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Title: 2D and 3D Simulations of Damage in 5-Grain Copper Gas Gun Sample

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Form 836 (7/06)

2D and 3D Simulations of Damage in 5-Grain Copper Gas Gun Sample

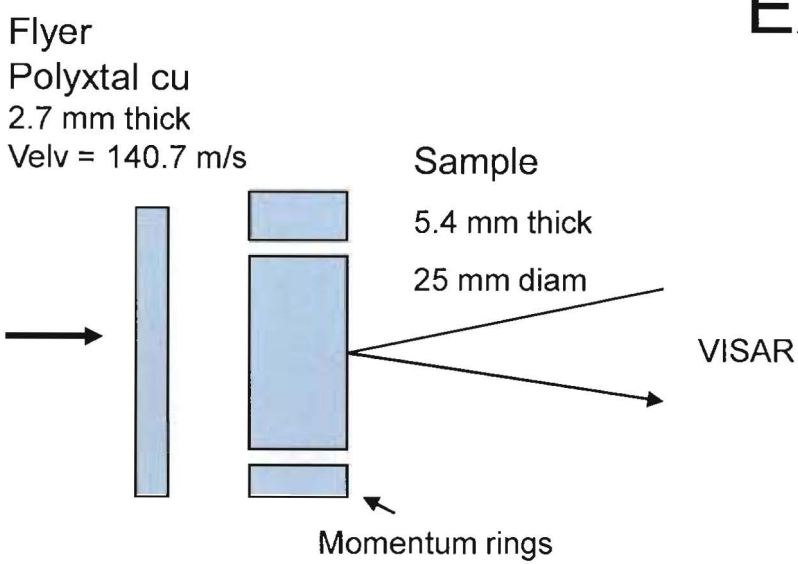
Calc: D. Tonks, S. Luo Exper: H Cerreta,
D. Dennis-Koller, P. Escobedo-Diaz,
C. P. Trujillo, J. Bingert
LANL

- study spall damage initiation at discrete grain boundaries in Cu.
  - free surface VISAR and metallurgy of recovered samples
- 2D and (new) 3D simulations
  - single crystal Cu plasticity model
  - porosity, pressure based damage model

Abstract

2D and 3D Hydrocode simulations were done of a gas gun damage experiment involving a 5 grain sample with a polycrystalline flyer with a velocity of about 140 m/s. The simulations were done with the Flag hydrocode and involved explicit meshing of the 5 grains with a single crystal plasticity model and a pressure based damage model. The calculated fields were compared with two cross sections from the recovered sample. The sample exhibited grain boundary cracks at high angle and tilt grain boundaries in the sample but not at a sigma 3 twin boundary. However, the calculation showed large gradients in stress and strain at only the twin boundary, contrary to expectation. This indicates that the twin boundary is quite strong to resist the predicted high gradients and that the calculation needs the addition of a grain boundary fracture mode . The 2D and 3D simulations were compared.

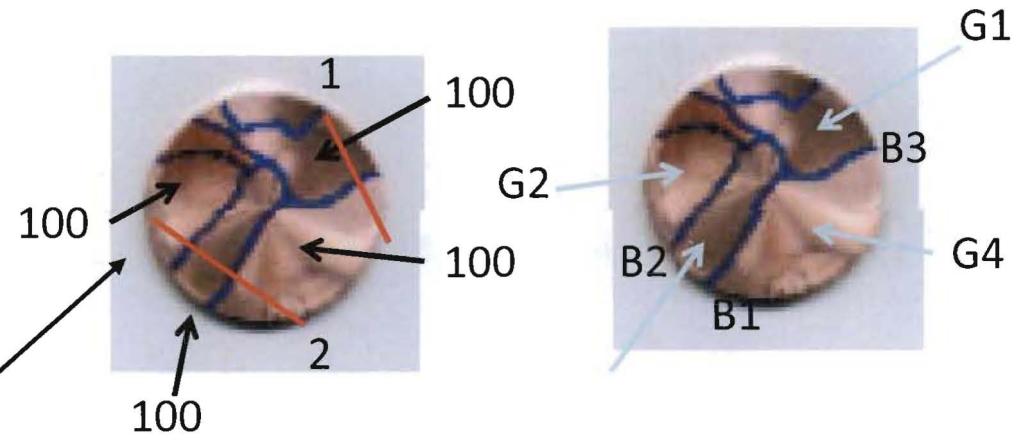
Experiment



Shock pressure about 3 GPa

Sample grain structure:

- Grain sides are ~ vertical (axial)



Cut 2 was simulated in 2D.

- Contains boundary B1 (high angle) and boundary B2 (twin)
- Boundary B3 is tilt

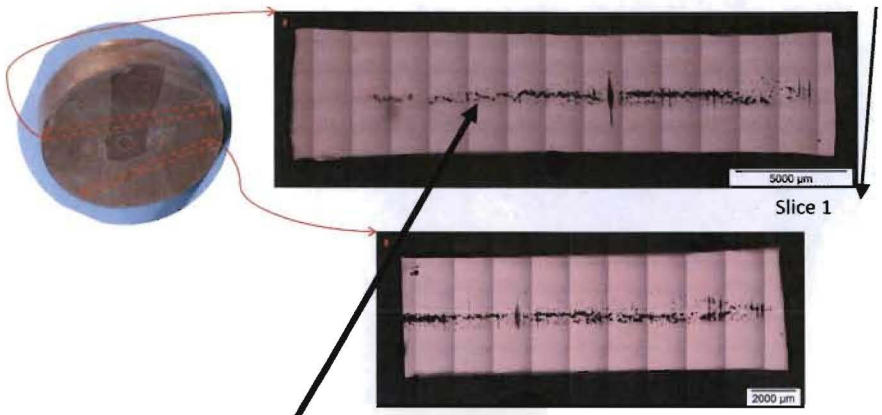
Code Used

- Flag: 2 and 3D LANL ASC code
- Single crystal plasticity model and pressure only damage model created and installed by Tonks
- Meshing done with CUBIT (Sandia)
  - CUBIT -> Flag mesh conversion done in house (Carrington, T-3, LANL)
- 3D Flag slip surfaces problematic
  - 3D code seems robust otherwise
  - Work around possible

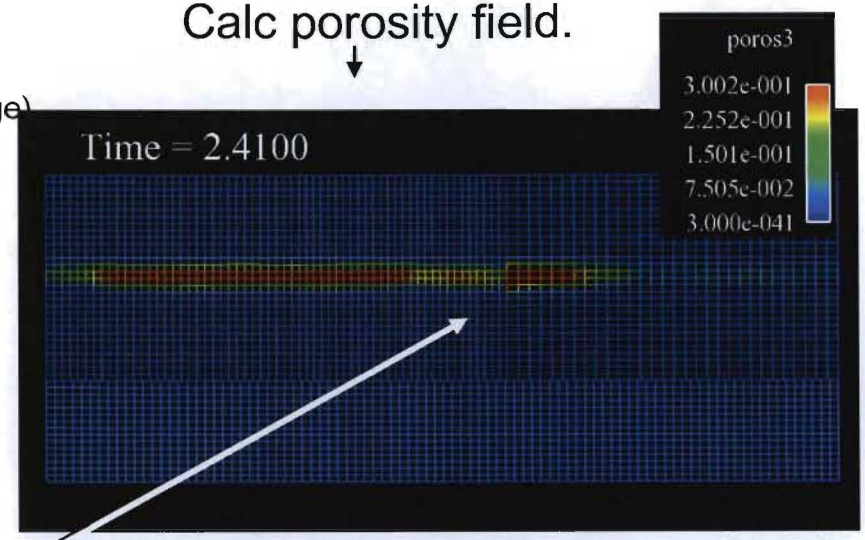
Damage in slice 2: comparison of exper and 2D calc

Recovered Damage, slice 2

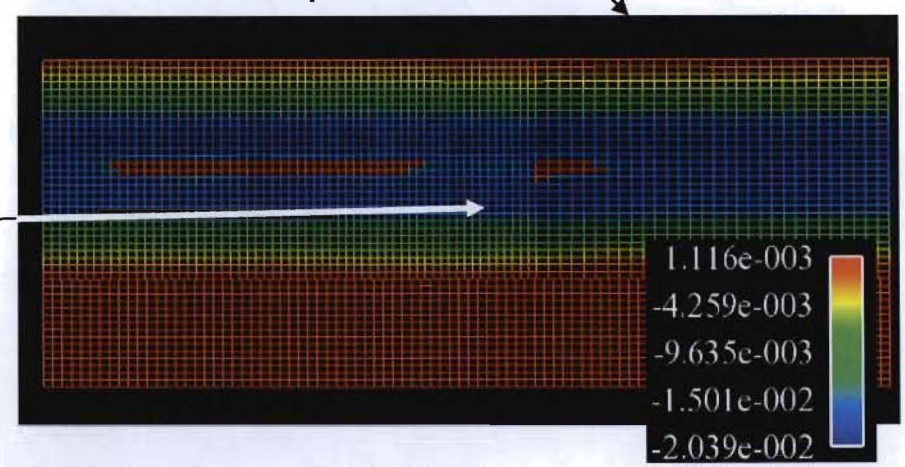
(Labeled slice 1 in image)



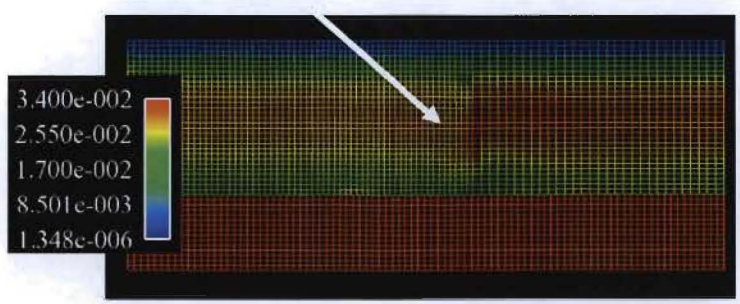
Calc porosity field.



Calc pressure field



Note experimental crack and calc discontinuities across grain boundary

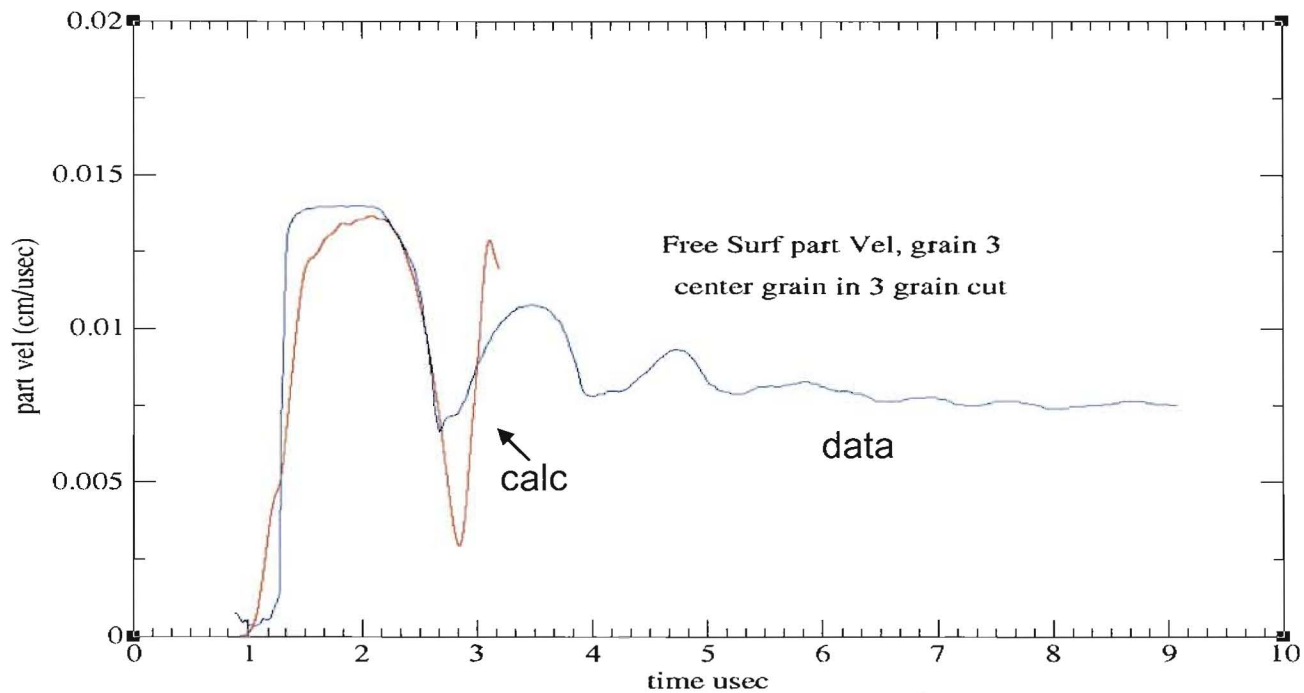


← Calc plas strain field

(units: 100 GPa)

Calc free surf vel of central grain vs VISAR

(slice 2, 2D calculation)

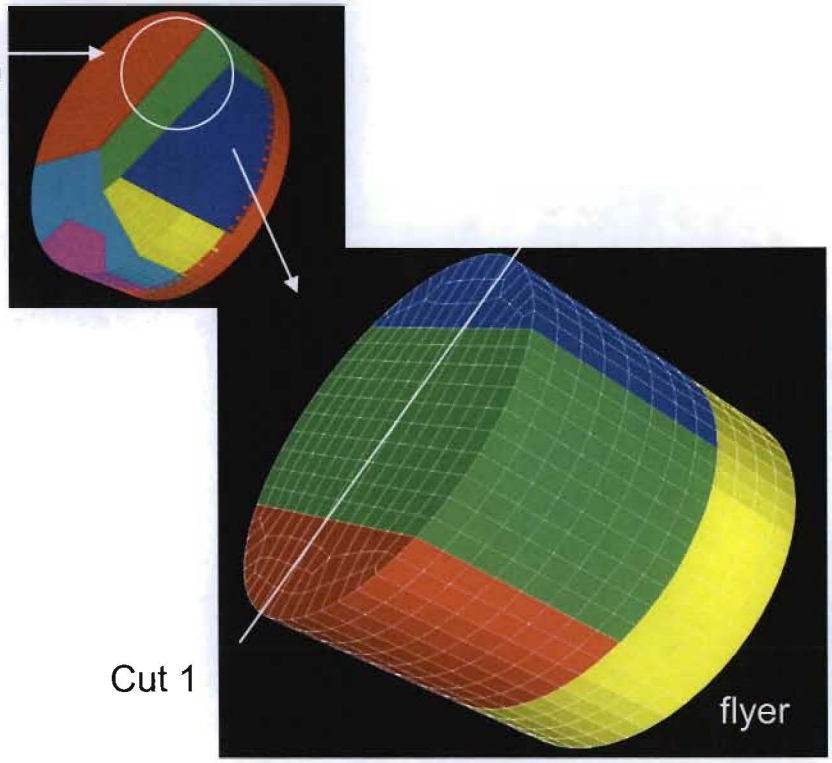


- Calc single crystal plasticity in shock rise too "soft"
- Release modeled well
- Model damage threshold stress too high

<u>Future plasticity and damage model tuning will enhance knowledge</u>

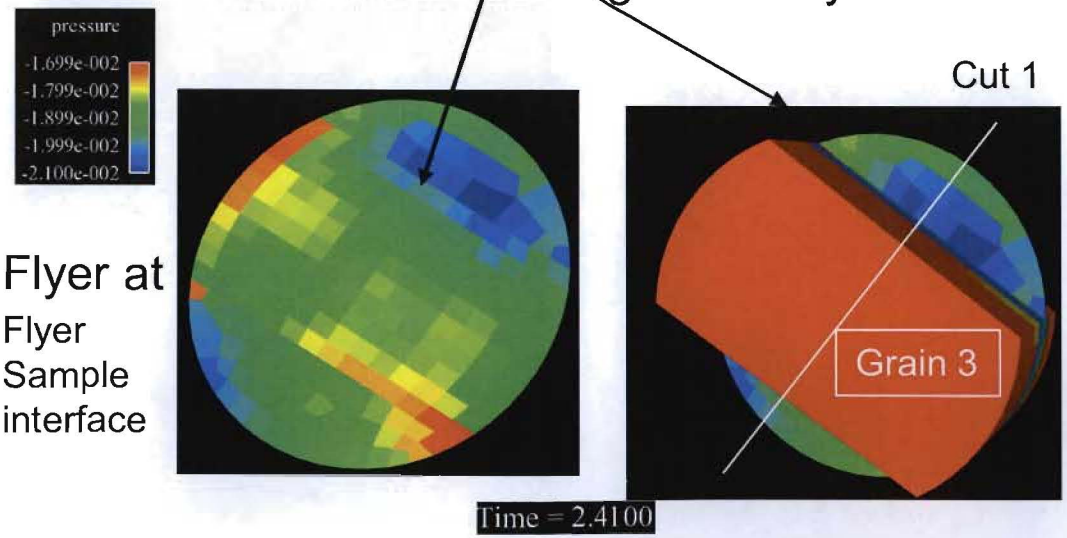
3D calc of flyer – sample core, containing Cut 1

- Smaller mesh, better for scoping
- troublesome slip surface removed
  - Still realistic for Cu on Cu – no flyer separation
- Meshing somewhat coarse, but ran to 3.5 μs in about 7 hours with 32 processors
- 3742 zones



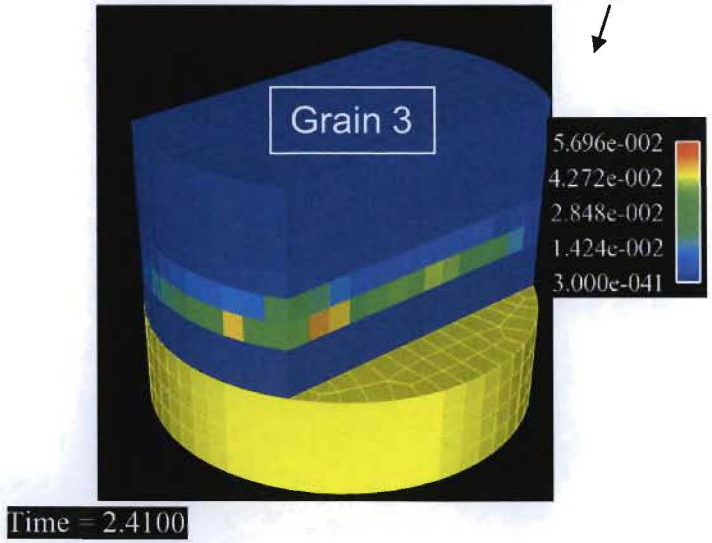
Calculated pressure:
2D slice-view at flyer- sample interface

Grain boundary pressure concentration seen in 2D at twin grain bndry



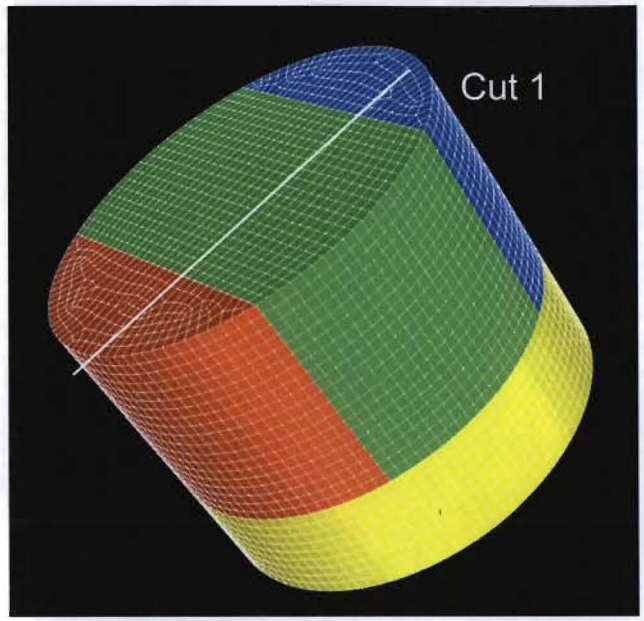
Flyer at
Flyer
Sample
interface

Calculated porosity in grain 3



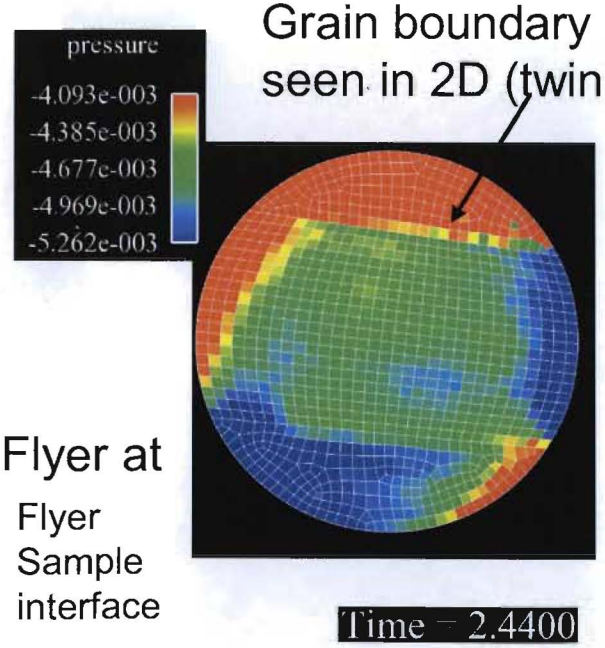
3D calc of flyer – sample core, containing Cut 1 more finely zoned

- 33,252 zones - versus 3742 zones prev slide
- Ran to 3.4 μs in 10 hours with 96 processors.
- Mesh coarser than 2D but acceptable

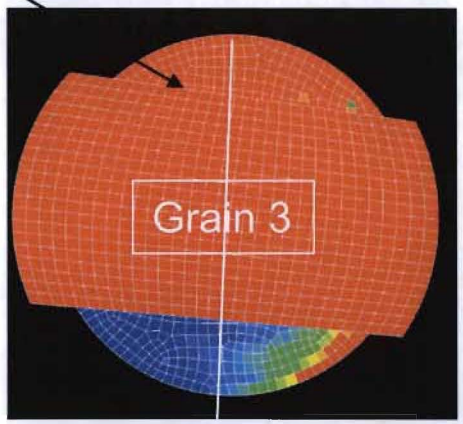


Calculated pressure:
Z-axis section at flyer sample interface

Grain boundary pressure concentration seen in 2D (twin bndry).

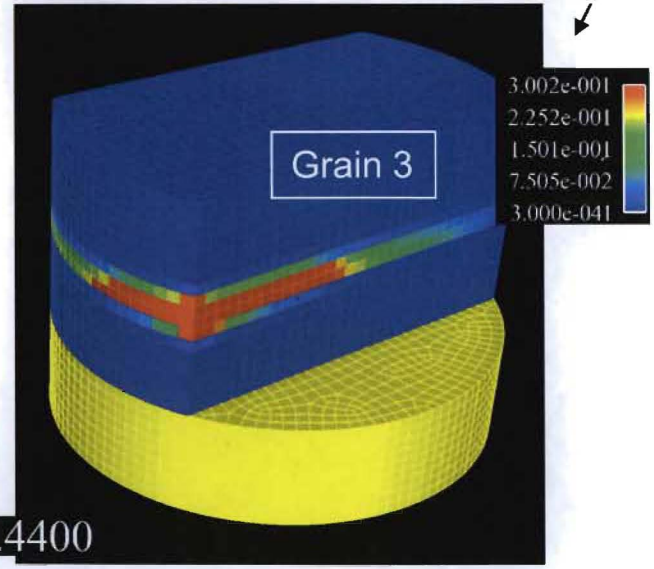


Flyer at
Flyer Sample interface



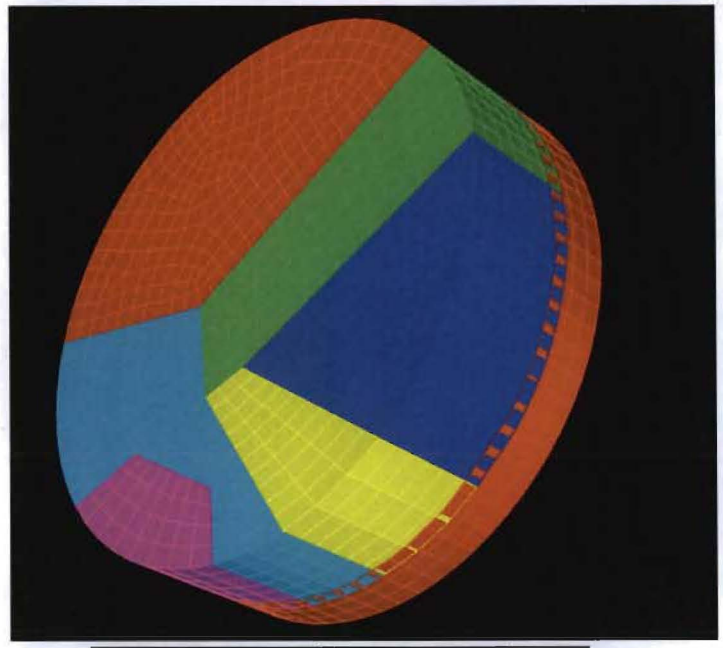
Cut 1

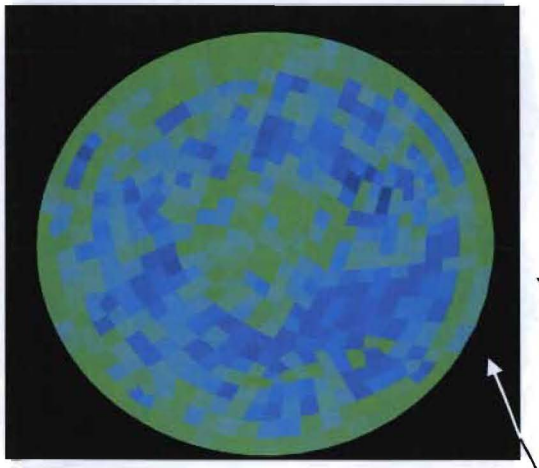
Calculated porosity in grain 3



Whole sample - flyer 3D simulation

- First attempt, work in progress
- Fairly coarse (5 zones in flyer thickness)
- Ran 1.95 ms before **slip surface problem**
- Grain 4 shows some neg pressure grain concentration in pressure at 1.95 μs
- Took about 21 hours with 32 processors,
  8118 zones
  - Need to try 128 or 256 processors with finer mesh.

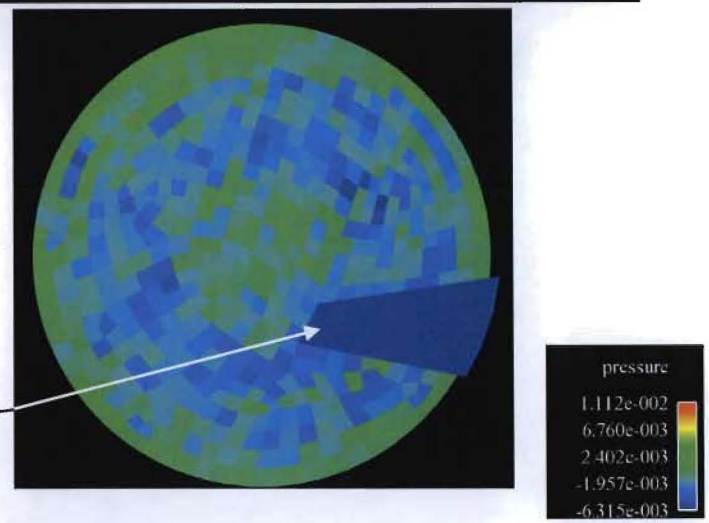




Calc pressure at 1.95 μs

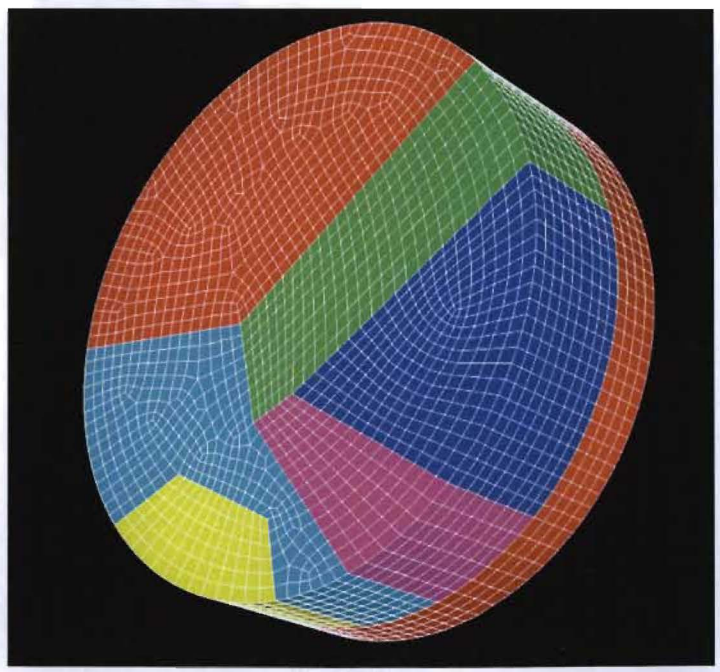
Z axis sections

Grain 4 "shadow"

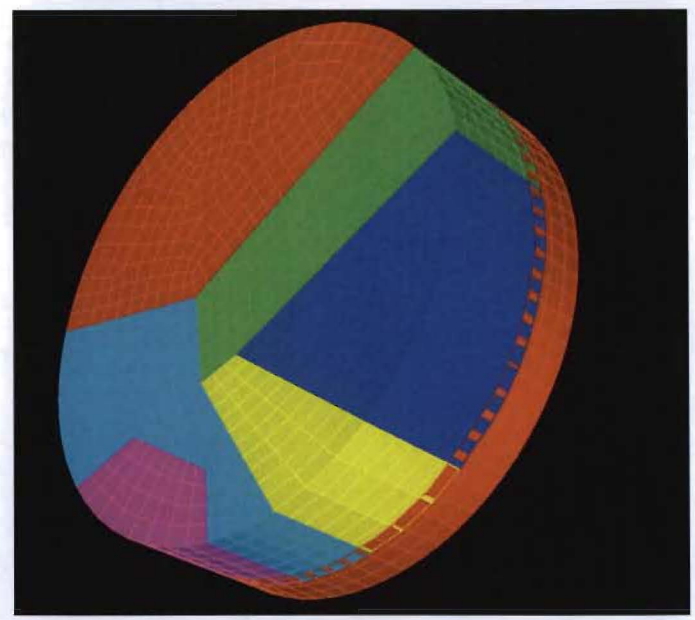


Whole sample - flyer 3D simulation finer mesh

- Grains welded, no penetration problem
- Resolution almost adequate
  - 9 zones in flyer thickness
- Ran 4.0 μs in 7 hours with 128 processors
- 23224 zones, about 3x number of 1st attempt
- Marked grain effects in stress, porosity fields (pressure gradients even)



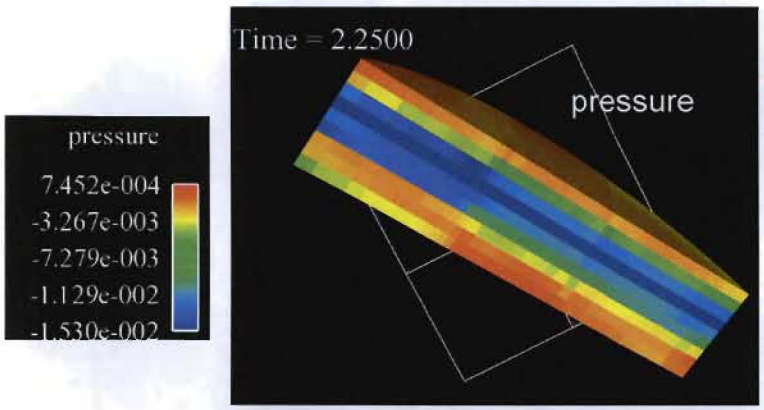
new

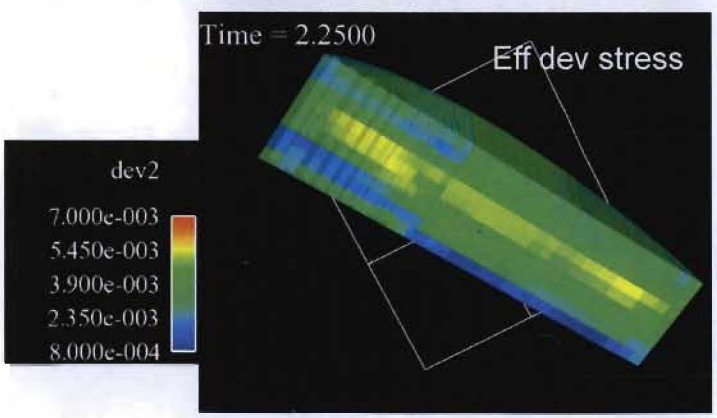


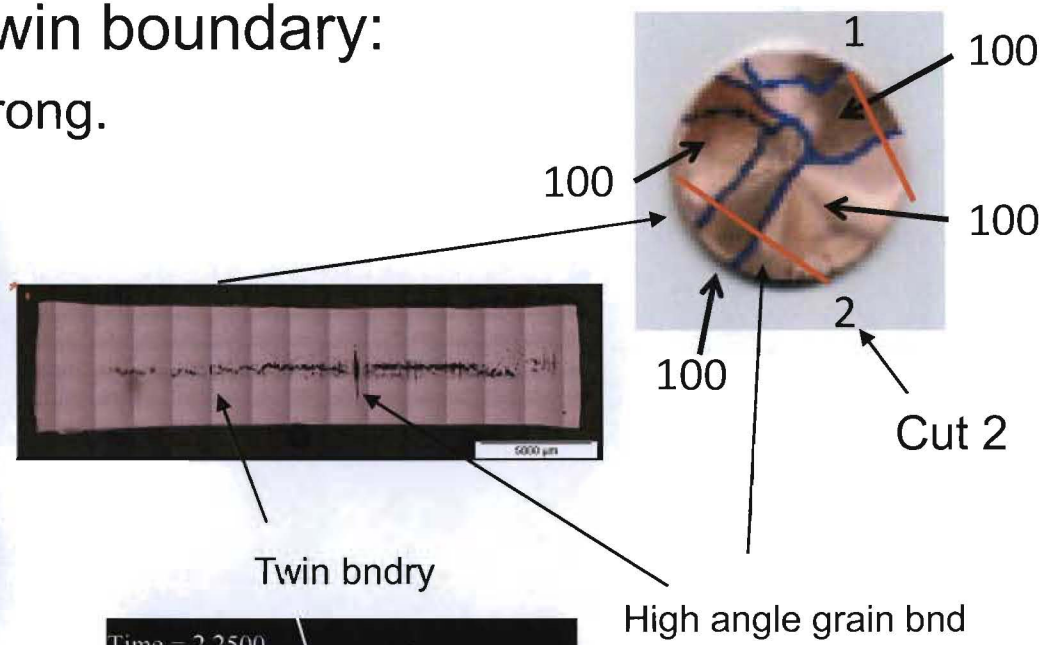
1st attempt

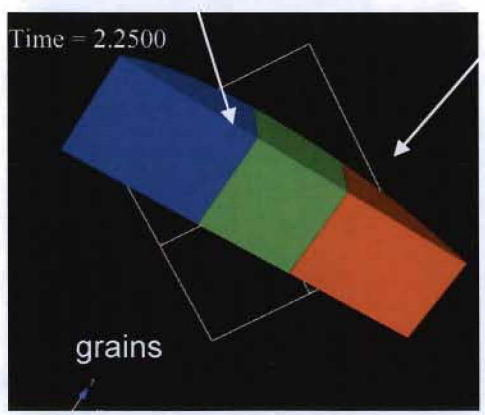
Calculated stresses from cut 2 from recovered sample

- Calc grad largest at twin boundary:
  - Implies twin bdry is strong.



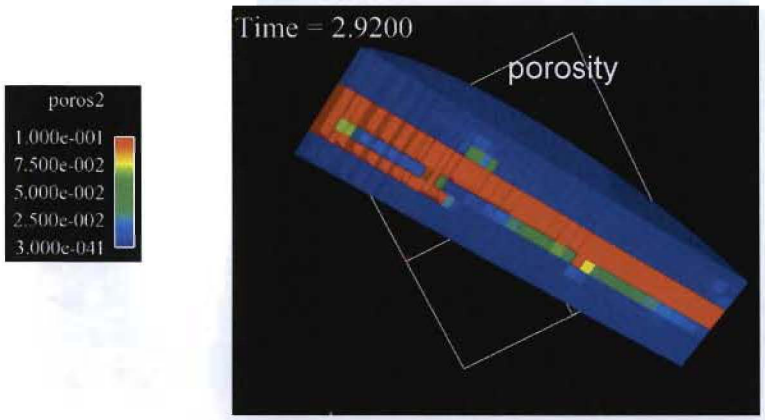


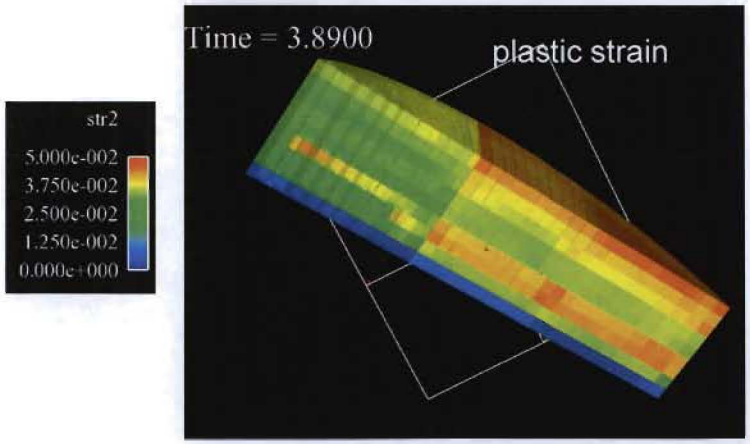


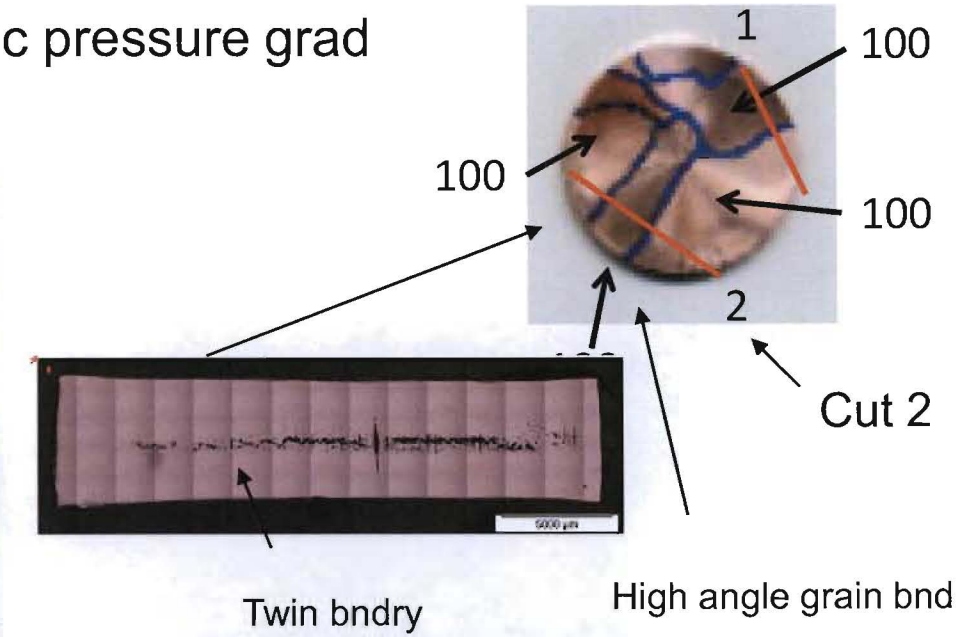


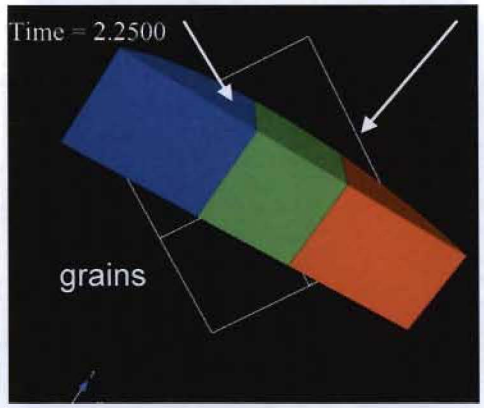
Calculated porosity & plas strain from cut 2 from recovered sample

- Calc gradient largest at twin boundary:
  - Implies twin bdry is strong.
- Cal porosity grad due to calc pressure grad



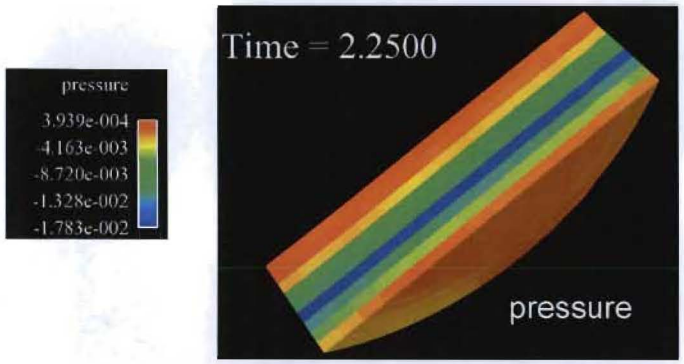


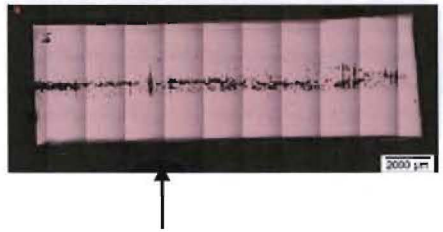




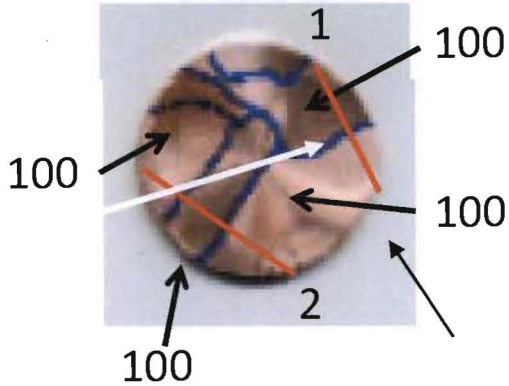
Calculated stresses vs cut 1 from recovered sample

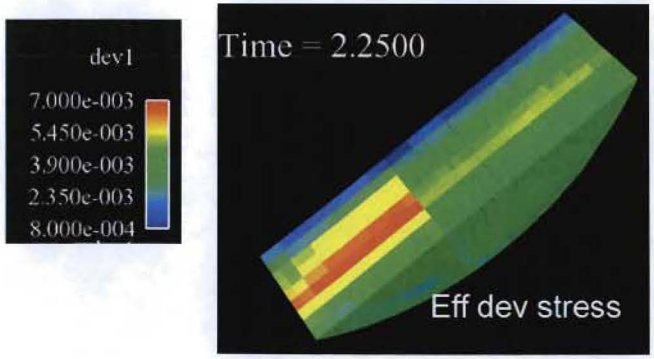
- large dev stress gradient at tilt bndry but not pressure grad
  - Implies dev stress effects important, but not pressure

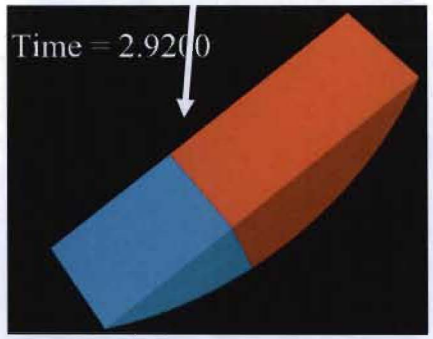




Tilt grain bnd

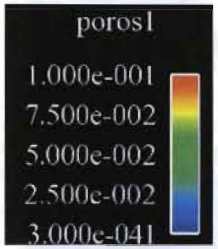


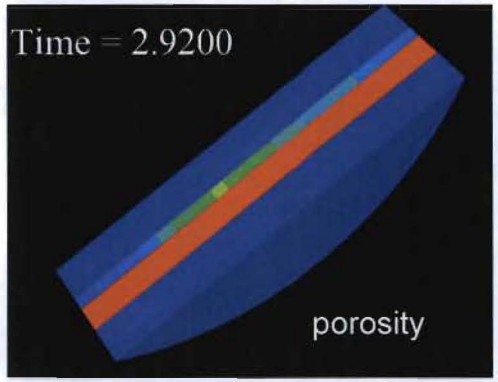


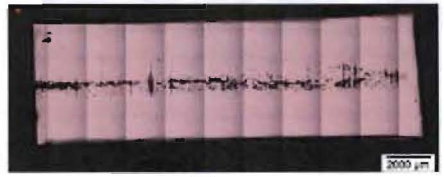


Calculated stresses vs cut 1 from recovered sample

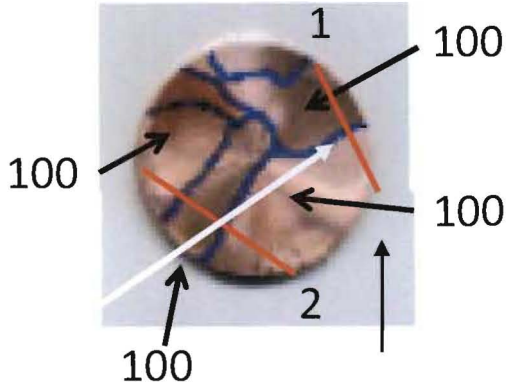
- No large gradient at high angle grain bndry
  - Implies tilt bdry is strong.



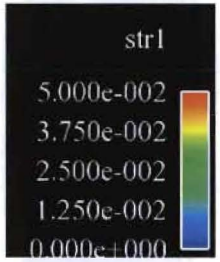


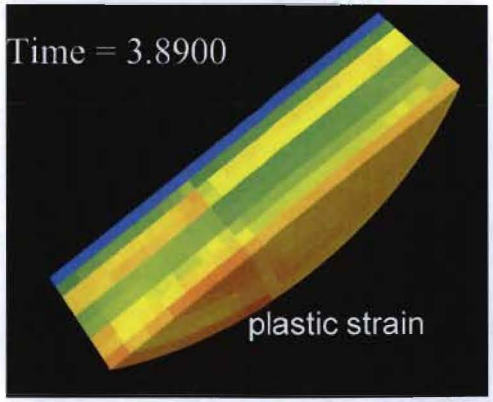


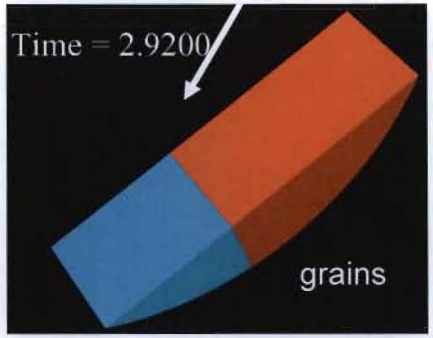
tilt grain bnd



Cut 1







Conclusions

- Exper twin grain bndry able to "stand"calculated gradients in pressure and plastic strain without fracture
  - Twin grain boundary is strong
- In this case, high angle grain bndry experiences gradient in only deviatoric stress
  - Fractures nevertheless
  - High angle grain bndy weaker than twin boundary
- High angle boundary crack not explained by calculated interior grain fields

– **explicit crack failure model needed**