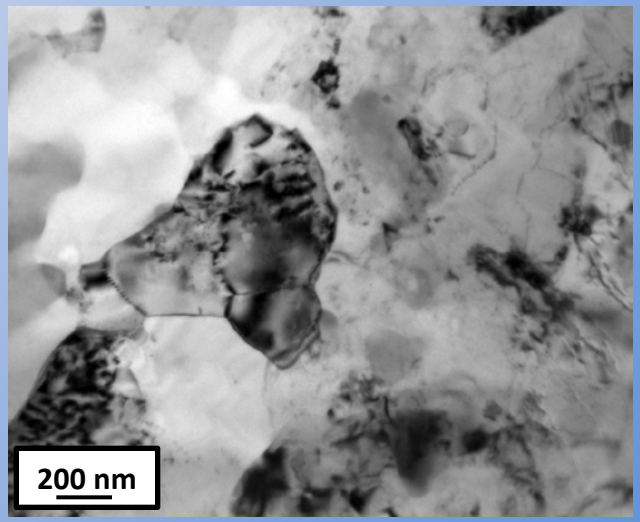
Vacuum Hot Press Results



Aluminum 7075 LaRC cryo-ball milled powder

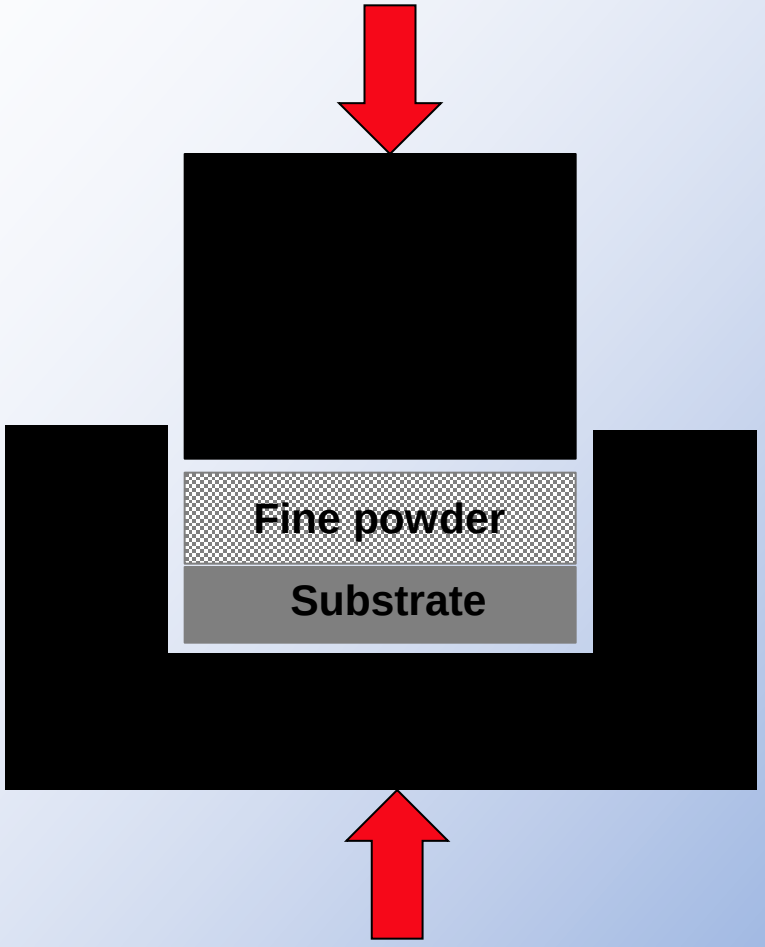


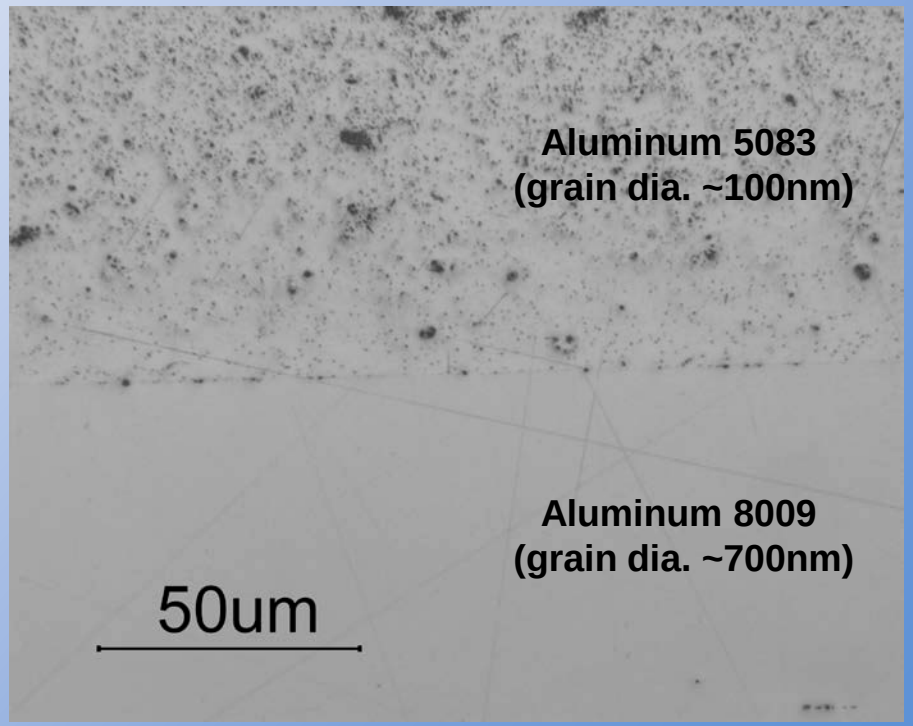
Aluminum 5083 UC Davis cryo-ball milled powder



Graded Material Approach

- Fine powder bonded to relatively-coarse substrate
  - Cryo-ball-milled Aluminum 5083 powder (~100 nm) on Aluminum 8009 sheet (~700 nm)

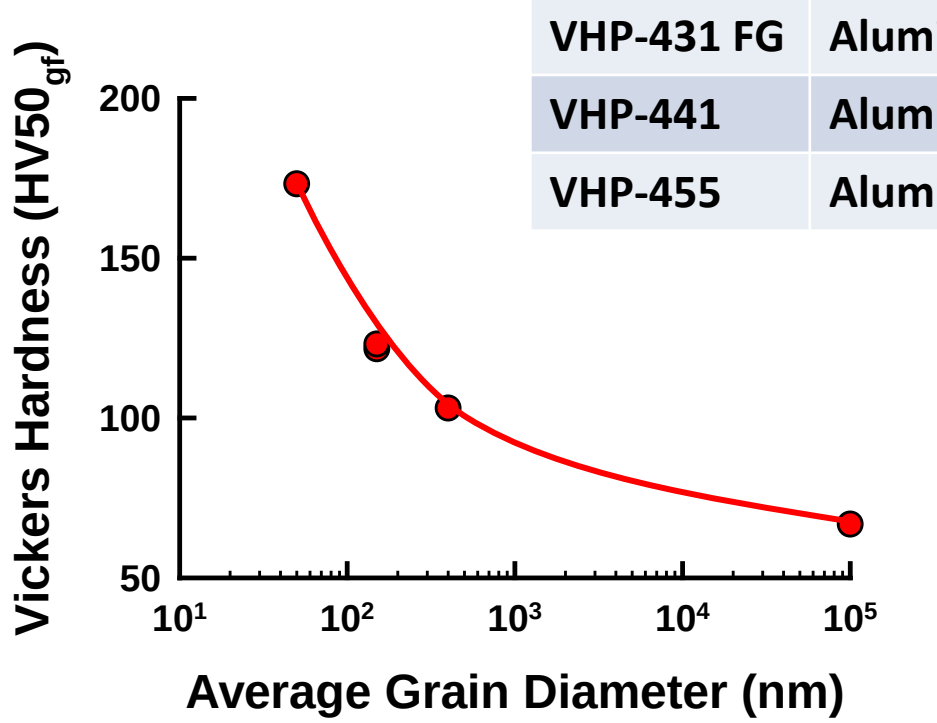




Results – Nano-indentation

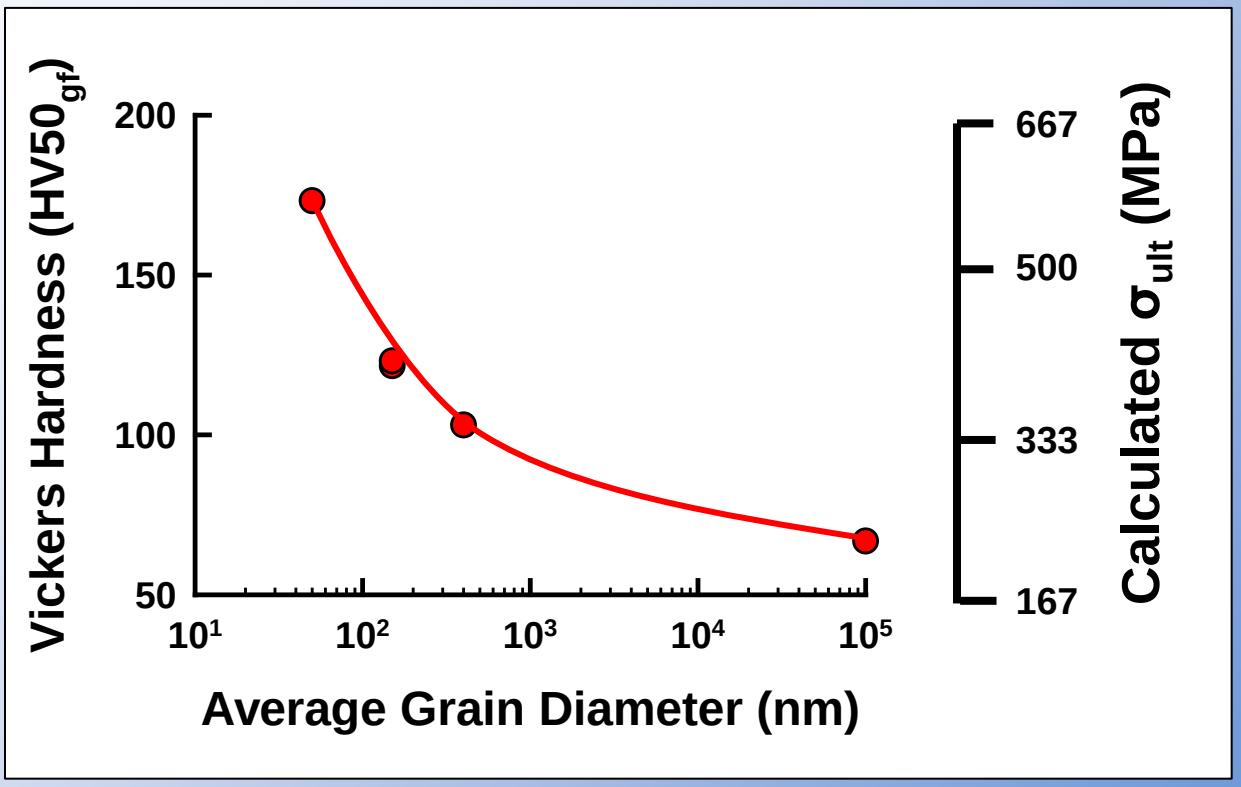
SAMPLE	DESCRIPTION	VICKERS HARDNESS
VHP-428	Aluminum 7075; D ~ 100 μm	66.8
VHP-429	Aluminum 7075; D ~ 400 nm	103.1
VHP-431 CG	Aluminum 8009; D ~ 700 nm	143.9*
VHP-431 FG	Aluminum 5083; D ~ 150 nm	121.6
VHP-441	Aluminum 5083; D ~ 150 nm	123.1
VHP-455	Aluminum 5083; D ~ 50 nm	173.2

* Not powder consolidated material



Corroboration of Analysis and Experiment

$$\sigma_{ult} \sim 3.33\ H_v$$



Experiments show greater strength and less ductility with decreasing grain size. This behavior agrees with both MD and DD computational results.

Concluding Remarks

- Multiscale modeling capabilities were extended to incorporate GB strengths from MD simulations. Analyses were performed on a cylindrical specimen with three different microstructures and a size that is accessible to experimental validation.
- MD simulations were used to quantify stress-strain behavior, deformation and failure processes for various uniform and graded microstructures.
- MD models were created to determine GB strength for different GB orientations in graded materials.
- DD simulations were performed using a variety of structurally-graded models with parametrically varied GB strengths to develop a catalogue of stress-strain predictions.
- MD and DD analyses showed through limiting strain localization and load transfer from coarse to nanograin regions a mechanistic support for structurally-graded (SG) metallic materials offering the promise of combining the strength of nanocrystalline materials with the ductility and toughness of coarse grained materials.
- The fabrication processes examined and analytical results obtained provide trends that can be used to guide development of future SGNC microstructures.

Opportunity for Continued Development

- With additional development….
  - the analysis methods discussed here can provide guidance for material design and shorten the material development and qualification cycle
  - the processing methods used to develop graded/layered SGNC materials will be capable of producing the engineered microstructures needed to meet NASA's unique mission demands
- Potential sources of future support include ARMD's Fundamental Aeronautics program and the Materials Genome Initiative (MGI)
- The nascent capability developed here is the basis for collaboration with other government agencies such as DoE, DoD and NIST
  - working similar materials problems
  - complementary, not duplicative goals