
Ercan Gürses

California Institute of Technology

Graduate Aeronautical Laboratories

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1 Configurational Force Driven Brittle Fracture
   - Motivation and Overview
   - Variational Formulation of Brittle Crack Propagation
   - Algorithmic Treatment of Configurational Force Driven Fracture
   - Numerical Examples of Configurational Force Driven Fracture
Outline

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2. Evolution of Deformation Microstructures
   - Motivation and Overview
   - Incremental Variational Formulation of Inelasticity
   - Relaxation Theory and Microstructures
   - Single Crystal Plasticity
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   - Single Crystal Plasticity

3 Multiscale Modeling of High Energetic Materials
   - Motivation and Overview
   - Modeling at Polycrystal Level
   - Modeling at Single Crystal Level
   - Modeling at Microstructure Level
Motivation and Overview

What are Configurational Forces:

- Configurational forces are results of *inhomogeneities* in solids.
- Grain boundaries in polycrystals, phase boundaries in multiphase materials, cracks, voids and inclusions are all examples of inhomogeneities.

Grain boundaries

Dislocations

Phase boundaries

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http://www.tf.uni-kiel.de/matwis/amat/def_en/

Chu and James [1995]

Crack propagation  Gürses and Miehe [2008]
Motivation and Overview

What are Configurational Forces:

- **Physical forces** $f_{phy}$ perform work on variations in actual placement of material points

- **Configurational (material) forces** $f_{con}$ perform work on variations of material points in the reference configuration

  \[
  \delta W \bigg|_x = f_{phy} \cdot \delta x \quad \text{and} \quad \delta W \bigg|_x = f_{con} \cdot \delta X
  \]

- In other words, configurational forces define an energy release associated by a translation of the defect

  \[
  f_{phy} = \frac{\partial W}{\partial x} \bigg|_x \quad \text{and} \quad f_{con} = \frac{\partial W}{\partial X} \bigg|_x
  \]

- Forces can be considered as work conjugate variables to variations of particular displacements
Driving Forces for Dislocation Movement:

- A traction force $T_x$ is applied to top surface and bottom surface is kept fixed.
- An edge dislocation nucleates from left side and runs through the crystal.
- Top half of the crystal is displaced by the amount of Burgers vector $\mathbf{b} = [b_x \ 0 \ 0]$.
- Total work done by the surface traction is

$$W = b_x \cdot T_x$$
Driving Forces for Dislocation Movement:

- $W$ has to be equal to the work done by the dislocation driving force on the dislocation

$$W = L_x \cdot f_x L_z$$

where $f_x$ is the driving force per unit length of dislocation line

- Dislocation driving force is then obtained as

$$f_x = \frac{W}{L_x L_z} = \frac{b_x T_x}{L_x L_z} = b_x \sigma_{xy}$$

- This is the Peach-Koehler force acting at a point of dislocation line with tangent $\xi$

$$f = (\sigma \cdot b) \times \xi$$
The response of an elastic continuum $\mathcal{B} \subset \mathbb{R}^3$ with boundary $\partial\mathcal{B} = \partial\mathcal{B}_\varphi \cup \partial\mathcal{B}_t$ under quasi-static loading conditions parametrized by $t \in \mathcal{R}_+$ is governed by

- **Deformation Map of the Continuum**
  maps reference positions $X \in \mathcal{B}$ of material points onto their spatial positions $x \in S_t$

  $\varphi_t : \left\{ \begin{array}{l c l} \mathcal{B} & \rightarrow & S_t \\ X & \mapsto & x = \varphi_t(X) \end{array} \right.$

  with $F := \nabla \varphi_t(X)$ and $\det[F] > 0$

- **Variational Principle of Elastostatics**
  minimizes potential energy storage $E$ for a specific free Helmholtz energy density $\psi$

  $$E(\varphi_t) = \int_{\mathcal{B}} \psi(F) dV \rightarrow \text{Min!}$$

  for prescribed loading $\varphi_t = \bar{\varphi}_t$ on $\partial\mathcal{B}_\varphi$
Consider time-dependent parameterizations $\Xi_t$ and $\xi_t$ of the material and spatial configurations, governing the current deformation $\varphi_t$ and the energy $E_t(\varphi_t)$.

- **Material Configurational Map**
  maps initial positions $\theta \in \Omega$ of material points onto current material positions $X \in B_t$
  $\Xi_t : \begin{cases} \Omega \to B_t \\ \theta \mapsto X = X_t(\theta) \end{cases}$
  with $J_t := \nabla_\theta \Xi_t(\theta)$ and $\det[J_t] > 0$

- **Spatial Configurational Map**
  maps initial positions $\theta \in \Omega$ of material points onto current spatial positions $x \in S_t$
  $\xi_t : \begin{cases} \Omega \to S_t \\ \theta \mapsto x = \xi_t(\theta) \end{cases}$
  with $j_t := \nabla_\theta \xi_t(\theta)$ and $\det[j_t] > 0$
Variational Formulation of Brittle Crack Propagation

**Definition of Kinematic Objects**
as compositions of the time-dependent spatial and material configurational maps

\[ \varphi_t := \xi_t \circ \Xi_t^{-1}, \quad F_t := j_t \circ J_t^{-1}, \quad dV_t = \det[J_t]d\Omega \]

**Rates of Basic Kinematic Objects**
contain contributions form spatial and material configurational changes

\[ \frac{d}{dt} \varphi_t = \nu - F_t \cdot V, \quad \frac{d}{dt} F_t = \nabla \nu - F_t \cdot \nabla V, \quad \frac{d}{dt} dV_t = (I : \nabla V)dV_t \]

with admissible spatial and material velocity fields \( \nu \) and \( V \).
Energy $E_t(\varphi_t)$ depends on time-dependent material and spatial configurational maps $\Xi_t$ and $\xi_t$

- **Rate of Bulk Energy**
  - is governed simultaneously by local spatial and material stress powers
  
  \[
  \frac{d}{dt}E_t := \frac{d}{dt} \int_{B_t} \psi(F_t) dV_t = \int_{B_t} \{ P : \nabla v + \Sigma : \nabla V \} dV_t
  \]

- **Definition of Stress Tensors**
  - 1st PK stress $P$ and Eshelby stress $\Sigma$ drive spatial and material configurational changes

  \[
  P := \partial_{F_t} \psi(F_t) \quad \text{and} \quad \Sigma := \psi(F_t) I - F_t^T \partial_F \psi(F_t)
  \]
Global Dissipation Postulate
positive difference between external stress power and change of bulk energy storage

\[ \mathcal{D} := \mathcal{P} - \frac{d}{dt} E_t = \int_{\partial B} \mathbf{t} \cdot \mathbf{v} dA - \frac{d}{dt} \int_{\mathcal{B}_t} \psi(F_t) dV_t \geq 0 \]

for all admissible spatial and material configurational changes

\[ v \in \{v \mid v = \bar{v} \text{ on } \partial \mathcal{B}_\varphi\}, \quad V \in \{V \mid V = 0 \text{ on } \partial \mathcal{B}, \ V \cdot n = 0 \text{ on } \Gamma_t, \ V = \dot{a} \text{ on } \partial \Gamma_t\} \]

Conditions form Spatial Configurational Changes

\[ \text{Div } \mathbf{P} = 0 \text{ in } \mathcal{B}_t, \quad \mathbf{P} \cdot n = t \text{ on } \partial \mathcal{B} \quad \mathbf{P} \cdot n = 0 \text{ on } \Gamma_t^{-/+} \]

Conditions form Material Configurational Changes

\[ \text{Div } \mathbf{\Sigma} = 0 \text{ in } \mathcal{B}_t \]
**Reduced Global Dissipation Inequality**

\[ D = \int_{\partial \Gamma_t} g \cdot \dot{a} dL_t \geq 0 \quad \text{with} \quad g := \lim_{|c|\to 0} \int_c \Sigma \cdot n dS \]

**Constitutive Formulation of Crack Propagation**

Normality rule obtained from a principle of maximum dissipation yields

\[ \dot{a} = \dot{\gamma} \frac{g}{|g|} \quad \text{locally on} \quad \partial \Gamma \]

with discontinuous local evolution of the crack surface

\[ \dot{\gamma} \geq 0, \quad [ |g| - g_c ] \leq 0, \quad \dot{\gamma}[ |g| - g_c ] = 0 \]
Global Disipation Postulate
positive difference between external stress power and change of bulk energy storage

\[ D^h := P^h - \frac{d}{dt} E^h = \sum_{I=1}^{N_{node}} \left\{ [p_I + f_I] \cdot \mathbf{v}_I + g_I \cdot \mathbf{V}_I \right\} \geq 0 \]

with the discrete nodal forces at the node \( I \)

\[ p_I := \sum_{e=1}^{N_{elem}} \int_{\partial B^e} N^T_I t dA, \quad f_I := -\sum_{e=1}^{N_{elem}} \int_{B^e_{\Gamma_I}} B^T_I P dV, \quad g_I := -\sum_{e=1}^{N_{elem}} \int_{B^e_{\Gamma_I}} B^T_I \Sigma dV \]

has to be satisfied for any admissible spatial and material configurational changes \( \mathbf{v}_I, \mathbf{V}_I \)
Exploitation of the dissipation postulate in a sense of a Coleman method gives

- **Spatial Configurational Change:** Conditions of Equilibrium
  \[ f_I = 0 \text{ in } B^h_{\Gamma_I}, \quad f_I + p_I = 0 \text{ on } \partial B^h, \quad f_I = 0 \text{ on } \Gamma^h_I \]

- **Material Configurational Change:** Conditions for optimal mesh
  \[ g_I = 0 \text{ in } B^h_{\Gamma_I} \]

- **Reduced Dissipation Inequality:** Condition for Crack Propagation
  \[ D^h = \sum_{i \in \partial \Gamma^h_I} g_I \cdot \dot{a}_I \geq 0 \]
1. **Energy Minimization.** For frozen crack solve

\[ E_{n+1}^h = \int_{B_{\Gamma_{n+1}}} \psi(F_{n+1})dV \rightarrow \text{Min!} \quad \iff \quad f_I = 0 \quad \text{in} \quad B_{\Gamma_{n+1}}^h \]

2. **Global Fracture Criterion.** Find the maximum loaded node

\[ J = \arg\{ \max_{I=1...N_{\text{node}}} (|g_I|) \} \quad \text{If} \quad |g_J| < g_c \quad \text{EXIT.} \]

3. **Segment Reorientation.** Loop over the segments \( S = 1...n_{\text{seg}} \) emanating from \( J \) and find the critical segment \( S_{\text{cr}} \). Reorient it s.t. \( S_{\text{cr}} \) is aligned to the material force \( g_J \)

4. **Segment Release and Node Doubling.** Release \( S_{\text{cr}} \), double \( J \) and extend the crack

\[ \Delta a_J = h g_J / |g_J| \quad \text{Go to Step 1.} \]
Numerical Examples of 2-D Configurational Force Driven Fracture

Asymmetric Three Point Bending Test
Bittencourt et al. [96]

![Diagram of asymmetric three point bending test](image)

- The notch is parameterized by $a$ and $b$
- Geometry I: $a = 5.0$, $b = 1.5$
  - 3205 elements
- Geometry II: $a = 6.0$, $b = 1.0$
  - 3080 elements

Double Notched Specimen in Tension
Bouchard et al. [03]

![Diagram of double notched specimen in tension](image)

- Two symmetric notches and two holes
- Two separate cracks advance symmetrically
- 2394 elements
- 4170 elements
Numerical Examples of 2-D Configurational Force Driven Fracture

Comparison with Experiments  Bittencourt et al. [96], Miehe and Gürses [07]
Notch Geometry I with 2021, 3205, 4042 and 4912 elements

Notch Geometry II with 1664, 2652, 3080 and 4642 elements
Tension Test of Notched Specimen: Discretizations with 3738 and 3486 elements.
Two different boundary conditions are investigated by varying the spring constant $K$

- Boundary Condition I: $K = 0$ (no support) and II: $K = \infty$ (roller support)

Two different discretizations with 3448 and 5811 elements are considered

- **BC I** deformation crack surface
- **BC II** deformation crack surface
### Comparison of Crack Trajectories with Experiments

**BC I**  
3448 elements | 5811 elements | Experiment

![Front](image1)  ![Rear](image2)  ![Front](image3)  ![Rear](image4)

**BC II**  
3448 elements | 5811 elements | Experiment

![Front](image5)  ![Rear](image6)  ![Front](image7)  ![Rear](image8)
Numerical Examples of 3-D Configurational Force Driven Fracture

Torsion Test of Notched Prismatic Concrete Beam
Brokenshire [96], Gürses and Miehe [08]

- The notch with 45° to the longitudinal axis of the beam
- Formation of a crack surface with double curvature
- Two different discretizations with 4510 and 4943 elements are considered

Mesh I: 3D $x - y$  
Mesh II: 3D $x - y$
Numerical Examples of 3-D Configurational Force Driven Fracture

Comparison of Crack Trajectories with Experiments  Brokenshire [96]
Deformed mesh with 4510 elements (Deformation is 10 times magnified)

Experimental Pictures
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Motivation and Overview

What is a Microstructure?

- Microstructures are patterns that are observed in nature and possess length scales much smaller than characteristic macroscopic dimensions of the problem considered.

(i) Optical micrograph of the twin microstructures in biaxially loaded Cu-Al-Ni

(ii) Parallel wall structures and labyrinth formed in twins in fatigued polycrystalline copper

(iii) Light micrograph of microstructures in a polycrystalline ferroelectric ceramic
Motivation and Overview

Characteristic Features and Mathematical Realization of Microstructures

- Fine scale oscillatory patterns with some level of periodicity are observed
- Mathematical description of these microstructures by non-convex variational problems
- Non-existence of minimizers in these variational problems are associated with fine scale oscillatory infimizing sequences which are interpreted as microstructures

Consider a non-convex energy $W : \mathcal{R} \rightarrow \mathcal{R}$

$$W(\varepsilon) = (\varepsilon^2 - 1)^2 \geq 0 \quad \text{with} \quad \varepsilon = \frac{du}{dx}$$

and minimize the functional

$$E(u) = \int_0^1 (W(\varepsilon) + u^2) \, dx$$

For scalar problems: if $W(\varepsilon)$ is convex then there exists at least a minimizer of $E(u)$
Motivation and Overview

Non-Existence of Minimizers and Microstructures

- Both terms in $E(u)$ are non-negative and $\inf_u \{E(u)\} = 0$. However, the infimal energy will be never attained. One can form sequences $u_i$ such that
  \[ \varepsilon_i = \frac{du_i}{dx} = \pm 1 \text{ almost everywhere} \quad \text{and} \quad u_i(0) = u_i(1) = 0 \]

- Finer the oscillations smaller the functional, i.e. $\lim_{n \to \infty} E_n = 0$. There exists no solution!

\[ E_1 = 8.33 \times 10^{-2} \]
\[ E_2 = 6.94 \times 10^{-3} \]
\[ E_4 = 4.82 \times 10^{-5} \]
\[ E_8 = 2.33 \times 10^{-9} \]
Motivation and Overview

FEM simulations of a non-convex material with different meshes

Finite element computations of materials having non-convex energy storage functions yield

- very bad oscillatory convergence behavior, finer the mesh more difficult the convergence,
- non-smooth, strongly mesh-dependent and physically meaningless results

due to existence of several local minima.

**Remedy:** Relaxation methods based on construction of generalized convex envelopes and energy minimization.
Fundamental Equations for Standard-Dissipative Materials

- **Free Energy Function** $\psi$ yields stresses $P = \partial_F \psi(F, I)$
- **Dissipation Function** $\phi$ describes evolution $0 \in \partial_I \psi(F, I) + \partial_I \phi(\dot{I}, I)$

Incremental Variational Formulation for Standard-Dissipative Materials

- **Minimization Problem** defines minimizing path $W(F_{n+1}) = \inf_{I \in G} \int_{t_n}^{t_{n+1}} [\dot{\psi} + \phi] \, dt$
- **Quasi-hyperelastic Potential** $W$ yields stresses $P_{n+1} = \partial_F W(F_{n+1})$
Local Constitutive Minimization Problem of Standard Materials determines the current internal state of the material

\[ W(F_{n+1}) = \inf_{\mathcal{I} \in \mathcal{G}} \int_{t_n}^{t_{n+1}} \left\{ \dot{\psi} + \phi \right\} dt \quad \text{at given state } (F_n, \mathcal{I}_n) \]

Global Minimization Problem for Incremental BVPs of Standard Solids determines the current admissible deformation field of the solid

\[ I(\varphi_{n+1}^*) = \inf_{\varphi_{n+1} \in \mathcal{W}} \left\{ \int_{\mathcal{B}} W(F_{n+1}) dV - \Pi_{\text{ext}}(\varphi_{n+1}) \right\} \]
Incremental minimization formulation implies existence result for regular solutions of the time-discrete problem

- **Global Minimization Problem for Incremental BVPs of Standard Solids**
  determines the current admissible deformation field of the solid

\[
I(\varphi_{n+1}^*) = \inf_{\varphi_{n+1} \in \mathcal{W}} \left\{ \int_{\mathcal{B}} W(F_{n+1}) \, dV - \Pi_{\text{ext}}(\varphi_{n+1}) \right\}
\]

- **Main Theorem for Existence of Regular Minimizers of Incremental BVP**

\[
I(\varphi_{n+1}) \text{ s.w.l.s. } \iff W(F_{n+1}) \text{ quasiconvex + growth (coercivity) conditions}
\]
Energy Relaxation Theory and Microstructures

\[ \partial D \]

homogeneous deformation

\[ D \]

arbitrary fluctuation

\[ F^- \]

rank-1 fluctuation

**Quasiconvexity Condition** Morrey [1952]. For all \( w \) with support on \( \partial D \), the homogeneous deformation \( F_{n+1} \) provides an absolute minimizer of the incremental potential \( W \):

\[
W(F_{n+1}) \leq \inf_{w_{n+1} \in \mathcal{W}} \frac{1}{|D|} \int_D W(F_{n+1} + \nabla w_{n+1})dV
\]

**Rank-One Convexity Condition** For laminate deformations \( F^+ \) and \( F^- \), the homogeneous deformation \( F_{n+1} = \xi F^+ + (1 - \xi) F^- \) provides an absolute minimizer of potential \( W \):

\[
W(F_{n+1}) \leq \inf_{\xi,F^+,F^-} \{ \xi W(F^+) + (1 - \xi) W(F^-) \} \quad \text{with} \quad \text{rank}[F^+ - F^-] \leq 1
\]
Time-discrete incremental minimization problems determine developing microstructure of instable material at $t_{n+1}$ relative to given previous state at $t_n$ in two steps:

- **Local Minimization Problem of Relaxed Material Response**
  Quasiconvexification determines microstructural fluctuation field

  \[
  W_Q(F_{n+1}) = \inf_{w_{n+1} \in \mathcal{W}_w} \frac{1}{|D|} \int_D W(F_{n+1} + \nabla w_{n+1})dV \quad \text{at given} \quad (\phi_n; w_n)
  \]

- **Global Minimization Problem of Relaxed Standard Solid**
  determines the current admissible deformation field

  \[
  I_Q(\phi_{n+1}^*) = \inf_{\phi_{n+1} \in \mathcal{W}_\phi} \left\{ \int_B W_Q(F_{n+1})dV - \Pi_{ext}(\phi_{n+1}) \right\}
  \]
Energy Relaxation Theory and Microstructures

**Rank–One Convexification**

\[
W_{R_k}(F_{n+1}) = \inf_{\xi, F^+, F^-} \{ \xi W_{R_{k-1}}(F^+) + (1 - \xi) W_{R_{k-1}}(F^-) \}
\]

Construction of rank–one convex envelope with recursion formula. For level \( k = 1, 2, \ldots \) minimizing first–order laminate is determined.

\[
W_R(F_{n+1}) = \lim_{k \to \infty} W_{R_k}(F_{n+1})
\]

**Mechanical Interpretation**

Decomposition of unstable state \( F_{n+1} \) into laminates \( F^\pm, A^\pm, B^\pm, \ldots \) on levels \( k = 1, 2, \ldots \).

Determination of developing micro–phases which form sequential laminates.
Model Problem: Single Crystal Plasticity

Micro-Scale: Dislocation Movements
Plastic deformation through dislocations

Average slip is through Orowan-equation

\[ \dot{\gamma} = b \rho_d \dot{x} \quad \text{with} \quad \dot{x} = \frac{1}{n} \sum_{i=1}^{n} \dot{x}_i \]

Macro-Scale: Continuum Slip Theory
Multiplicative decomposition

\[ F = F^e F^p \quad \text{with} \quad F^p = I + \gamma^\alpha (S^\alpha \otimes T^\alpha) \]
Model Problem: Single Crystal Plasticity

IBVP Tension Test: Objectivity (Mesh-Invariance) of Load Displacement Curves
Considered discretizations 6x12, 8x16, 12x24, 16x32, 20x40

Non-Relaxed Analysis
without microstructures is non-objective

Relaxation Analysis
with microstructures is objective

Development of Microstructures
Model Problem: Single Crystal Plasticity

**Deformed Meshes**
Considered discretizations 6x12, 8x16, 12x24, 16x32, 20x40

**Non-Relaxed Analysis**
without Microstructures yields
Stiff Response

**Relaxation Analysis**
with Microstructures yields
Soft Response
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Motivation and Overview

What are High Energetic (HE) Materials?

- Class of materials with high amount of stored chemical energy that can be released by an external stimulus
  - thermal stimulus
  - mechanical stimulus in the form of a shock generated by an impact
- HE materials exist in an energetically metastable state, they do not undergo chemical decomposition unless sufficient energy is provided
- The decomposition is referred to as initiation or ignition
- Examples of HE materials: Explosives, Propellants and Pyrotechnics
- Explosives can be liquid or solid (single- and poly-crystals)
- Solid explosives are often produced in polycrystalline forms and called as polymer bonded explosives (PBX) which consist of molecular crystalline grains and inert polymer binder matrix
Motivation and Overview

Initiation of High Energy Materials

- HE materials initiate for an energy input much less than to heat bulk explosive
- Localized hot-spots are considered to cause detonation in HE materials
- Microscopic defects are thought to be a prime source for hot-spots
- Initiation of defect-free HE crystals are not very clear

- Inhomogeneous nature of plastic deformation at sub-grain level (microstructures with localized deformation) and heterogeneity of polycrystals could cause initiation

Cracks in pressed PBX 9501,
Borne et al. [05]
Multiscale Model of Initiation in HE Polycrystals

Microscale

Chemical decomposition in hot-spots

Optimal subgrain microstructures (relaxation)

Mesoscale

Single crystal plasticity of individual grains

Direct numerical simulation of polycrystal

Macroscale

Plate impact test of explosive polycrystal
Modeling at Polycrystal Level

Barycentric Subdivision

Coarse mesh → Refined mesh → Subdivision mesh → Subdivision dual

Bisection → Barycentric subdivision → Definition of the dual

Grain Boundary Area Minimization

Polycrystal Evolution
Modeling at Single Crystal Level

- Displacement gradient \( \beta = \nabla u \) is decomposed additively \( \beta = \beta^e + \beta^p \)
- Due to crystallographic nature of crystals \( \beta^p(\gamma) = \sum_{\alpha=1}^{N} \gamma^\alpha s^\alpha \otimes m^\alpha \)
- Slip Systems of body centered tetragonal PETN Single Crystals

<table>
<thead>
<tr>
<th>Slip System</th>
<th>I</th>
<th>II</th>
<th>III</th>
<th>IV</th>
<th>V</th>
<th>VI</th>
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<td>( \pm[1\bar{1}\bar{1}] )</td>
<td>( \pm[111] )</td>
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<td>(1\bar{1}0)</td>
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<td>(1\bar{1}0)</td>
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</tbody>
</table>
Modeling at Single Crystal Level

Variational Formulation, Relaxation and Microstructures

- The energy density has additive structure of elastic and plastic parts
  \[ A(\beta, \gamma) = W^e(\beta - \beta^p(\gamma)) + W^p(\gamma) \] with \( \gamma = \{\gamma^1, \gamma^2, \ldots \gamma^N\} \)
- Plastic parameters are condensed out by a local minimization
  \[ W(\beta) = \min_{\gamma \in \mathbb{R}^N} A(\beta, \gamma) \]
- \( W(\beta) \) is non-convex and ill-posed for FEM. Relaxation of \( W^p(\gamma) \) gives well-behaved softest average response
  \[ W^p_Q(\gamma) = \sum_{\alpha} \tau^\alpha_c |\gamma^\alpha| \]  
  Conti and Ortiz [05]

- Heterogeneous microstructures allow highly localized slip lines \( \Rightarrow \text{Hot-Spots} \)
Modeling at Microstructure Level

Construction of Optimal Microstructure

- Macroscopic deformation $\beta$ decomposes into first order laminates

$$\beta_1 = \beta^e + \sum_{\alpha=1}^{I-1} \gamma^\alpha s^\alpha \otimes m^\alpha \quad \text{and} \quad \beta_2 = \beta_1 + \frac{1}{\epsilon} \gamma^I s^I \otimes m^I$$

and second order laminates

$$\beta_3 = \beta^e + \sum_{\alpha=2}^{I-1} \gamma^\alpha s^\alpha \otimes m^\alpha + \frac{1}{\epsilon} \gamma^I s^I \otimes m^I \quad \text{and} \quad \beta_4 = \beta_3 + \frac{1}{\epsilon} \gamma^I s^I \otimes m^I$$

satisfying the rank one connectivity conditions

$$(1 - \epsilon)\beta_1 + \epsilon \beta_2 = \beta \quad \text{and} \quad (1 - \epsilon)\beta_3 + \epsilon \beta_4 = \beta_2$$
Thermal Softening and Chemical Decomposition Model

- Elastic constants $C_{ij}$ depend on temperature and vanish at melting temperature $\theta_{melt}$
  \[
  C_{ij}(\theta) = C_{ij}(\theta_0) \left[ \theta - \theta_{melt} \right] / \left[ \theta_0 - \theta_{melt} \right]
  \]

- CRSS values $\tau^\alpha_c$ depend on temperature, Stainier et al. [02]
  \[
  \tau^\alpha_c(\theta) = \tau^\alpha_c(0) \frac{k_B \theta}{G^\alpha} \text{asinh} \left( \xi^\alpha \exp \left( \frac{G^\alpha}{k_B \theta} \right) \right)
  \]

- Temperature of hot-spot is computed assuming adiabatic heating
  \[
  \Delta \theta_{hs} = \tau^\alpha \Delta \gamma^\alpha / \rho c_v
  \]

- Chemical reaction is modeled by an Arrhenius type depletion law
  \[
  \frac{d\lambda}{dt} = Z(1 - \lambda) \exp \left( - \frac{E}{R \theta_{hs}} \right)
  \]
Plate Impact Test of PETN Polycrystal

Flyer and PETN Plate

Computational Model

Polycrystal Model: Discretization and Grains

- 817 grains with maximum grain size of 0.1 mm
- Impact velocities in the range of 500 - 800 m/s
- Simulation of total 0.3 \( \mu s \) with \( \Delta t = 1 \times 10^{-4} \mu \text{sec} \)
Plate Impact Test of PETN Polycrystal

- Simulation results for \( v = 700 \text{m/s} \)

Axial Velocity

Surface Temperature

Temperature Threshold

Temperature MRI
Plate Impact Test of PETN Polycrystal

Microstructure Evolution

Temperature and Chemical Reaction in a Hot-Spot

Aspects of Energy Minimization in Solid Mechanics

Graduate Aeronautical Laboratories
Plate Impact Test of PETN Polycrystal

- Hot-spots based on minimum temperature criterion

Surface temperature for different impact velocities

Aspects of Energy Minimization in Solid Mechanics  Ercan Gürses  Graduate Aeronautical Laboratories
Plate Impact Test of PETN Polycrystal

- Comparison with experiments, impact pressure vs. distance to detonation

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Pop-plots for several HE materials, *Sheffield and Engelke [09]*

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Number of hot-spots vs impact velocity
Collaborations and Future Plans

• Computational homogenization techniques for fracture and delamination in composites
  Joint work together with M. Birkle and C. Miehe (University of Stuttgart)

• Multiscale material modeling and scale bridging techniques
  Joint work together with C. Miehe (University of Stuttgart)

• Fracture and fragmentation of solids under dynamic loads
  Joint work together with A. Karakaya and C. Miehe (University of Stuttgart)

• Numerical computation of anisotropically evolving yield surfaces for polycrystals
  Joint work together with M. Becker and C. Miehe (University of Stuttgart)

• Micromechanical modeling and anisotropic response of single crystals
  Joint work together with M. Ortiz (Caltech)

• Grain boundary energy, misorientation and grain growth simulations
  Joint work together with M. Ortiz (Caltech) and J. Rimoli (MIT)

• Constitutive modeling of shape memory polymers
  Joint work together with S. Göktepe (Stanford)