Solid Dynamics
Detonation-Driven Tube Fracture Modeling and Simulation

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Detonation-driven tube fracture

strain (0.1%)

(a) (b) (c) (d)

time (ms)

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

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

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

5184 shell elements

20736 shell elements

(Cirak et al., 2004)
Shell-Fluid Coupled Simulation

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

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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
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.)
Porous plasticity - Damage

(Courtesy Hans Hermann, University of Stuttgart, Germany)
Spall – Engineering model - Validation

U6Nb ring expansion
(Becker LLNL ‘02)

FE simulation
(Weinberg et al ‘04)

(time s)

(velocity m/s)

(movie)

Rich Becker, LLNL
Validation – Impact Test – Band speed

Shear band speed $\sim 500 \text{ m/s}$

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

(Guduru et al., 2001)
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

- **Vacancy generation**
- **Void growth, coalescence**
- **Damage localization**
- **Dislocation emission, nanovoid cavitation**
- **Vacancy clustering, nanovoid nucleation**
- **Ductile fracture**
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 \(\rightarrow\) decreasing formation energy
- Calculated diffusion barrier (E.A.Carter):
  - Barrier = 0.25-0.65eV
  - Open volume (tensile stress or grain boundary) \(\rightarrow\) low barrier
Vacancy clusters in Al – KMC

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

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

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First principles

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

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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

\[ p \text{ (GPa)} \]

\[ \varepsilon_v \text{ (%)} \]

1st yield point

\[ A - \frac{1}{2}\langle 110 \rangle \{111 \} \]

\[ B - \frac{1}{2}\langle 110 \rangle \{001 \} \]

2nd yield point

Cavitation

(J. Marian, J. Knap and M. Ortiz, PRL ’04)
Nanovoid cavitation in Al – Shear

Shear stress-strain curve

(1/6 (110) \{111\})

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.

Void growth and coalescence – level set

(A. Cuitiño and K. Dhruva, 2005)
Void growth – TODO list

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