ANALYTICAL MODEL DEVELOPMENT RELATED TO MECHANICAL DEFORMATION AND INITIATION OF PBXs

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Introduction

- Goal: understanding of mechanical deformation and initiation of PBXs below shock initiation threshold
- Secondary goal: understanding the role of crystal quality

- Example of mechanical deformation test
- Intra- and/or intergranular sliding friction
  - Intra ➔ model with shear rate dependence
  - Inter ➔ model with pressure, shear rate and duration dependence
    - Analytical model for thermo-chemical decomposition due to local heat flux is needed
    - Experiment and model of laser heating of metal covered materials

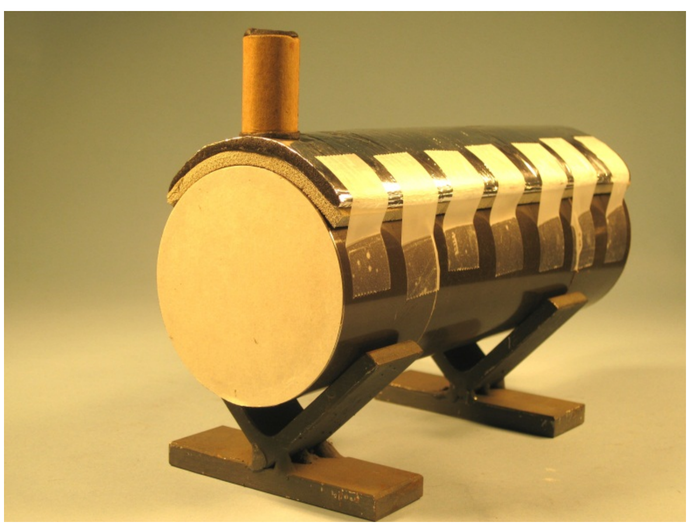
Deformation in energetic materials

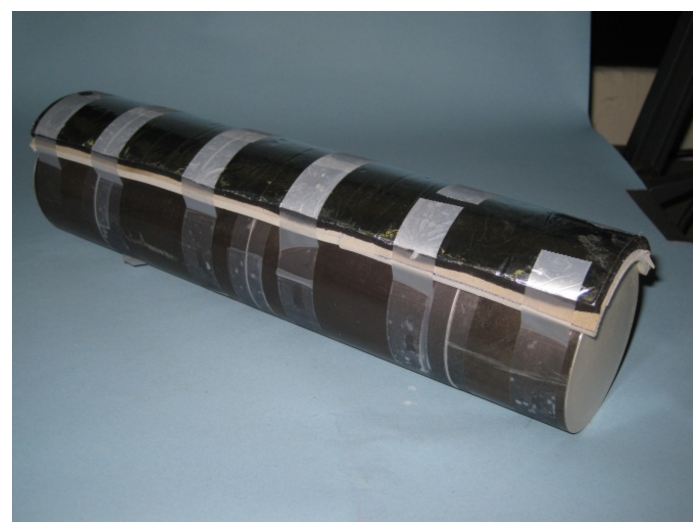
- Examples of deformation of energetic materials in munitions
  - Accidental deformation
  - Imposed deformation during functioning
  - Deformation required before functioning
  - Deformation-induced functioning

- Scales of deformation processes
  - Macro >> meso >> micro
  - Munition with energetic material >> plastic bonded explosive with particulate features >> crystal

Explosion-driven deformation

- From left to right:
  - 5 cm steel tube filled with sand
  - 10 cm steel tube filled with PBX
  - 5 cm steel tube filled with sand
  - Rubber + plastic explosive layer on full length to create deformation
    - Thickness plastic explosive layer is varied





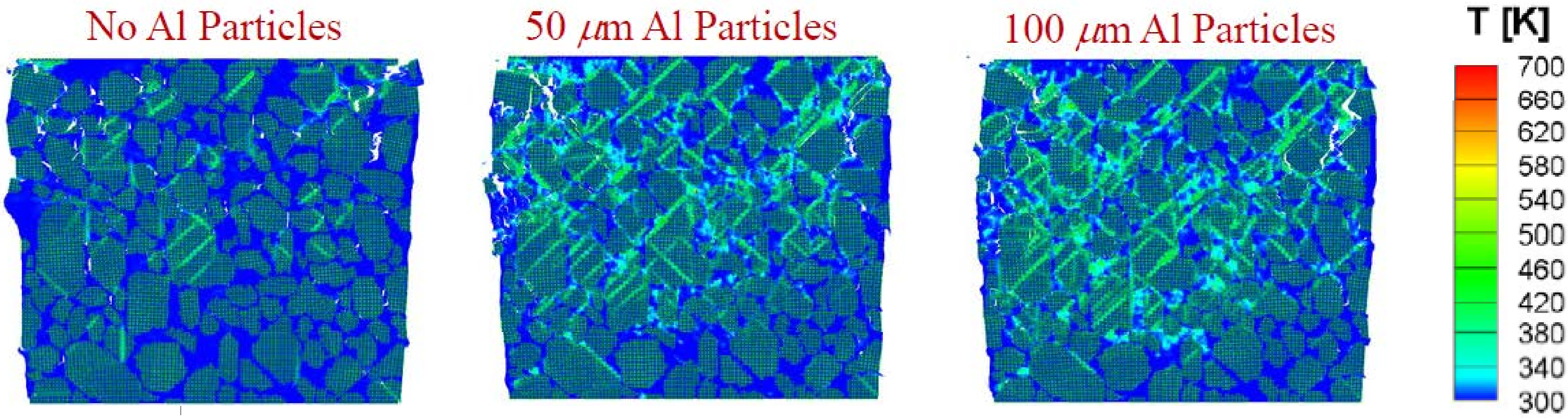
PBXN-109

- 3, 4 and 5 mm deformation charge

Meuken *et al.*, shear initiated reactions in energetic and reactive materials, 2006

Modeling of energetic materials at the meso-scale

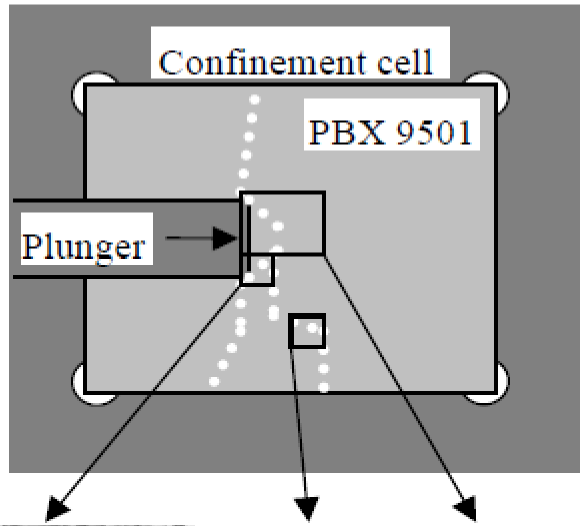
- 1) fit continuum model with particle-specific features to experimental data
- 2) simulate representative volume element and determine collective mechanical behaviour
- 3) simulate the mechanical behaviour with spatially resolved explosive grains and binder



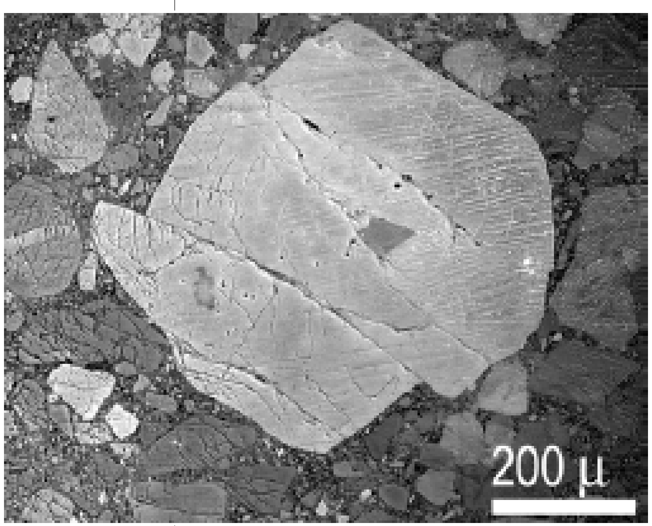
$(\eta_{Al} = 0.1,\ \eta_{HMX} = 0.64,\ T_i = 300\ K,\ v = 150\ m/s,\ \varepsilon = 0.1,\ \dot{\varepsilon} = 50\times10^3\ s^{-1})$

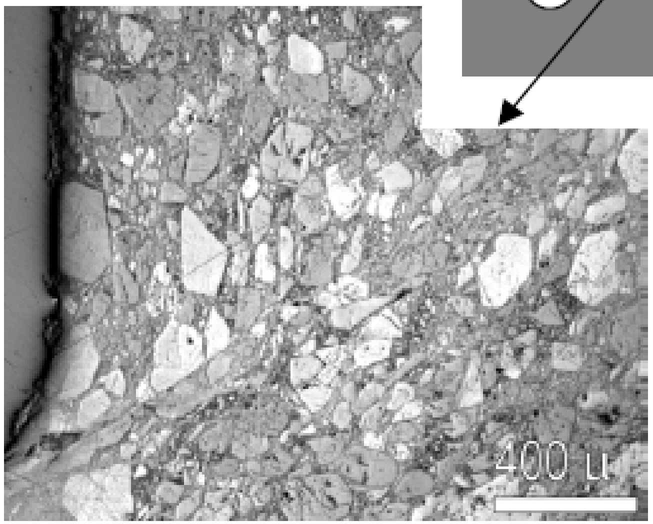
Zhou *et al*., a Langrangian framework for analyzing fracture and heating of PBXs under impact loading, 2011

Intra- and intergranular sliding friction sensitivity



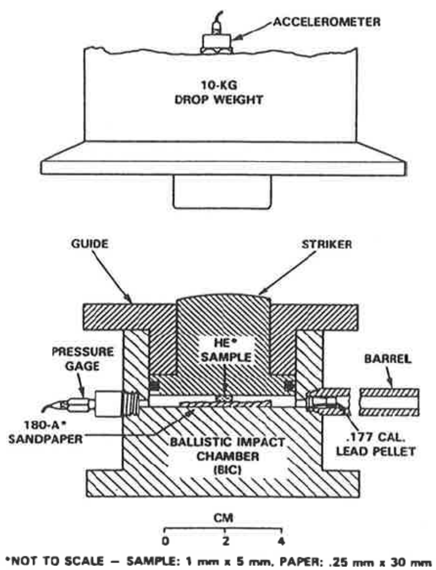
Skidmore *et al.*, Microstructural effects in PBX9501 damaged by shear impact, 1999





Intragranular sliding friction
Ballistic Impact Chamber

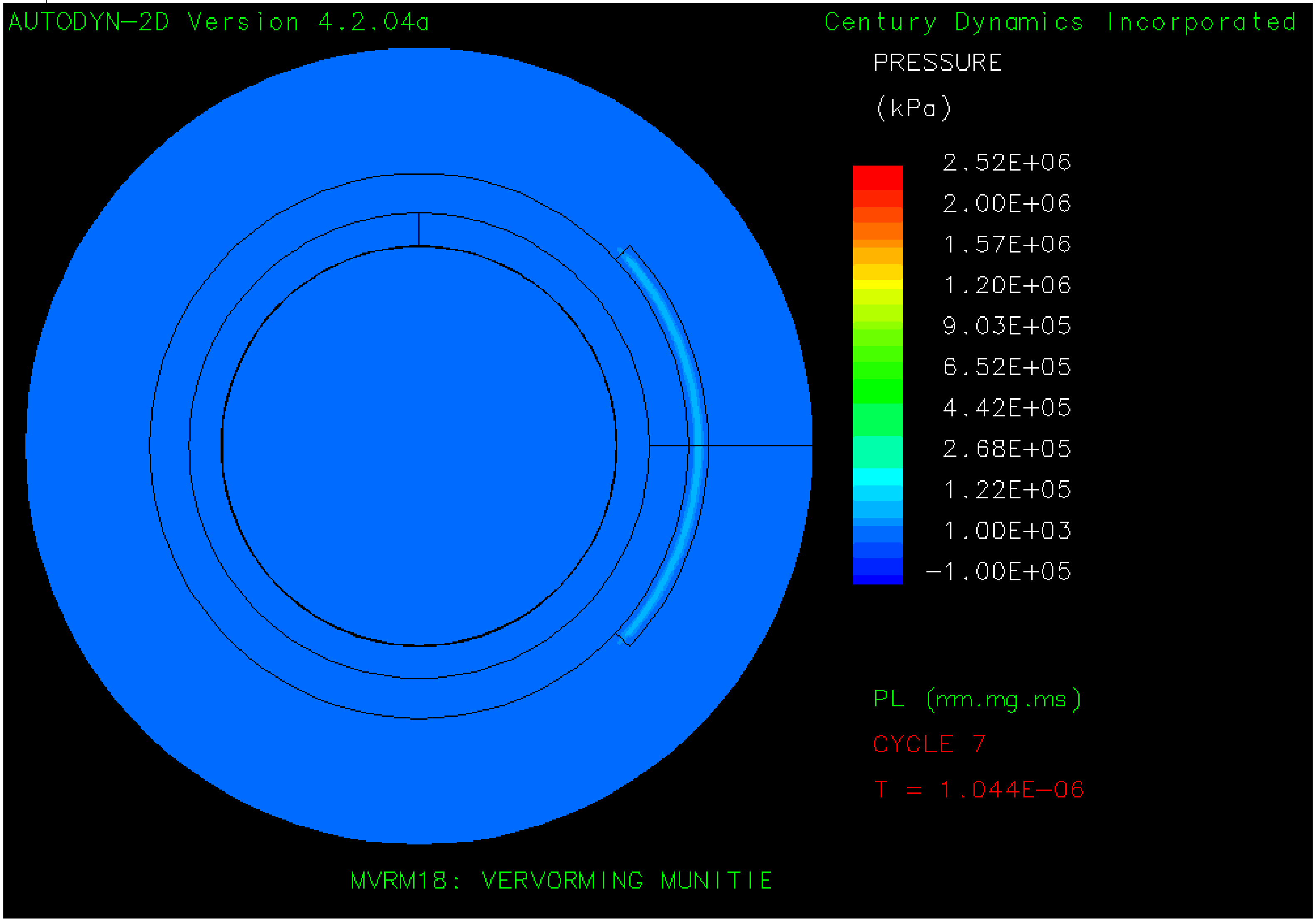
- Background is 1) relation between rate of energy dissipation and rate of plastic deformation of **deforming crystal**, and 2) determined deformation rates at initiation.
- Experiment is attempt to measure plastic deformation rate at initiation site at moment of initiation of polymer and explosive crystal compound.
- Namkung *et al*., Plastic deformation rate and initiation of crystalline explosives, 2002



HMX(125 μ)	$.7 \times 10^4$
HMX(5 μ)	$.8 \times 10^4$
HMX(5 μ, calculated)	1×10^4
RDX(calculated)	1×10^4
IH-H7-D	2×10^4
IH-H7-D2	2×10^4
IH-H7-F	7×10^4
Comp B	7×10^4
TNT	$> 2 \times 10^5$
TNT(calculated)	2×10^5
PBXN-109(heated)	1.4×10^5
PBXN-109	1.7×10^5
PBXW-128	2×10^5
TATB(calculated)	$> 2 \times 10^5$
PBX-9502	$> 3 \times 10^5$
Detonation (All Materials, calculated)	a few times 10^6

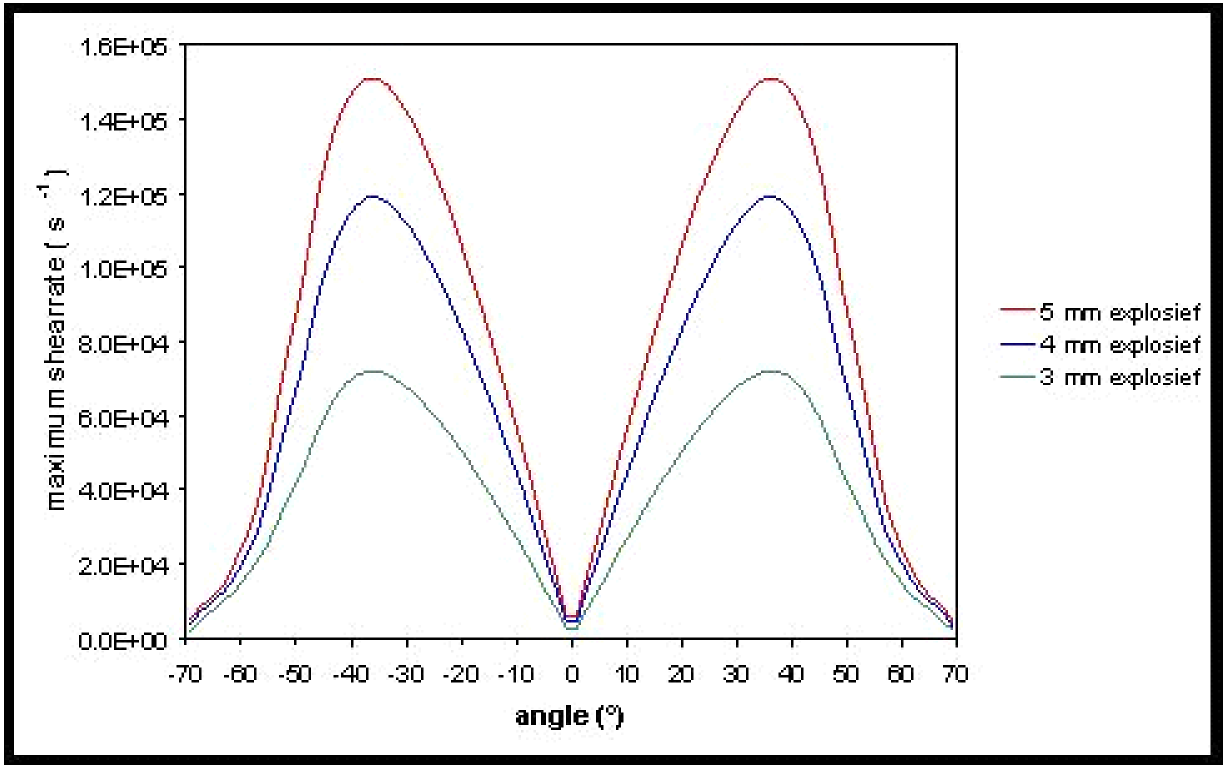
PBXN-109

- 3, 4 and 5 mm deformation charge

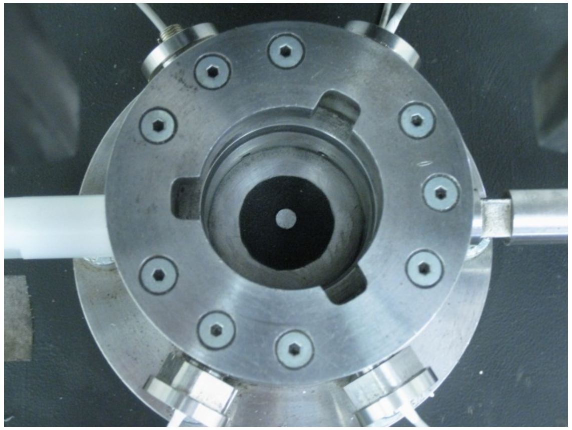

AUTODYN-2D Version 4.2.04a
Century Dynamics Incorporated
PRESSURE
(kPa)
2.52E+06
2.00E+06
1.57E+06
1.20E+06
9.03E+05
6.52E+05
4.42E+05
2.68E+05
1.22E+05
1.00E+03
-1.00E+05
PL (mm.mg.ms)
CYCLE 7
T = 1.044E-06
MVRM18: VERVORMING MUNITIE

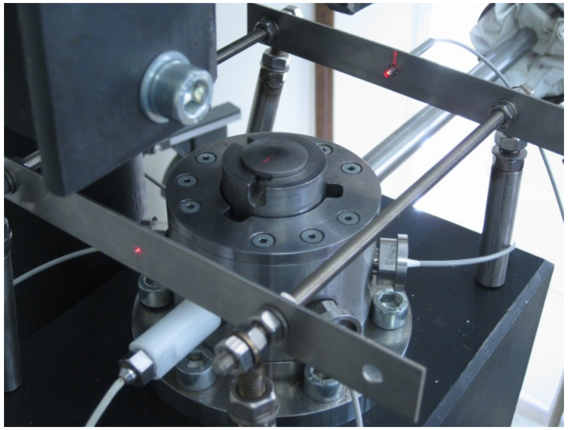
PBXN-109, maximum shear rate

- 3 mm, 7.2 10^4 s^{-1}
- 4 mm, 1.19 10^5 s^{-1}
- 5 mm, 1.51 10^5 s^{-1}

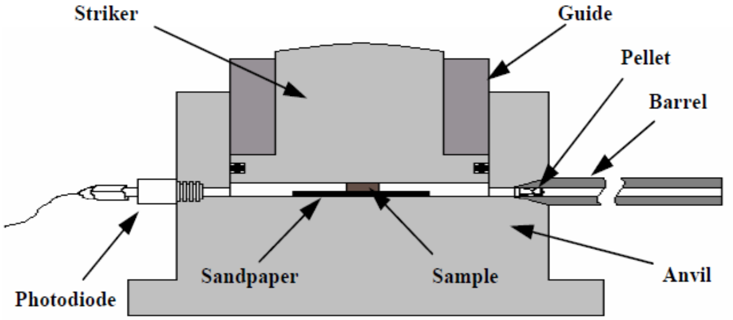


BIC





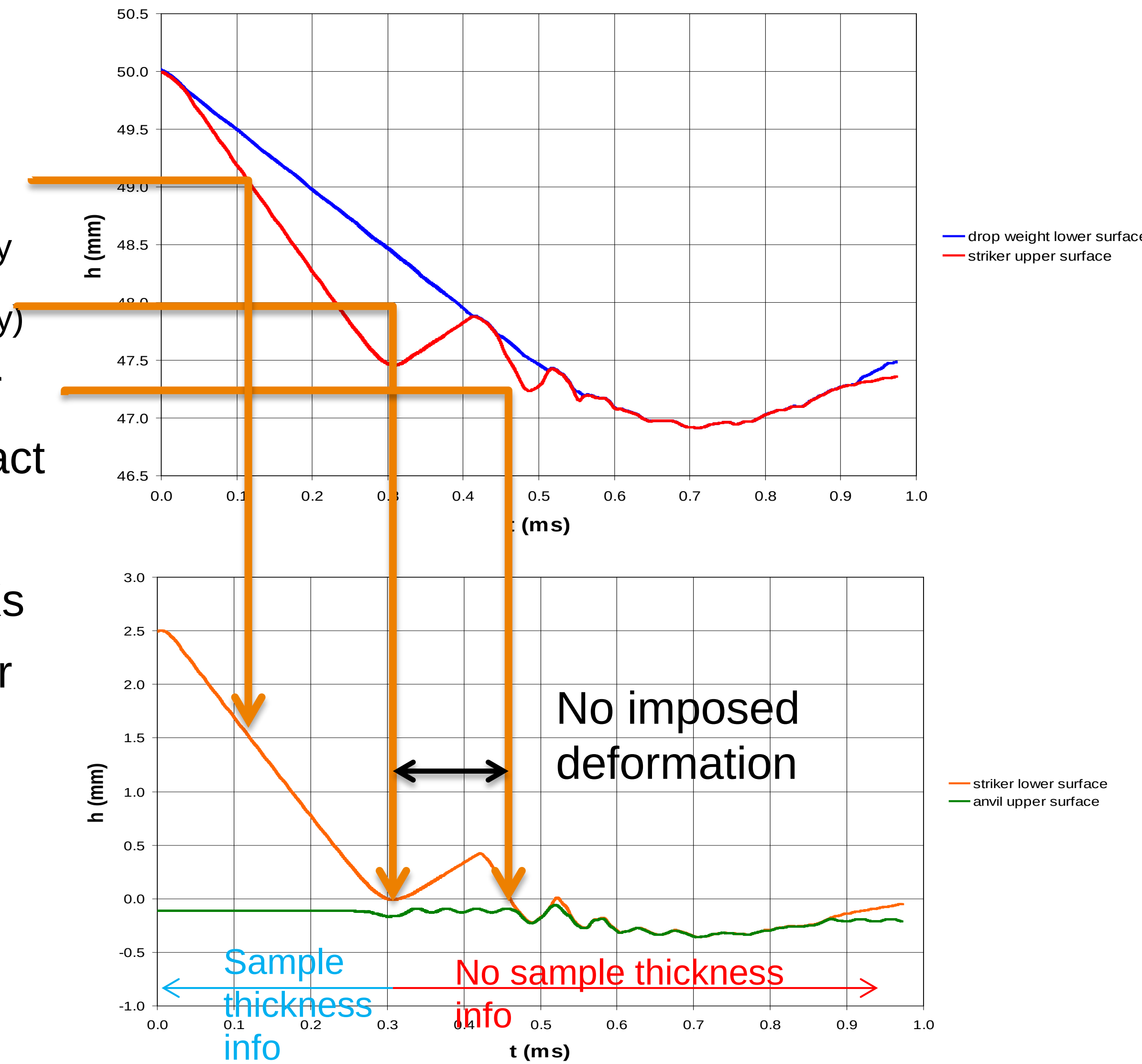
$$\frac{d\gamma}{dt} \approx \frac{r_0}{h^2}\sqrt{\frac{h_0}{h}}\,\frac{dh}{dt}$$

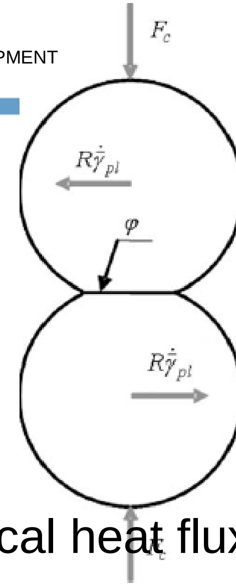


Compression sequence

- Primary compression by striker (equation by Namkung and Coffey)
- Rebound striker
- Secondary impact

- Initiation in PBXs often noted after primary compression

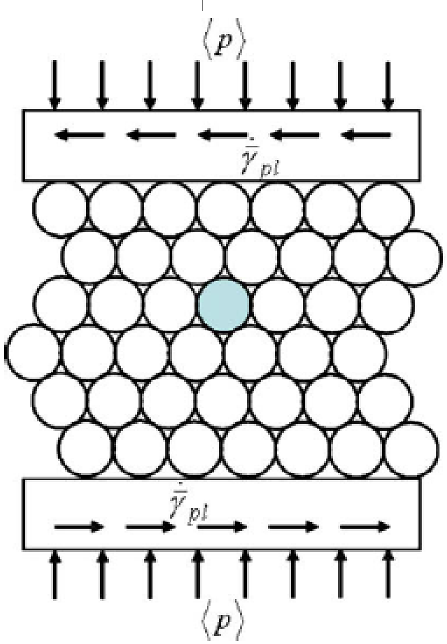


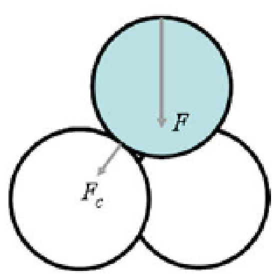


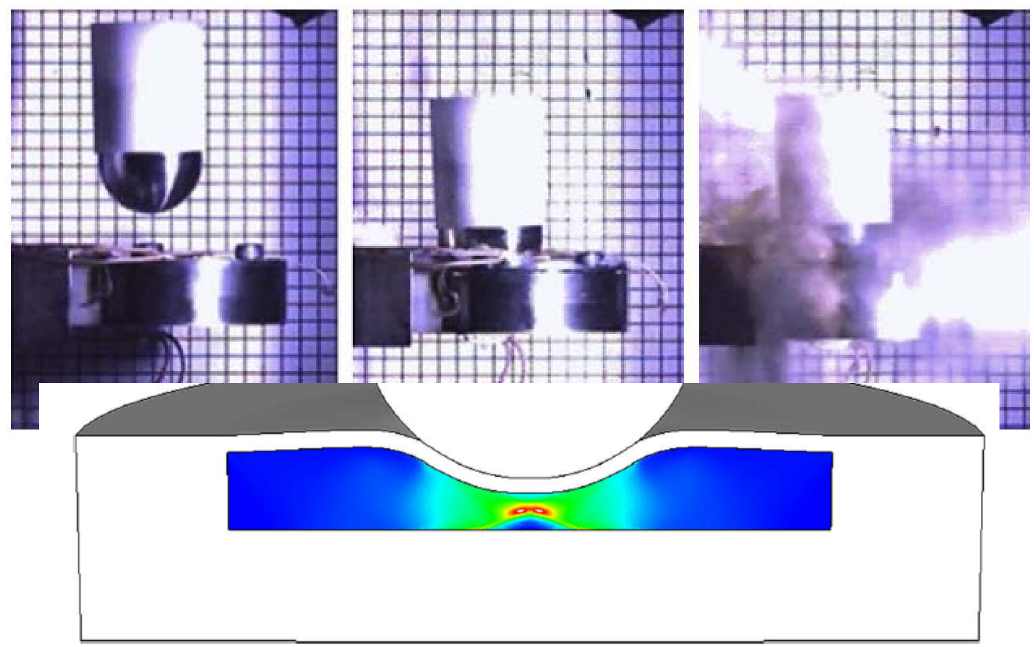
Intergranular sliding friction
Friction between particles

- 1) Hertz contact stress
- 2) Work due to sliding motion
- 3) Thermo-chemical decomposition due to local heat flux

Browning, microstructural model of mechanical initiation of energetic materials, 1995
Gruau *et al*., ignition of a confined high explosive under low velocity impact, 2009







Intergranular sliding friction
Browning model

- 1) Hertz contact stress ➔ analytical
- 2) Work due to sliding motion ➔ analytical
- 3) Thermo-chemical decomposition due to local heat flux ➔ numerical

  - Today: only model for HMX-PBX and applied to Steven impact test

- Typical outcome of modelling effort is a threshold that demonstrates influence of pressure, shear rate and duration, e.g. $p^{2/3}\left(\frac{d\gamma}{dt}\right)_{max}^{1.27} t_{ign}^{1/4}$

- An analytical model for thermo-chemical decomposition due to a local heat flux is needed for wider applicability

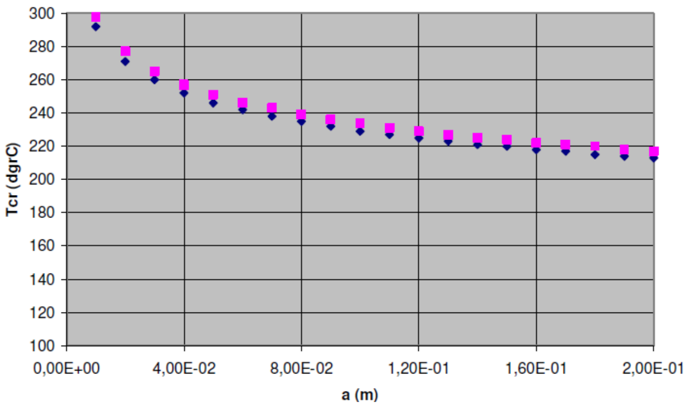
Local heat flux – initiation of energetic materials

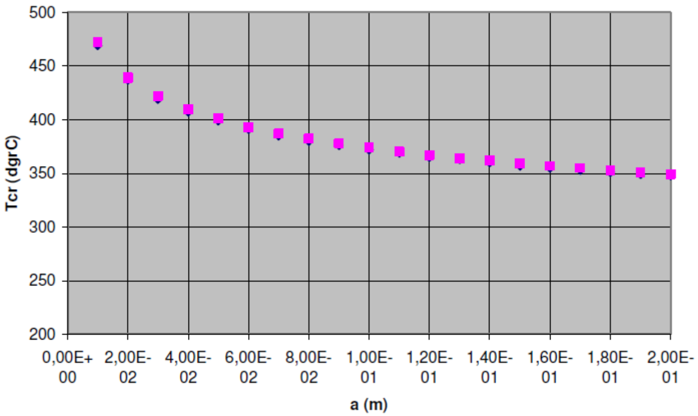
- Thermal explosion where thermal diffusion within explosive is rate limiting step
  - Frank-Kamenetskii, calculation of thermal explosion limits, 1939

$$\frac{E_a}{RT_{cr}} = \ln\left(\frac{a^2 \rho QZE_a}{\delta \lambda RT_{cr}^2}\right)$$

- Critical temperature applied locally to an explosive covered with a thin metal sheet, and
  - Rubencik, on the initiation of high explosives by laser radiation, 2007

$$\frac{E_a}{RT_{cr}} = \ln\left(\frac{2a^2 \rho QZR^2 T_{cr}}{\lambda E_a^2}\right)$$





- Infinite cylinder with TNT of radius a (left), laser illumination of TNT with spot of radius a (right)

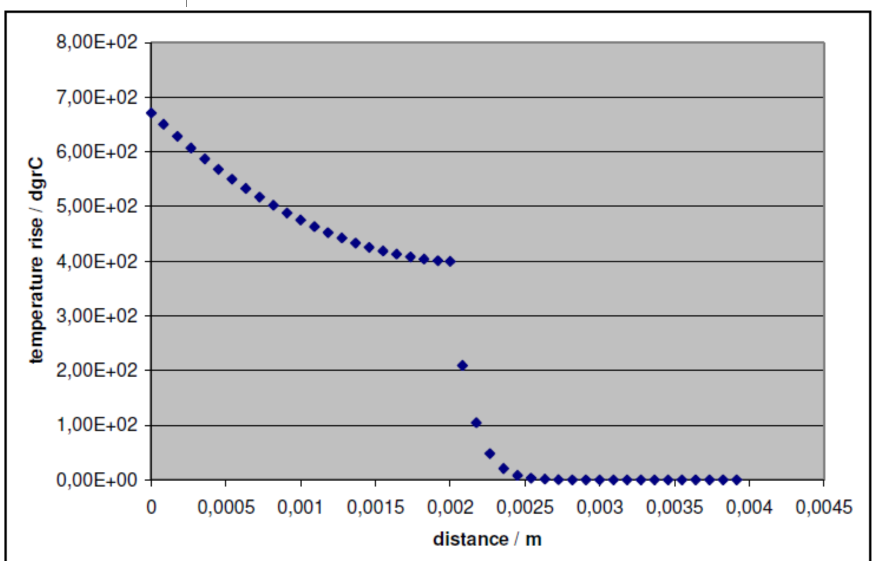
Richard Bouma
ANALYTICAL MODEL DEVELOPMENT

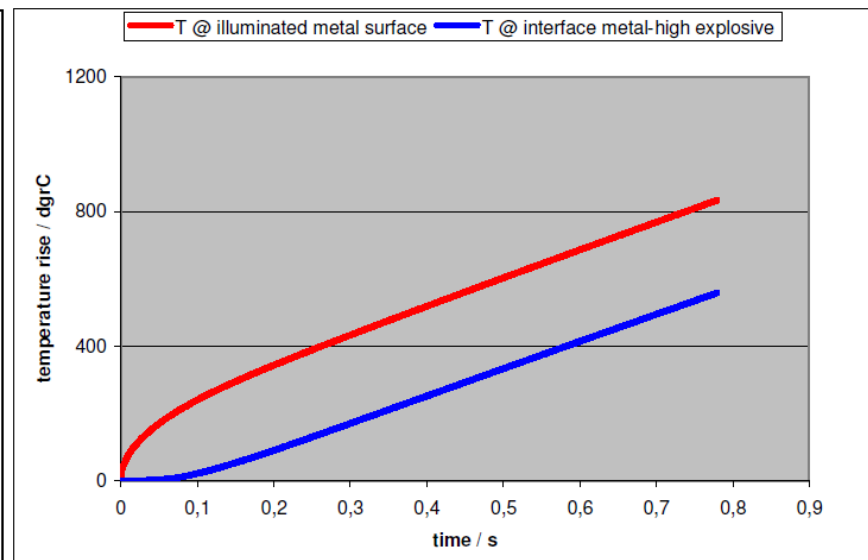
Local heat flux – laser initiation of munitions

- Time to ignition needs to be considered
- In laser initiation of munitions the approach by Rubencik *et al*. is to calculate required temperature rise ΔT, and then calculate the time-lag τ related to a finite casing thickness l (note that radius laser beam is neglected)

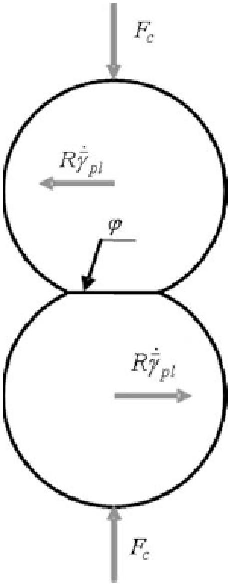
$$\tau = \frac{\rho c l \Delta T}{\alpha I} + \frac{l^2}{6D}$$

- Time lag equation is verified through numerical simulation
  - Stuivinga, future use of HE laser systems, 2011





Local heat flux



- Heat will diffuse laterally from contact area of two crystals, heat will also diffuse radially because of small dimension of contact area
- Hypothesis taking into account finite radius and thickness effects

$$\tau = \tau_1 + \frac{l^2}{6D} \qquad \tau_1 = \frac{\rho c l \Delta T}{\alpha l\left(1 - \exp\left(-\frac{a^2}{4D\tau_1}\right)\right)}$$

- αl is to be replaced by the rate at which work due to sliding friction is dissipated in Hertz contact area of radius a and which is function of normal pressure p
- Definition of thickness l is still a problem in crystal-crystal contact


Local heat flux with temperature measurement compared to model

- Experimental laser radiation onto 4 mm steel with PMMA backing
  - 100, 200, or 300 W and 10, 25 or 50 mm diameter spot
  - Thermocouples at steel/PMMA interface at 10 mm distances
  - 2D-calculations with one set of thermal properties reproduce all experimental data