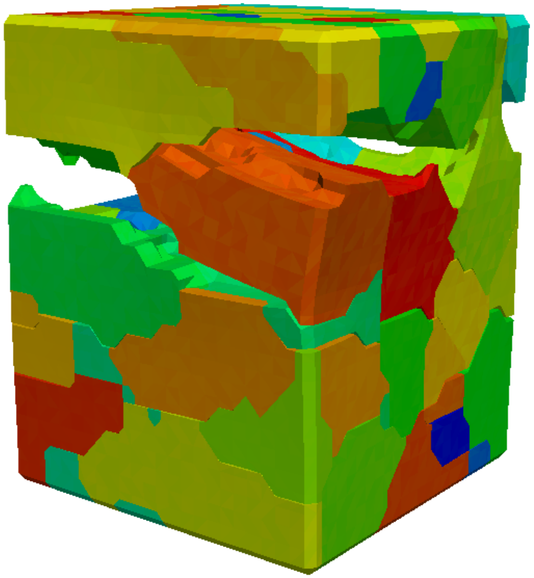
Grain Boundary Decohesion and Particle-Matrix Debonding in Aluminum Alloy 7075-T651 using the PPR Potential-Based Cohesive Zone Model



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Outline

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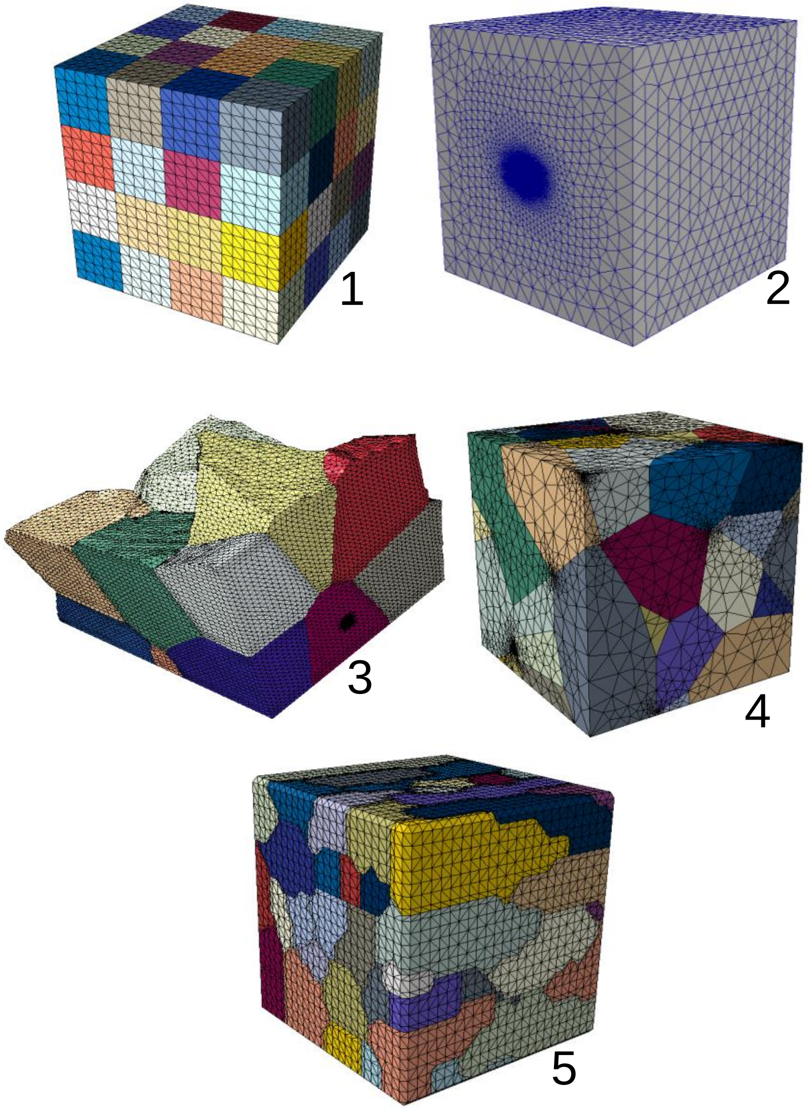
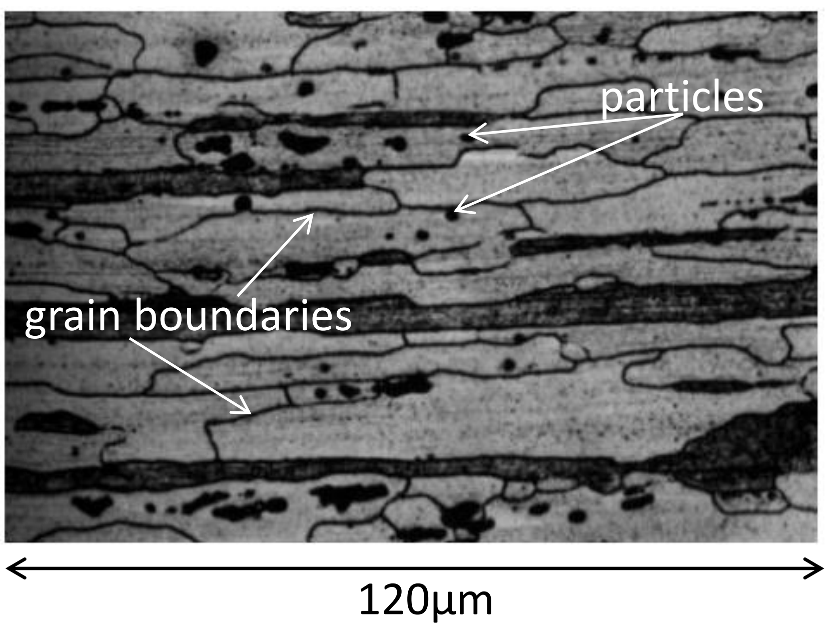
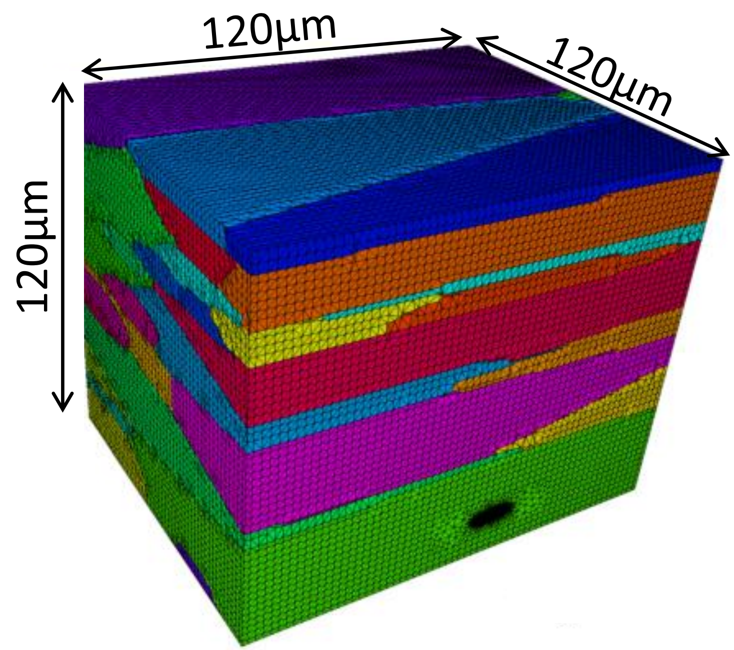
- Material Models
- Computational Considerations
- Case Studies
  1. idealized cubical polycrystal
  2. cracked particle embedded in single grain
  3. equi-axed grain polycrystal
  4. irregular-shaped-grain polycrystal
  5. rolled-grain polycrystal
- Conclusions



Problem Description

- Majority of a fatigue crack's life spent in the microstructurally small fatigue crack (MSFC) phase. Estimates as high as 90%.
- Grain boundary decohesion (intergranular fracture) and particle - matrix debonding occur in some aluminum alloys.
- To model accurately MSFC behavior in aluminum microstructures, must account for these interface mobilizations.





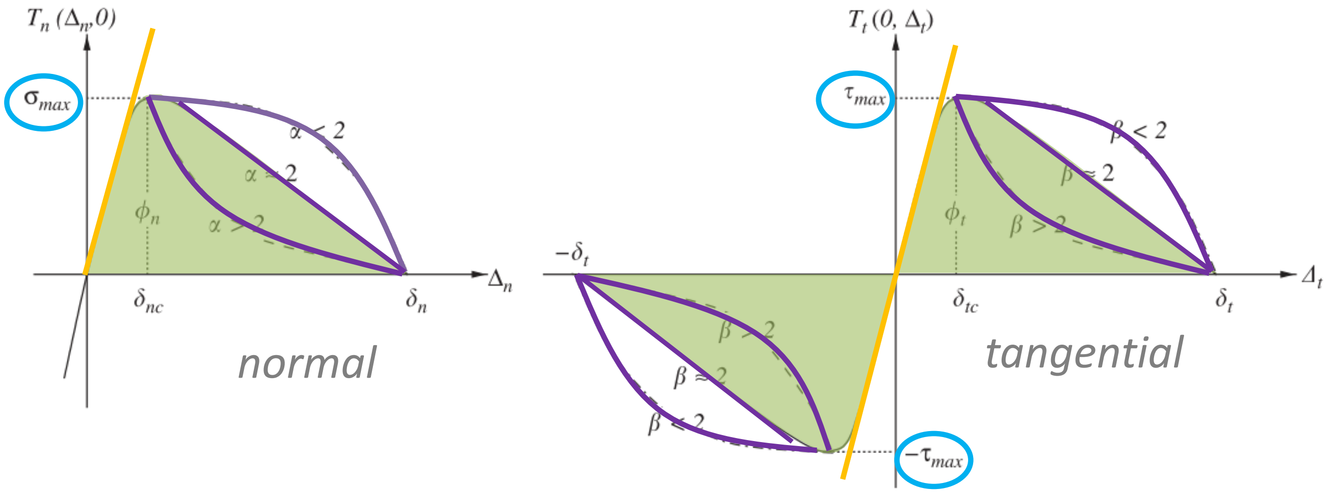
Left Image: *J.E. Hatch. Aluminum: properties and physical metallurgy. ASM International, 1984.*

Material Models

Interfaces

PPR CZM

- PPR used to account for interface mobilizations.
- Published in 2009. Generalized to 3D at Cornell.
- Robust in mixed-mode analyses.



Grains

elasto-viscoplastic, rate-dependent FCC crystal plastic

- Euler angles define grain orientations; orientations are randomized
- precipitation hardening applied
- slip metrics are queried → direction of nucleation from cracked particles

linear elastic, isotropic

- E = 72GPa, ν = 0.33

Computational Considerations

Solver Specifics

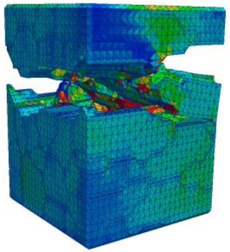
- FEAWD is the FE driver.
  - A parallel, C++ code.
  - Built on PETSc, BLAS/LAPACK, and FemLib.
- Nonlinear Solver: Newton method with trust region
  - preferred over line search
  - line search unable to follow negative global stiffness

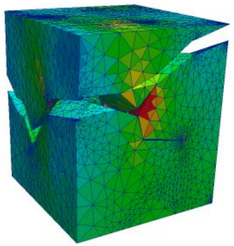
Cluster Specifics

- Analyses run on Cornell Fracture Group's ADMMII cluster and Texas Advanced Computing Center's cluster Ranger.
- FEAWD scales to as little as 4,000 DOFs/core on Ranger.

Visualization

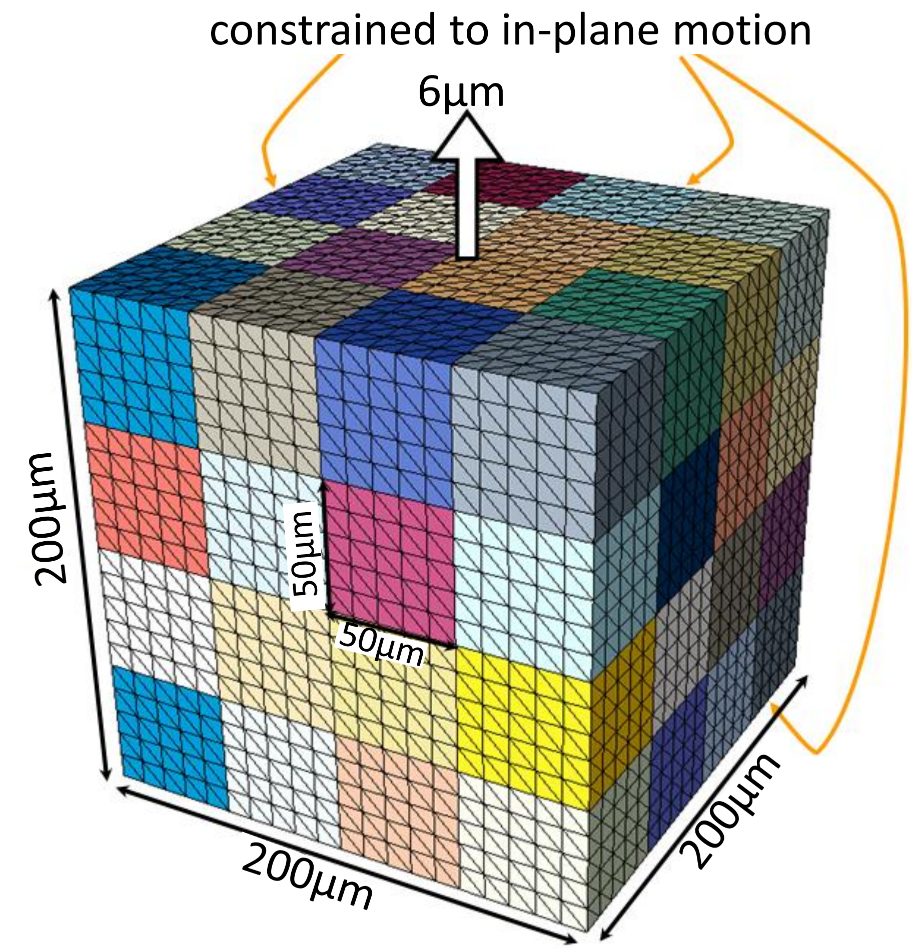
- All models visualized in ParaView.





Case Study 1: Grain Boundary Decohesion, Idealized Polycrystal

- 64 cubical grains.
- Simple tension loading w/ 3% applied strain.
- Cohesive elements placed along all grain boundaries. Cohesive strengths = 450MPa.
- Bulk material modeled as elasto-viscoplastic, rate-dependent FCC crystal plastic. Initial slip resistance = 220MPa.
- Grains have randomized crystallographic orientations.



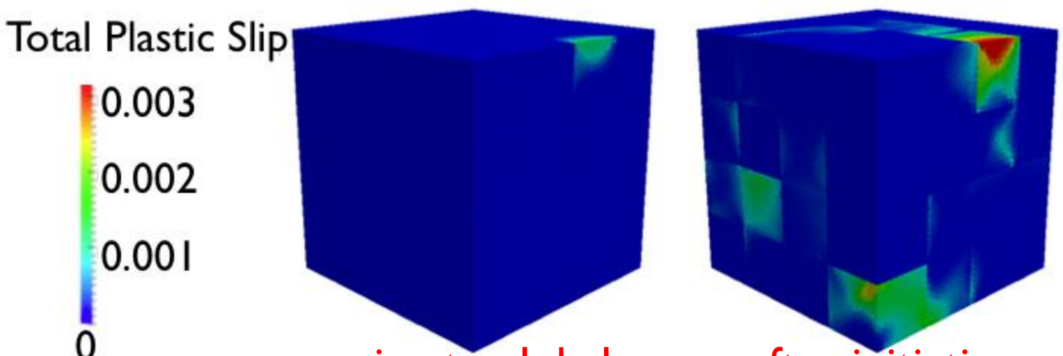
Case Study 1: Interplay between plasticity in grains and cohesive softening of grain boundaries

Competition between cohesive softening and plastic slip is a highly nonlinear process.

Cohesive Softening Dominates

cohesive strength = 450MPa

initial slip resistance = 220MPa



prior to global cohesive softening

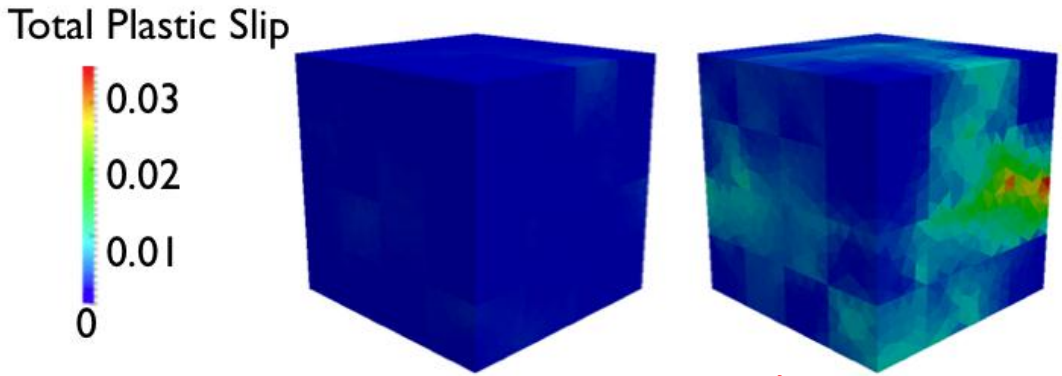
after initiation of softening

Slip Dominates

cohesive strength = 450MPa

initial slip resistance = 200MPa (9% reduction)

increases in slip as high as 35x



prior to global cohesive softening

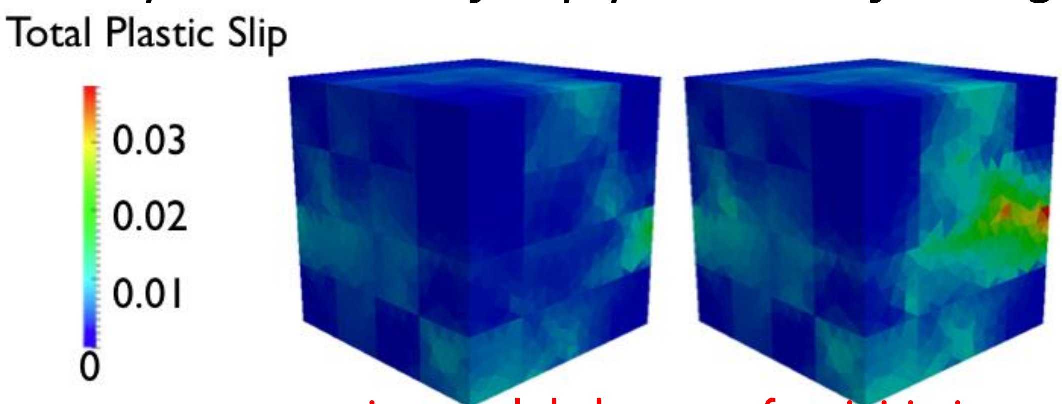
after initiation of softening

Stalemate

cohesive strength = 495MPa

initial slip resistance = 220MPa

note prevalence of slip prior to softening

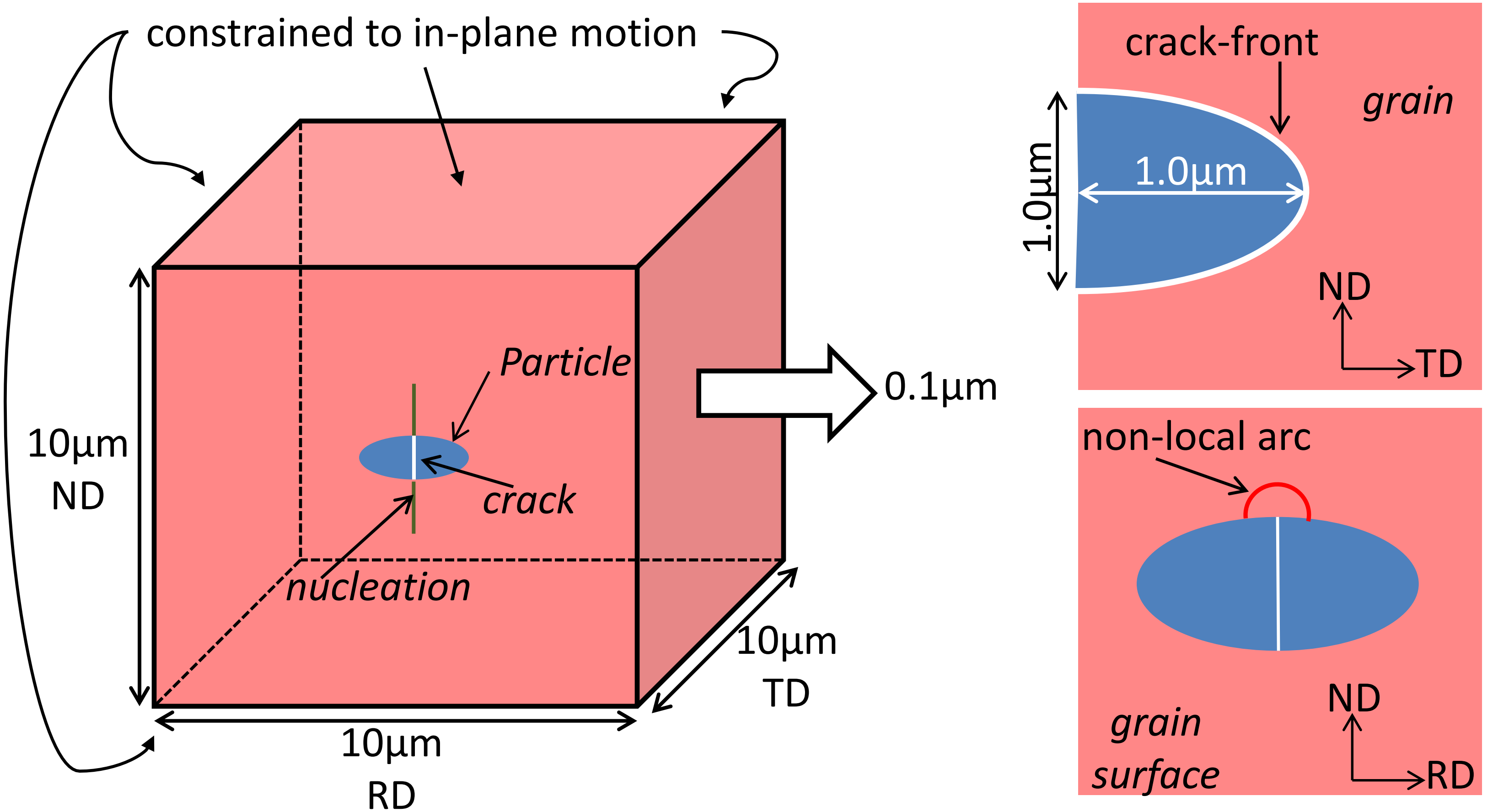


prior to global cohesive softening

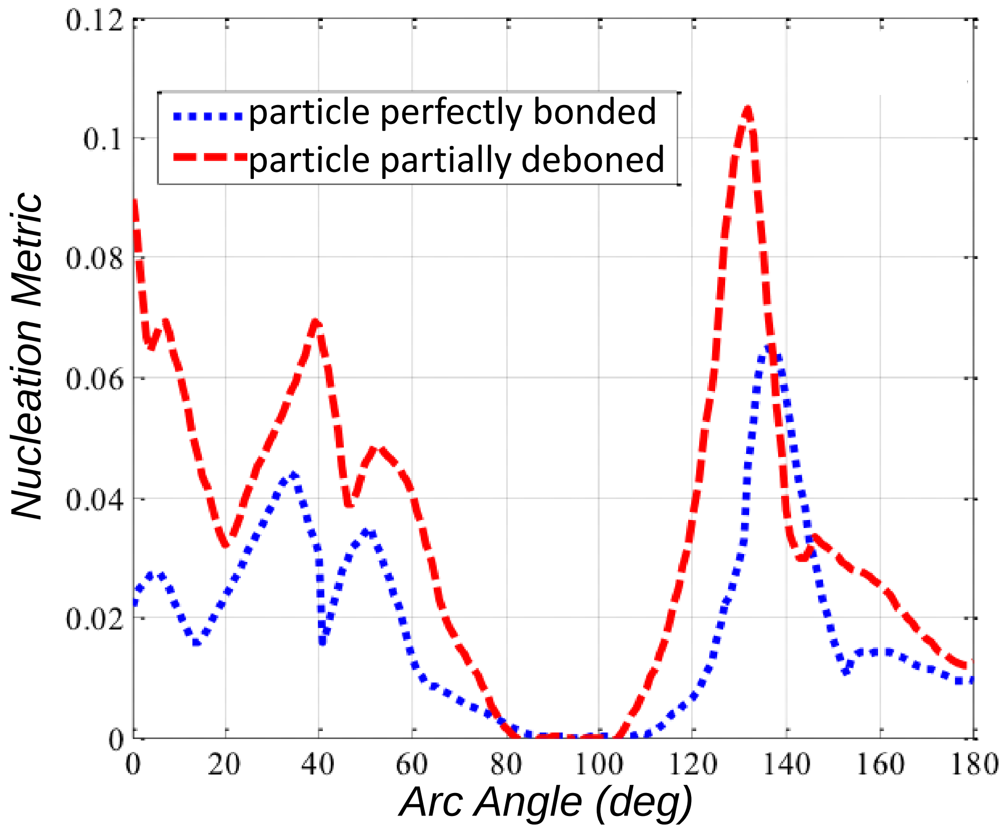
after initiation of softening

Case Study 2: Debonding of Cracked Particle in Single Idealized Grain

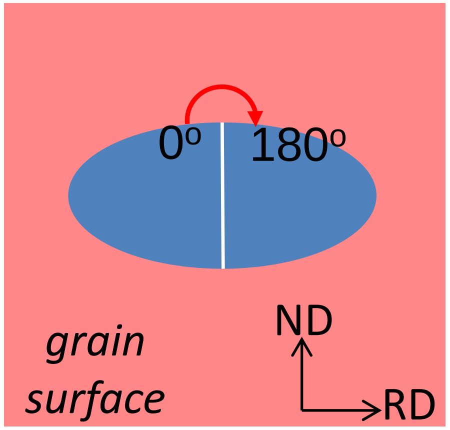
- Emulates grain containing a cracked, semi-elliptical, second-phase particle located on the surface of the grain.
- Cohesive elements placed along the grain - particle interface.
- Investigation into nucleation of crack from particle into grain.
- Nucleation metric mapped to non-local arc to avoid crack-front dominance.



Case Study 2: Tendency for Nucleation With and Without Particle Debonding



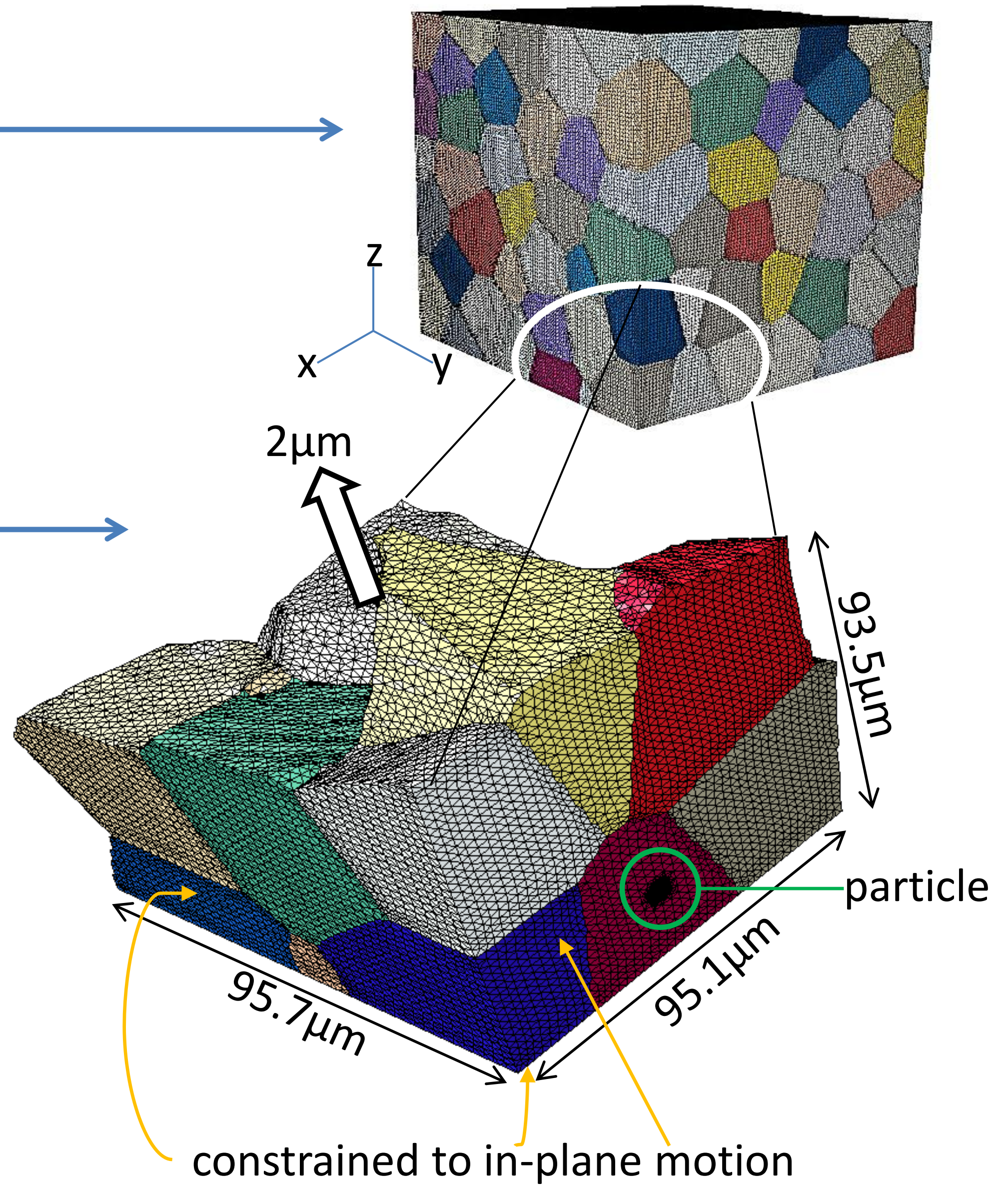
- Definite correlation between bonded and partially debonded scenarios.
- Slip around partially debonded particle generally higher.
- Predicted direction of nucleation from particle similar.



Case Study 3: Realistic Polycrystal Sub-Model

Start with 222-grain synthetic polycrystal.

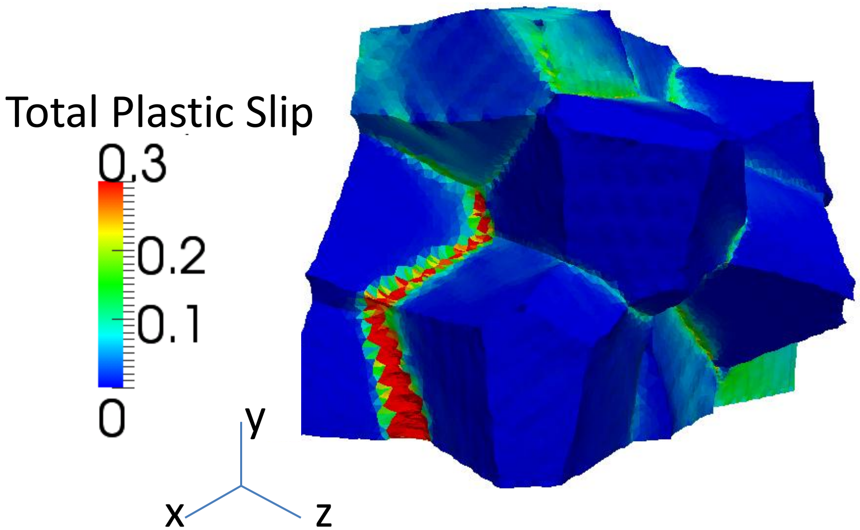
Extract 12-grain submodel.

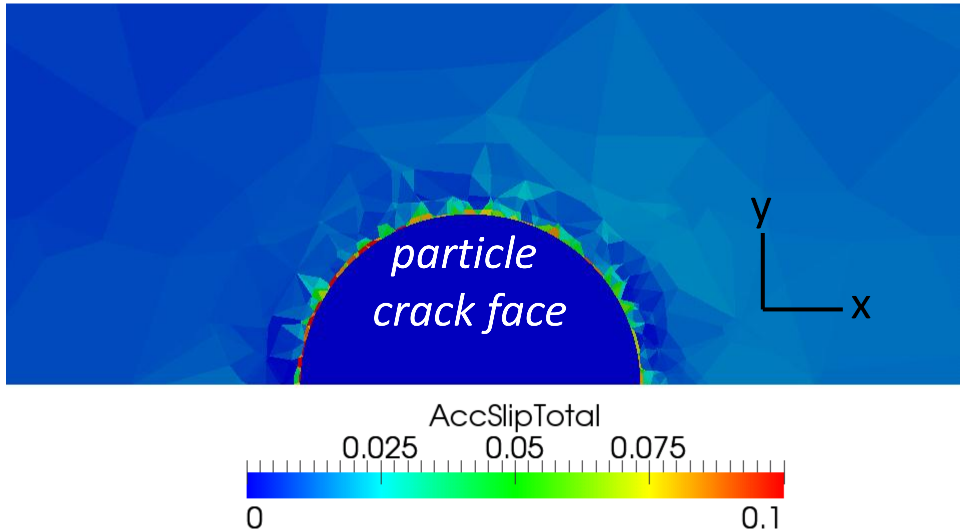


- 12 crystal plastic grains, 1 cracked particle, PPR cohesive model on all interfaces
- 2% strain applied to z-max surface, indicated by arrow

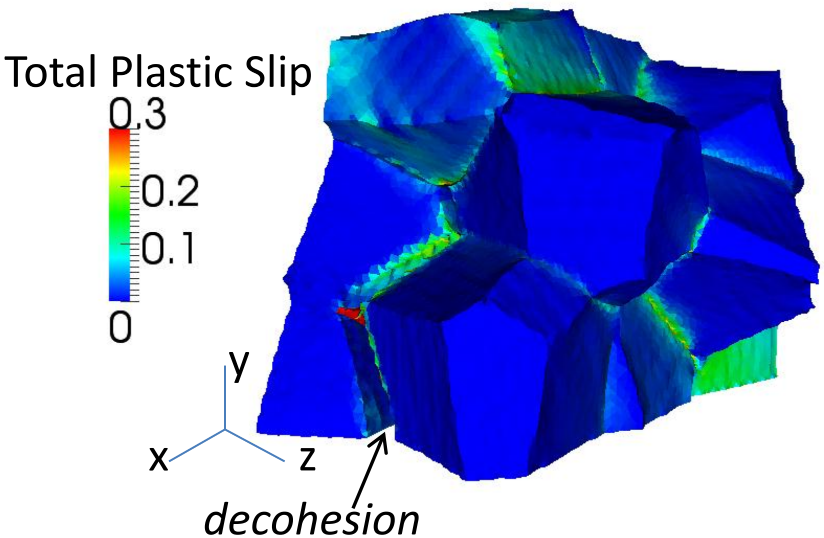
Case Study 3: Plastic Slip in Polycrystal at 45% of Applied Strain

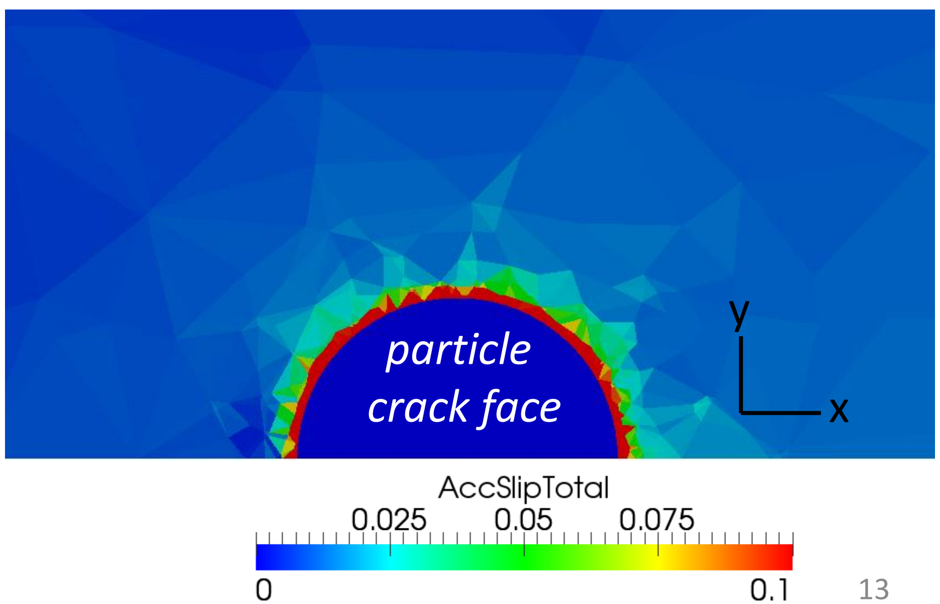
Interfaces Perfectly Bonded





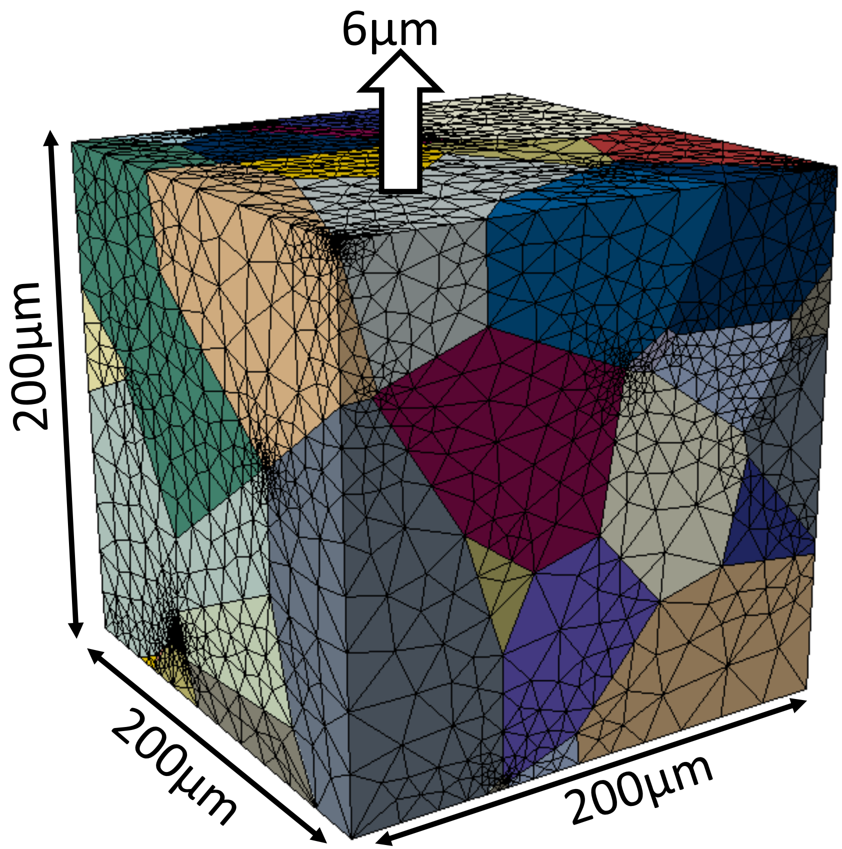
Cohesive Interfaces

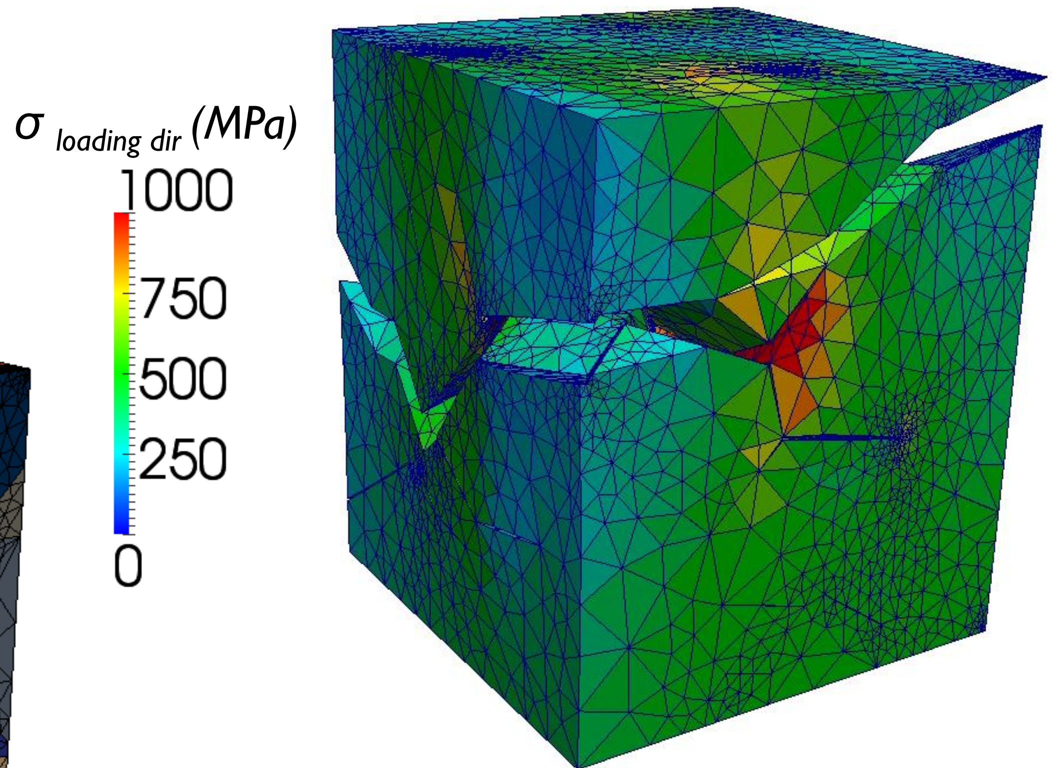




Case Study 4: Irregular-Shaped-Grain Polycrystal

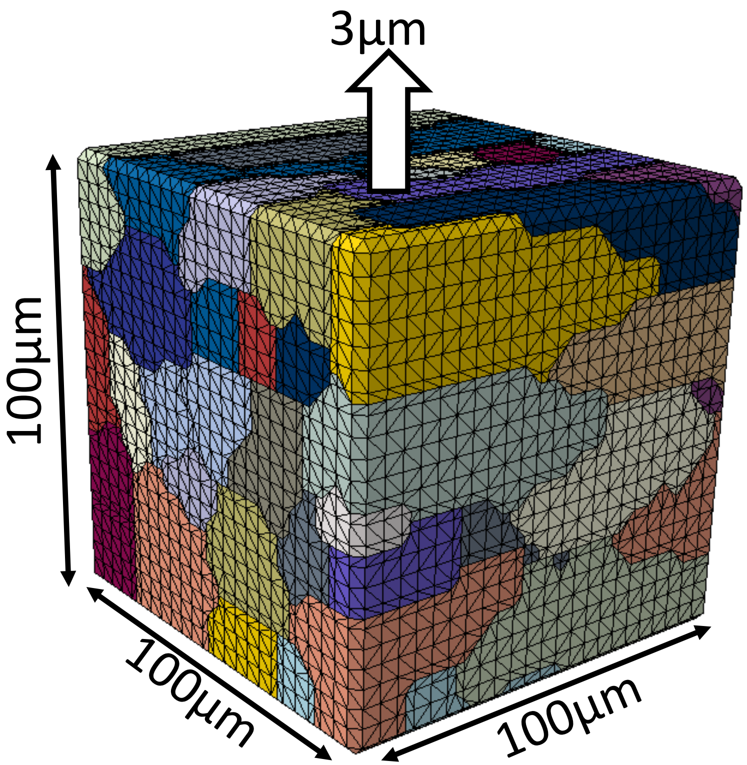
- 64 LEI grains
- Synthetic Microstructure
- Loaded in simple tension

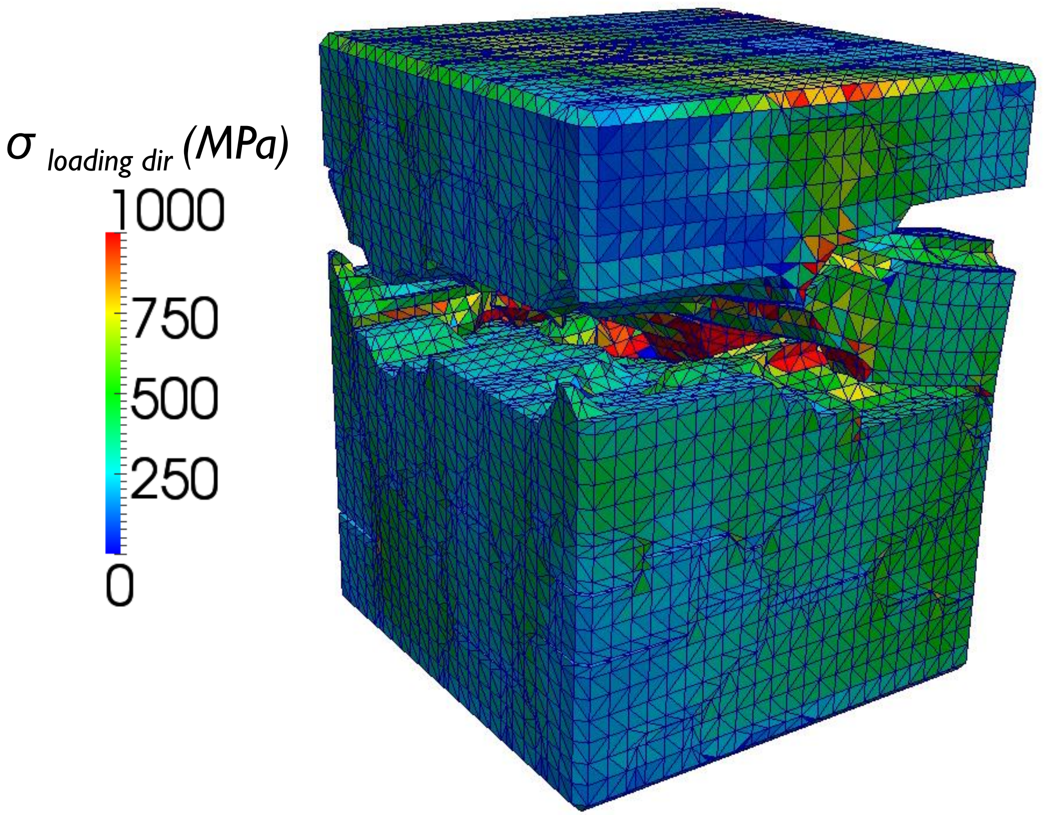




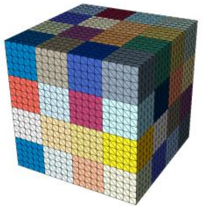
Case Study 5: Rolled-Grain Polycrystal

- 60 LEI grains
- Loaded in simple tension
- Model-Making Procedure
    1. Statistics (GSDF, ODF, MODF)
    2. Micro Generation (DREAM.3D)
    3. Surface Meshing (DREAM.3D)
    4. Volumetric Meshing (Polymesh)
    5. Cohesive Element Insertion

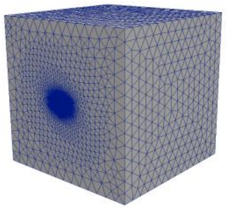




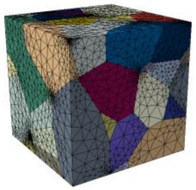
Conclusions of Five Case Studies



Interplay between plastic slip in grains and cohesive softening modeled without numerical difficulties.



Particle debonding significantly alters the magnitude and location of plastic slip in vicinity of the particle.



When paired with a scalable finite element solver, the cohesive finite element method with the PPR CZM is an efficient, stable approach to modeling interface mobilizations in microstructures.

Future Plans

Grow transgranular cracks in conjunction with modeling interface mobilizations.

Backup

Crystal Plasticity Model

precipitation hardening is applied to represent the strong self-hardening typical of Orowan looping evident in AA7075-T651 (dislocation loops around the particles)

parameter	value	
m	0.005	strain rate sensitivity parameter
g_0	220 MPa	initial slip resistance
$\dot{\gamma}_0$	$1.0\ \mathrm{s}^{-1}$	reference shear rate parameter
G_0	120 MPa	hardening rate parameter
g_s	250 MPa	Saturation hardening
μ	28300 MPa	C44
λ	60900 MPa	C12
η	5100 MPa	[2*C44 + C12 – C11] / 2

Mesh Details

Case I

Mesh ID	# of Bulk Elements	# of Cohesive Elements	# of DOF
1	4,056	1,152	27,840
2	15,494	2,856	88,386
3	129,900	11,232	615,642
4	504,482	32,022	2,283,576

Analysis	# of Nodes	# of Cores	Approx. Wall Clock Time
Mesh 1	1	4	~ 12 hours
Mesh 2	1	4	2 days
Mesh 3	6	24	7 days
Mesh 4	16	96	42 days

Case II

# of Bulk Elements	# of Cohesive Elements	# of DOF
625,690	17,956	2,669,526

Case III

# of Bulk Elements	# of Cohesive Elements	# of DOF
330,976	21,754	1,550,151

Microstructure Generation

statistics

- orientation distribution
- misorientation distribution
- grain size distribution

mbuilder

- equiaxed, rolled, twins
- ellipse packing
- user defines ellipse geometry

surface meshing

- marching cubes algorithm
- various smoothing techniques used

DREAM.3D

- supports reconstruction from serial sectioning
- synthetic builder generates equiaxed and rolled grains
- surface meshing supported, but not volumetric

volumetric meshing

- polymesh
- produces high quality finite element meshes
- post-process for cohesive element and/or crack insertion

Case Study 1: Mesh Considerations

Mesh ID	# of Bulk Elements	# of Cohesive Elements	# of DOF
1	4,056	1,152	27,840
2	15,494	2,856	88,386
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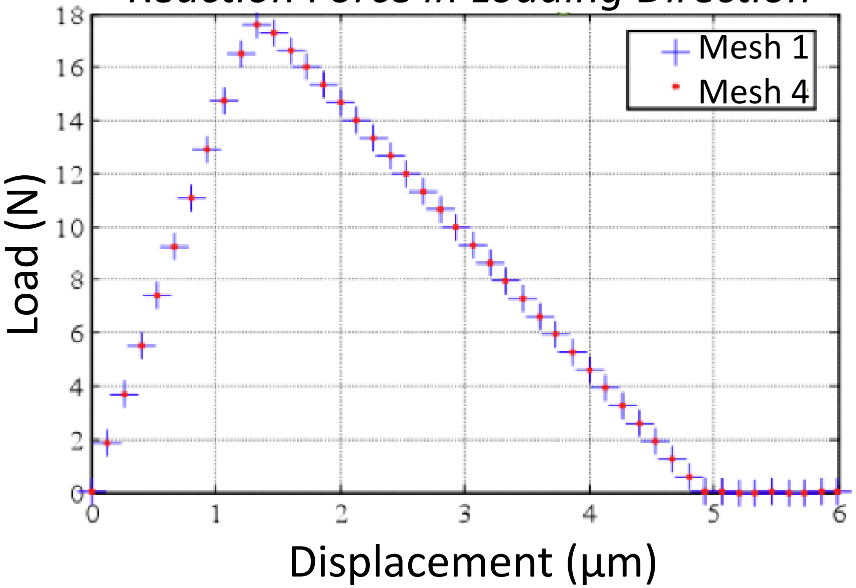

Total Accumulated Plastic Slip