Solid Dynamics
Detonation-Driven Tube Fracture Modeling and Simulation

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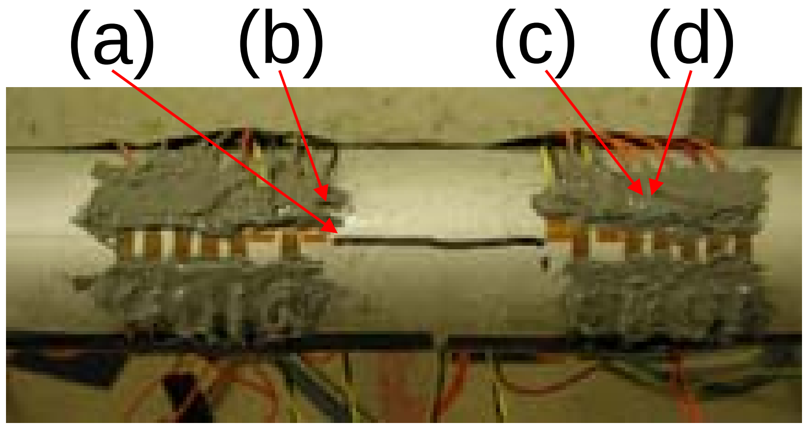
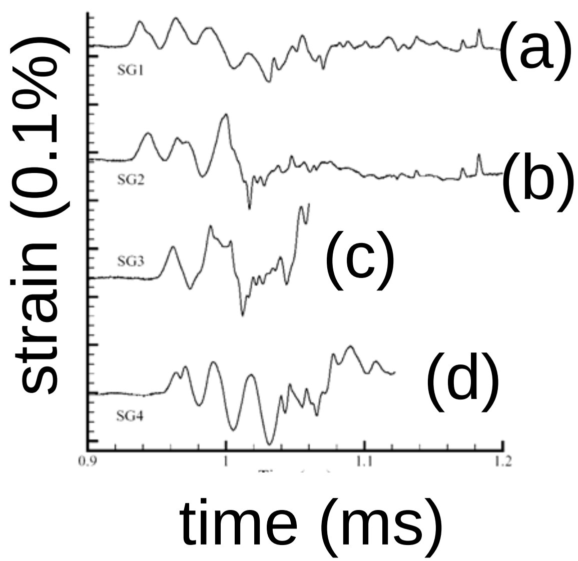
In collaboration with: J.E. Shepherd, F. Cirak…

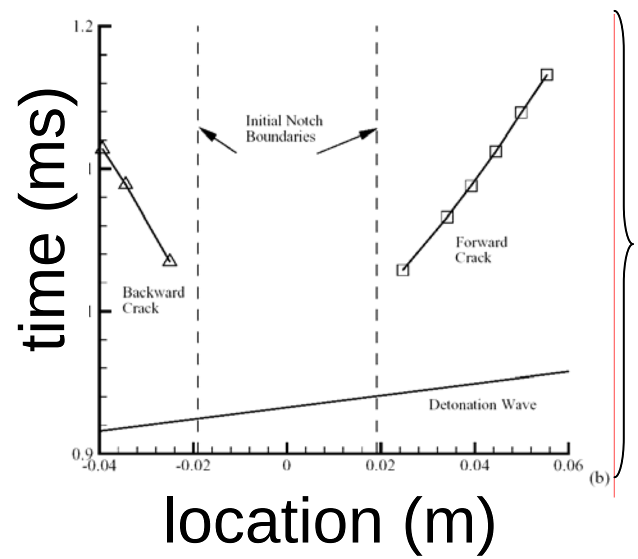
Caltech ASC Center – Midyear review

April 13-24, 2005

Detonation-driven tube fracture







metrics

(J. E. Shepherd, T.-W. Chao, J. Austin)

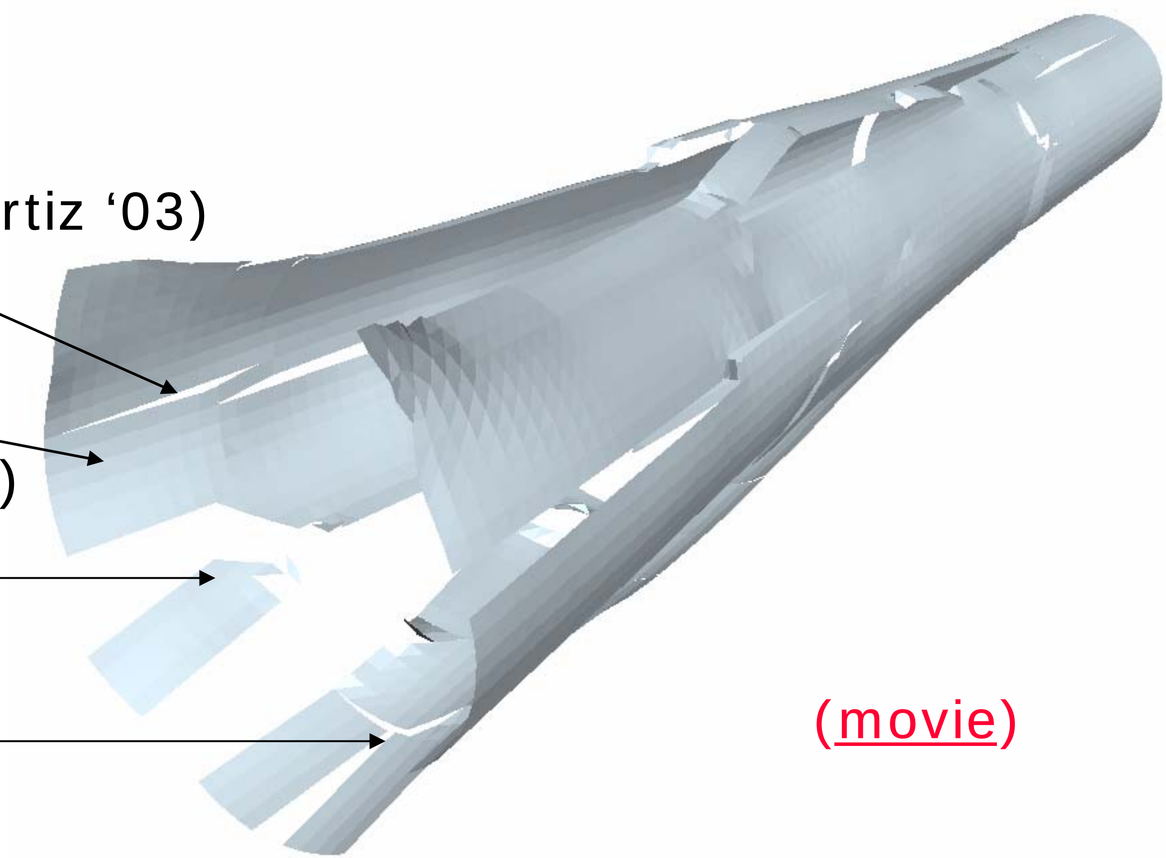
Engineering capability

Cohesive elements (Cirak, Pandolfi and Ortiz ‘03)

Subdivision shell elements (Cirak, Ortiz and Schröder ‘00)

branching, fragmentation

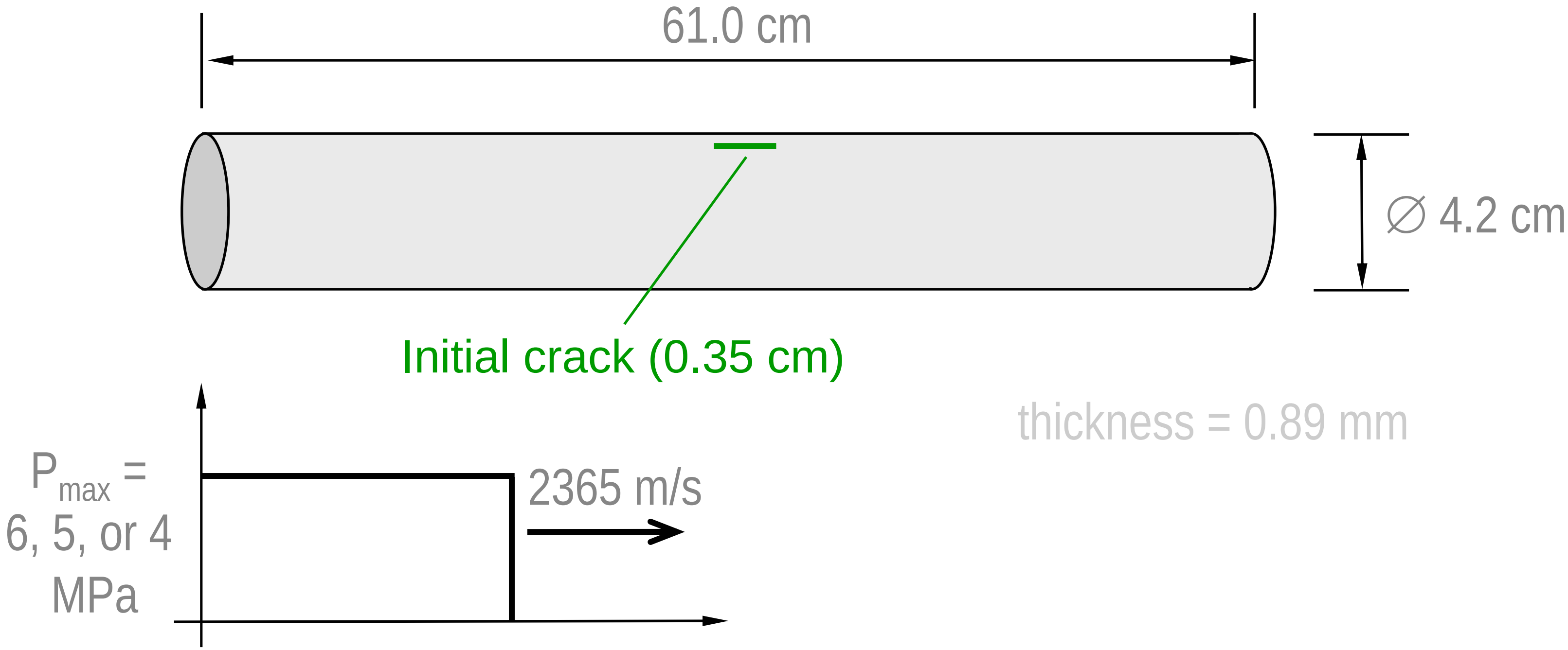
crack tracking



(movie)

Fracture of tube under blast loading (Cirak, 2004)

Shell-Fluid Coupled Simulation

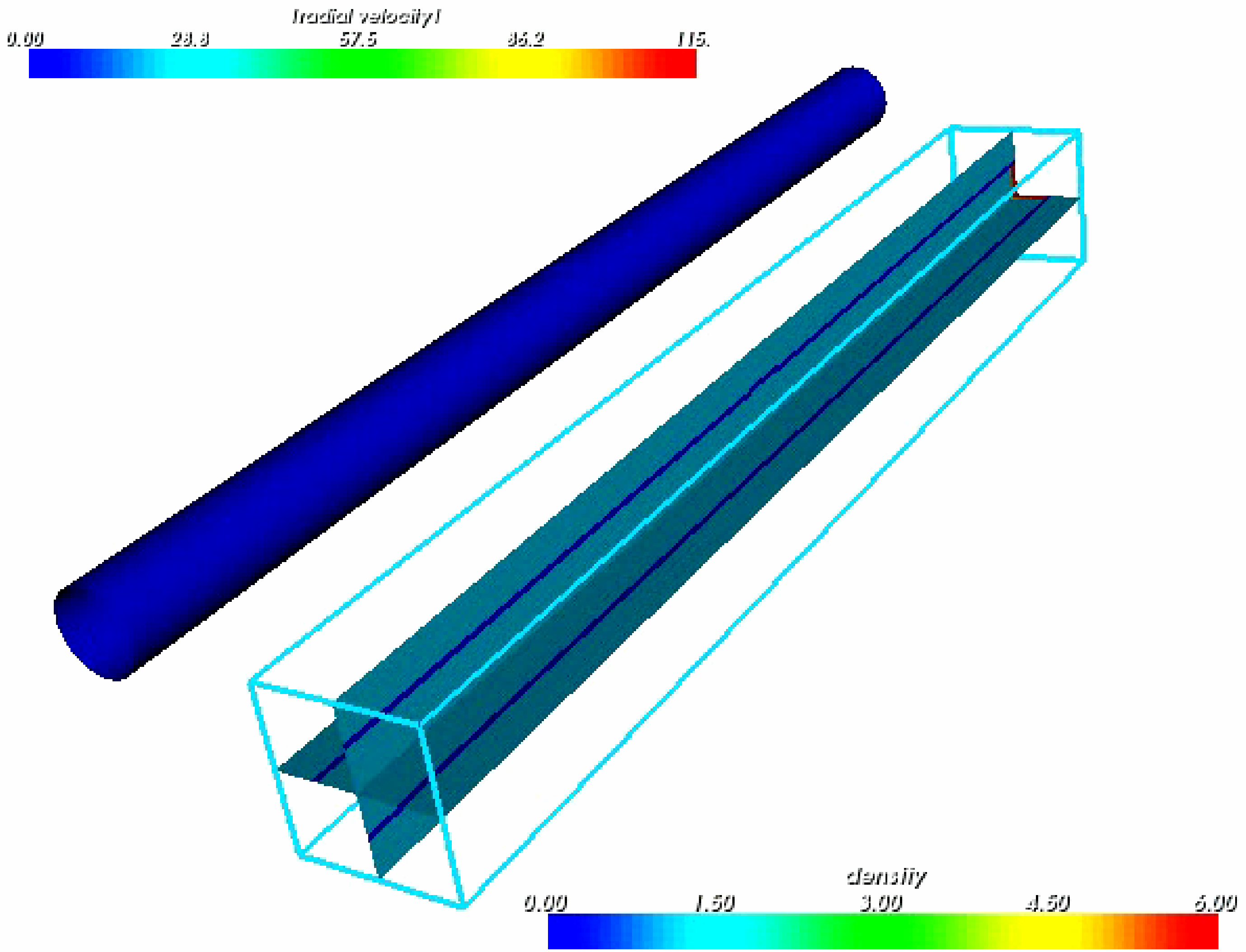


Material model for Al 6061-T6:
J_2 - plasticity with viscosity

Cohesive interface model:
Linearly decreasing envelope
with loading and unloading

(Cirak et al., 2004)

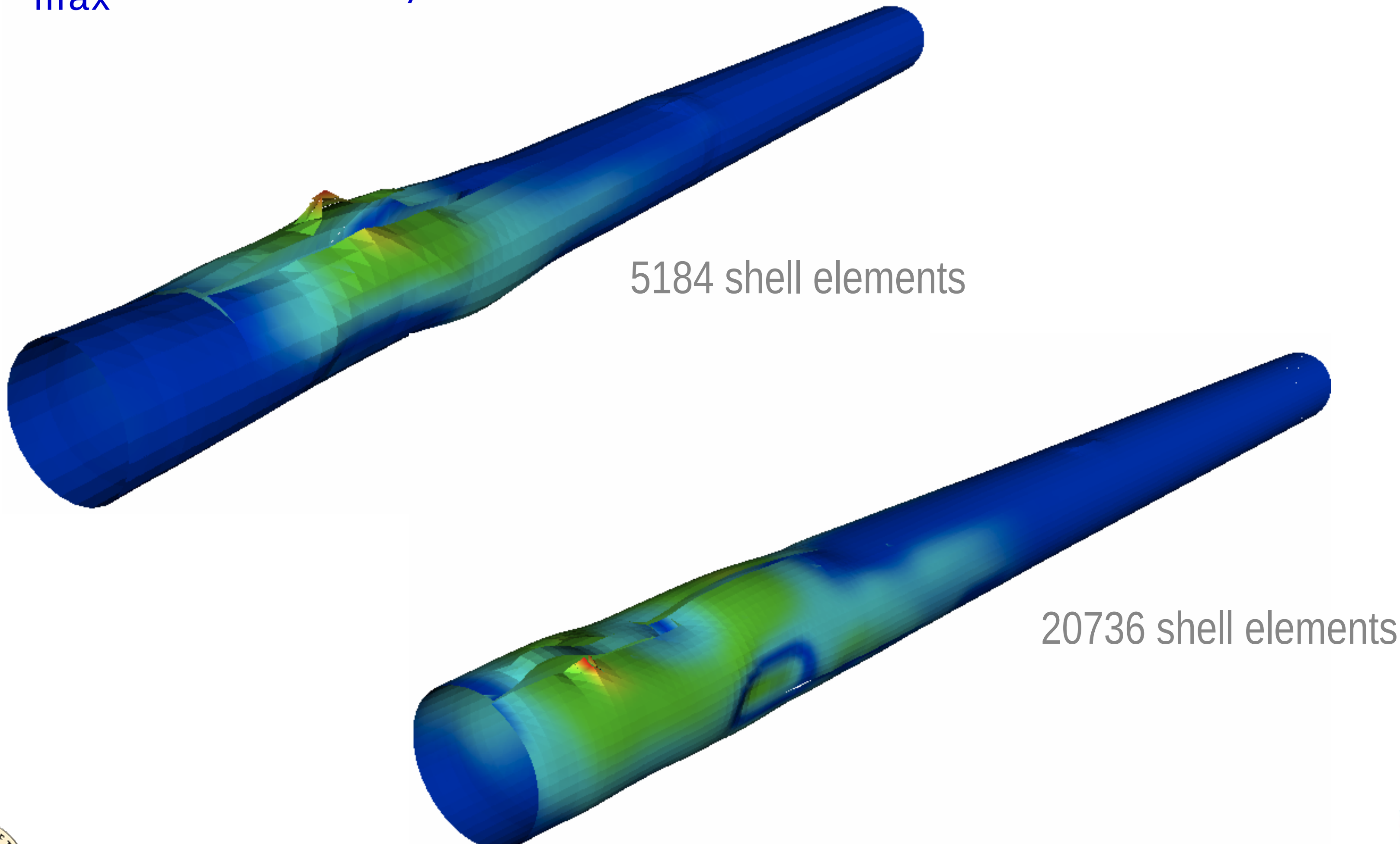
Engineering capability



(Cirak et al., 2004)

Shell-Fluid Coupled Simulation

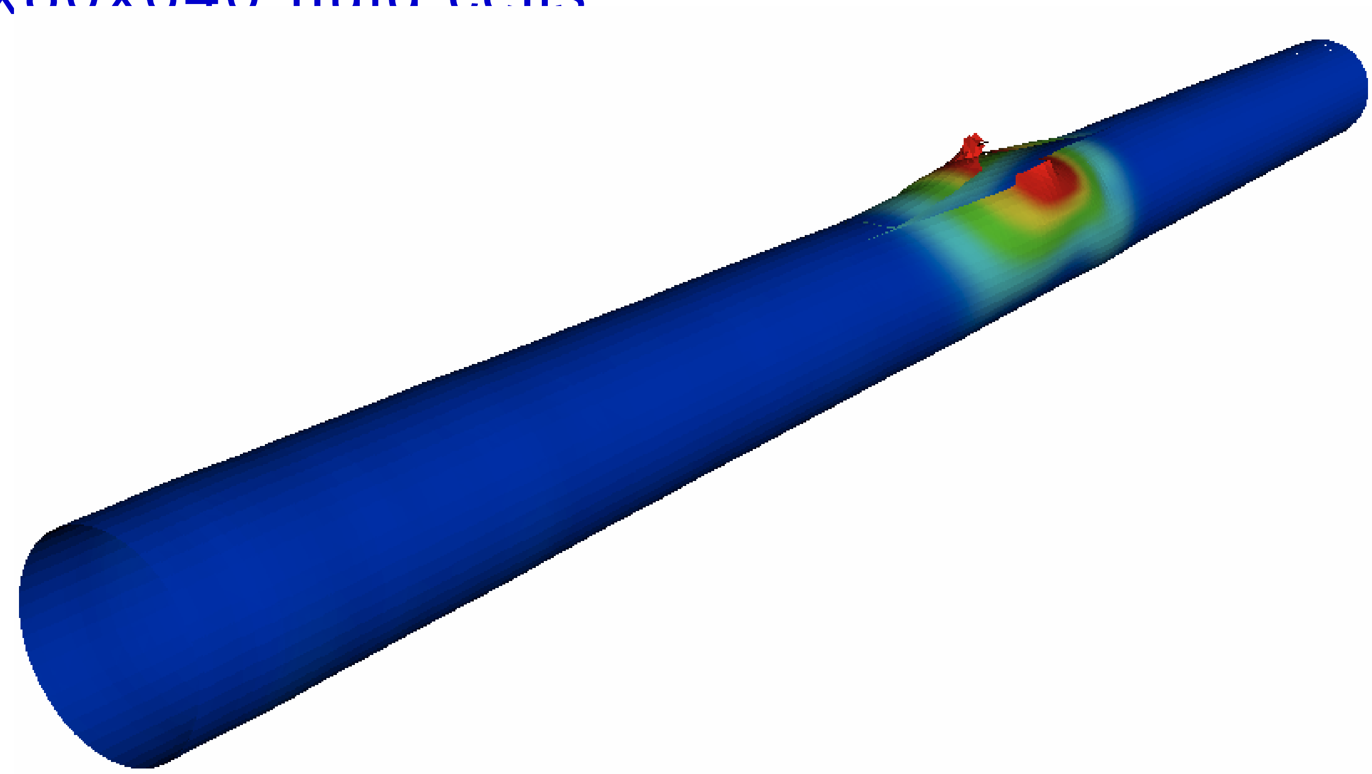
- P_{max} = 6.0MPa, 40x40x320 fluid cells



(Cirak et al., 2004)

Shell-Fluid Coupled Simulation

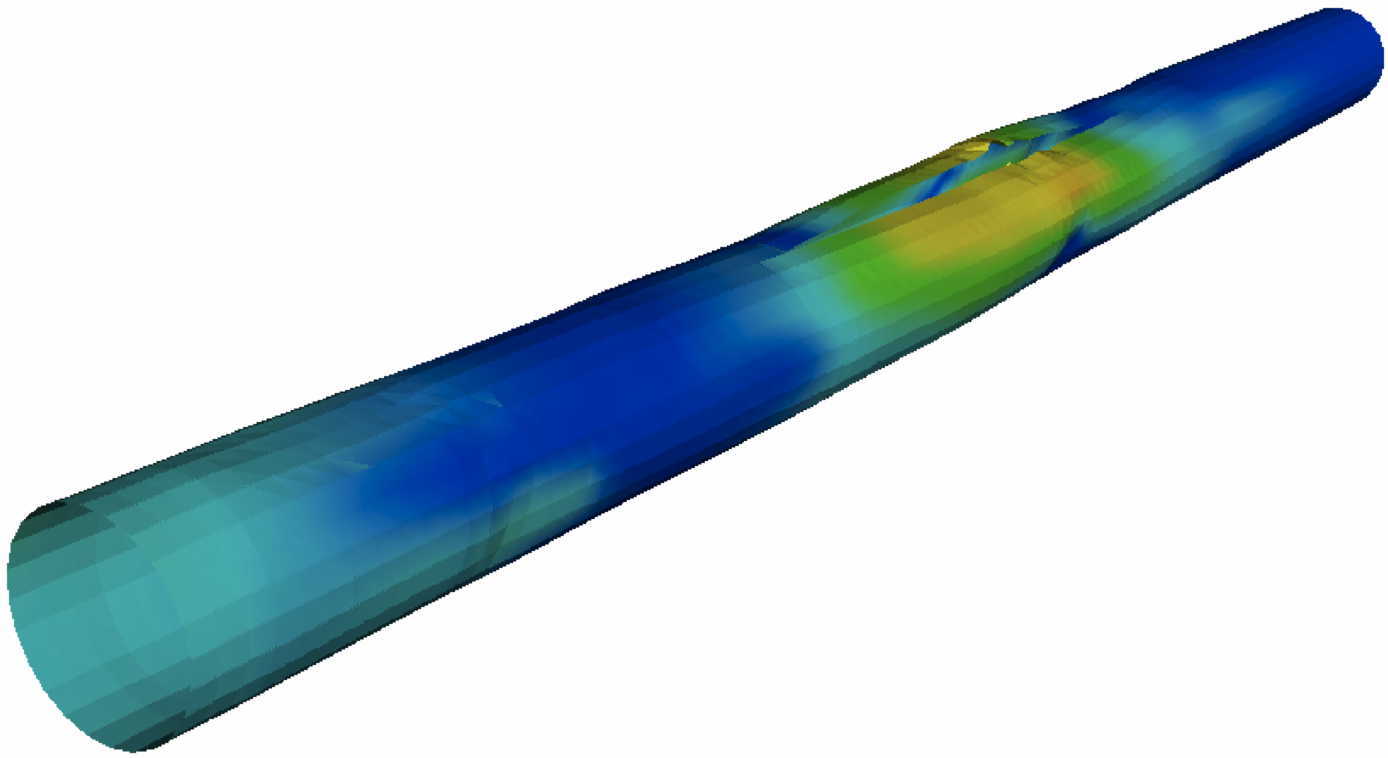
- P_{max} = 5.0MPa, 20736 shell elements, 80x80x640 fluid cells



(Cirak et al., 2004)

Shell-Fluid Coupled Simulation

- P_{max} = 5.0MPa, 5184 shell elements, 40x40x320 fluid cells



(Cirak et al., 2004)

Shell-Fluid Coupled Simulation

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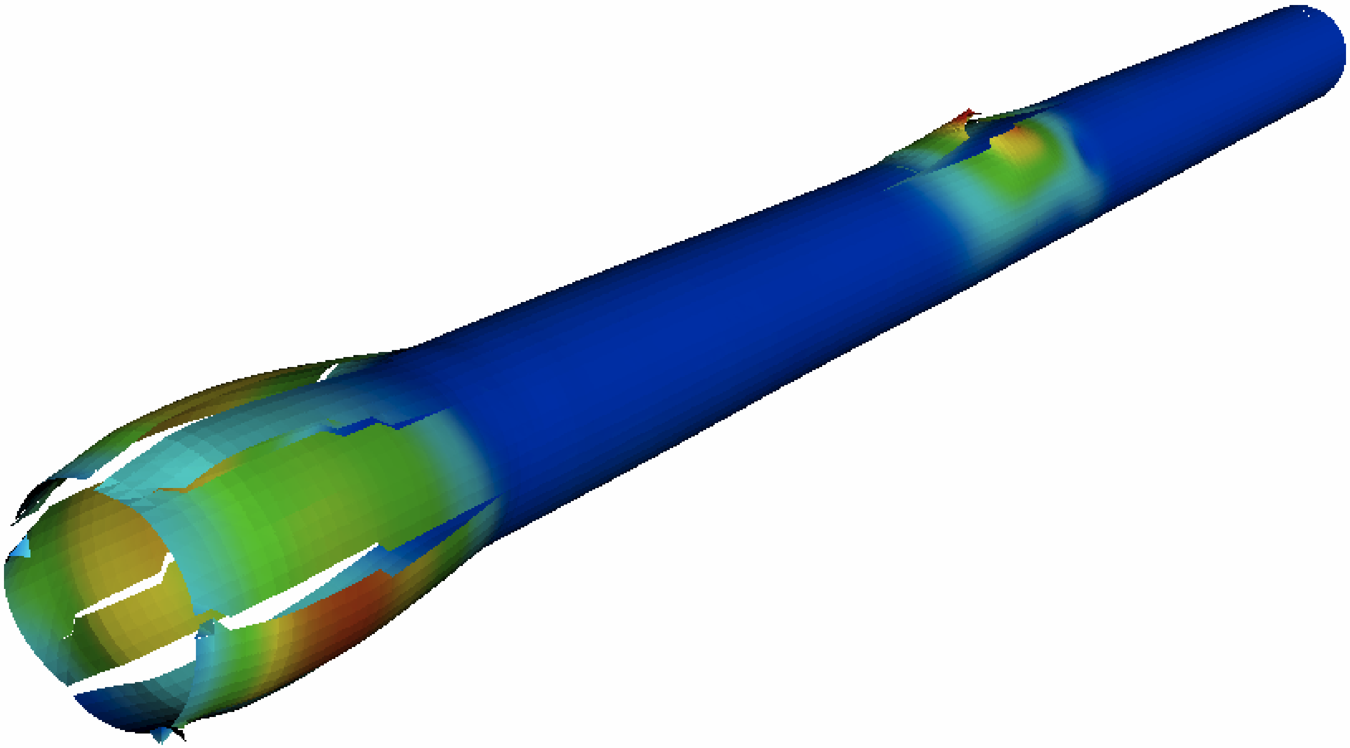


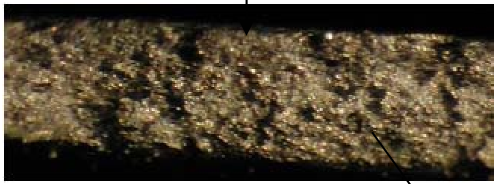
(Cirak et al., 2004)

Path forward

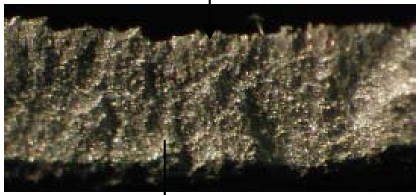
- Engineering calculations are based on:
  - *J2-plasticity model for aluminum*
  - *Cohesive model of fracture*
  - *Ideal gas law*
- Engineering calculations lack:
  - *Thermo-mechanical coupling*
  - *Localization of deformation into shear bands*
  - *Void nucleation, growth, coalescence*
  - *Damage localization into spall planes*

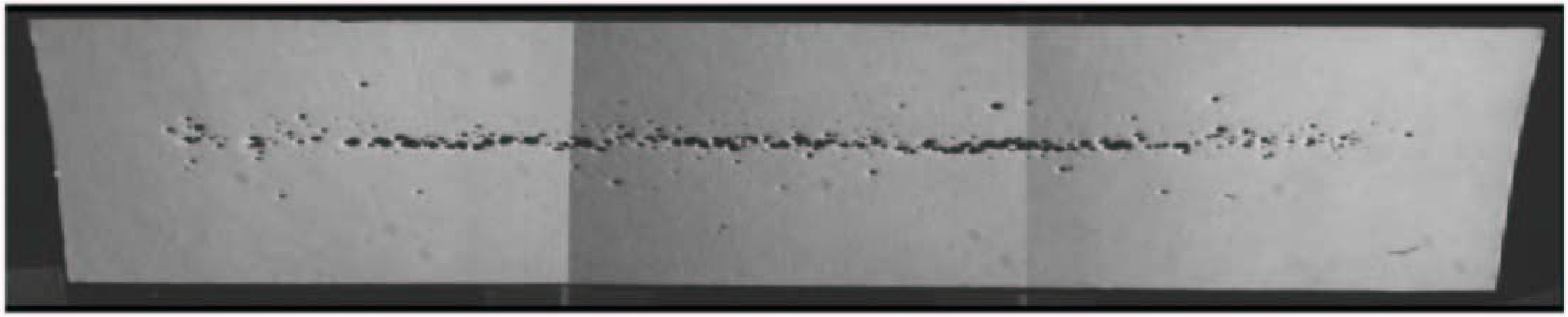
Ductile fracture - Damage

fractography shows profuse dimpling!



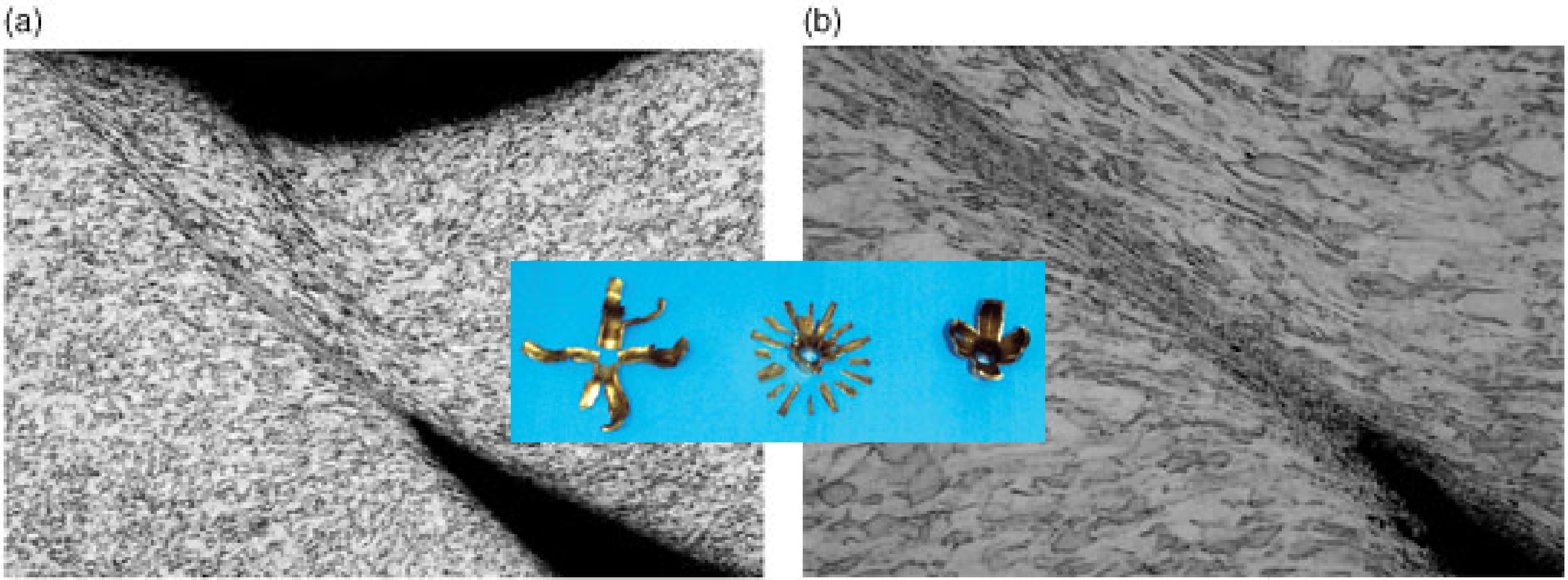
(JE Shepherd *et al.*)





Shock-driven spall fracture
(R. Becker, “How Metals Fail”, UCRL-52000-02-7/8 | July 12, 2002)

Ductile fracture – Shear bands



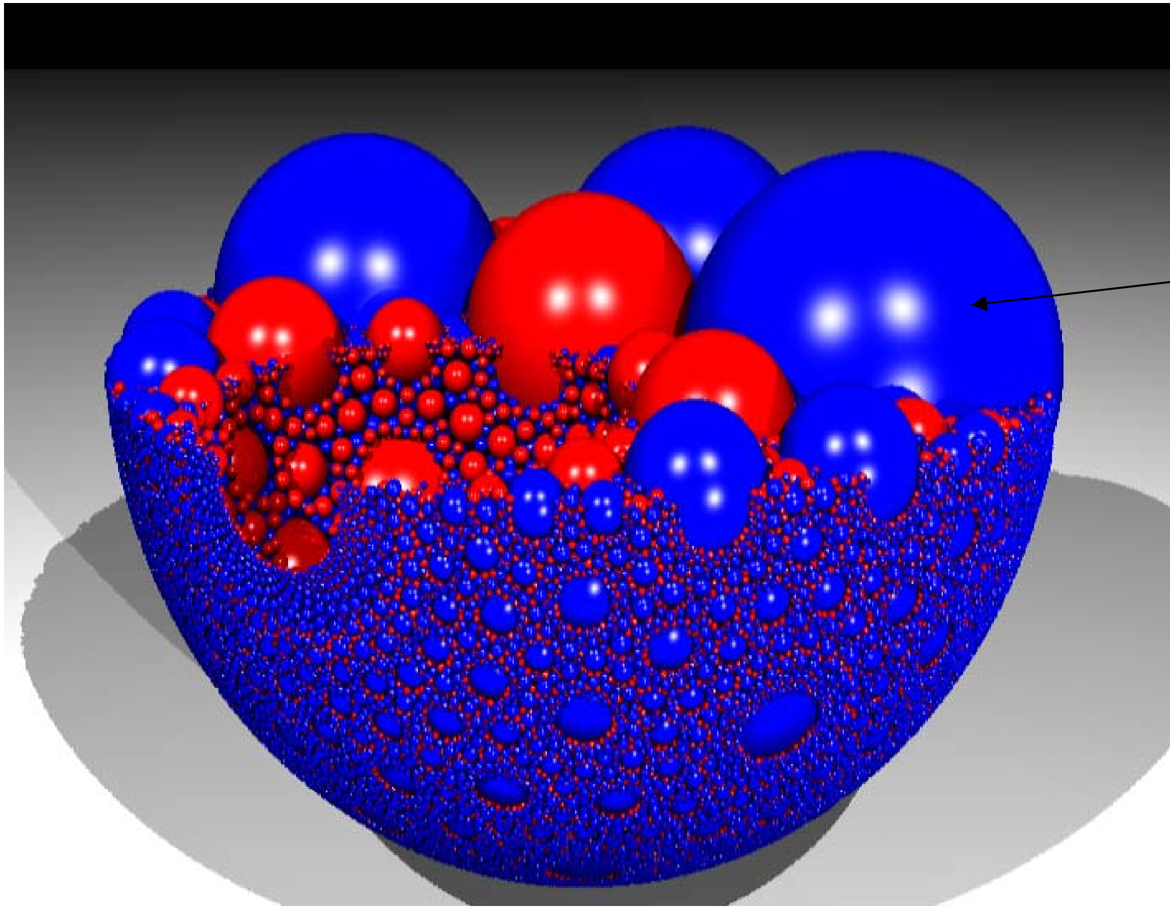
(a) This micrograph of a tantalum–tungsten alloy cylinder driven by a gas gun shows that the material breaks along shear bands (darker diagonal line).

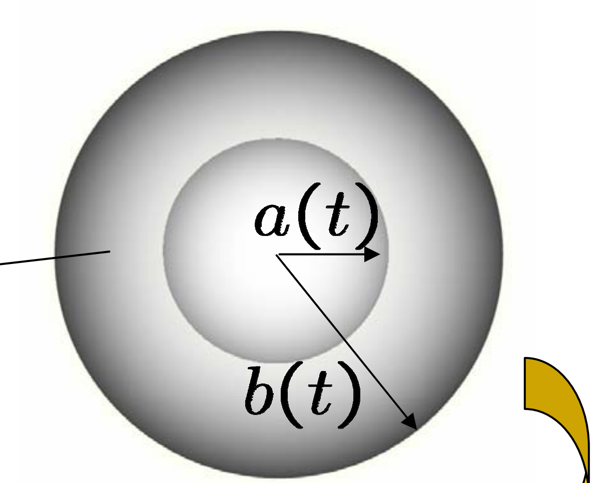
(b) The crack tip at a higher magnification.

(Micrograph produced by Anne Sunwoo.)

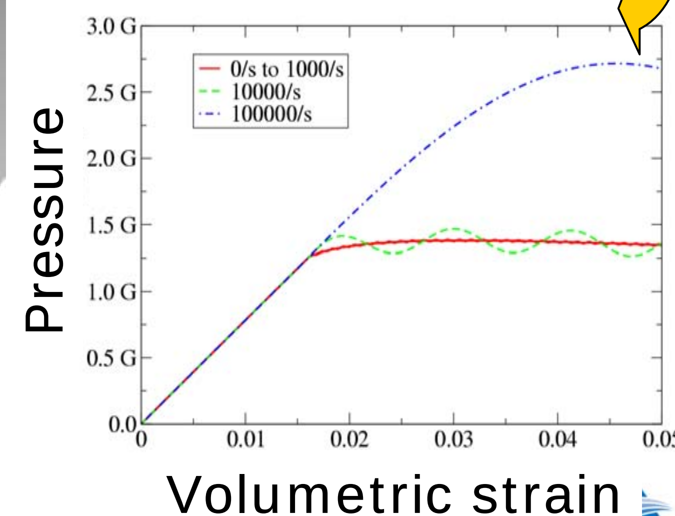
(R. Becker, “How Metals Fail”, UCRL-52000-02-7/8 | July 12, 2002)

Porous plasticity - Damage



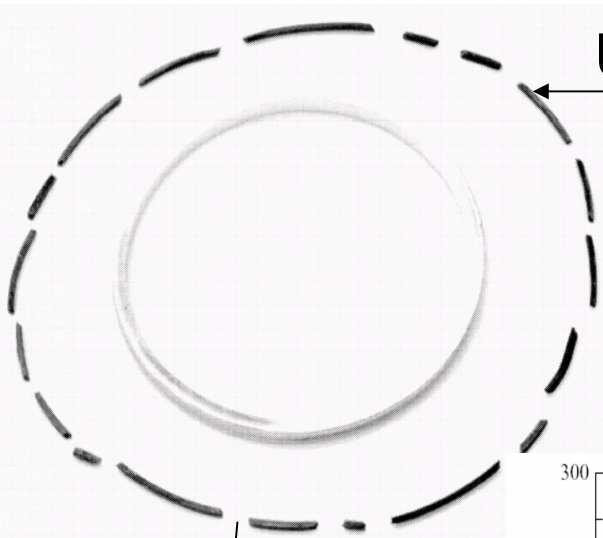


Shell model



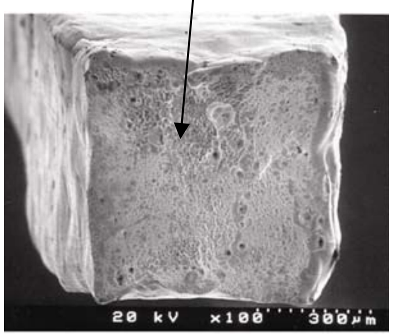
(Courtesy Hans Hermann, University of Stuttgart, Germany)

Spall – Engineering model - Validation

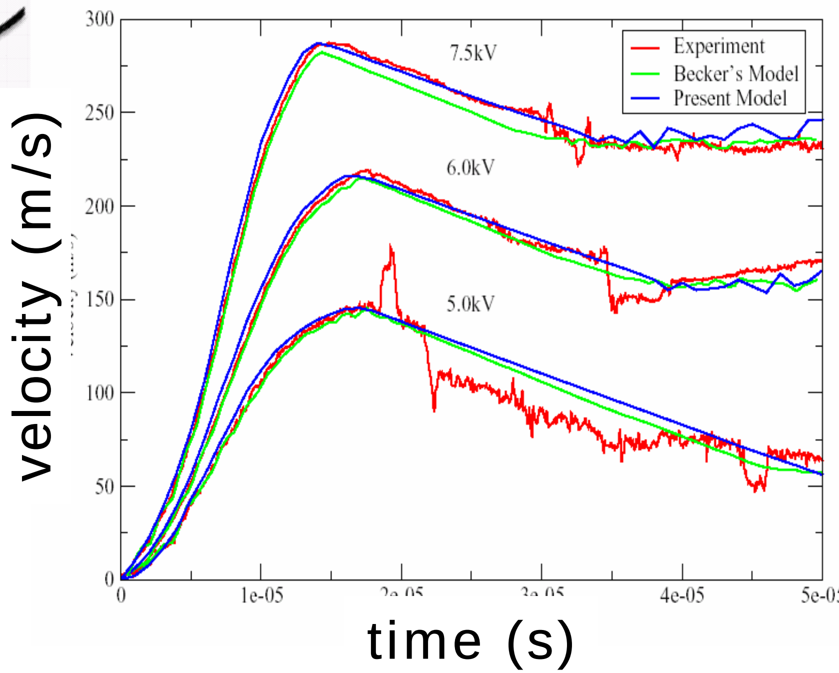


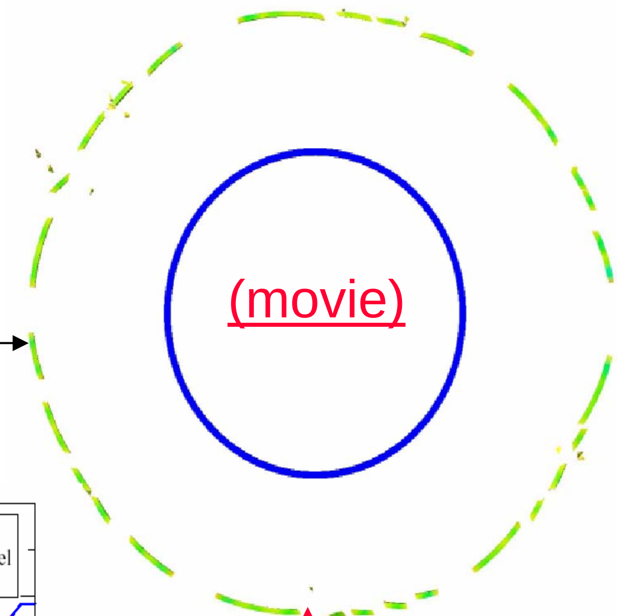
U6Nb ring expansion (Becker LLNL ‘02)

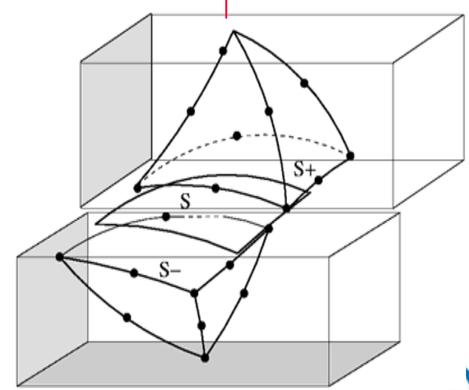
FE simulation (Weinberg *et al* ‘04)



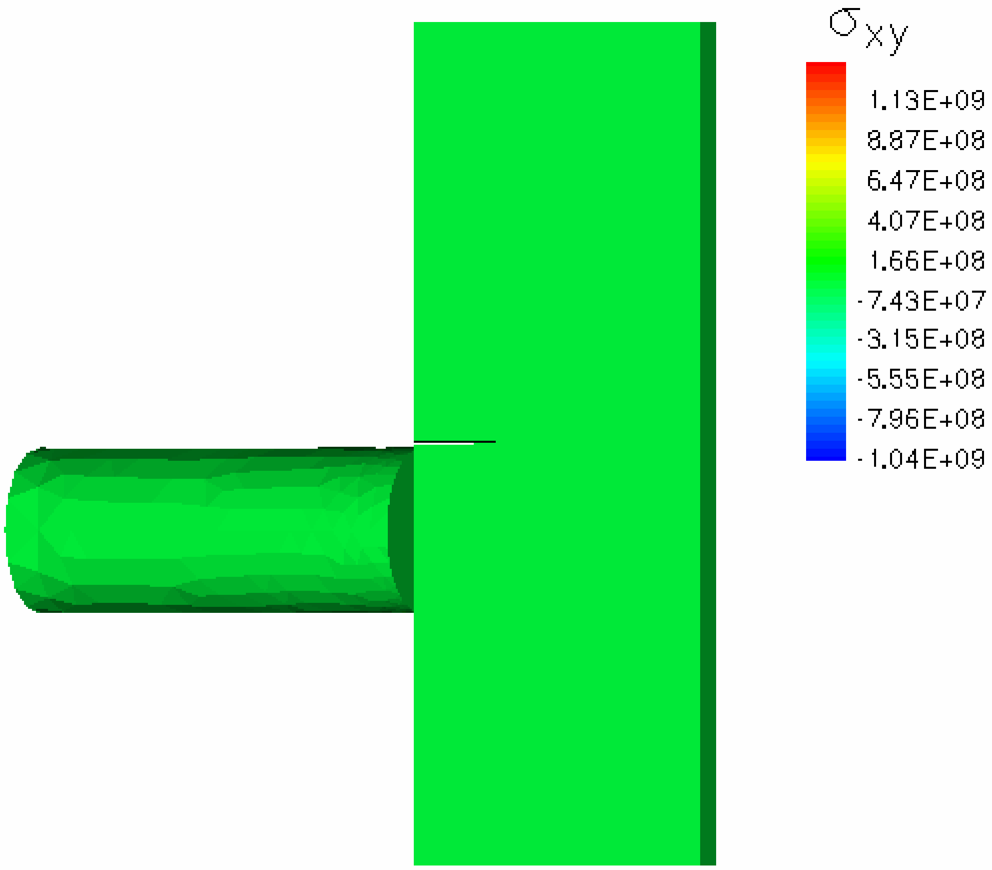
Rich Becker, LLNL)

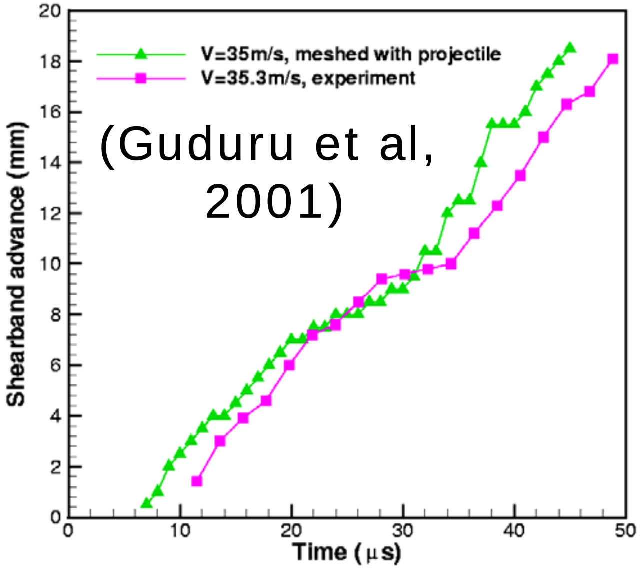






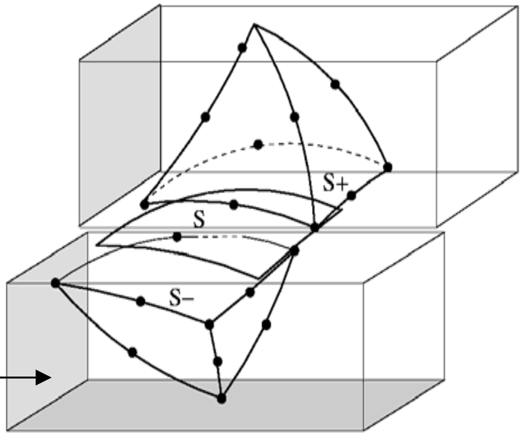
Validation – Impact Test – Band speed





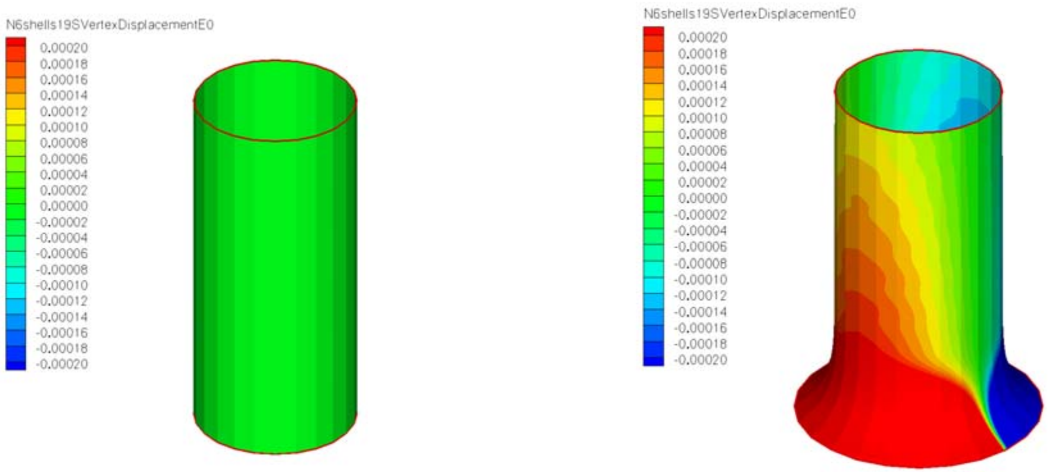
Shear band speed ~ 500 m/s

Shear-band elements (Yang et al., 2004)



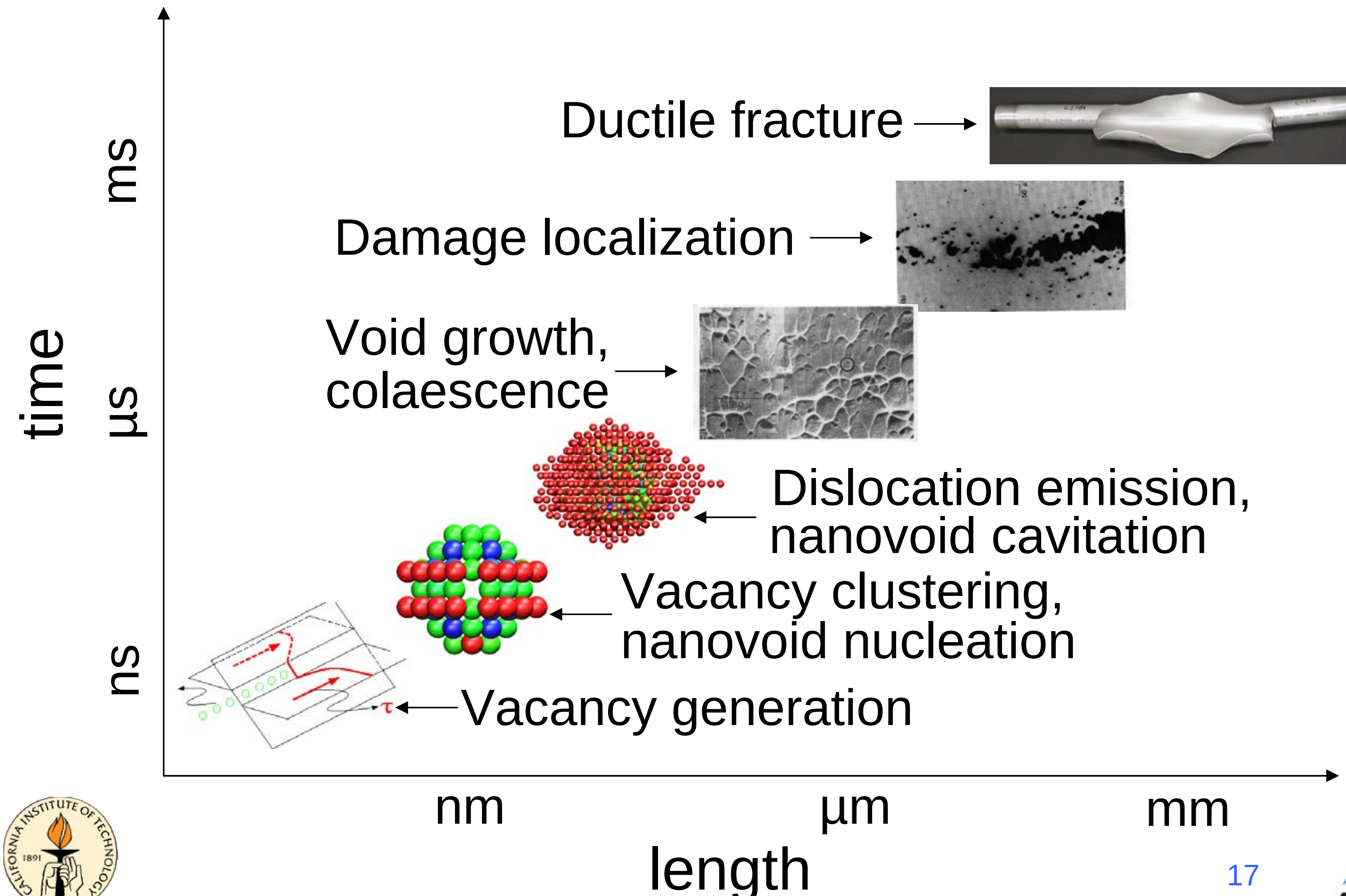
Engineering models - TODO list

- Integrate damage model into VTF
- Integrate localization elements into VTF
- Integrate shear-band elements into VTF
- Add thermo-mechanical coupling
- Re-run tube detonation calculations



(Mota, 2005)

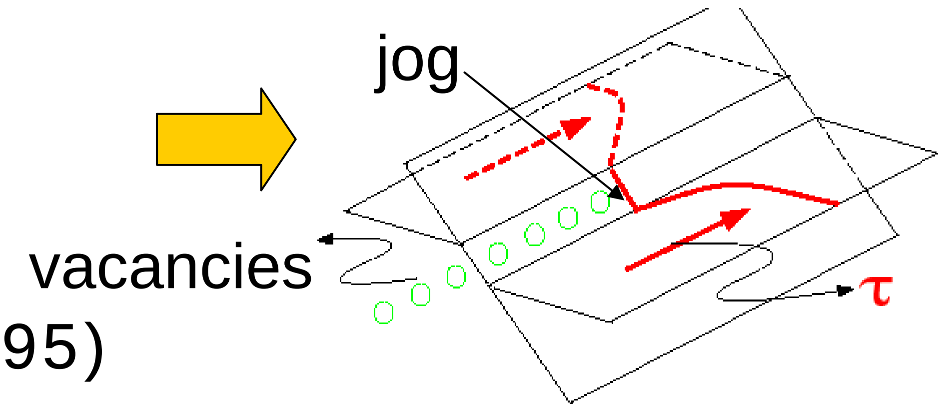
Ductile fracture – Lengthscale hierarchy



Nanovoid nucleation mechanism

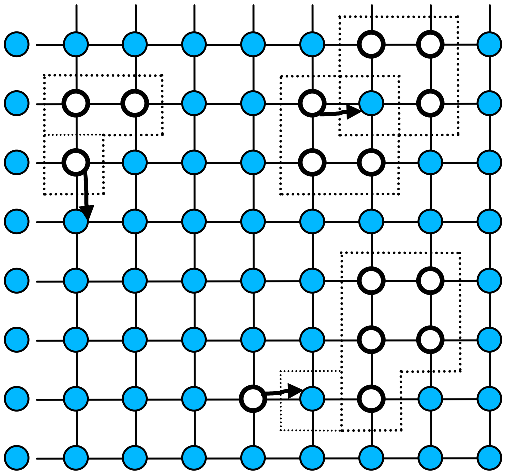
- Vacancy generation:
  - *Cross slip*
  - *Dislocation intersection*

(Cuitino and Ortiz, 1995)



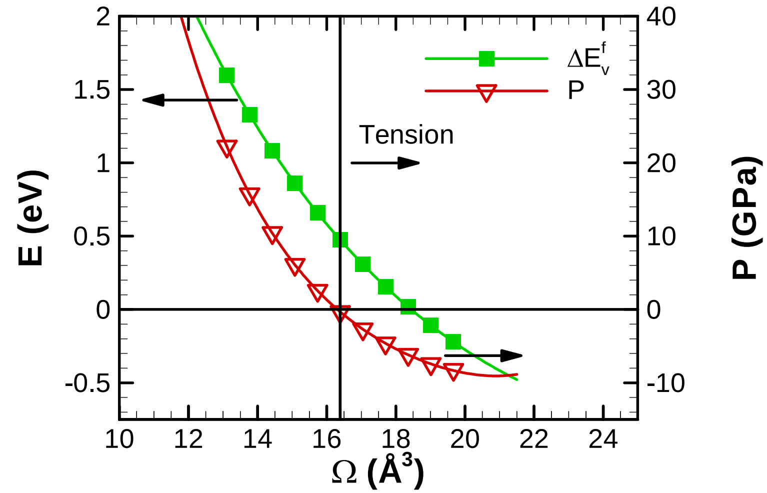
- **Vacancy aggregation**:
  - *Vacancy diffusion*
  - *Attachment and detachment*
  - *Large scale cluster statistics*

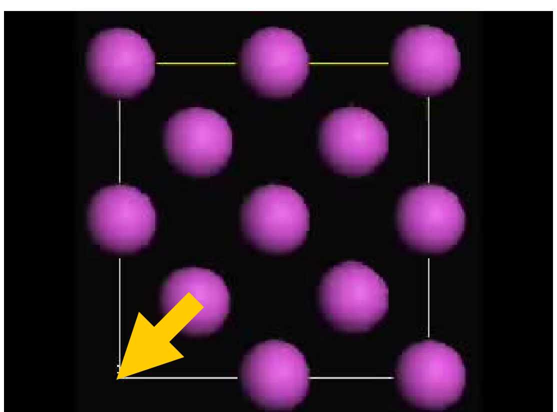
(S. Serebrinksy, M. Ortiz, E.A. Carter)

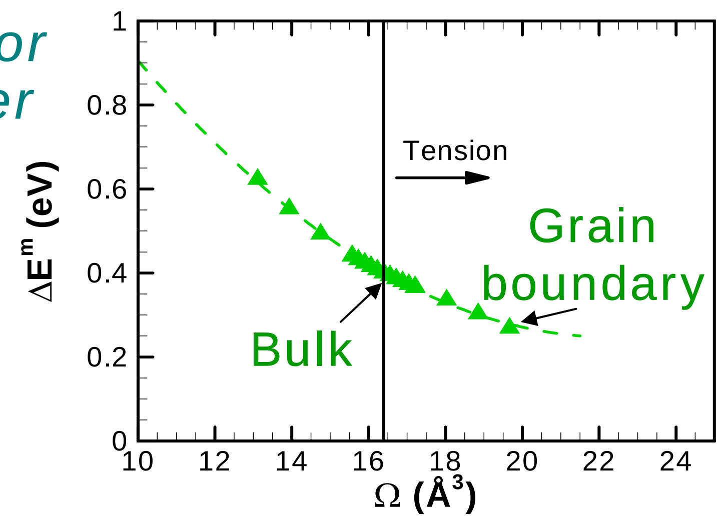


Vacancies in bulk Al – OFDFT

- Calculated formation energy (E.A.Carter):
  - *Open volume → decreasing formation energy*
- Calculated diffusion barrier (E.A.Carter):
  - *Barrier = 0.25-0.65eV*
  - *Open volume (tensile stress or grain boundary) → low barrier*







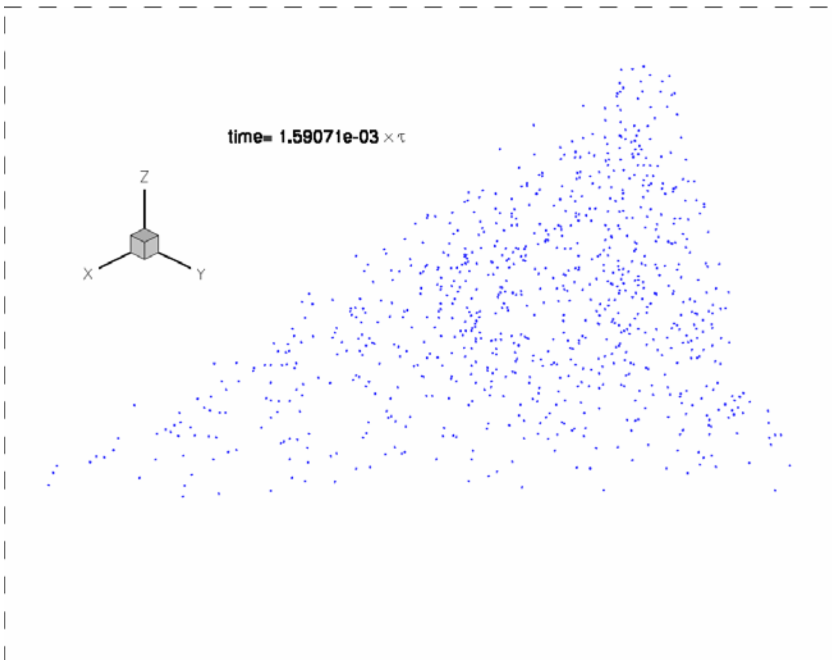
E.A. Carter, G. Ho, M. Ong, K. Caspersen

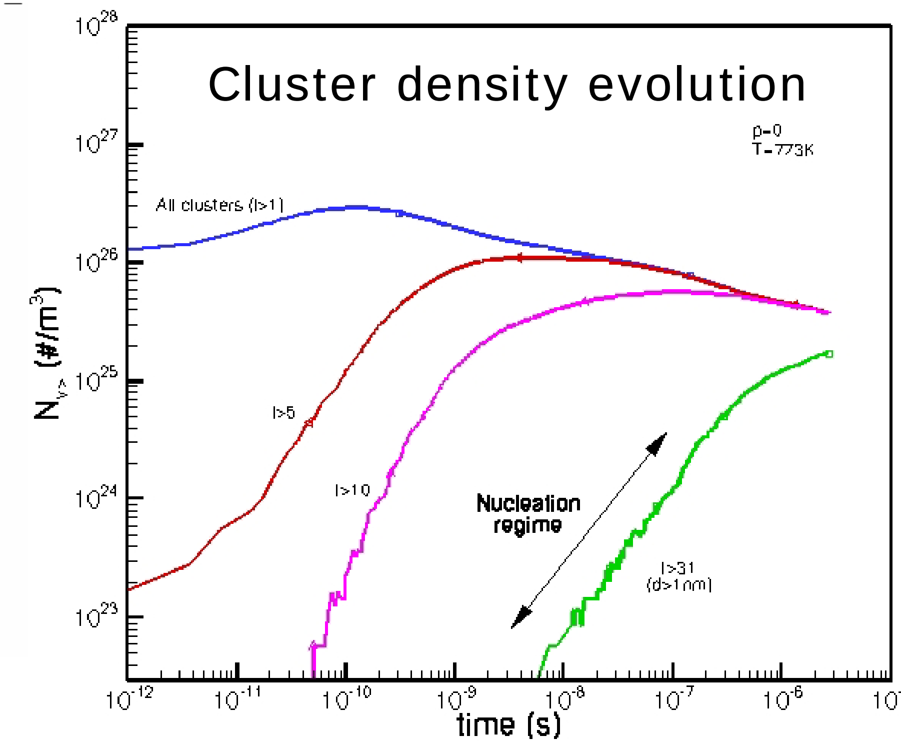
Vacancy clusters in Al – KMC

- Markov chain Monte Carlo
  - *Ising Hamiltonian*
  - *Transition rate probabilities q determined by first principles*

$$q_{ij} = \nu e^{-\beta \Delta E_0^m} \min(e^{-\beta(H_j - H_i)}, 1)$$

First principles





(S. Serebrinksy, M. Ortiz, E.A. Carter)

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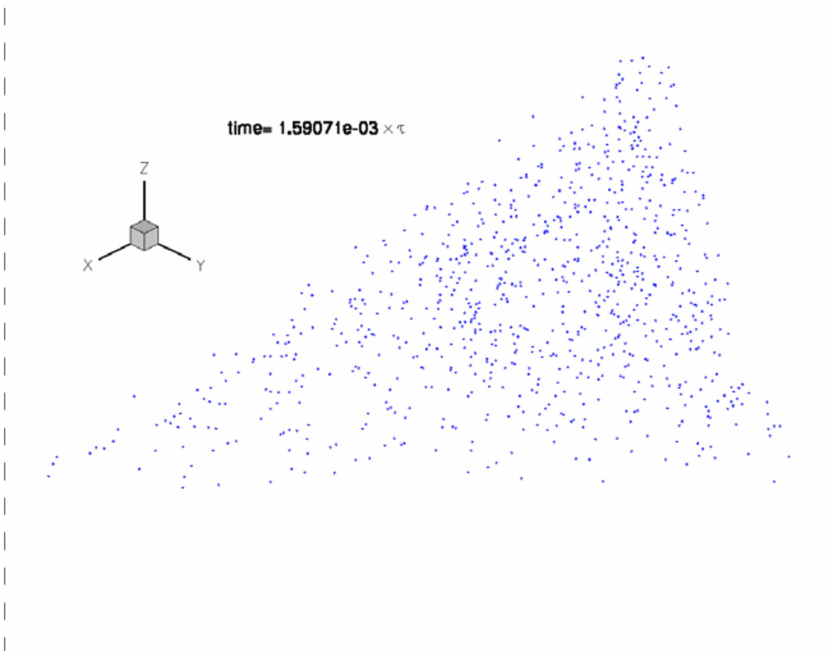
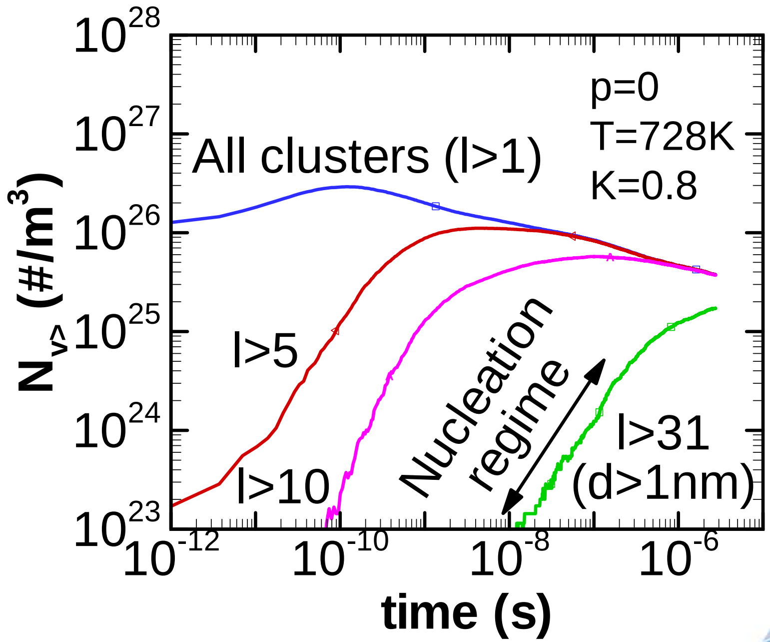


Evolution of densities of clusters larger than a given size l

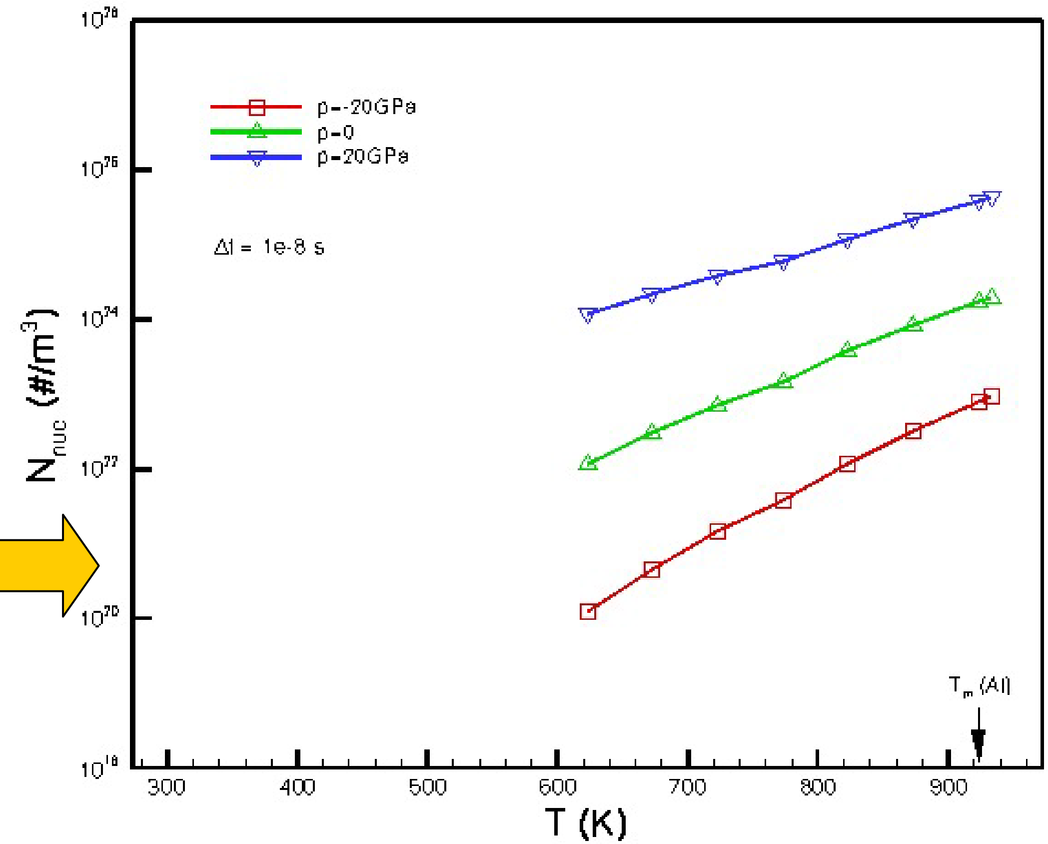


(S. Serebrinksy, M. Ortiz, E.A. Carter)

Nanovoid nucleation rate in Al

- Shock conditions
  - *High temperature*
  - *High stress*
  - *Large effect on nucleation rate*

Density of voids that can cavitate plastically (diameter>1nm) formed in 10^{-8}s



(S. Serebrinksy, M. Ortiz, E.A. Carter)

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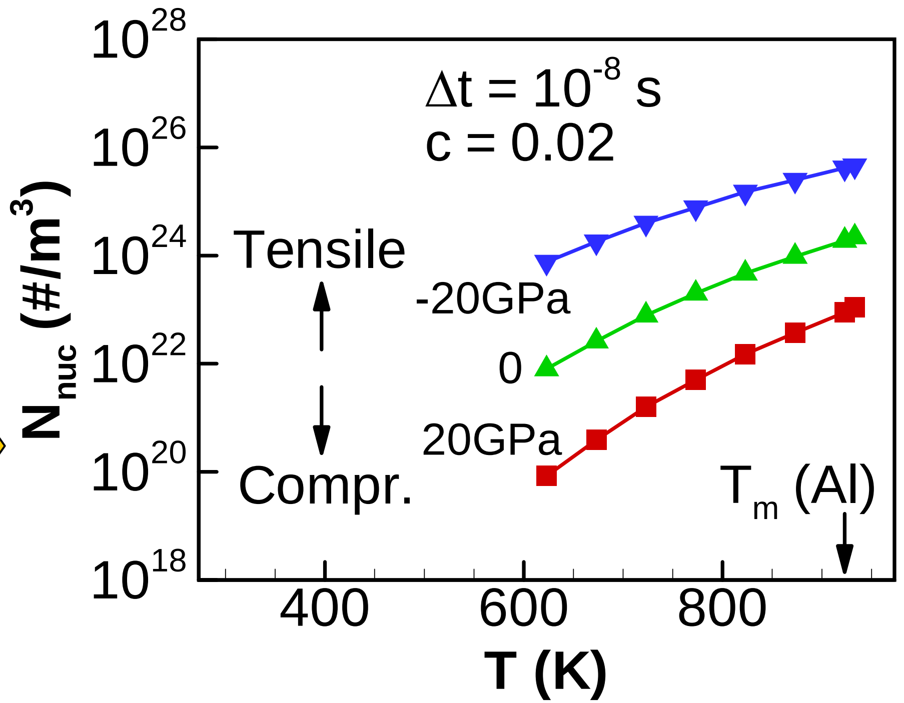
Number of critical voids

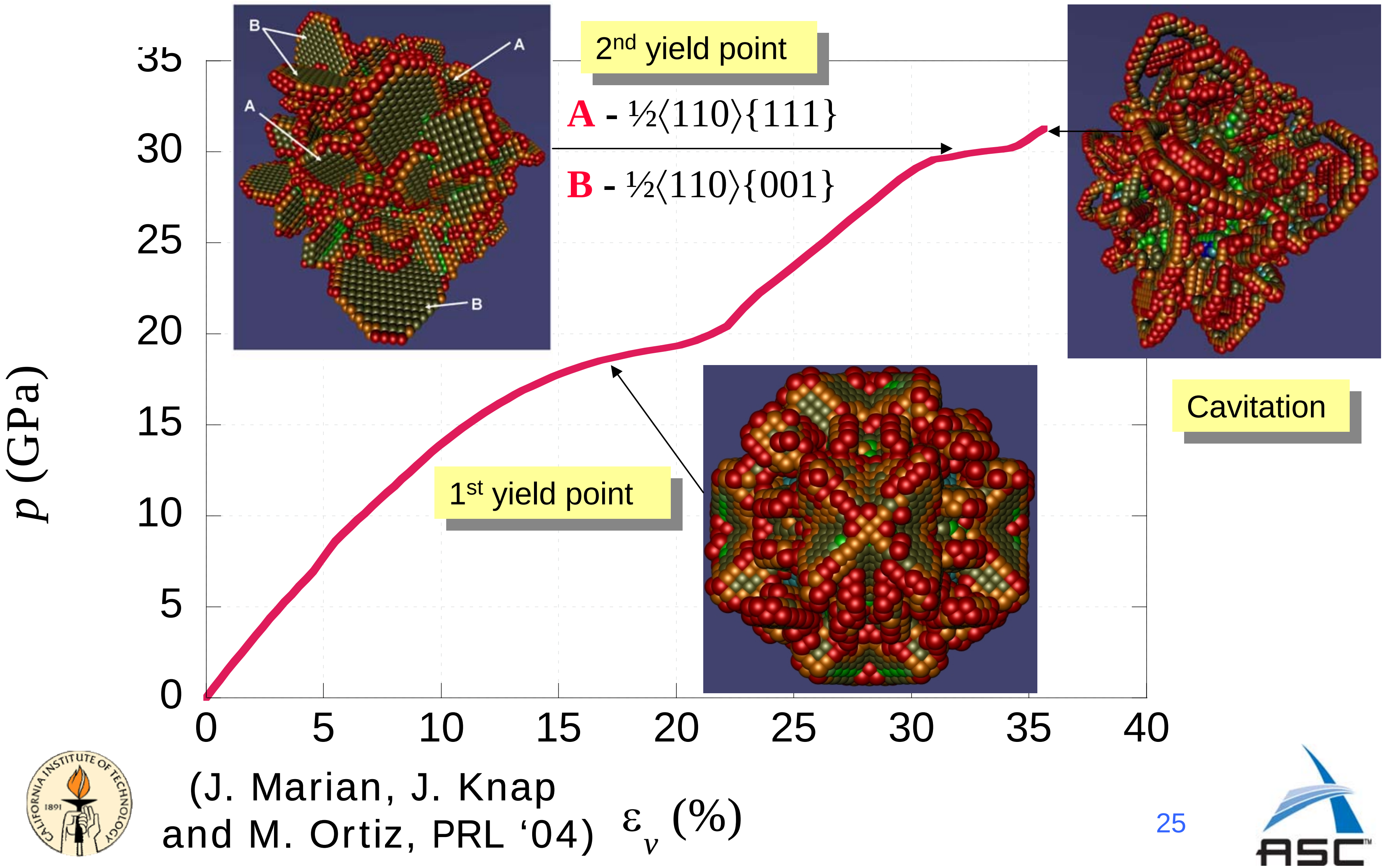


(S. Serebrinksy, M. Ortiz, E.A. Carter)

Nanovoid nucleation – TODO list

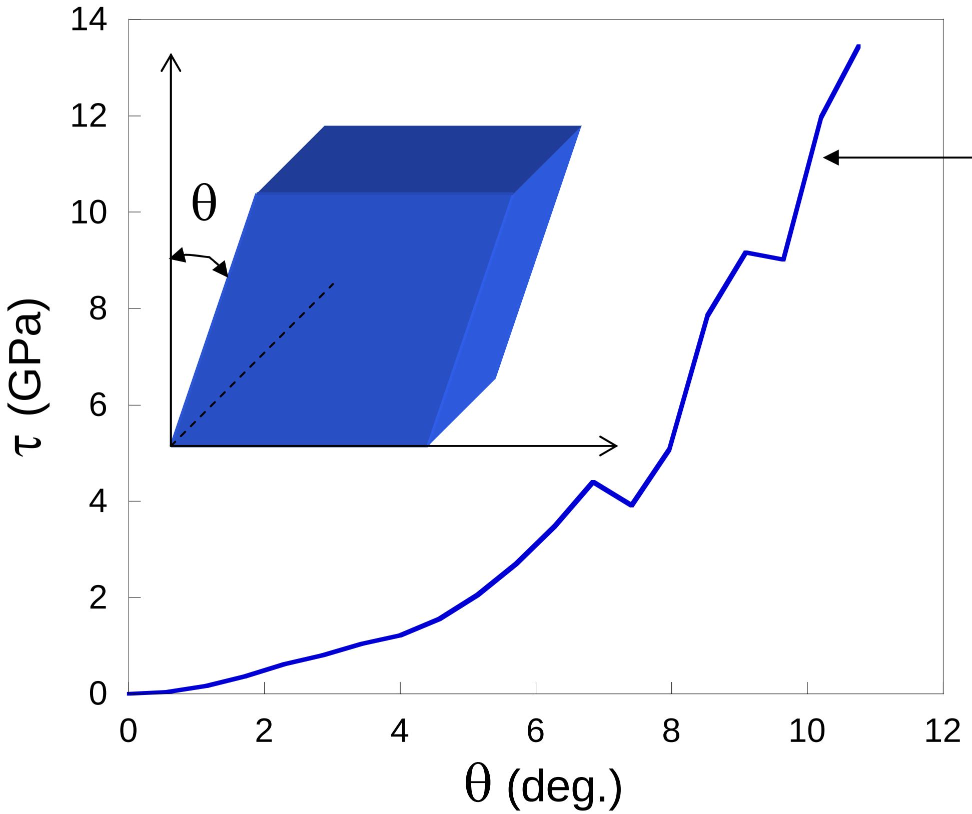
- Integrate volume dependence of attempt frequency, migration barrier, di-vacancy binding energy in MC simulations
- Pipe diffusion (inhomogeneous volume)
- Grain boundaries (inhomogeneous volume)
- Integrate into engineering model

Nanovoid cavitation in Al – Hydrostatic

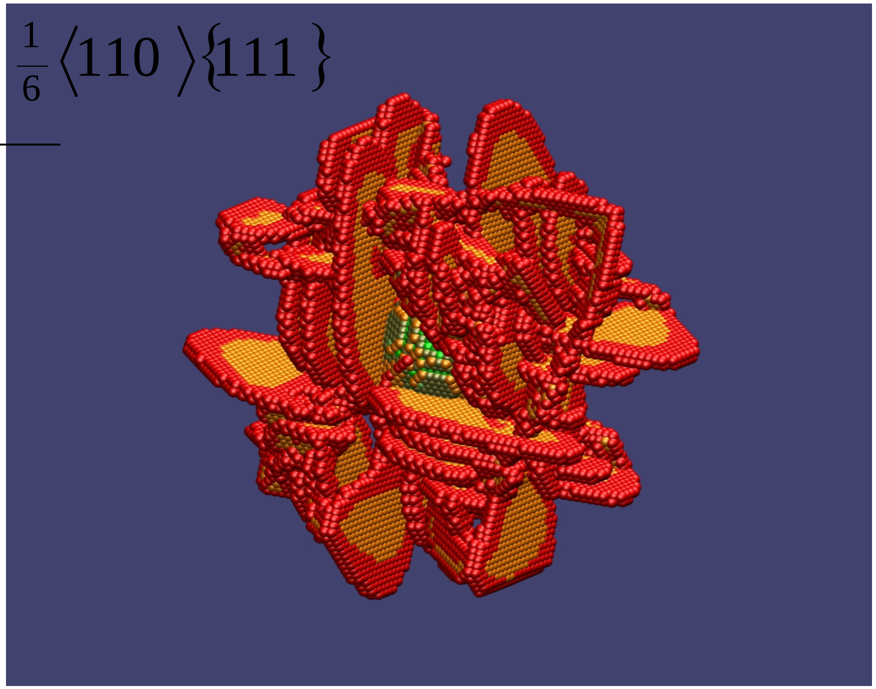


(J. Marian, J. Knap and M. Ortiz, PRL '04)

Nanovoid cavitation in Al – Shear



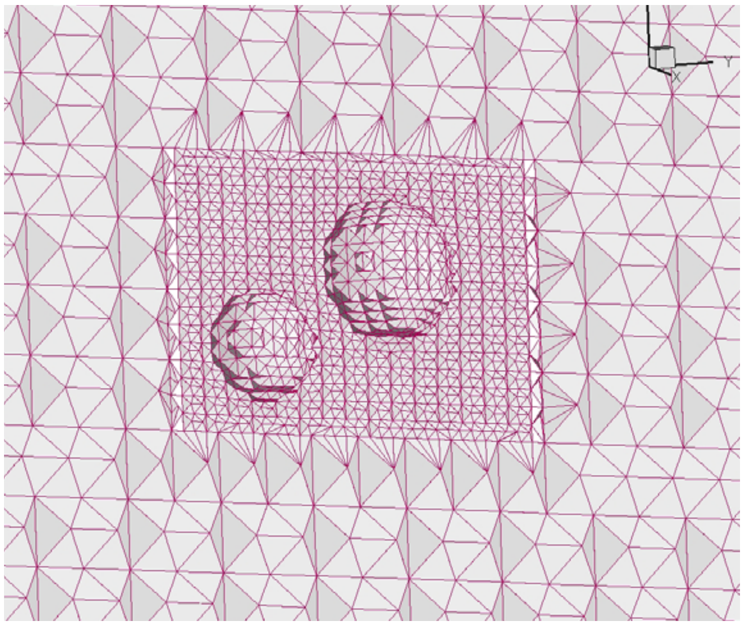
Shear stress-strain curve



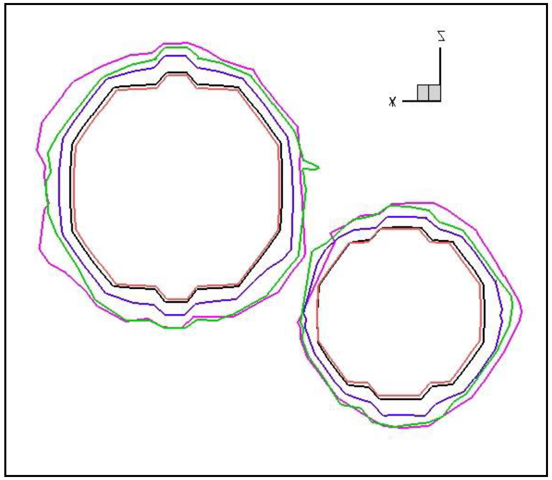
Dislocation structures

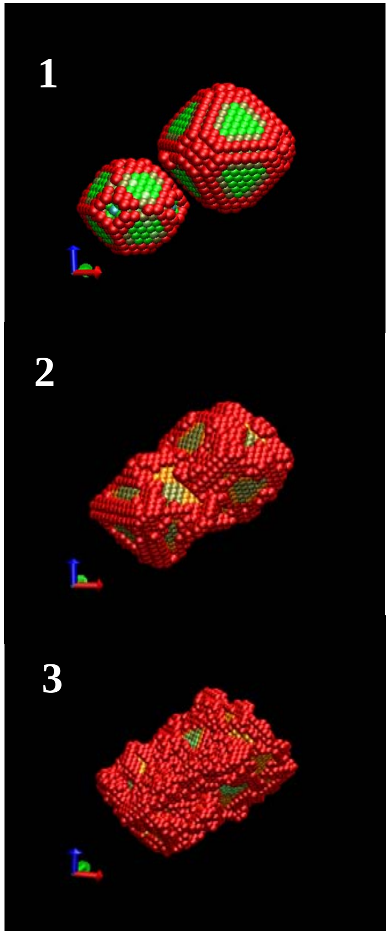
(J. Marian, J. Knap and M. Ortiz, 2004)

Nanovoid coalescence in Al



- **2 Spherical** (5 and 4-nm) **voids** under tri-axial tension



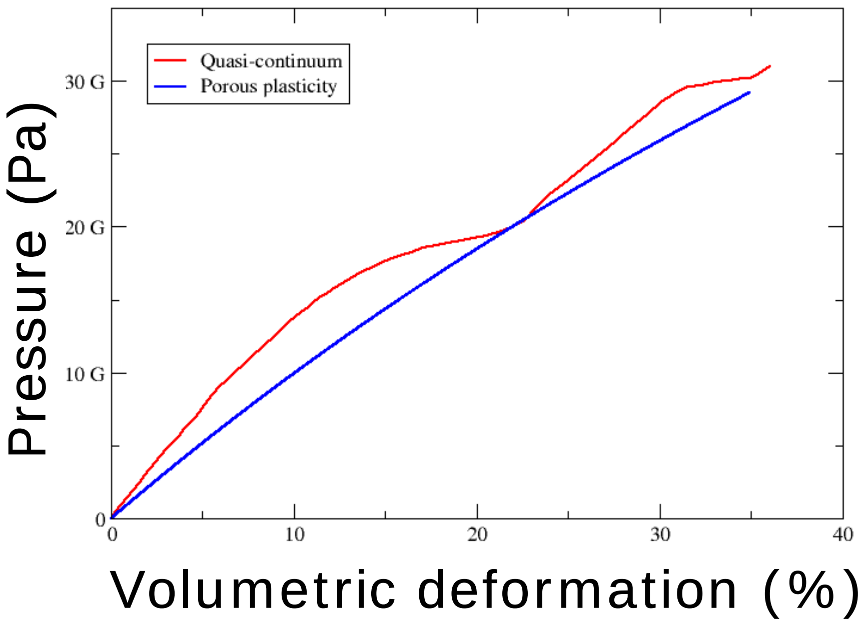


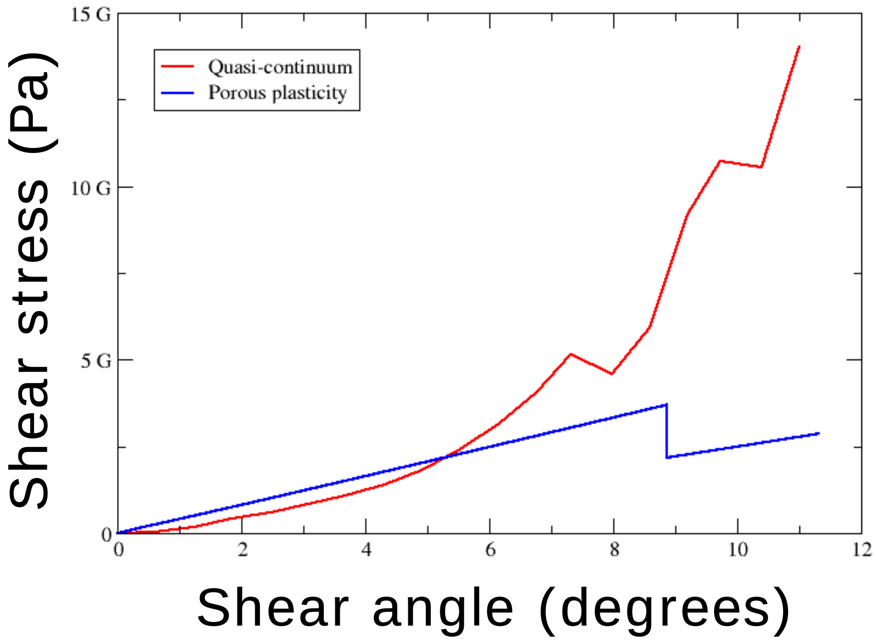
- Symmetry-breaking conditions
- Cavitation occurs at ~8 GPa (as opposed to 19 GPa for a single void)

(J. Marian, J. Knap and M. Ortiz, 2005)

Nanovoid cavitation – TODO list

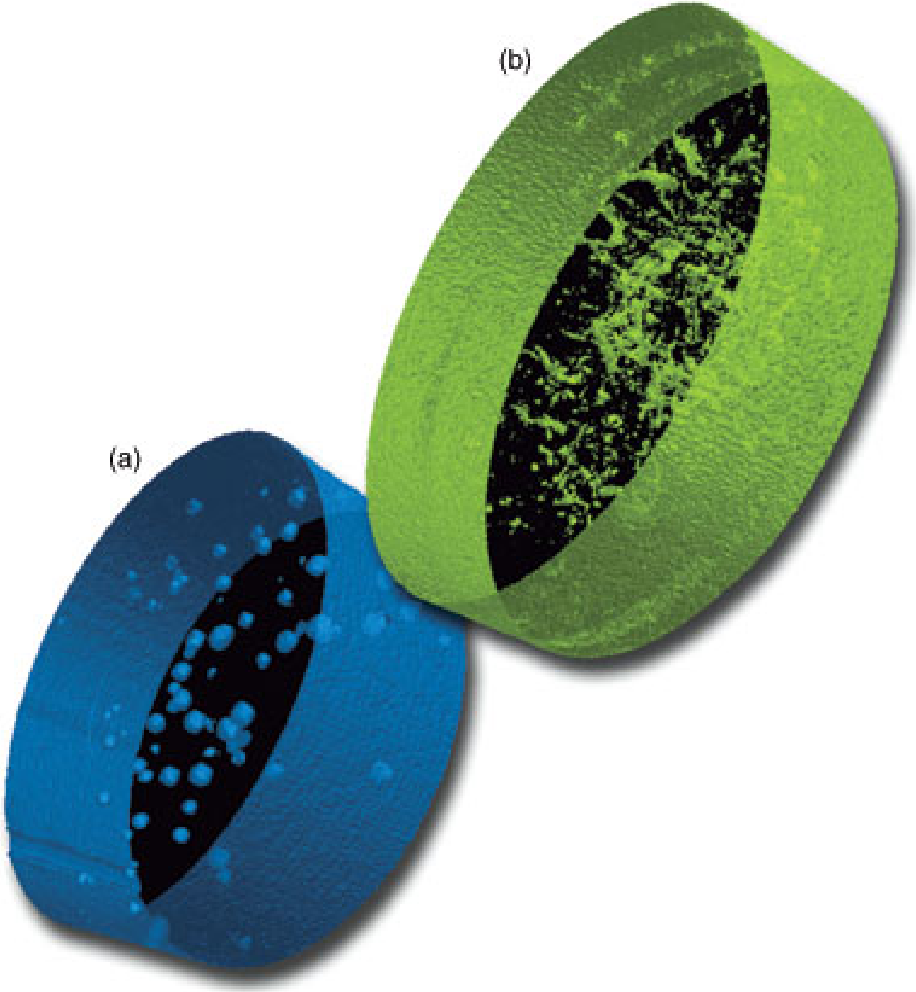
- Use nanoscale results to inform engineering model of porous plasticity





(A. Mota J. Marian, J. Knap and M. Ortiz)

Void growth and coalescence

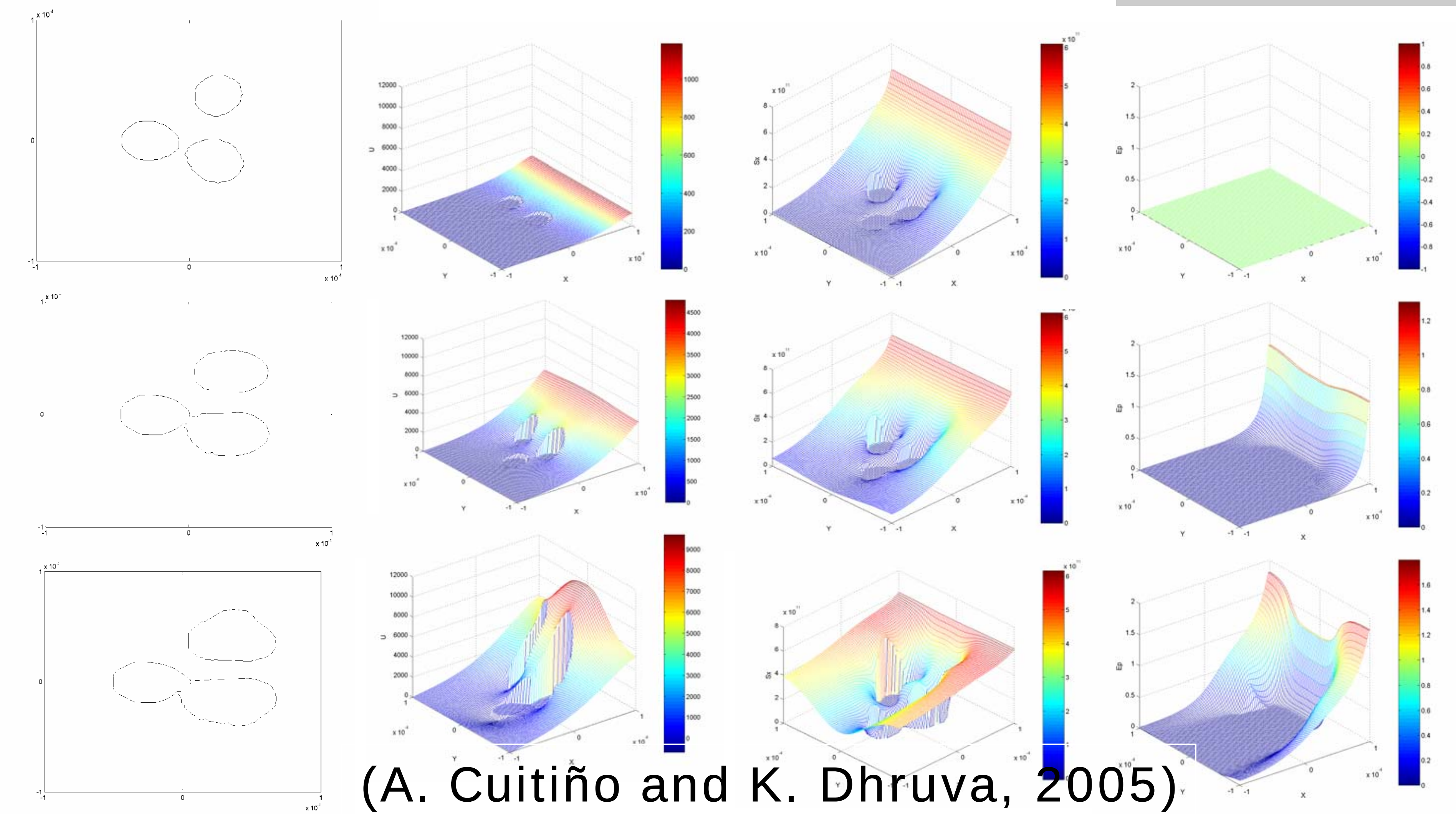


The Stanford Synchrotron Radiation Laboratory is used to obtain three-dimensional x-ray tomographic images of experimentally produced incipient spallation. The images are from a 6-millimeter region in the center of the spall plane in (a) single-crystal aluminum and (b) polycrystalline aluminum.

(R. Becker, “How Metals Fail”, UCRL-52000-02-7/8 | July 12, 2002)

Void growth and coalescence – level set

Void Interface	U-velocity	Stress Along x-axis (S_x)	Effective Plastic Deformation



(A. Cuitiño and K. Dhruva, 2005)

Void growth – TODO list

- Extend to three dimensions
- Use mesoscopic information to inform engineering models of porous plasticity