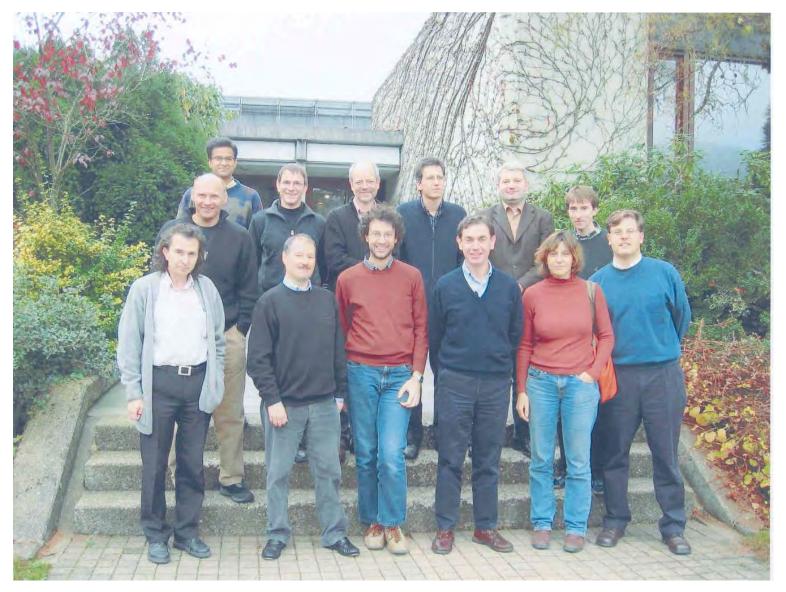
# Optimal scaling in plasticity and fracture

## M. Ortiz California Institute of Technology

Workshop on Analysis and Computation of Microstructure in Finite Plasticity
Bonn, Germany, 4-8 May 2015







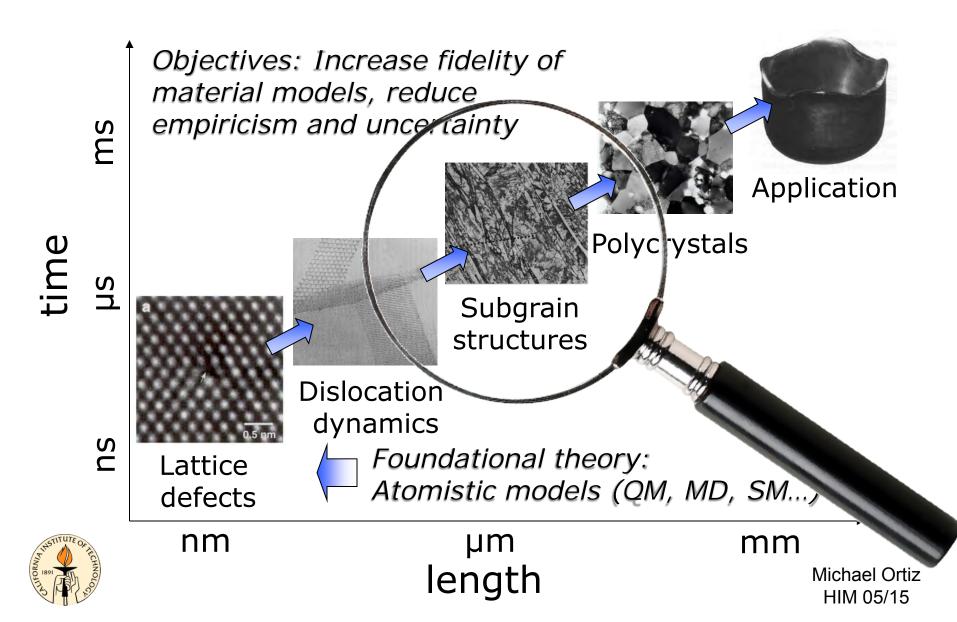
Mini-Workshop on Analysis and Computation of Microstructures in Finite Plasticity Mathematisches Forschungsinstitut Oberwolfach Oberwolfach, Germany, Nov. 14-18, 2005





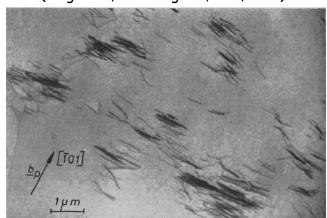
The Genesis of the program: Mathematicians and engineers puzzle over microplasticity...

#### The framework: Multiscale physics



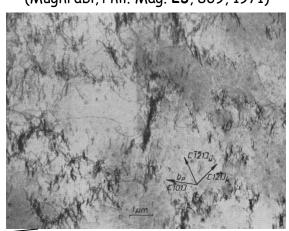
## The question: Evolving microstructures

Copper single crystal (Mughrabi, Phil. Mag. 23, 869, 1971)



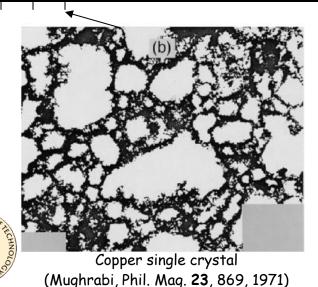
1%

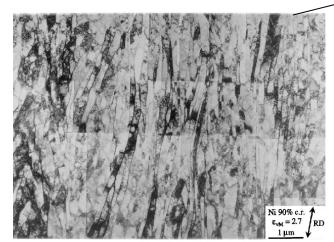
Copper single crystal (Mughrabi, Phil. Mag. 23, 869, 1971)



deformation

100%





90% cold-rolled Ni (Hansen, Huang and Hughes, Mat. Sci. Engin. A 317, 3, 2001)

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#### The promise: Nonlinear analysis

Can analysis shed light on the experimental record? (e.g., can some of the observed microstructures be understood as energy minimizers?)

Can analysis inform modeling and simulation? (e.g., homogeneization, multiscale modeling, relaxation, acceleration...)



#### Ten Years Later...

#### The well-understood setting:

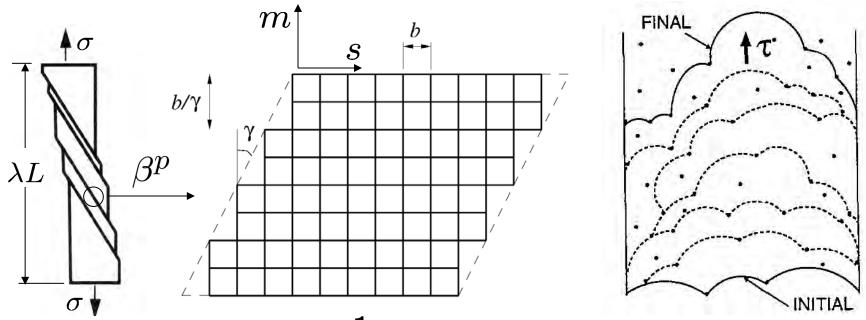
Rate-independent, proportional loading and local behavior (deformation theory of plasticity + relaxation)

#### Still open:

Rate-dependent, non-proportional loan and non-local or localized behavior



#### Crystal plasticity – Linearized kinematics



• Kinematics: 
$$\epsilon^p(\gamma) = \frac{1}{|\Omega|} \int_{J_u} \llbracket u \rrbracket \odot m \, d\mathcal{H}^2 \equiv \sum \gamma s \odot m$$

• Energy: 
$$E(u,\gamma) = \int_{\Omega} [W^e(\nabla u - \epsilon^p(\gamma)) + T |\nabla \gamma \times m|] dx$$

ullet Dissipation:  $\psi(\dot{\gamma}) = \left\{egin{array}{l} au_c |\dot{\gamma}|, & ext{single slip}, \ +\infty, & ext{otherwise}. \end{array}
ight.$ 



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## Crystal plasticity – Deformation theory

• Energy-dissipation functional<sup>1</sup>:

$$F_{\epsilon}(u,\gamma) = \int_{0}^{T} e^{-t/\epsilon} \left[ \Psi(\dot{\gamma}(t)) + \frac{1}{\epsilon} E(u(t),\gamma(t)) \right] dt \to \text{inf!}$$

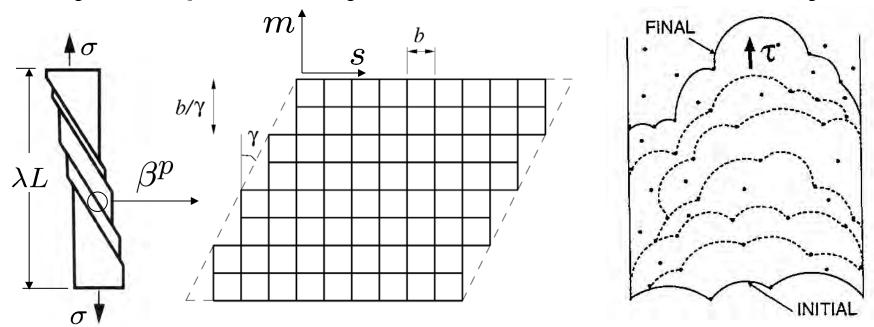
- Assume:  $\gamma(t)$  monotonic (proportional loading).
- Plastic work density:  $W^p(\gamma) = \begin{cases} \sum \tau_c \gamma, & \text{single slip}, \\ +\infty, & \text{otherwise}. \end{cases}$
- Then:  $\Psi(\dot{\gamma}(t)) = \frac{d}{dt} \int_{\Omega} W^p(\gamma(t)) dx = \frac{d}{dt} P(\gamma(t))$
- Energy-dissipation functional: minimize pointwise!

$$F_{\epsilon}(u,\gamma) = \int_0^T \frac{\mathrm{e}^{-t/\epsilon}}{\epsilon} [E(u(t),\gamma(t)) + P(\gamma(t))] dt \to \inf!$$

<sup>1</sup>A. Mielke and M. Ortiz, *ESAIM COCV*, **14** (2008) 494.

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#### Crystal plasticity – Deformation theory



- Incremental flow rule:  $\epsilon^p(\gamma) = \sum \gamma s \odot m$
- Pseudo-elastic strain energy density:

$$W(\epsilon) = \inf_{\gamma} \{ W^e(\epsilon - \epsilon^p(\gamma)) + W^p(\gamma) \}$$

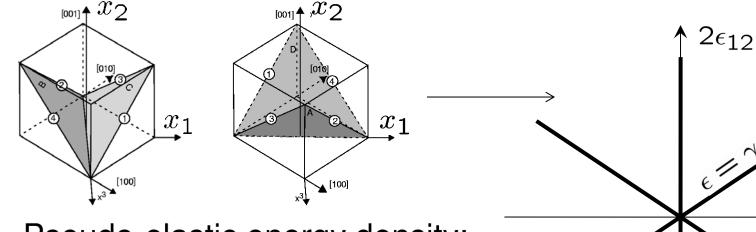
• Variational problem (static equilibrium):



$$F(u) = \int_{\Omega} W(\epsilon(u)) dx \to \inf!$$

## Crystal plasticity – Non-convexity<sup>1</sup>

• Example: FCC crystal deforming on  $(1\bar{1}0)$ -plane



Pseudo-elastic energy density:

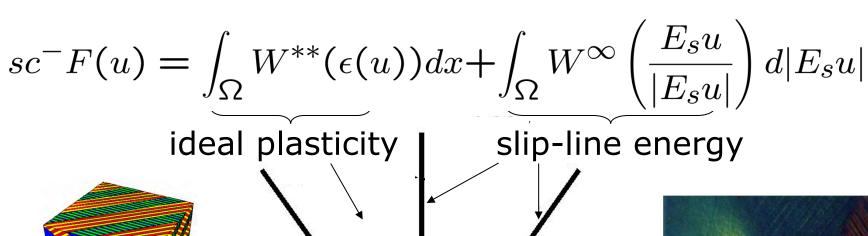
$$W = \begin{cases} \text{linear,} & \text{if } \epsilon = \gamma s \odot m \\ \text{quadratic,} & \text{otherwise.} \end{cases}$$

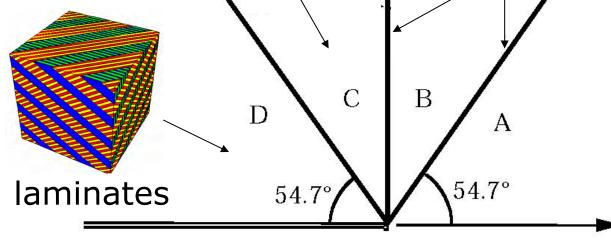
•  $W(\epsilon)$  non-convex!  $\Rightarrow$  Relaxation!



 $\epsilon_{11} - \epsilon_{22}$ 

## Crystal plasticity – Relaxation<sup>1</sup>





(Rice, Mech. Mat., 1987)

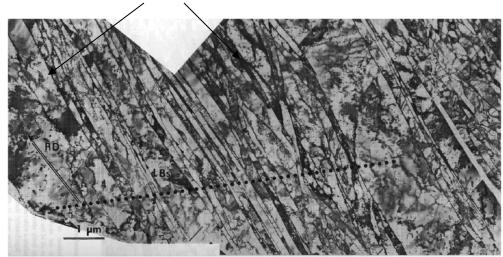
(Crone and Shield, *JMPS*, 2002)——



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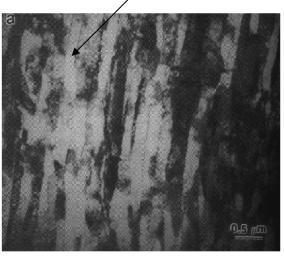
#### Crystal plasticity – Lamellar structures

Dislocation walls



Lamellar dislocation structure in 90% cold-rolled Ta (DA Hughes and N Hansen, Acta Materialia, 44 (1) 1997, pp. 105-112)

Dislocation walls



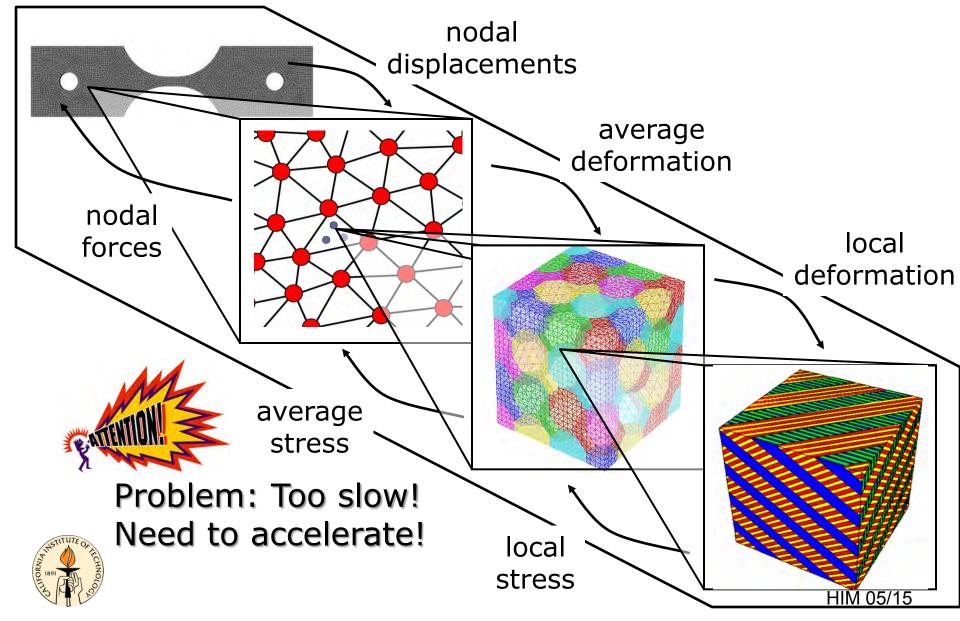
Lamellar structure in shocked Ta (MA Meyers et al., Metall. Mater. Trans., 26 (10) 1995, pp. 2493-2501)

Lamellar dislocation structures at large strains

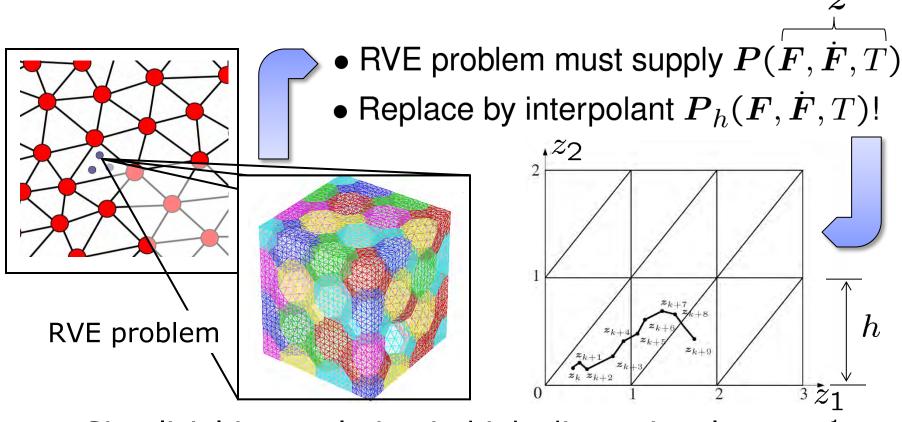


S. Conti, G. Dolzmann and C. Kreisbeck, *Math. Models Methods Appl. Sci.*, **23**(11) (2013) 2111.

## Polycrystals – Concurrent multiscale (C<sup>3</sup>)



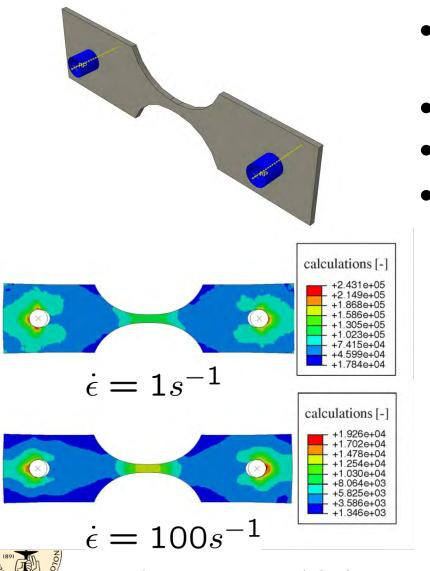
#### Acceleration: Phase-space interpolation



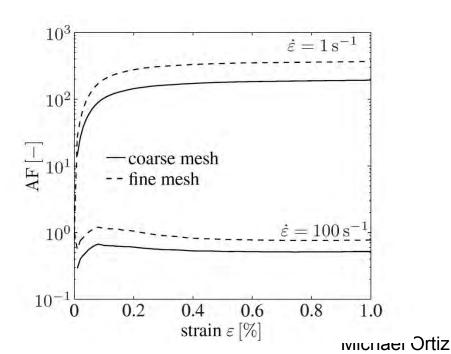
- Simplicial interpolation in high-dimensional spaces<sup>1</sup>
- One single RVE calculation per boundary crossing
  - Speed-up = #steps/simplex @ constant accuracy

<sup>1</sup>Chien, M.J. and Kuh, E., *IEEE Transactions*, 1978; **25**(11):938–940. Michael Ortiz Klusemann, B. and Ortiz, M., IJNME, 10.1002/nme.4887, 2015.

#### Acceleration: Phase-space interpolation



- Dynamic extension of tensile neo-Hookean specimen
- Explicit Newmark integration
- Hexahedral finite elements
- Quadratic:  $W(F) \rightarrow W_h(F)$



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Klusemann, B. and Ortiz, M., IJNME, 10.1002/nme.4887, 2015.

#### Ten Years Later...

#### The well-understood setting:

Rate-independent, proportional loading and local behavior (deformation theory of plasticity + relaxation)

#### Still open:

Rate-dependent, non-proportional loading and non-local behavior



#### **Pitfalls**

'Standard program' may fail due to:

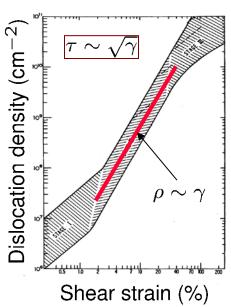
Non-proportional loading (unloading, cycling loading, change of loading path direction) leading to microstructure evolution

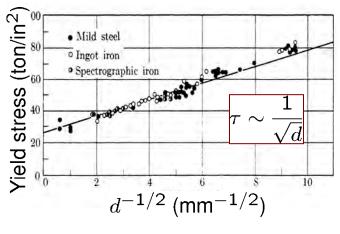
Departures from volume scaling (size effect, domain dependence, localization) leading to failure of homogeneization and relaxation

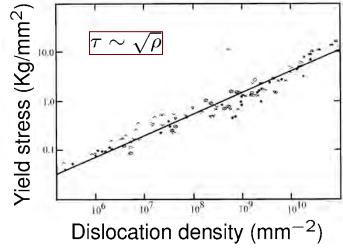


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#### Crystal plasticity – Scaling laws







Taylor hardening (RJ Asaro, Adv. Appl. Mech., 23, 1983, p. 1.)

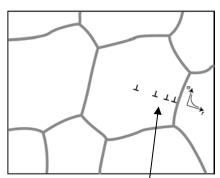
Hall-Petch scaling (NJ Petch, J. Iron and Steel Inst., 174, 1953, pp. 25-28.)

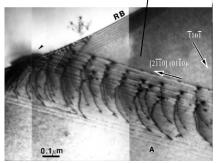
Taylor scaling
(SJ Basinski and ZS Basinski,
Dislocations in Solids,
FRN Nabarro (ed.)
North-Holland, 1979.)



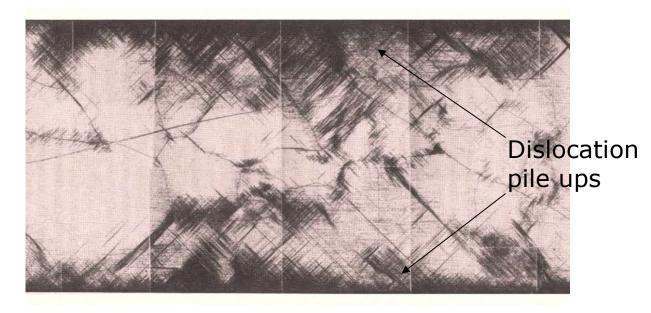
Classical scaling laws of crystal plasticity

#### Crystal plasticity – Effect of boundaries





Dislocation pile-up at Ti grain boundary (I. Robertson)

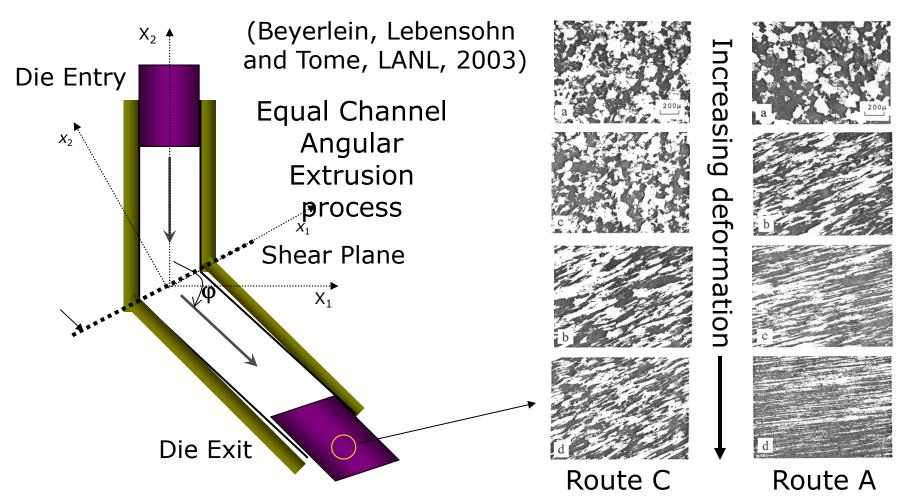


LiF plate impact experiment.
Dislocation pile-ups at surfaces
and grain boundaries
(G Meir and RJ Clifton, J. Appl. Phys.,
59 (1) 1986, pp. 124-148)



Dislocation pile-ups at grain boundaries, surfaces

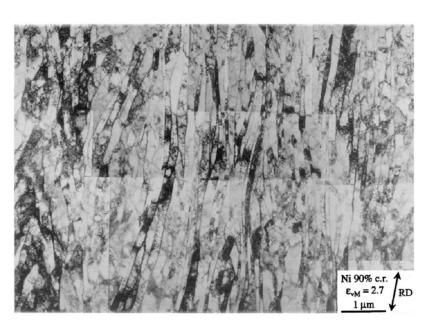
#### Crystal plasticity – Size effect



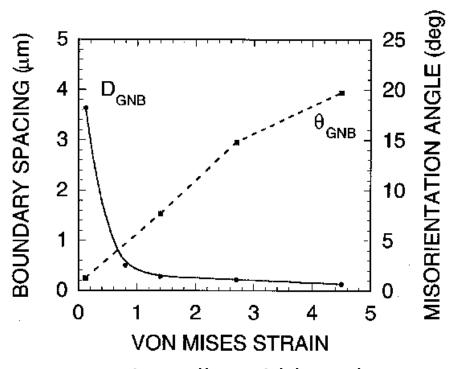


Evolution of dislocation structures in Cu specimen. Lamellar width:  $l \sim \gamma^{-0.6}$ 

#### Crystal plasticity – Size effect



Pure nickel cold rolled to 90% Hansen *et al.* Mat. Sci. Engin. A317 (2001).



Lamellar width and misorientation angle as a function of deformatation Hansen *et al.* Mat. Sci. Engin. A317 (2001).



Scaling of lamellar width and misorientation angle with deformation

#### Non-local microplasticity

Scaling laws such as Hall-Petch suggest the existence of an intrinsic material length scale

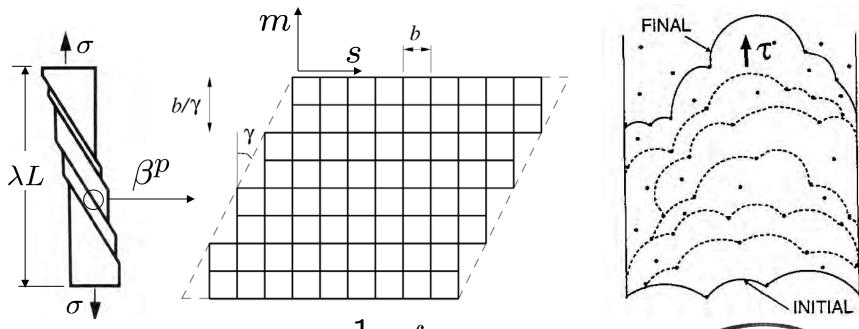
Modeling assumption: Account for dislocation self-energy using a line-tension approximation

The resulting deformation-theoretical energy is non-local (specifically, depends on  $\nabla \gamma$ )

Intrinsic length-scale: Burgers vector



### Crystal plasticity – Linearized kinematics



• Kinematics: 
$$\epsilon^p(\gamma) = \frac{1}{|\Omega|} \int_{J_u} \llbracket u \rrbracket \odot m \, d\mathcal{H}^2 \equiv \sum \gamma s \odot m$$

$$\bullet$$
 Energy: 
$$E(u,\gamma) = \int_{\Omega} [\,W^e(\nabla u - \epsilon^p(\gamma)) + T\,|\nabla\gamma \times m|\,]\,dx$$

• Dissipation:  $\psi(\dot{\gamma}) = \left\{ \begin{array}{l} \tau_c |\dot{\gamma}|, & \text{single slip,} \\ +\infty, & \text{otherwise.} \end{array} \right.$ 

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#### Crystal plasticity – Optimal scaling

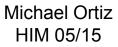
**Theorem** [Conti & MO, ARMA, 2005] *There are constants* c *and* c' *such that* 

$$cE_0(T, \gamma, \tau_0, \mu, d) \le \inf E \le c'E_0(T, \gamma, \tau_0, \mu, d)$$

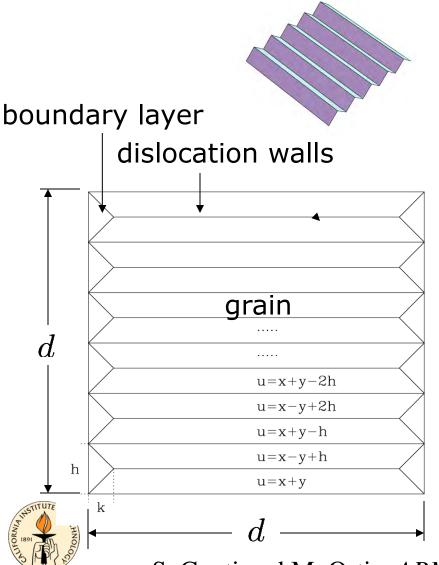
where 
$$E_0(T, \gamma, \tau_0, \mu, d)/G\gamma^2 d^3 =$$

$$\min\left\{1,\frac{\mu}{G},\frac{\tau_0}{G\gamma}+\left(\frac{\mu}{G}\right)^{1/2}\left(\frac{T}{G\gamma bd}\right)^{1/2},\frac{\tau_0}{G\gamma}+\left(\frac{T}{G\gamma bd}\right)^{2/3}\right\}$$

- Upper bounds determined by construction
- Lower bounds: Rigidity estimates, ansatz-free lower bound inequalities (Kohn and Müller '92, '94; Conti '00)



#### Optimal scaling – Laminate construction



Energy:

$$W \equiv \frac{E_0}{d^3} \sim \tau_0 \gamma + \left(\frac{\mu T \gamma^3}{bd}\right)^{1/2}$$

Yield stress:

$$\tau \equiv \frac{\partial W}{\partial \gamma} \sim \tau_0 + \frac{1}{2} \left( \frac{\mu T \gamma}{b d} \right)^{1/2}$$

parabolic hardening +

Hall-Petch scaling

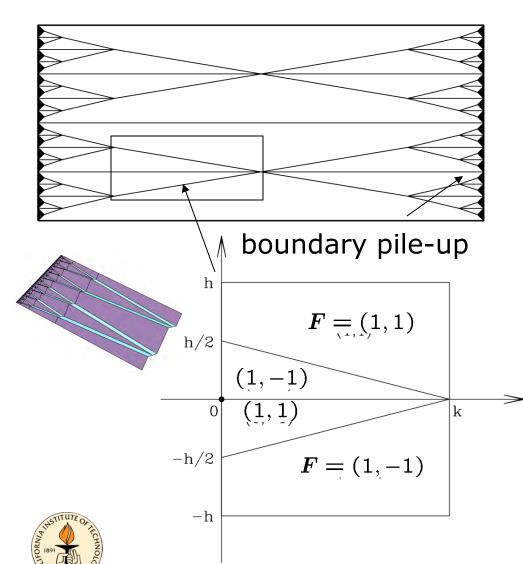
Lamellar width:

$$l \sim \left(\frac{\mu T d}{\mu \gamma b}\right)^{1/2}$$

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S. Conti and M. Ortiz, *ARMA*, **176** (2005), pp. 103–147

### Optimal scaling – Branching construction



• Energy:

$$W \sim \tau_0 \gamma + G \left( \frac{T \gamma^2}{Gbd} \right)^{2/3}$$

Yield stress:

$$\tau \sim \tau_0 + \left(\frac{T}{bd}\right)^{2/3} (G\gamma)^{1/3}$$

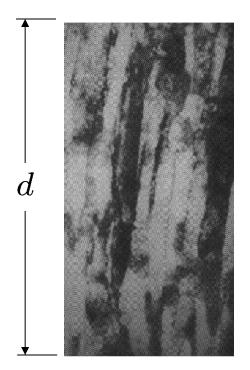
Microstructure size:

$$l \sim \left(\frac{Td^2}{G\gamma b}\right)^{1/3}$$

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S. Conti and M. Ortiz, ARMA, 176 (2005), pp. 103–147

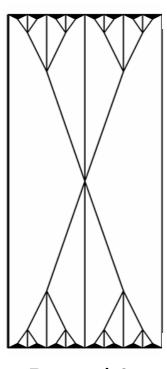
#### Optimal scaling – Microstructures



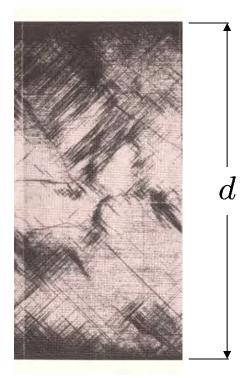
Shocked Ta (Meyers et al '95)



Laminate



Branching



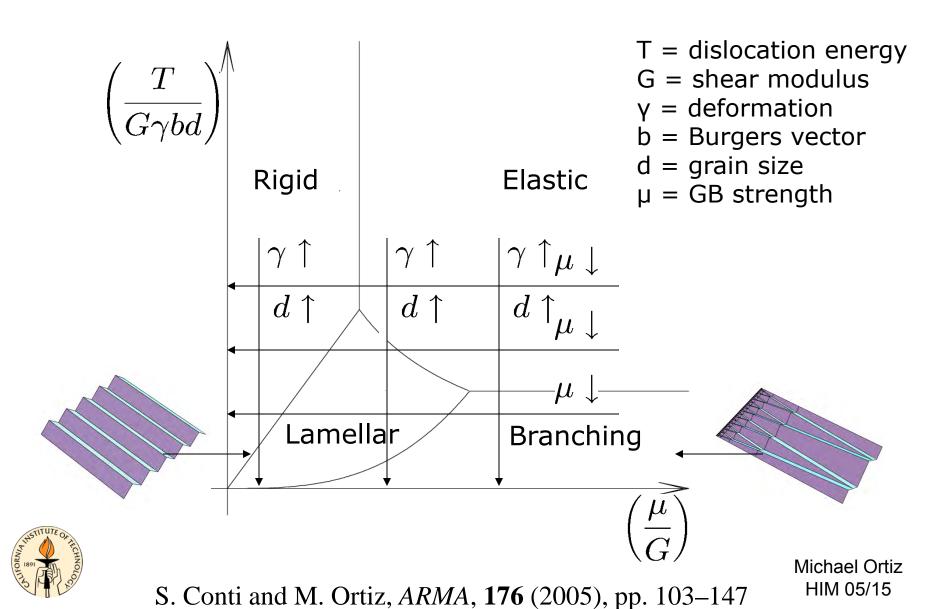
LiF impact  $au \sim d^{-1/2} \quad au \sim d^{-2/3}$  (Meir and Clifton '86)

Dislocation structures corresponding to the lamination and branching constructions

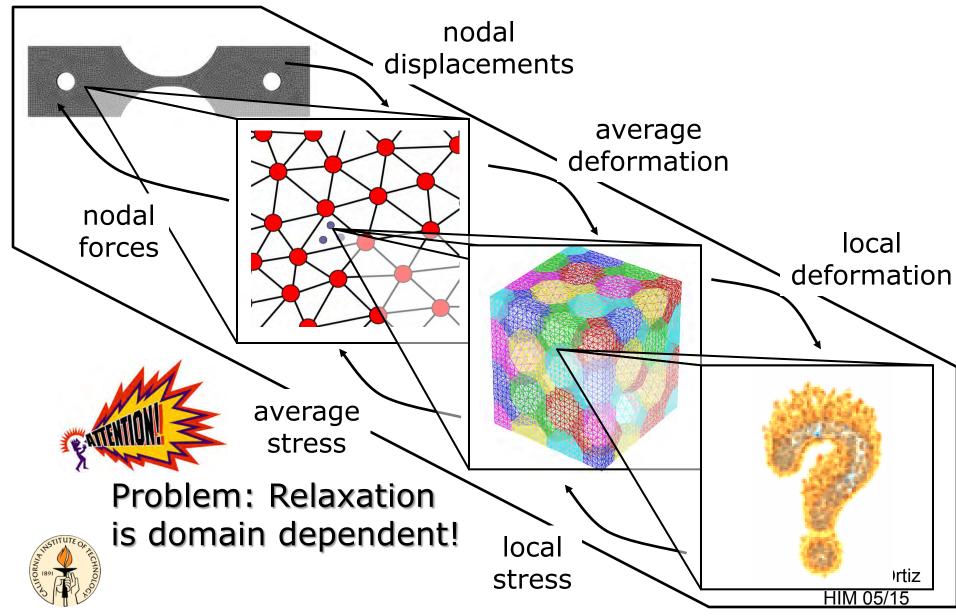
S. Conti and M. Ortiz, *ARMA*, **176** (2005), pp. 103–147

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#### Optimal scaling – Phase diagram



## Polycrystals – Concurrent multiscale (C<sup>3</sup>)



#### **Pitfalls**

'Standard program' mail fail due to:

Non-proportional loading (unloading, cycling loading, change of loading path direction) leading to microstructure evolution

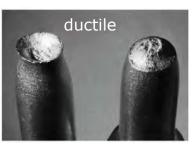
Departures from volume scaling (size effect, domain dependence, localization) leading to failure of homogeneization and relaxation



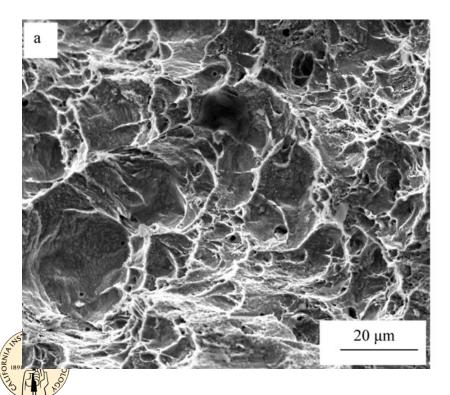
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#### Localization – Fracture scaling





(Courtesy NSW HSC online)

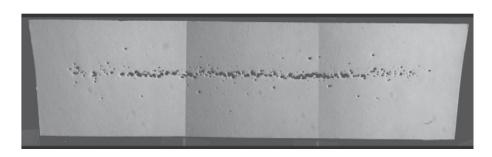


- Ductile fracture in metals occurs by void nucleation, growth and coalescence
- Fractography of ductilefracture surfaces exhibits profuse dimpling, vestige of microvoids
- Ductile fracture entails large amounts of plastic deformation (vs. surface energy) and dissipation.

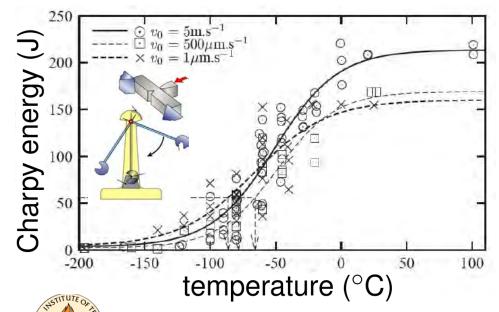
Fracture surface in SA333 steel, room temp.,  $d\epsilon/dt=3\times10^{-3}s^{-1}$  (S.V. Kamata, M. Srinivasa and P.R. Rao, Mater. Sci. Engr. A, 528 (2011) 4141–4146)

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#### Localization – Fracture scaling



Void sheet in copper disk<sup>1</sup>

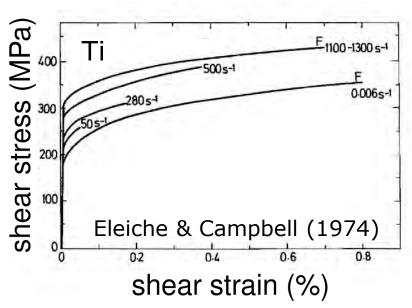


arpy energy of A508 steel<sup>2</sup>

- Fracture energy scales with crack area:  $E \sim L^2$
- A number of ASTM
   engineering standards are
   in place to characterize
   ductile fracture properties
   (J-testing, Charpy test)
- In general, the specific fracture energy for ductile fracture is greatly in excess of that required for brittle fracture...

<sup>1</sup>Heller, A., Science & Technology, LLNL, pp. 13-20, July/August, 2002 <sup>2</sup>Tanguy *et al.*, *Eng. Frac. Mechanics*, 2005

### Naïve model: Local plasticity

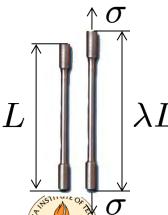


Deformation theory: Minimize

$$E(y) = \int_{\Omega} W(Dy(x)) dx$$

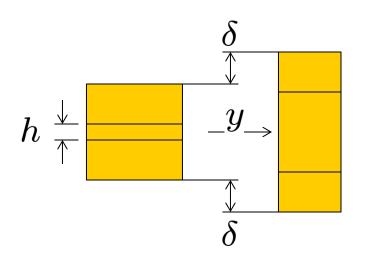
- Growth of W(F)?
- Asume power-law hardening:

$$\sigma \sim K\epsilon^n = K(\lambda - 1)^n$$



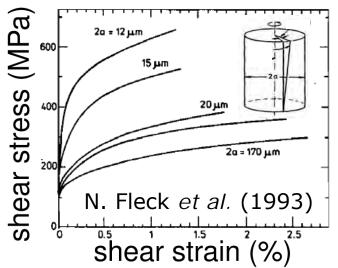
- Nominal stress:  $\partial_{\lambda}W = \sigma/\lambda = K(\lambda-1)^{n}/\lambda$
- For large  $\lambda$ :  $\partial_{\lambda}W \sim K\lambda^{n-1} \Rightarrow W \sim K\lambda^n$  In general:  $W(F) \sim |F|^p, \ p=n \in (0,1)$
- - ⇒ Sublinear growth!

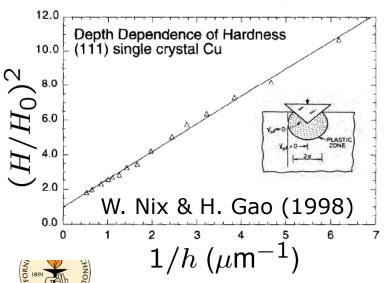
#### Naïve model: Local plasticity



- Example: Uniaxial extension
- Energy:  $E_h \sim h \left(\frac{2\delta}{h}\right)^p$
- For p < 1:  $\lim_{h \to 0} E_h = 0$
- Energies with sublinear growth relax to 0.
- For hardening exponents in the range of experimental observation, local plasticity yields no useful information regarding ductile fracture properties of materials!
- Need additional physics, structure...

#### Strain-gradient plasticity





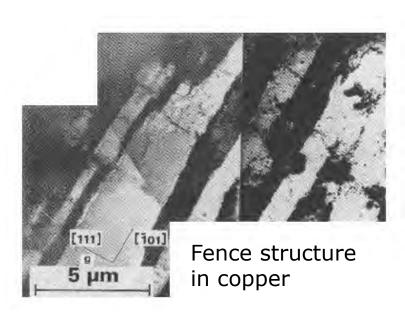
- The yield stress of metals is observed to increase in the presence of strain gradients
- Deformation theory of straingradient plasticity:

$$E(y) = \int_{\Omega} W(Dy(x), D^2y(x)) dx$$

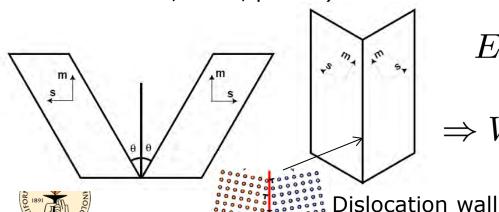
 $y:\Omega\to\mathbb{R}^n$ , volume preserving

- Strain-gradient effects may be expected to oppose localization
- Question: Can fracture scaling be understood as the result of strain-gradient plasticity?

# Strain-gradient plasticity



(J.W. Steeds, *Proc. Roy. Soc. London*, **A292**, 1966, p. 343)



- Growth of  $W(F, \cdot)$ ?
- For fence structure:

$$F^{\pm} = R^{\pm} (I \pm \tan \theta \, s \otimes m)$$

Across jump planes:

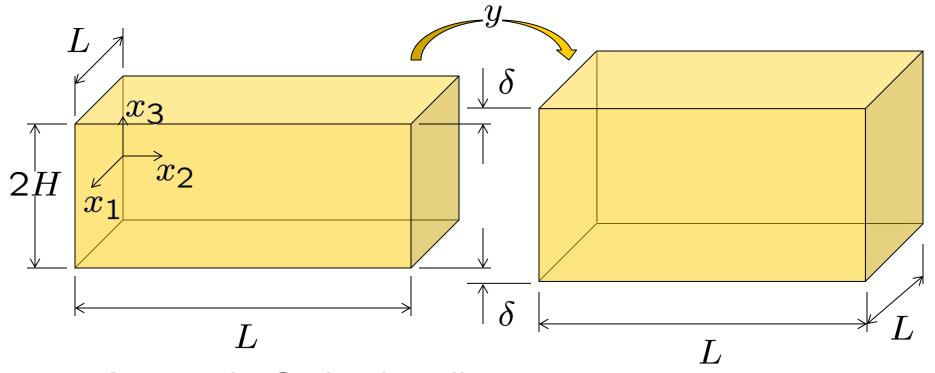
$$|\llbracket F \rrbracket| = 2 \sin \theta$$

• Dislocation-wall energy:

$$E = \frac{T}{b} 2 \sin \theta = \frac{T}{b} | \llbracket F \rrbracket |$$

 $\Rightarrow W(F, \cdot)$  has linear growth!

# Optimal scaling – Ductile fracture



- Approach: Optimal scaling
- Slab:  $\Omega = [0, L]^2 \times [-H, H]$ , periodic
- Uniaxial extension:  $y_3(x_1, x_2, \pm H) = x_3 \pm \delta$

# Optimal scaling – Ductile fracture

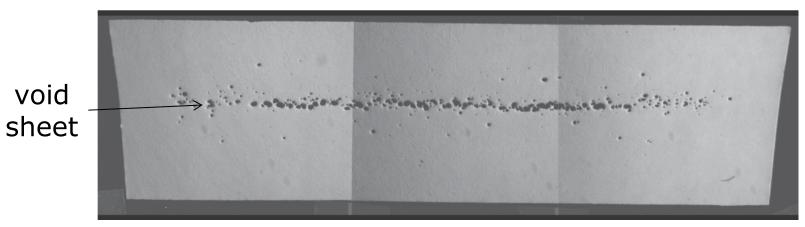
- $y: \Omega \to \mathbb{R}^3$ ,  $[0, L]^2$ -periodic, volume preserving
- $y \in W^{1,1}(\Omega; \mathbb{R}^3), Dy \in BV(\Omega; \mathbb{R}^{3\times 3})$
- Growth: For  $p \in (0,1)$ , intrinsic length  $\ell > 0$ ,

$$E(y) \sim K\left(\int_{\Omega} (|Dy|^p - 3^{p/2}) dx + \ell \int_{\Omega} |D^2y| dx\right)$$

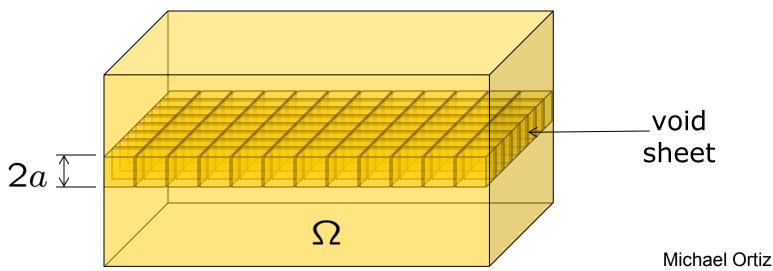
**Theorem** [Fokoua, Conti & MO, ARMA, 2013]. For  $\ell$ sufficiently small,  $p \in (0, 1), 0 < C_L(p) < C_U(p),$ 

$$C_L(p)L^2\ell^{\frac{1-p}{2-p}}\delta^{\frac{1}{2-p}} \leq \inf E \leq C_U(p)L^2\ell^{\frac{1-p}{2-p}}\delta^{\frac{1}{2-p}}$$
 Fracture!

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Heller, A., Science & Technology Review Magazine, LLNL, pp. 13-20, July/August, 2002



L. Fokoua, S. Conti and M. Ortiz, *ARMA*, **212** (2014) pp. 331-357. HIM 05/15

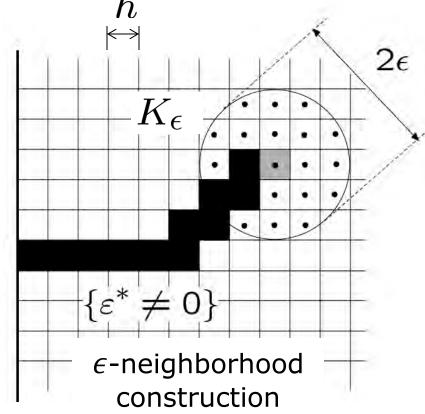
• In every cube: void

• Calculate, estimate:  $E \leq CL^2 \left(a^{1-p}\delta^p + \ell\delta/a\right)$ 

• Optimize:  $a = (\ell \delta^1 + p)^{1/(2-p)} \Rightarrow E \le C_U L^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}$  void growth!

L. Fokoua, S. Conti and M. Ortiz, ARMA, 212 (2014) pp. 331-357. HIM 05/15

# Numerical implementation Material-point erosion



- $\epsilon$ -neighborhood construction: Choose  $h \ll \epsilon \ll L$
- Erode material point if

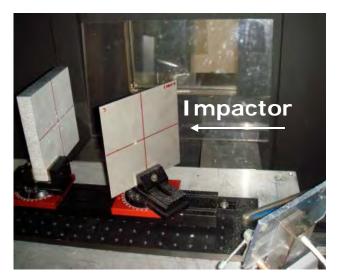
$$\frac{h^2}{|K_{\epsilon}|} \int_{K_{\epsilon}} W(\nabla u) \, dx \geq J_c$$

 For linear elasticity, proof of Γconvergence to Griffith fracture

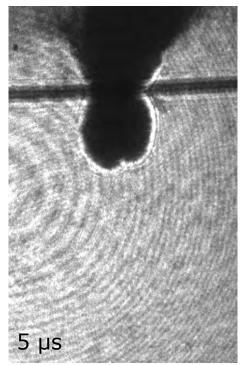
<u>Theorem</u><sup>1</sup>: Suppose  $\epsilon = \epsilon(h)$  and  $h/\epsilon(h) \to 0$  as  $h \to 0$ . Then,  $\Gamma - \lim_{h \to 0} E_{h,\epsilon(h)} =$  Griffith energy

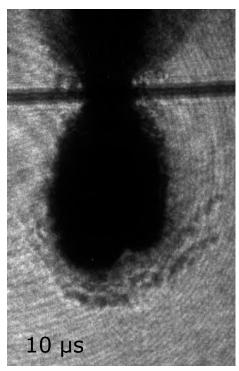


# Application to hypervelocity impact









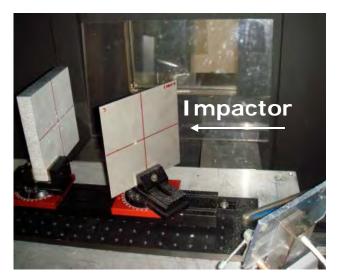
Hypervelocity impact (5.7 Km/s) of 0.96 mm thick aluminum plates by 5.5 mg nylon 6/6 cylinders (Caltech)



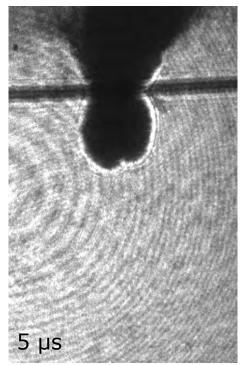
Pandolfi, A. & Ortiz, M., IJNME, 92 (2012) 694.

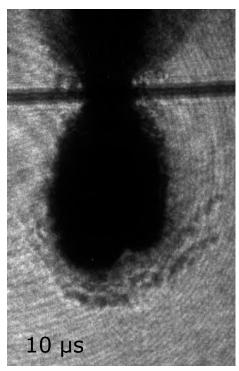
Pandolfi, A., Li, B. & Ortiz, M., *Int. J. Fract.*, **184** (2013) 3. Li, B., Stalzer, M. & Ortiz, M., *IJNME*, **100** (2014) 40.

# Application to hypervelocity impact









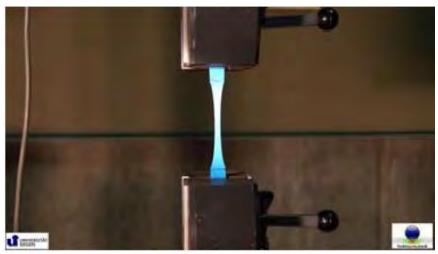
Hypervelocity impact (5.7 Km/s) of 0.96 mm thick aluminum plates by 5.5 mg nylon 6/6 cylinders (Caltech)



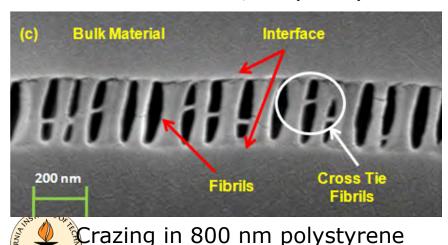
Pandolfi, A. & Ortiz, M., IJNME, 92 (2012) 694.

Pandolfi, A., Li, B. & Ortiz, M., *Int. J. Fract.*, **184** (2013) 3. Li, B., Stalzer, M. & Ortiz, M., *IJNME*, **100** (2014) 40.

# Fracture of polymers



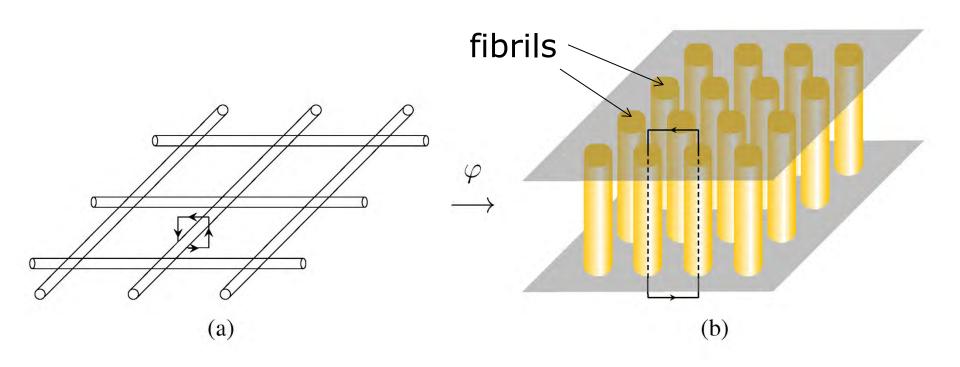
T. Reppel, T. Dally, T. and K. Weinberg, Technische Mechanik, 33 (2012) 19-33.



film (C. K. Desai et al., 2011)

- Polymers undergo entropic elasticity and damage due to chain stretching and failure
- Polymers fracture by means of the crazing mechanism consisting of fibril nucleation, stretching and failure
- The free energy density of polymers saturates in tension once the majority of chains are failed: p=0!
- Crazing mechanism is incompatible with straingradient elasticity...

# Fracture of polymers - Topology



Formation of fibers from solid polymer entails a topological transition



# Fracture of polymers

• Suppose: For  $K_U > 0$ , intrinsic length  $\ell > 0$ ,

$$E(y) \le K_U \left( \int_{\Omega} (|Dy|^p - 3^{p/2}) dx + \ell \int_{\Omega} |D^2y| dx \right)$$

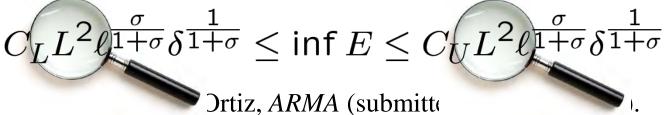
- If  $E(y) < +\infty \Rightarrow y$  continuous on a.e. plane!
- Crazing is precluded by the continuity of y!
- Instead suppose: For  $\sigma \in (0, 1)$ ,

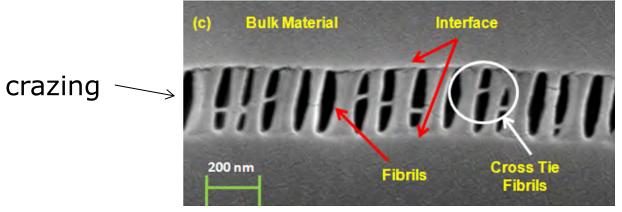
$$E(y) \le K_U \left( \int_{\Omega} (|Dy|^p - 3^{p/2}) dx + \ell^{\sigma} |y|_{W^{1+\sigma,1}(\Omega)} \right)$$

**Theorem** [Conti & MO, ARMA]. For ℓ sufficiently small,

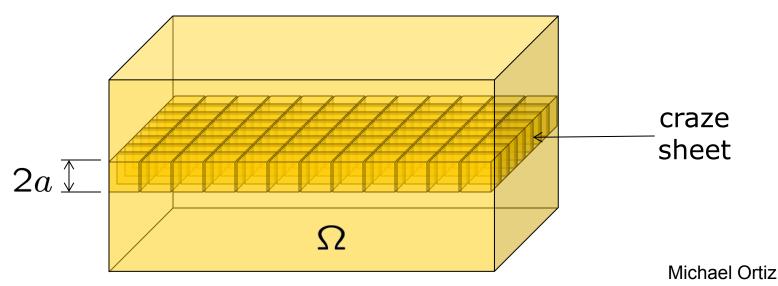
$$p = 0, \ \sigma \in (0,1), \ 0 < C_L < C_U,$$







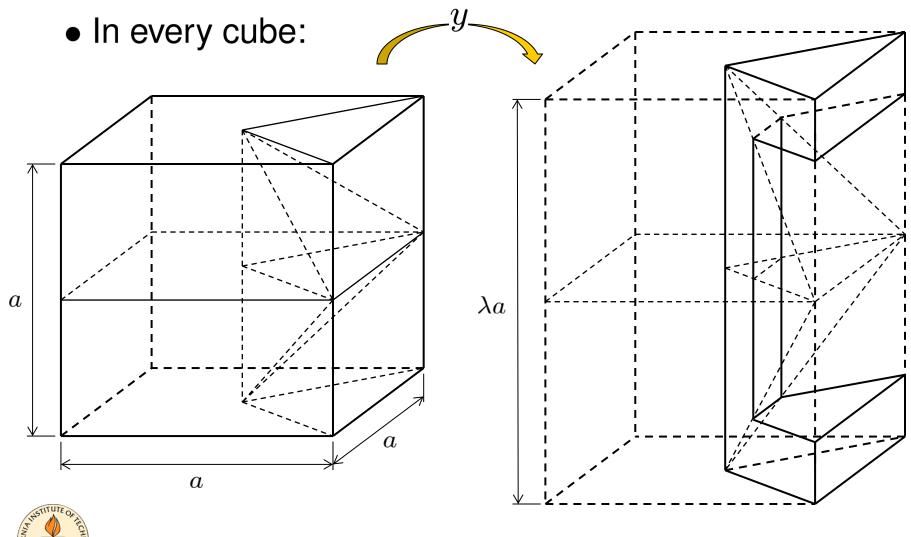
Crazing in 800 nm polystyrene thin film (C. K. Desai *et al.*, 2011)



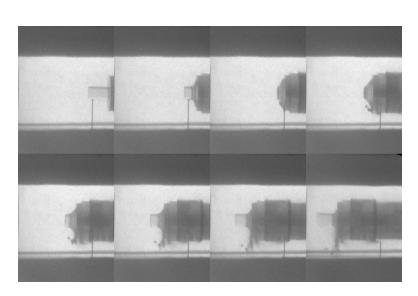
HIM 05/15



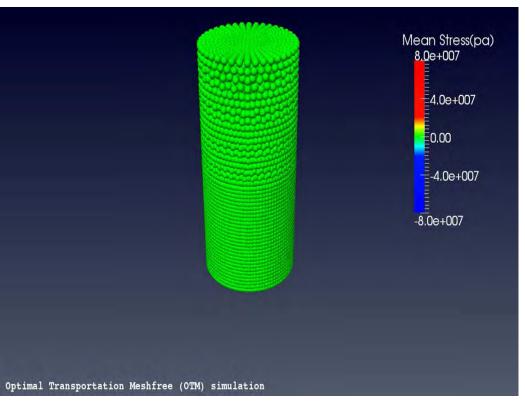
S. Conti and M. Ortiz, ARMA (submitted for publication).



## Taylor-anvil tests on polyurea



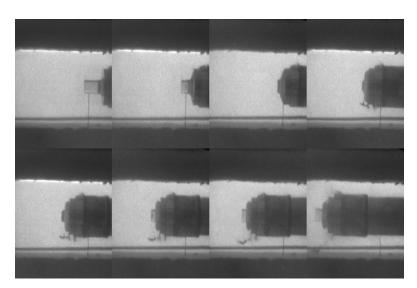
Shot #854: R0 = 6.3075 mm, L0 = 27.6897 mm, v = 332 m/s



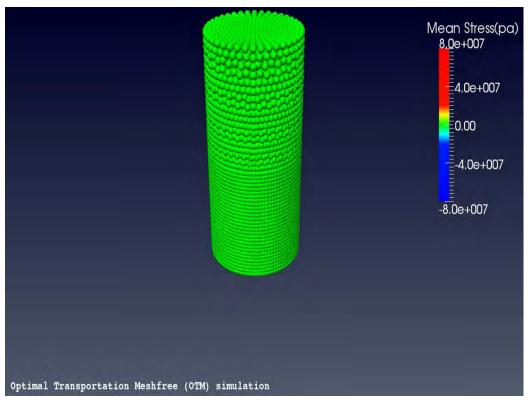


Experiments conducted by W. Mock, Jr. and J. Drotar, at the Naval Surface Warfare Center (Dahlgren Division) Research Gas Gun Facility, Dahlgren, VA 22448-5100, USA

## Experiments and simulations



Shot #861: R0 = 6.3039 mm, L0 = 27.1698 mm, v = 424 m/s





Experiments conducted by W. Mock, Jr. and J. Drotar, at the Naval Surface Warfare Center (Dahlgren Division) Research Gas Gun Facility, Dahlgren, VA 22448-5100, USA

## Concluding remarks

Can analysis shed light on the experimental record? (e.g., can some of the observed microstructures be understood as energy minimizers?)

Can analysis inform modeling and simulation? (e.g., homogeneization, multiscale modeling, relaxation, acceleration...)



#### Ten Years Later...

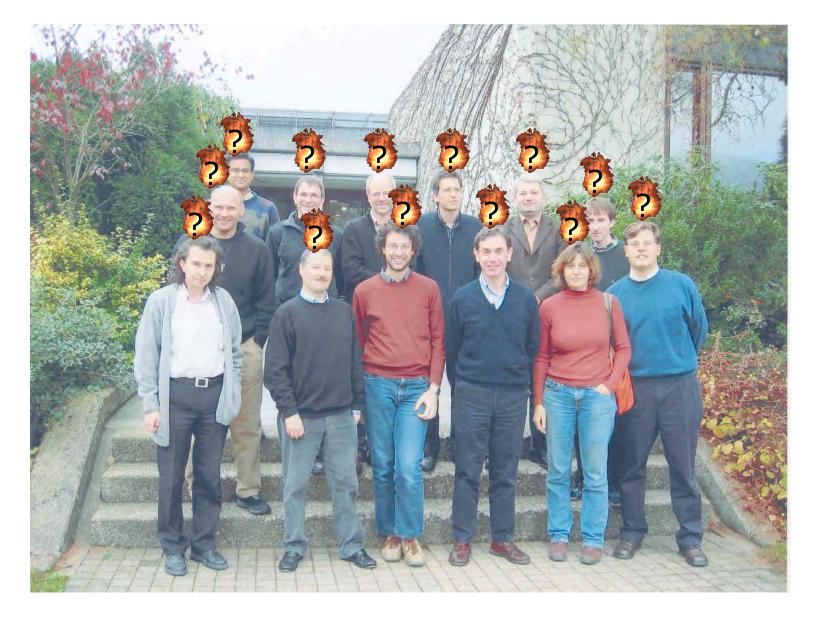
#### The well-understood setting:

Rate-independent, proportional loading and local behavior (deformation theory of plasticity + relaxation)

#### Still open:

Rate-dependent, non-proportional loading and non-local or localized behavior







The Apotheosis of the program: Mathematicians and engineers still puzzle over microplasticity...

# Thanks!

