Computational Modeling of Brittle Materials Under Dynamic Conditions

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Outline

• Experimental observations

• SCRAM and DCA (Dominant Crack Algorithm) Models:
  - Continuum-level models based on statistical consideration of defects.

• Calculations and data for explosives & ceramics

• Summary/discussions

Main Collaborators:
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Presented at 2012 Materials Science Symposium, UAH
December 5, 2012
Damage and Failure in Brittle Materials
(explosives, ceramics, propellants, concrete, sea ice, etc.)
Cracking in an Explosive (PBX 9501)

Heterogeneous:
HMX crystals & Polymer Binder

Distribution of HMX grains is random:
Bi-modal distribution (229/27.5 μm)

Microcracks in the “pristine” sample:
different sizes & orientations

size distribution of HMX Grains
(Bronkhorst et al.)

μ₁ = 27.5 μm
μ₂ = 229 μm

Data of Skidmore et al. (1997)
Dual Log-normal PDF

HMX Extracted

Processed, norm.
Model, norm.

Normalized Volume Fraction
Particle Size, microns

Disk of explosive after impact
Idar et al, 1998

Radial Cracks

Circumferential Cracks

Target 8
Ceramic Armor under Ballistic Impact

- **Ceramic** disk: Coors AD 995 (1/2” thick, 4 in diameter)

- Casing (3 pieces): Ti-6Al-4V
  2 cover plates (1/4 ” thick each)
  Ring (5” diameter, ½ ” thick)

- Impactor: Lexan rod
  1.5” long , ¾ ” diameter

- Impact velocity: 1.56 km/s

Can we predict the *location and size of the failed ceramic*?

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[Bingert et al](#)
Computational Modeling
Challenges

- Events taking place at length scales below the grid resolution can have significant effects on the damage and failure

- Challenges:
  - how far do we need to go down in scales (meso/micro scales?)
  - What about the history of defects?
  - How do we connect the mechanics/physics of different scales? (e.g., grain-level mechanics)
  - What about convergence and stability of the numerical solution (i.e., ill-posedness/Hadamard instability)?
Models based on statistical consideration of defects (cracks)

- SCRAM
- DCA
Superposition of Strain Rates

Defects idealized in the model

Difference in velocity

$$\Delta u \equiv u^2 - u^1 = \sum \Delta u^c + \sum \Delta u^d$$

Statistical averaging
(probability density function)

Total Stretch
(rate of deformation)
$$d = d_m + d_c + d_g + d_p$$

Matrix
Crack
Plastic
Crack growth
**SCRAM**: Model for damage, failure and initiation of brittle materials
Impact Initiation Scenario

Shock wave activates shear cracks.

Shear cracks grow easily in HMX, inhibited by binder.

Shear cracks grind and produce heat.

Heat conducted away from sliding interface; temperature rise causes cooking of HMX. \[ \dot{T} = DT_{xx} + qZe^{-E/kT} \]

HMX reaches ignition point (Linan & Williams or IGNC) \[ T > T_c \]

Burned gases open cracks, create initial high-pressure zone. Opening inhibited by inertia, stiffness, and damping.

\[ m \ddot{w} + c \dot{w} + k w = pA \quad p = f(M,T) \]

Burning increases general pressure, accelerating burn in adjoining hot spots.

Cracks coalesce when percolation threshold is exceeded, causing general explosion.
Dominant Crack Algorithm (DCA) Model (Zuo et al., 2006-)

- **Damage surface** is derived from the instability condition for the critical crack orientation;

- **New damage surface** has similar features to that in ISOSCM, but **removes a discontinuity** existed in ISOSCM;

- **Crack opening strain** is more consistent with physics-- only the **tensile** principal stresses contribute to the crack opening strain. Material response can be anisotropic.

- **Damage evolution** (growth rate of the mean crack radius) is given by the energy release rate for the crack along the **critical** (most unstable) orientation.

- Including a **nonlinear EOS** and porosity growth.

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Crack strain (damage)

Total strain is the sum of matrix strain and crack strain:

\[ \varepsilon = \varepsilon_m(\sigma) + \varepsilon_c(\sigma, \overline{c}) \]

Matrix strain:

\[ \varepsilon_m(\sigma) = C^m \sigma \quad C^m = \text{Matrix Compliance} \]

Crack strain:

\[ \varepsilon_c(\sigma, \overline{c}) = \sum_{\Omega_c} \Delta \varepsilon_c(\sigma, c, n) \]

For a crack set:

\[ \Delta \varepsilon_c(\sigma, c, n) = \beta c^3 \left( c^o + c^s \right) \sigma n(c, n, t) \Delta c \Delta \Omega \]

\[ n(c, n, t) : \text{crack number density dist.} \]

Fabric tensors:

\[ c^o = b - \nu a \quad c^s = b - 2a \]

\[ a = n \otimes n \otimes n \otimes n \quad b = \mathbf{i} \wedge n \otimes n + n \otimes n \wedge \mathbf{i} \]

Material damage:

\[ \varepsilon_c(\sigma, \overline{c}) = D\sigma = \left( C^o + C^s \right) \sigma \]

\[ C^o = (2 - \nu) \beta \int_\Omega \int_c n(c, n, t) c^o c^3 dcd\Omega \quad \text{open cracks} \]

\[ C^s = \beta \int_\Omega \int_c n(c, n, t) c^s c^3 dcd\Omega \quad \text{shear cracks} \]
Model calculations and data
(explosives & ceramics)
Comparison of the Stress-Strain Responses with Data

PBX (Plastic-Bonded eXplosive) 9501 at two strain rates (0.01/s and 1000/s)

Uniaxial (stress) Compression

Model captures the data, including peak stress, failure strain, and strain softening
Comparison with the Multiple-shock Experiment

- Experiment by Mulford et al. of LANL

- Composite Impactor: Vistal (Al₂O₃) and Plexiglas (Kel-F);

- Plate thicknesses (mm):
  11 (Vistal), 0.8 (Kel-F), 10 (HE);

- Impact velocity: 911 m/s

Calculated particle velocity histories agree with data reasonably well.
- Model calculation matches the **deformed profile**

- Calculated location of **failure** (maximum porosity) agrees with the post-mortem observation
Uniaxial Strain – Cyclic loading
Tension/Compression- I

Stress-strain

Evolution of crack size
Crack growth under *Uniaxial* strain compression

- Cracks becomes *unstable* when shear overcomes friction;
- Damage accumulates over a period;
- Stabilized as friction (pressure) takes over
Rate Effects

Uniaxial strain loading

Stress

$\sigma_{11}$ (Mbar)

strain

$\varepsilon_{11}$

rate

$10^5 / s$

$5 \times 10^4 / s$

$10^4 / s$

$\sim 10^3 / s$

$10^2 / s$
Summary/Discussions

• SCRAM: three-dimensional framework for anisotropic damage & failure of brittle materials. It also models the initiation of chemical reactions (explosion) of energetic materials.

• DCA: based on SCRAM model but is significantly simpler. It emphasizes on the growth of dominate (critical) crack. No chemical reactions.

• Many challenges exists both in fundamental understanding of the response of brittle materials under high rate conditions and in the representation in analysis (continuum-level) codes.
Extra: Supporting Modeling
ISO-SCM Model (Addessio-Johnson)

• A continuum damage model based on Dienes’ SCM work.

• Key assumptions/limitations: distribution of cracks remain isotropic. Damage is also isotropic.

• The size distribution remains exponential (Seaman et al, SRI), with the mean crack size (damage) evolving with loading.

• Simple damage surface based on averaging the instability conditions over all crack orientations. Damage surface is discontinuous at p=0.

• The crack strain is a simple function of stress and mean crack size. Crack opening strain accounted for p<0 (tension) only.
Crack Shear and Opening

- **Exponential crack size** (radius) distribution (Seaman et al, SRI):

\[
n(c, n, t) = \frac{N_0(n)}{\bar{c}(n, t)} \exp\left(-\frac{c}{\bar{c}(n, t)}\right)
\]

\[N_0(n) = N_0 \text{ Initial crack number density (# per unit vol.); isotropic}\]

\[\bar{c}(n, t) : \text{ Average radius of the cracks with normal (n)}\]

- **SCRAM** accounts for material **anisotropy** by allowing each direction has its own mean size: \(\bar{c}(n, t)\) depends on the crack normal (n)

- **ISO-SCM** (Visco-Scram, etc): the cracks remain **isotropic**:

\[\bar{c}(n, t) = \bar{c}\]

**Crack shear strain:**

\[\varepsilon_c^s(\sigma, \bar{c}) = \beta_1 d(\bar{c})\sigma^d\]

**Crack opening strain:**

\[\varepsilon_c^o(\sigma, \bar{c}) = (2 - \nu)\beta_1 d(\bar{c})\left(\sigma - \frac{3}{2} p i\right)\]

- For any \(p\)

- For \(p < 0\)

- For \(p \geq 0\)

\[\beta_1 = \frac{64(1 - \nu)}{5G(2 - \nu)}; \quad d(\bar{c}) \equiv N_0 \bar{c}^3 \text{-damage}\]
**Dominant Crack Model (DCA)**

- Crack Opening strain

**Mixed stress states:** \( \sigma_1 > 0; \sigma_3 < 0 \)

**Only the directions with** \( \sigma_n = n \cdot \sigma n > 0 \) **should contribute**

**ISO-SCM:**

\[
p = -\frac{\sigma_1 + \sigma_2 + \sigma_3}{3}
\]

\( p < 0, \quad \text{All directions contribute} \)

\( p \geq 0, \quad \text{No direction contributes} \)

**“Improved”:**

\[
\varepsilon_c^o (\sigma, \sigma_c) = 2 \beta_1 D(\sigma_c) \left( \sigma + \frac{1}{2} \text{tr}(\sigma) i \right)
\]

**Projection operators:**

\[
P^{sp} = \frac{1}{3} i \otimes i \quad P^d = I - P^{sp} \quad P^+ \equiv Q^+ \wedge Q^+
\]

**Positive spectral tensor:**

\[
Q^+ \equiv \sum_{i=1,3} H[\sigma_i] e_i \otimes e_i \quad \sigma_1 > \sigma_3 > 0
\]

\[
0 > \sigma_1 > \sigma_3 \quad \square \text{ISO-SCM!}
\]

**Only tensile principal stresses contribute to open strain**
Comparison of the Damage Surfaces

\[ F(\sigma, c) \equiv g(\sigma, n^c, c) / 2\gamma - 1 \Rightarrow \]

New damage surface is similar to that in ISO-SCM, but it is continuous.
Evolution equation for damage (Crack growth rate)

\[
\text{Dam. Surf. } F(\sigma, \bar{c}) = 0
\]

Damage increases for stress state outside the surface \((F(\sigma, \bar{c}) > 0)\):

Dynamic crack growth (Freund, 1990):

\[
\dot{c} = \dot{c}_{\text{max}} \left(1 - \frac{2\gamma}{g(\sigma, n^c, \bar{c})}\right)
\]

\(\dot{c}_{\text{max}}\): Terminal growth speed
(Rayleigh wave speed)

Damage function is also based on \(g(\sigma, n^c, \bar{c})\):

\[
F(\sigma, \bar{c}) \equiv \frac{g(\sigma, n^c, \bar{c})}{2\gamma} - 1
\]

Crack growth is related to the damage function:

\[
\dot{c} = \dot{c}_{\text{max}} \left(1 - \frac{1}{1 + \langle F(\sigma, \bar{c}) \rangle}\right)
\]

\(\bullet F(\sigma, \bar{c}) > 0 \Rightarrow \dot{c} > 0\)

\(\circ F(\sigma, \bar{c}) \leq 0\)

inelastic

elastic
Stress-strain Relationship

Given a total (applied) strain rate, we need to update stress and damage.

Recall:
\[
\varepsilon = \left( C^m + D(\bar{c}) \right) \sigma
\]

Damage:
\[
D(\bar{c}) = \beta^e N_0 \bar{c}^3 \left( \frac{3}{2 - \nu} P^d + P^+ \left( P^d + \frac{5}{2} P^{sp} \right) P^+ \right)
\]

Rate form:
\[
\dot{\varepsilon} = C^m \dot{\sigma} + \left[ D(\bar{c}) \dot{\sigma} + \dot{D}(\bar{c}) \sigma \right] = C^m \dot{\sigma} + \left[ \dot{\varepsilon}^c + \dot{\varepsilon}^{gr} \right] \tag{1}
\]

strain rate due to crack growth:
\[
\dot{\varepsilon}^{gr} = \dot{D}(\bar{c}) \sigma = \left( 3 \dot{\bar{c}} / \bar{c} \right) D(\bar{c}) \sigma
\]

Stress rate:
\[
\dot{\sigma} = -\dot{P} i + \dot{s}
\]

Deviatoric rate:
\[
P^d \text{ Eq.(1)} \Rightarrow \frac{1}{2G_s} \dot{s} + P^d D(\bar{c}) \left( \dot{s} - \dot{P} i \right) + \dot{\bar{c}} \frac{3}{\bar{c}} P^d D(\bar{c}) \left( s - \dot{P} i \right) = \dot{\varepsilon} \tag{2a}
\]

Degonis, L.E. and Q.H. Zuo (2011), JAP, 109, 073504
Volumetric Response

Pressure in the porous (voided) material

\[ P(\phi, \rho, e) = (1 - \phi)P_s(\rho_s, e_s) \]

The porosity:

\[ \phi = \frac{V_v}{V_s + V_v} \]

Pressure in the solid:

\[ P_s(\rho_s, e_s) = P_H(\mu_s) \left( 1 - \frac{1}{2} \Gamma_s \mu_s \right) + \Gamma_s \rho_s e_s \]

Hugoniot Pressure:

\[ P_H(\mu_s) = c_v \mu_s + d_v \mu_s^2 + s_v \mu_s^3 \]

Compression ratio:

\[ \mu_s = \frac{\rho_s}{\rho_{s0}} - 1 \quad \text{Nonlinear effect} \]

Porosity evolution:

\[ \dot{\phi} = (1 - \phi) \left( \dot{\varepsilon}_{kk}^c + \dot{\varepsilon}_{kk}^{gr} \right) \]

Rate form:

\[ \dot{P}(\phi, \rho, e) = -B\dot{\varepsilon}_{kk} + \alpha \left( \dot{\varepsilon}_{kk}^c + \dot{\varepsilon}_{kk}^{gr} \right) + \Gamma_s s : \dot{e} \quad (2b) \]

Mie-Gruneisen equation of state (Addessio and Johnson, 1990)

\[ (1 - \phi)(\phi - \phi^2) \]

TEPLA model:

\[ \dot{\phi} = (1 - \phi)\dot{\varepsilon}_{kk}^P \]

stationary
Vol. Tension/Compression

Load: ABC
Unload: CAD
Reload: DAC'E

Pressure-strain

Evolution of damage
Uniaxial (stress) tension and compression

Compression is much stronger than tension

\[ \frac{\sigma_c}{\sigma_t} = 2\sqrt{1 - \nu^2} \left( \sqrt{\mu^2 + 1 + \mu} \right) \]
The damage surface is continuous;

Size of the damage surface (in stress space) shrinks as cracks grow;

Stress path is above the damage surface, due to rate effects;

Pronounced strain softening right after the stress peak.
Cyclic loading - II

Cracks closing/reopening
Porosity growth

Evolution of porosity
Evolution of crack size
Large strain (10%) compression: *Hydrostatic* Loading

Cracks remain *stable* due to confinement:
No damage accumulation
Large strain compression: 
*Uniaxial* strain

\[ \sigma_{ij} \] (Mbar)

\[ \sigma_{11}, \sigma_{22} \]

DCA, DCA_NEOS

Nonlinear Terms

Why?
Multiphase Plasticity Model for Zirconium

The phase diagram of Zr

That the material experiences all three phases can have important implications...