Multiscale models of metal plasticity
Lecture I: Experimental and continuum thermodynamics basis

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Sixth Summer School in Analysis and Applied Mathematics

Rome, June 20-24, 2011

Outline of Lecture #1

- Applications of plasticity in engineering
- Empirical basis of plasticity
  - *Quasistatic uniaxial tests*
  - *Quasistatic multiaxial tests*
  - *Dynamic testing*
- The continuum thermodynamics framework
- Fidelity of engineering plasticity models
- Outlook for multiscale modeling

Applications of plasticity

What is plasticity good for?

Plasticity applications - Crashworthiness

Frontal crash test of
Volvo C30

Frontal crash test of
Chevrolet Venture

Offset frontal crash test of
1998 Toyota Sienna

Side-impact test of
1996 Ford Explorer vs.
2000 Ford Focus

Michael Ortiz
ROME0611

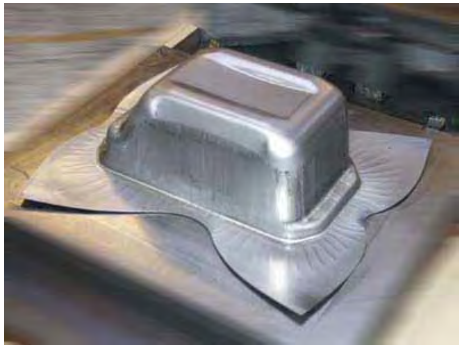
Source: http://en.wikipedia.org/wiki/Crash_test

Plasticity applications - Manufacturing

Metal ingot after forging

Lathe cutting metal from workpiece

Cold rolling of steel



Deep-drawing of blank metal sheet (source: ThomasNet)

Sources: http://en.wikipedia.org/wiki/Forging
http://en.wikipedia.org/wiki/Metal_forming
http://www.kanabco.com/vms/library.html

Plasticity applications – Metallic structures

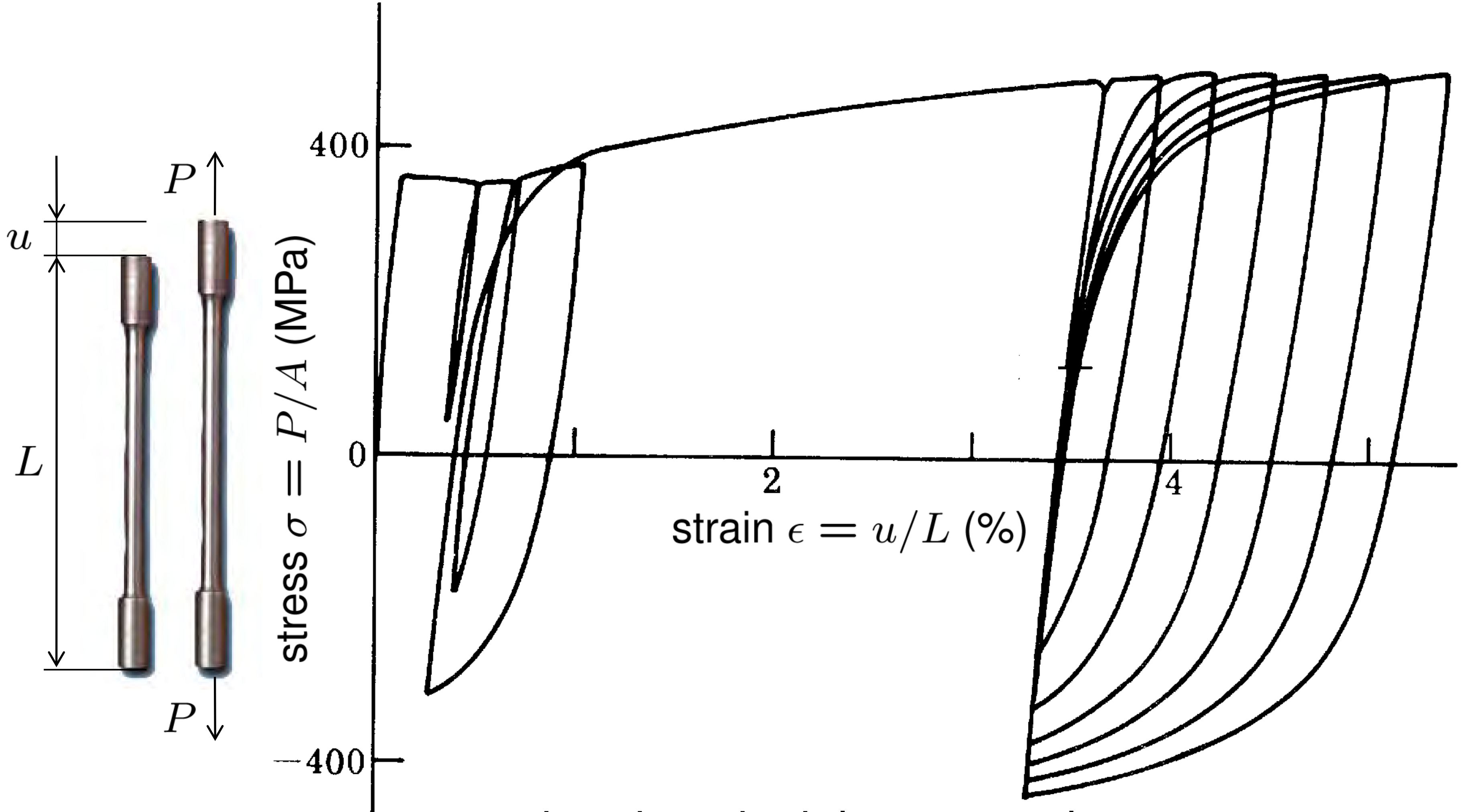
Plastic buckling of storage tank,
1999 Kocaeli earthquake
(PEER 2000/09, Dec. 2000)

Mid-story collapse,
1995 Kobe earthquake
(EQE Summary Rep., 1995)

Experimental basis of macrosocpic plasticity

- Quasistatic uniaxial tension/compression
  - *Elastic domain, yield point*
  - *Elastic-plastic decomposition of strain*
  - *Hooke's law for elastic unloading/reloading*
  - *Reverse yielding and Bauschinger effect*
  - *Unloading-point fading memory*
- Multiaxial loading, texture anisotropy
- Rate-sensitivity of the yield stress
- Temperature-dependence of the yield stress
- Fraction of work stored as internal energy
- Fraction of work dissipated as heat

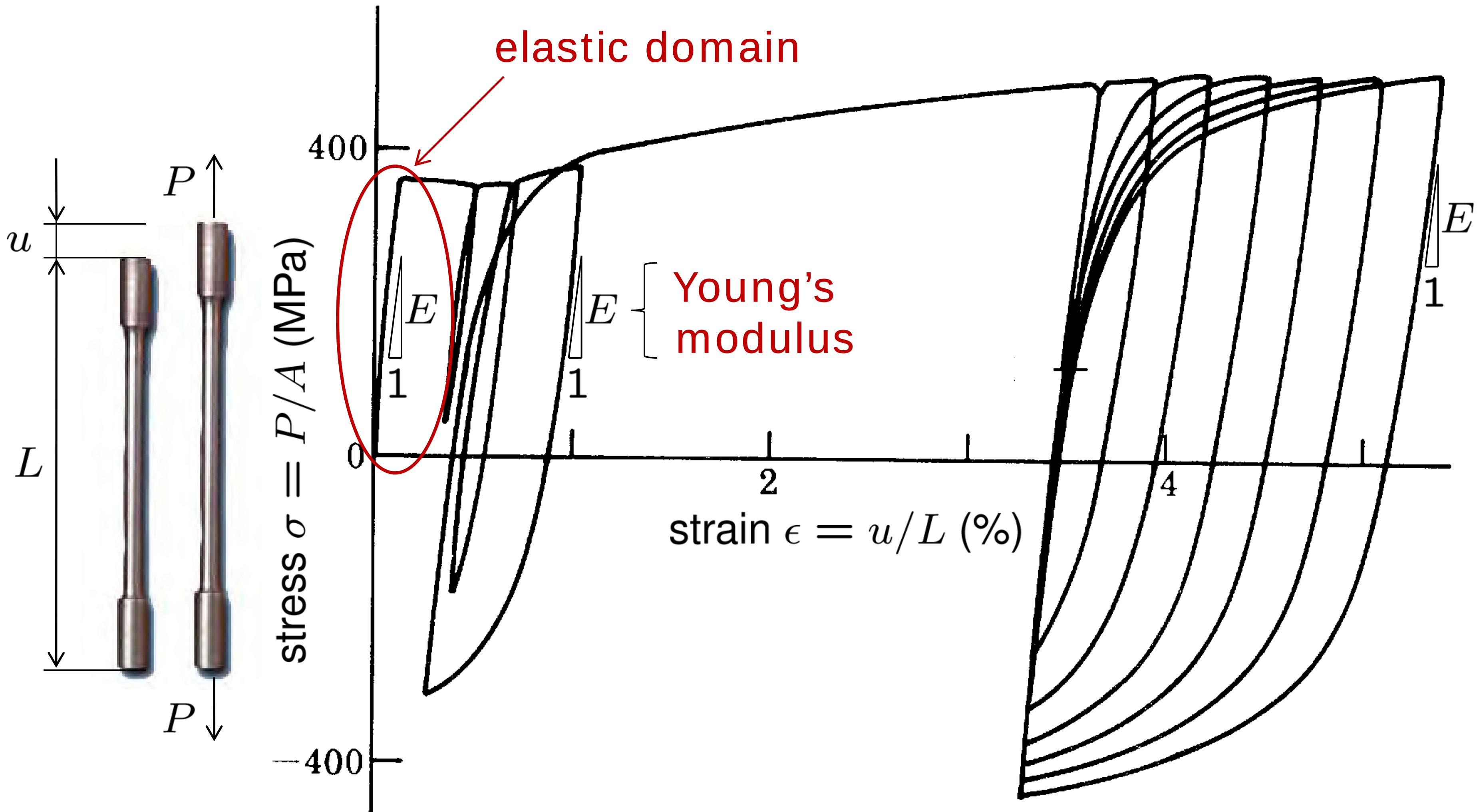
Quasistatic tension-compression test



Quasistatic uniaxial test, steel

M. Ortiz and E.P. Popov,
Proc. Roy. Soc. Lond. A **379**, 439-458 (1982)

Quasistatic tension-compression test



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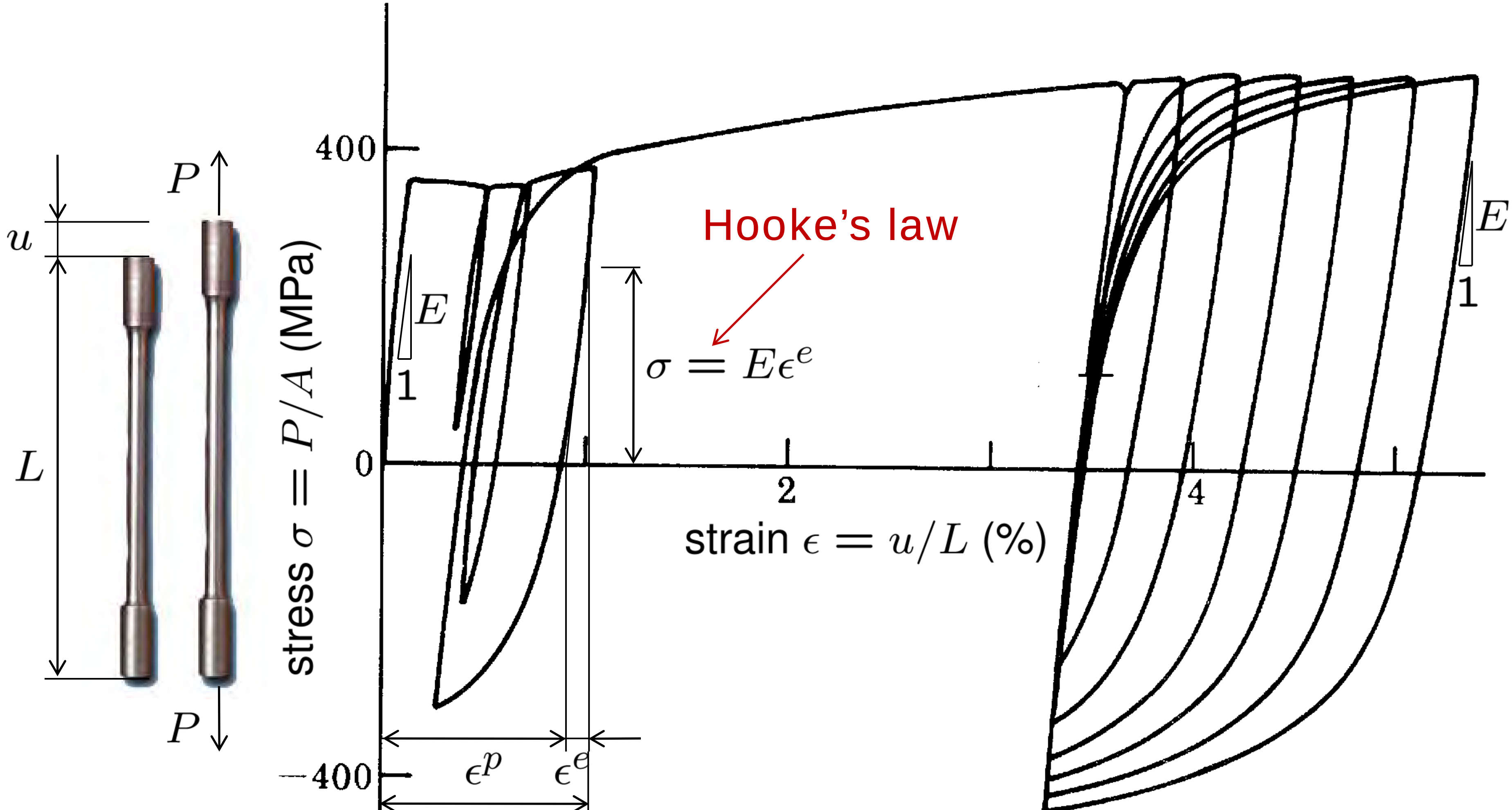
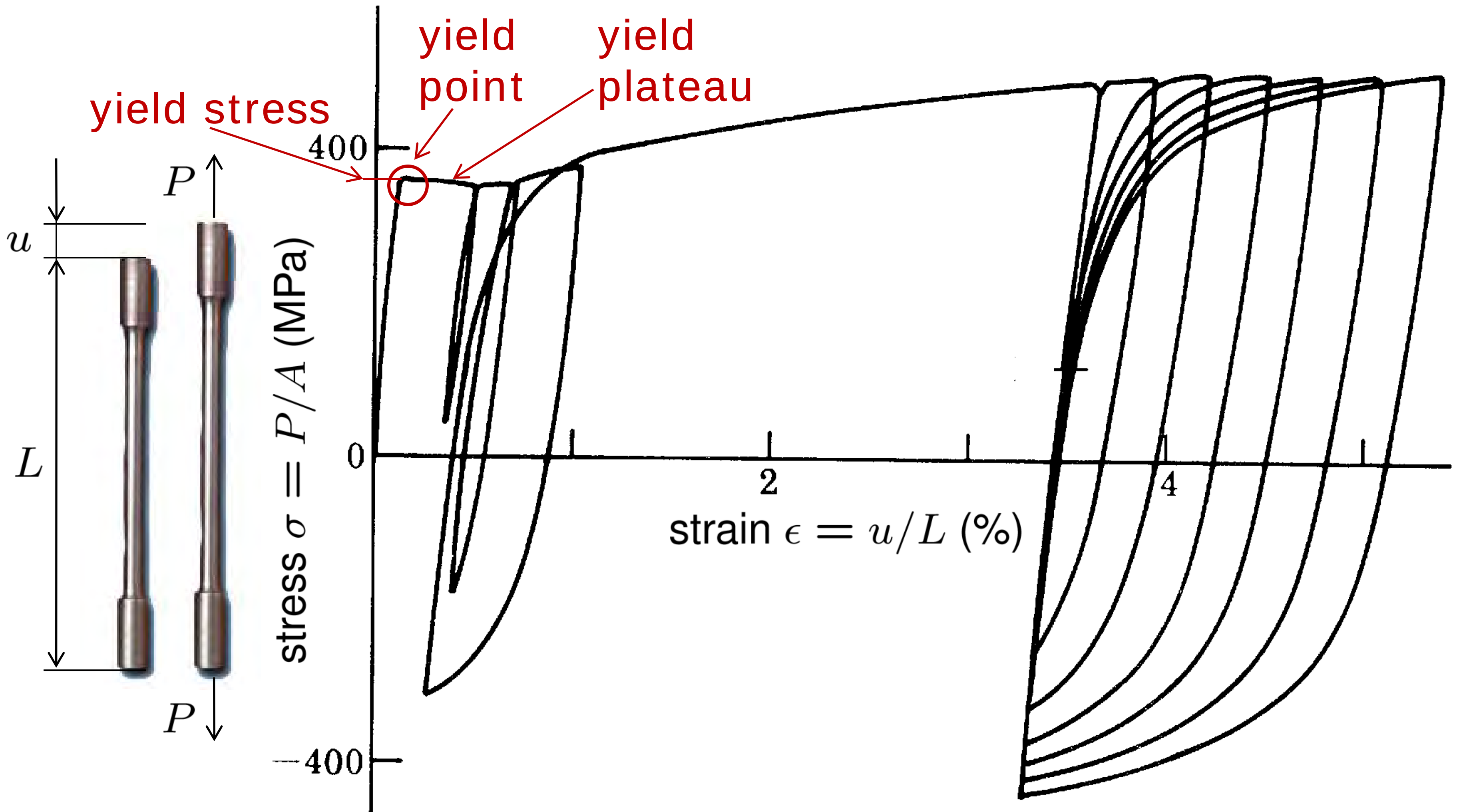


$\epsilon = \epsilon^e + \epsilon^p \leftarrow$ elastic-plastic decomposition of strain

M. Ortiz and E.P. Popov,
Proc. Roy. Soc. Lond. A **379**, 439-458 (1982)

Quasistatic tension-compression test



M. Ortiz and E.P. Popov,
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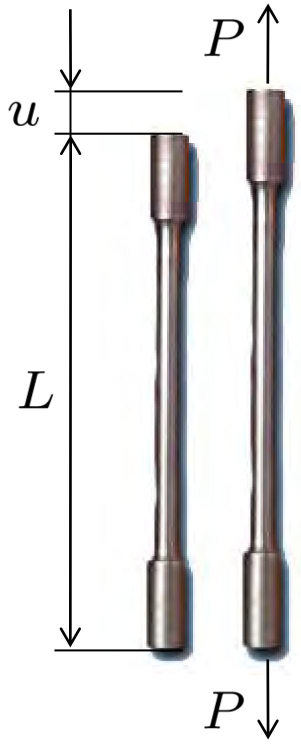

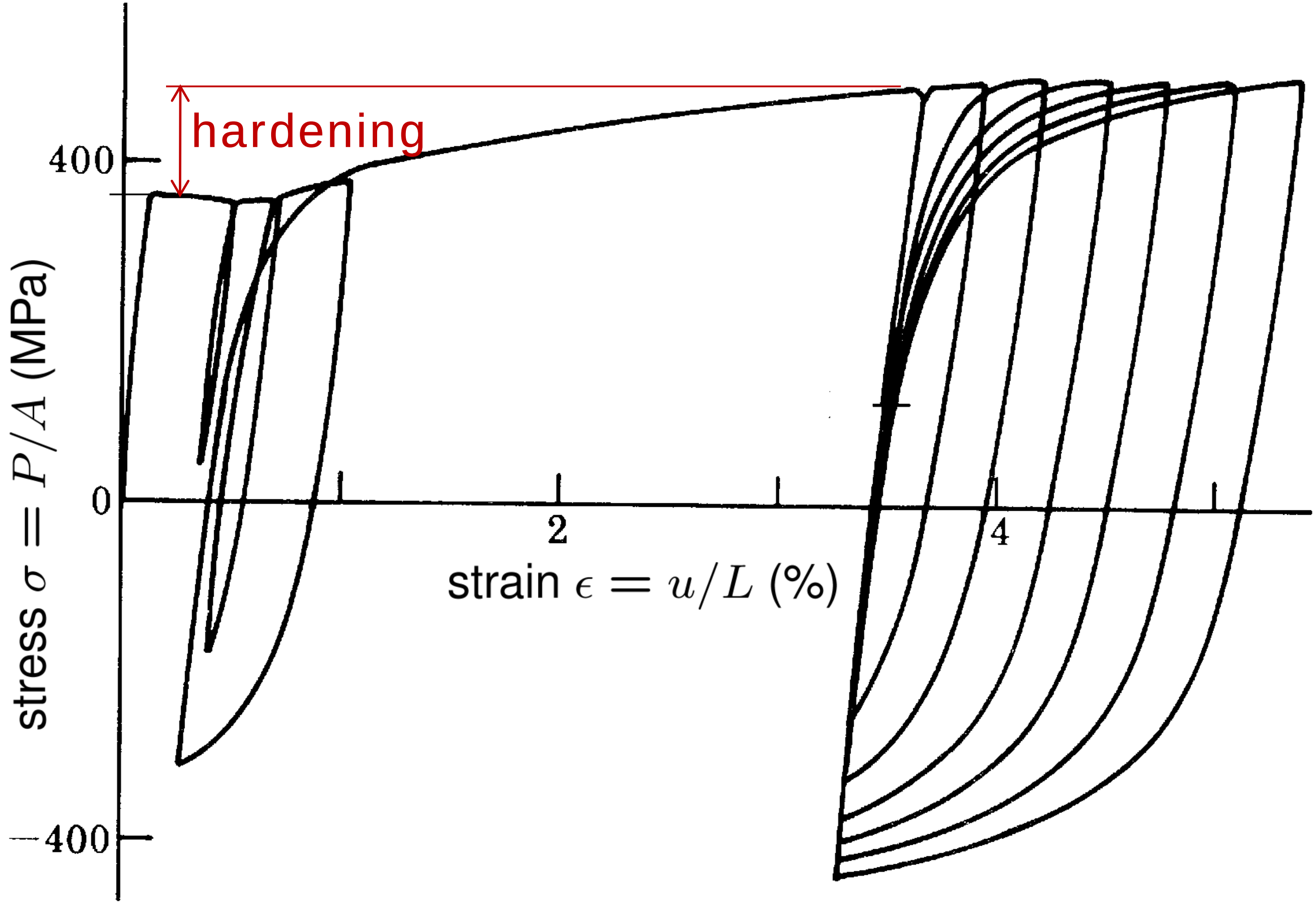

M. Ortiz and E.P. Popov,
Proc. Roy. Soc. Lond. A **379**, 439-458 (1982)

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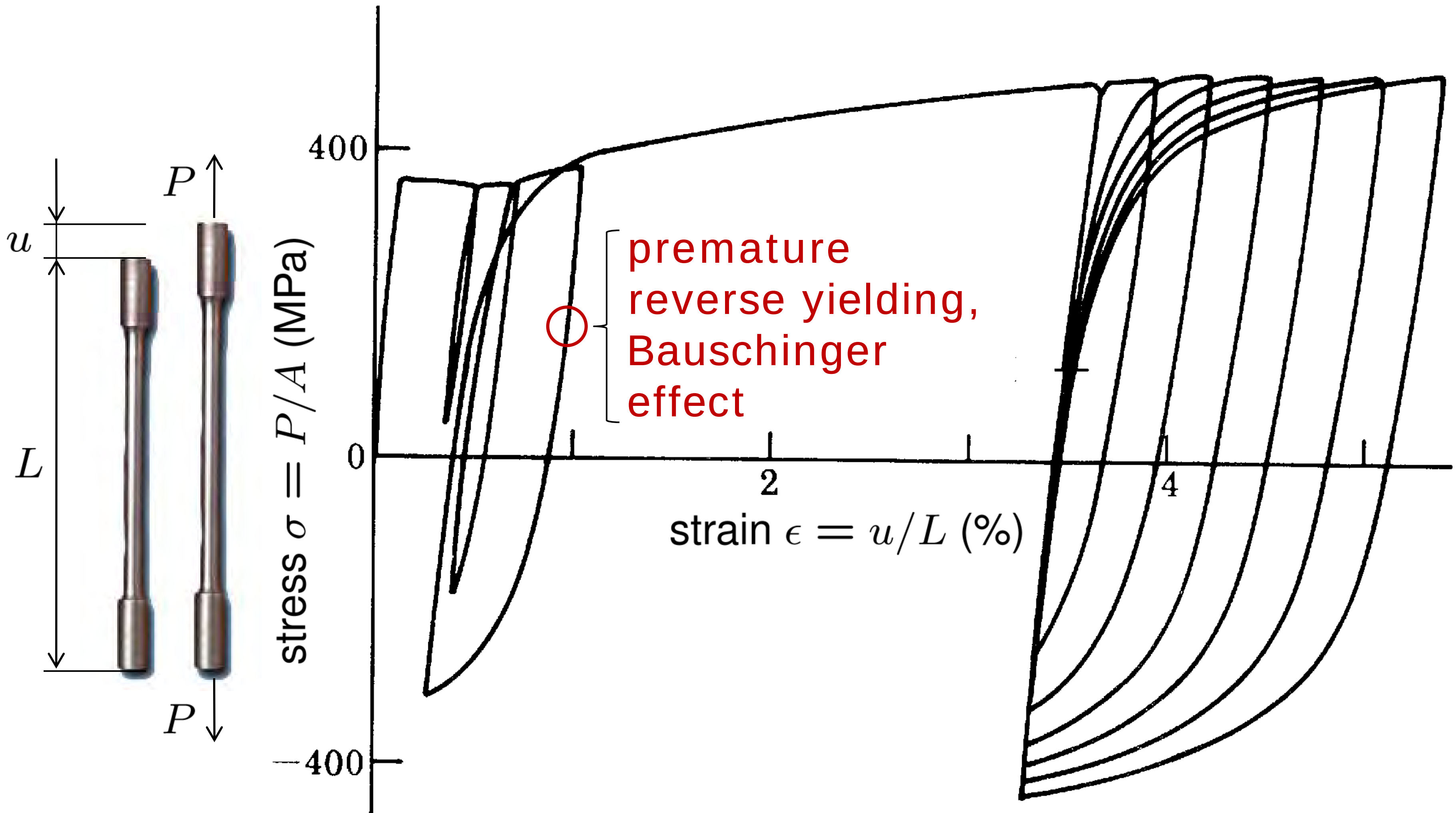

M. Ortiz and E.P. Popov,
Proc. Roy. Soc. Lond. A **379**, 439-458 (1982)

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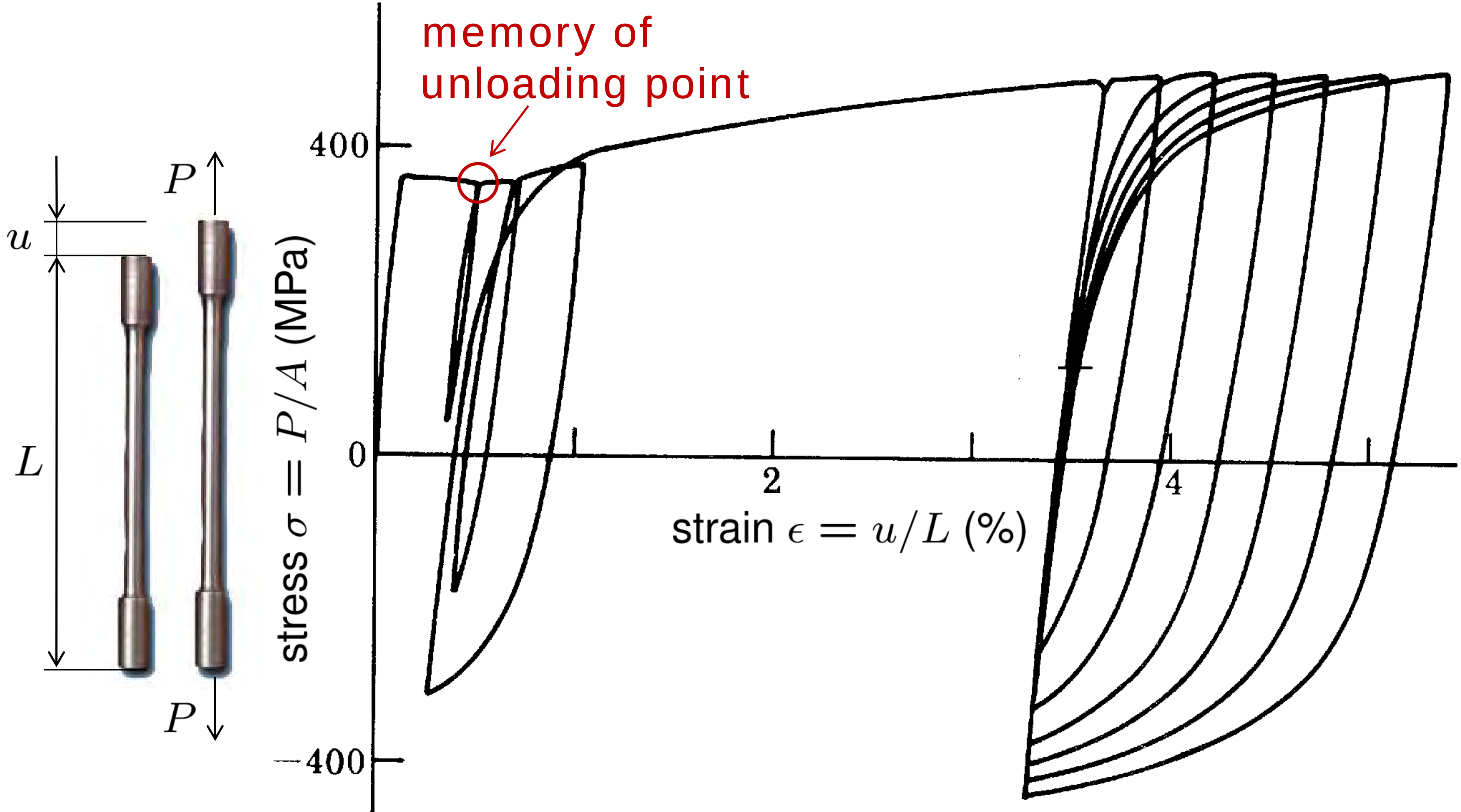

M. Ortiz and E.P. Popov,
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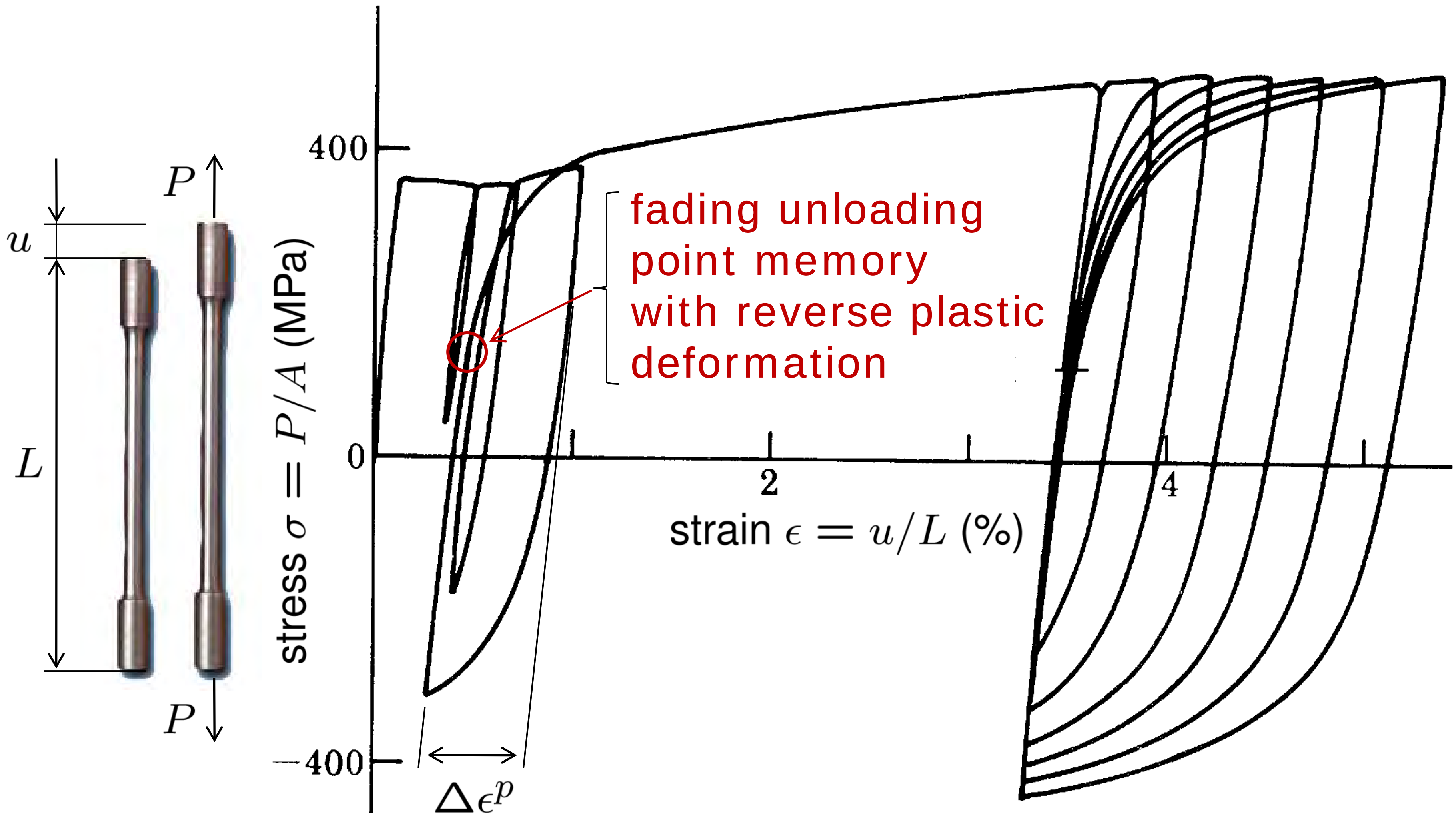

M. Ortiz and E.P. Popov,
Proc. Roy. Soc. Lond. A **379**, 439-458 (1982)

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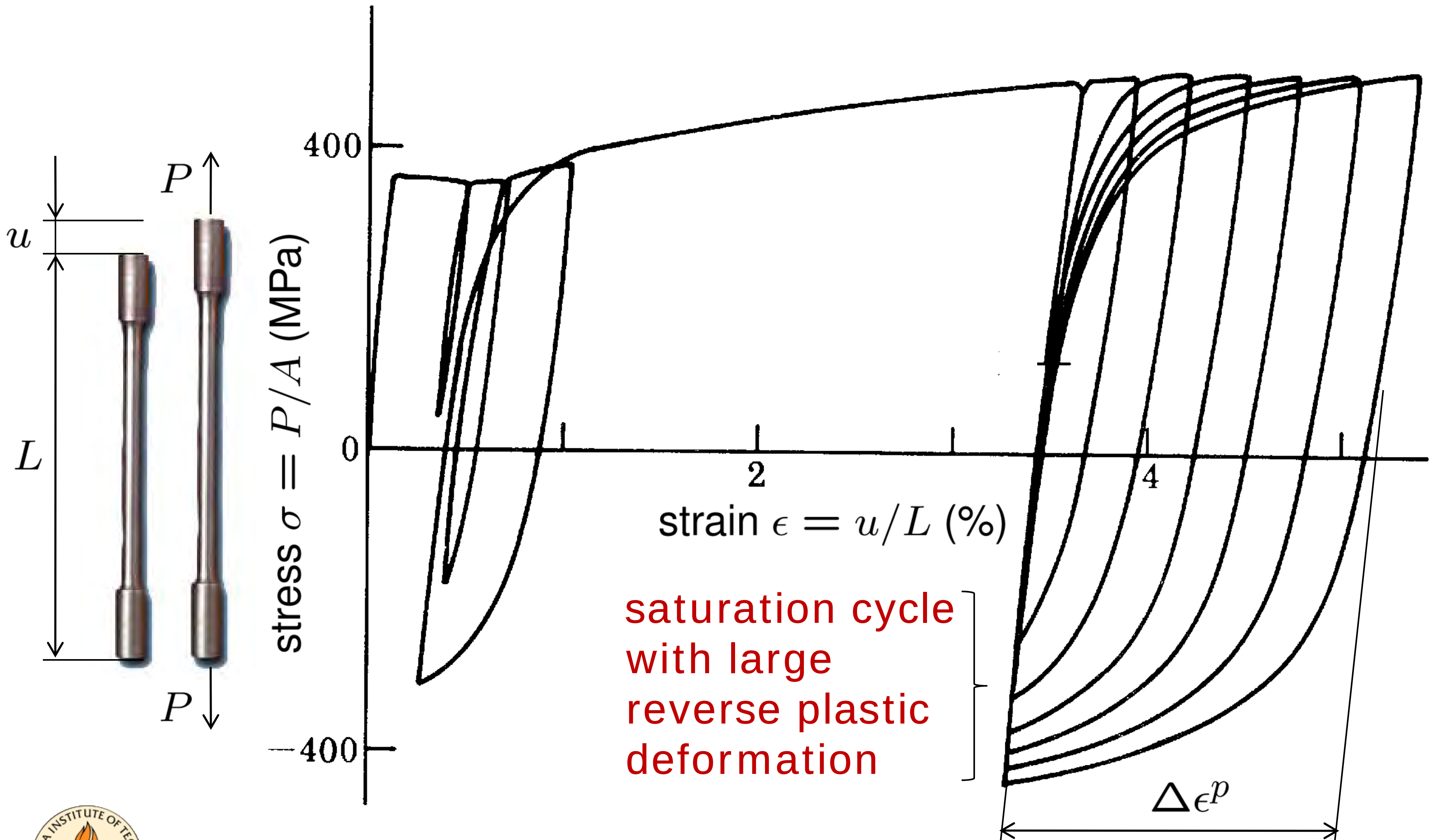
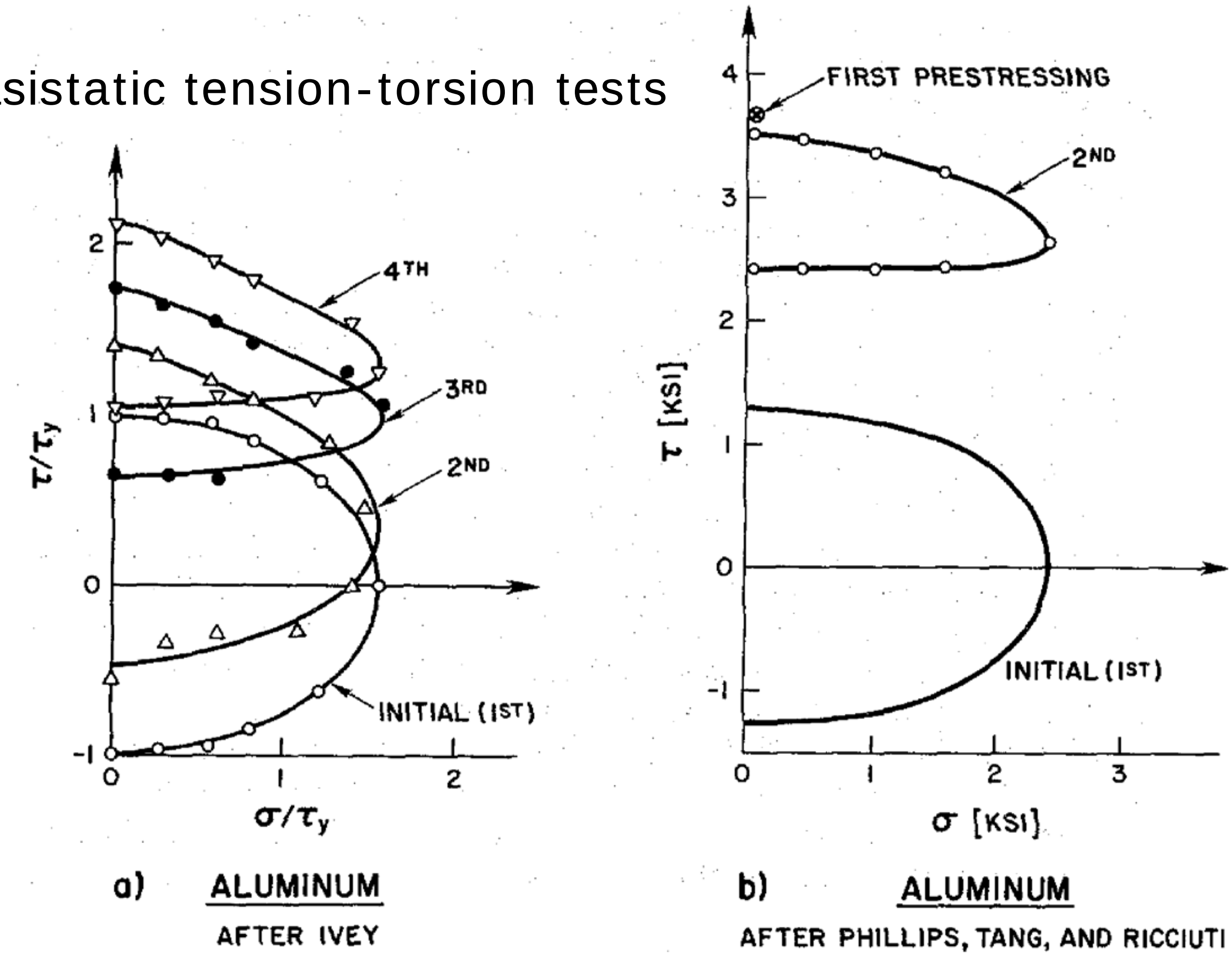


M. Ortiz and E.P. Popov, *Proc. Roy. Soc. Lond*. A **379**, 439-458 (1982)

Multiaxial elastic domain

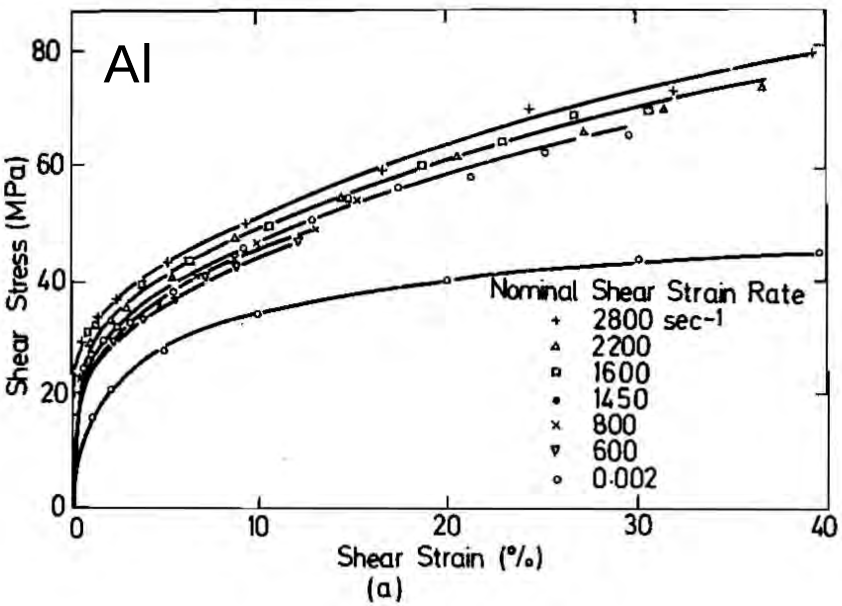
Quasistatic tension-torsion tests



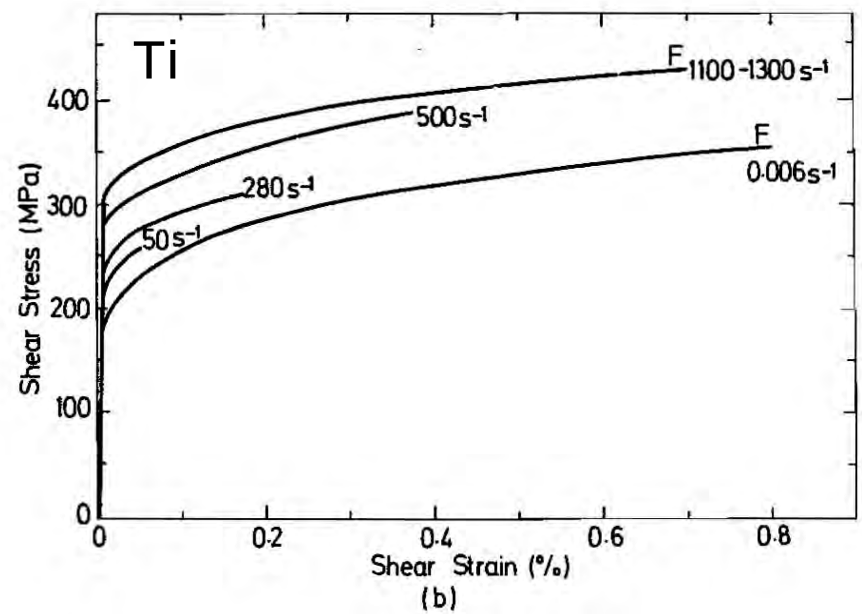
M. Ortiz and E.P. Popov,
J. Eng. Mech. ASCE **109** (4) 1042-1057 (1983)

Hardening and strain-rate dependence

Servo-hydraulic torsion tests



M.C.C. Tsao and J.D. Campbell, Oxford Eng. Lab. Report No. 1055 (1973)

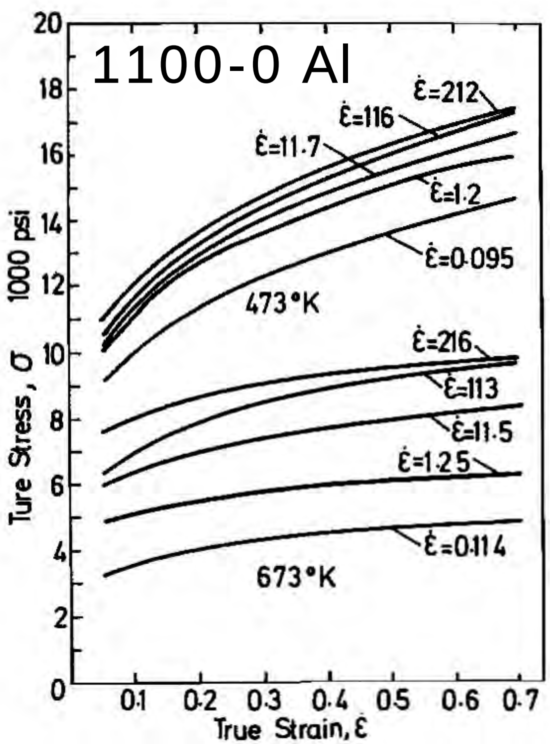


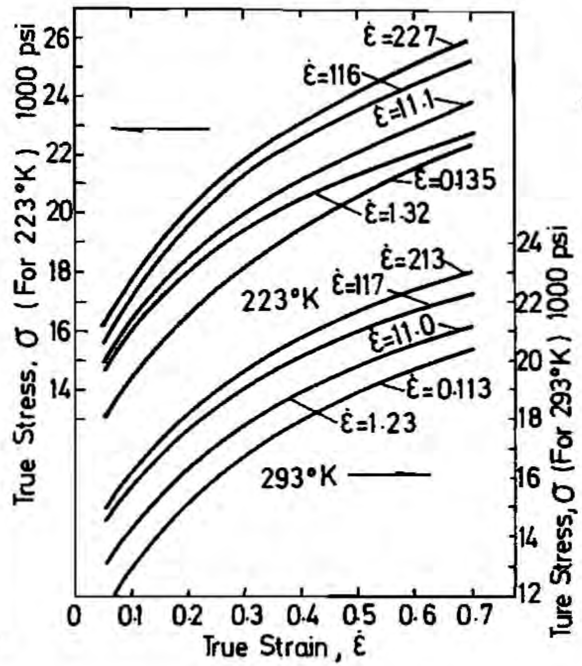
A.M. Eleiche and J.D. Campbell, Oxford Eng. Lab. Report No. 1106 (1974)

Y. Bai and B. Dodd, *Adiabatic Shear Localization,* Pergamon (1992)

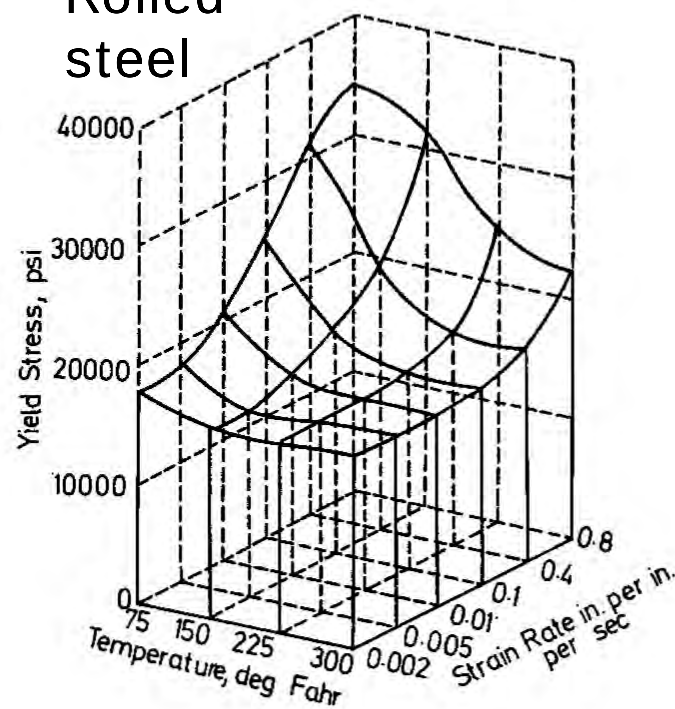
Thermal softening

Servo-hydraulic compression tests





Rolled steel



J.E. Hockett
Trans. AIME Metall. Soc., **239** (1967) 969-976.

Power-law fit:

$$\sigma = C(\epsilon^p)^n(\dot{\epsilon}^p)^m\theta^{-l}$$

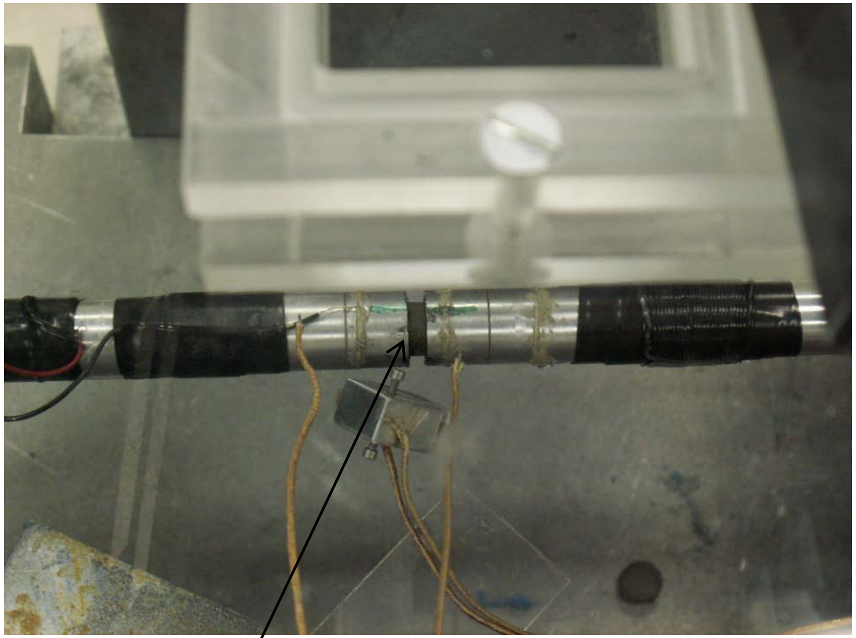
C.E. Work and T.J. Dolan
Proc. Am. Soc. Testing of Materials, **53** (1953) 611-656.

Y. Bai and B. Dodd,
Adiabatic Shear Localization, Pergamon (1992)

Dynamic testing

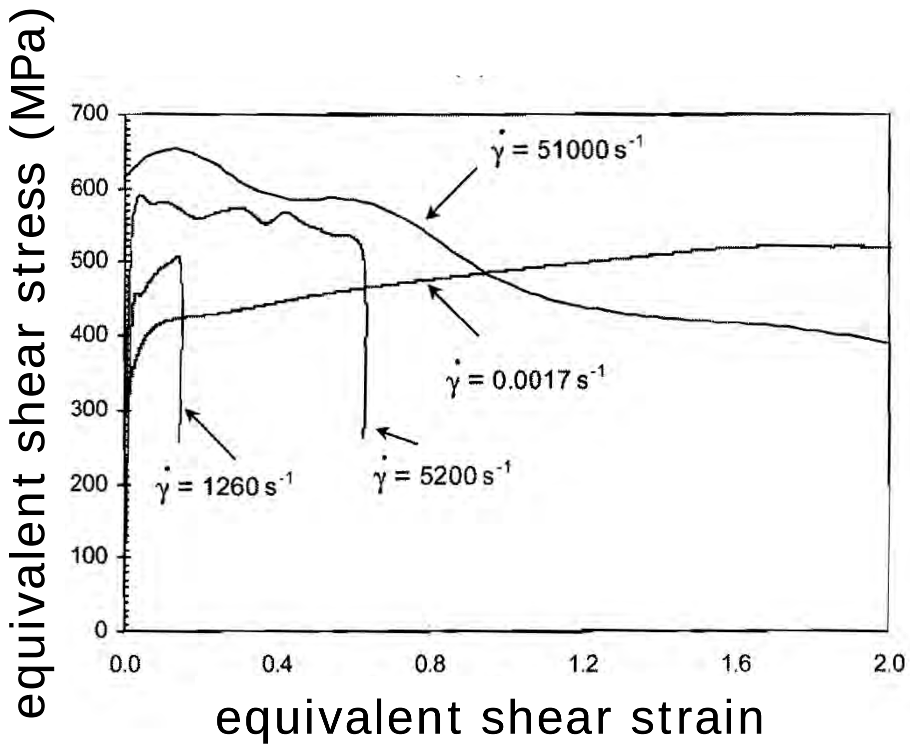
Split-Hopkinson (Kolsky) pressure bar

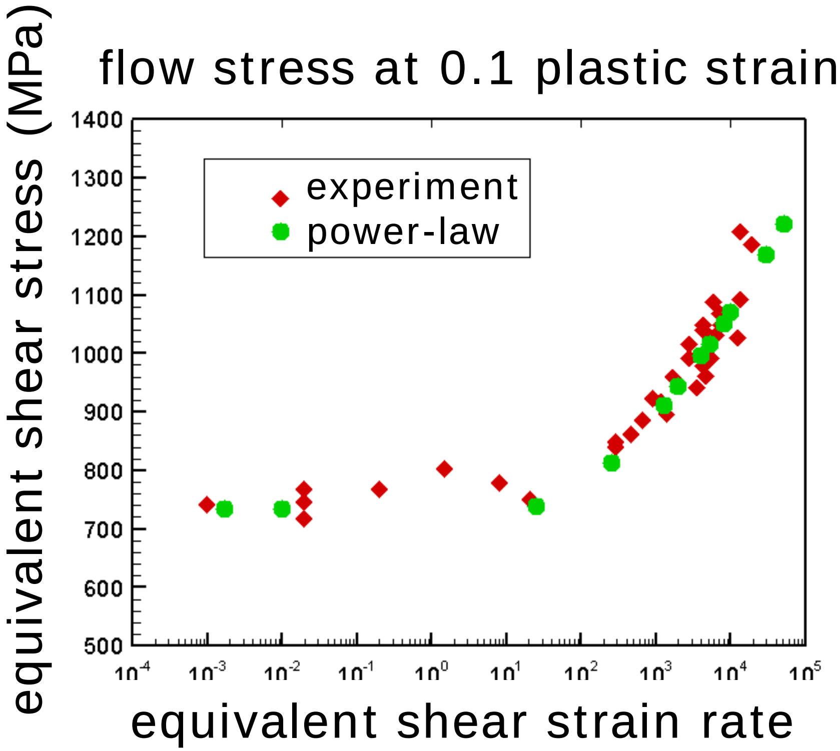
Independent measurements of stress, strain, temperature as functions of time



typical specimen

Strain-rate dependence of yield stress



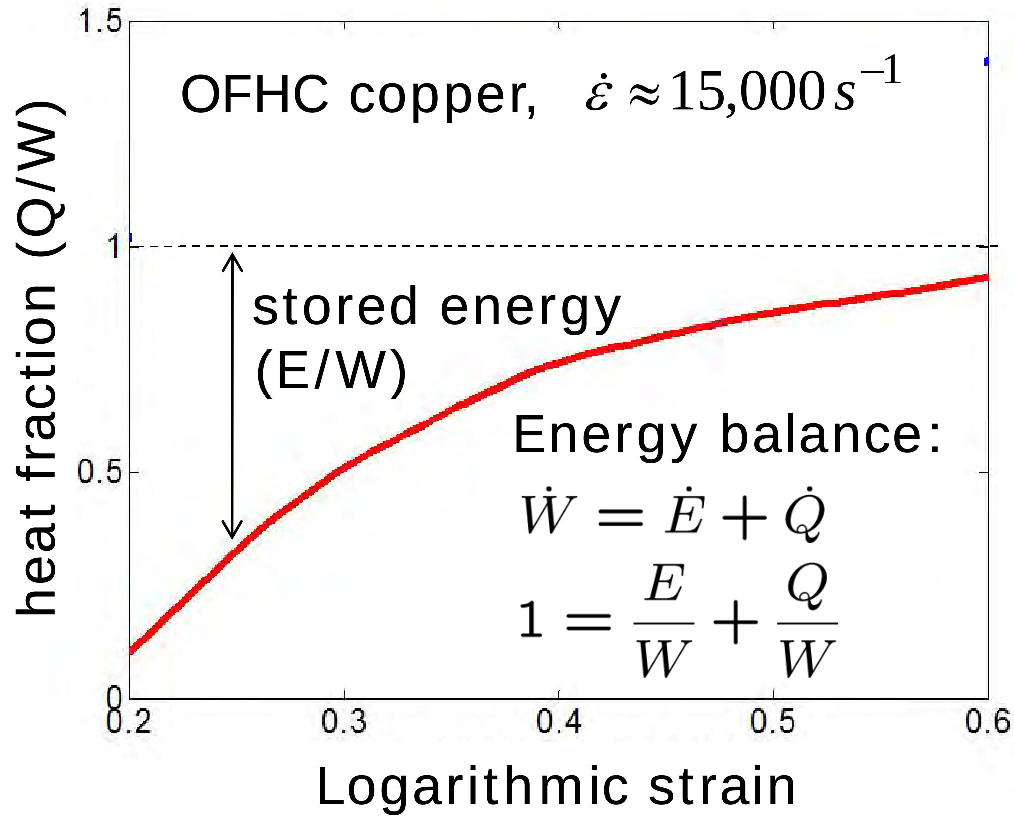


Shear-compression test

M. Vural, D. Rittel and G. Ravichandran, *Metall. Mater. Trans. A*, **34** (2003) 2873.

Energy storage and dissipation

Kolsky (split Hopkinson) pressure bar



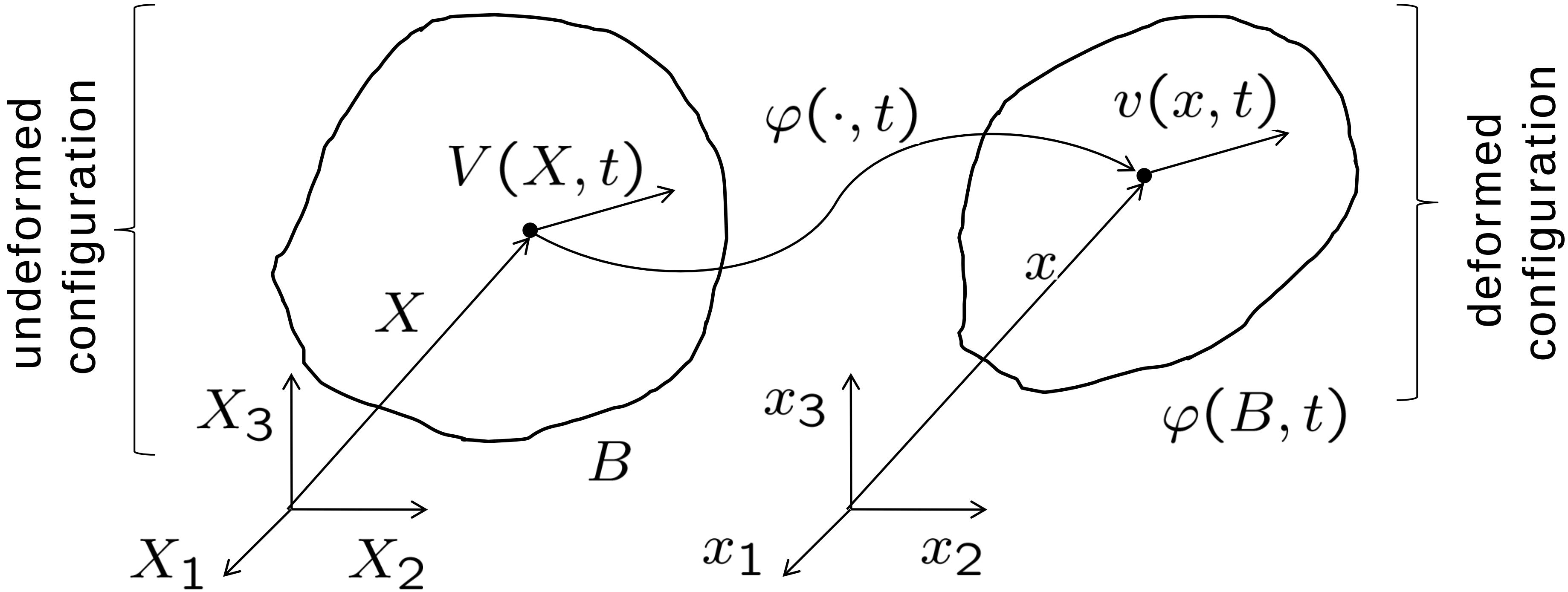
Fraction of total work dissipated as heat
Fraction of total work stored in lattice

D. Rittel, G. Ravichandran and S. Lee, *Mechanics of Materials*, **34** (2002) 627-642.

Continuum-thermodynamics framework

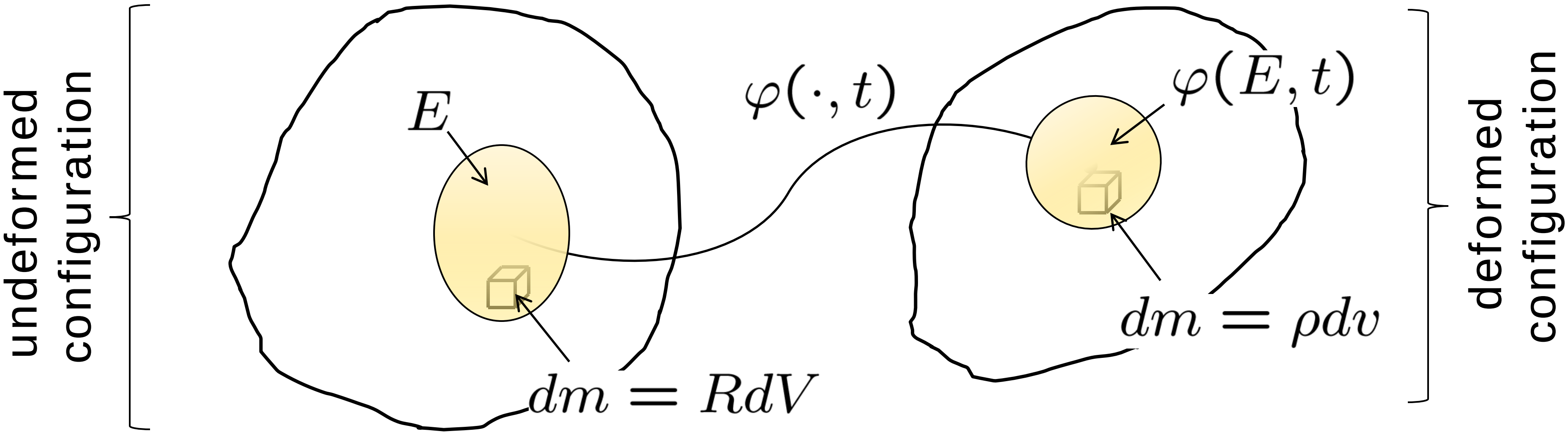
- Conservation laws:
  - *Conservation of mass*
  - *Conservation of linear momentum*
  - *Conservation of angular momentum*
  - *Conservation of energy*
  - *Second-law of thermodynamics*
- Onsager's theory of kinetic processes
- Application to finite-deformation plasticity
- Empirical engineering models
- Assessment of engineering models

Kinematics for finite deformation



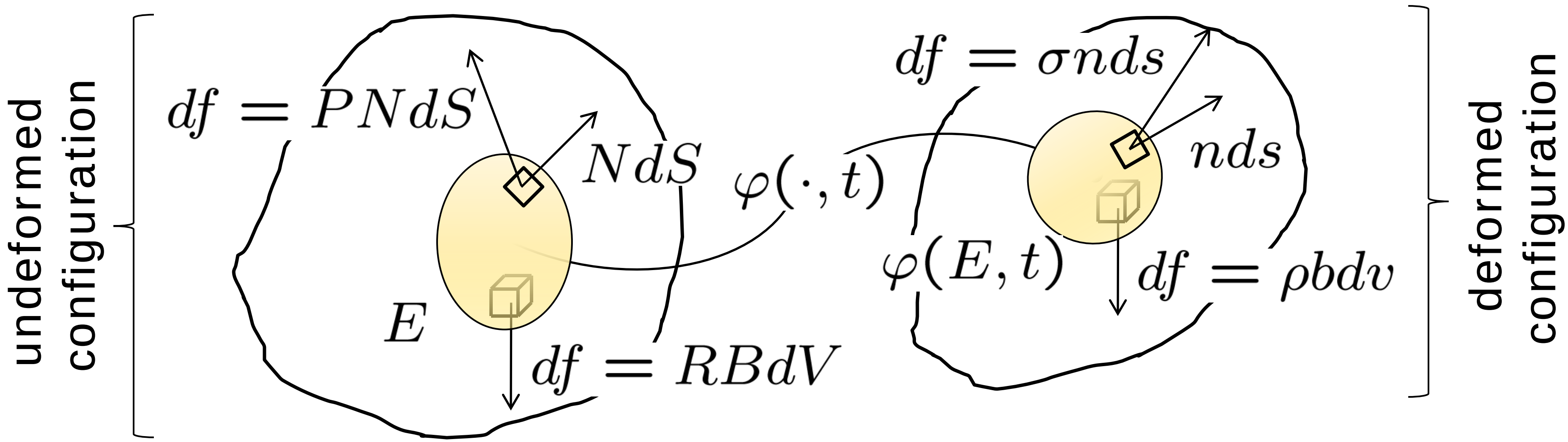
- Deformation mapping: $x = \varphi(X,t)$, $X \in B$, $t \geq t_0$
- Deformation gradient: $F(X,t) = \nabla\varphi(X,t)$
- Material velocity field: $V(X,t) = \dot{\varphi}(X,t)$
- Spatial velocity field: $v(x,t) = V(\varphi^{-1}(x,t),t)$
- Jacobian: $J(X,t) = \det(F(X,t))$

Conservation of mass



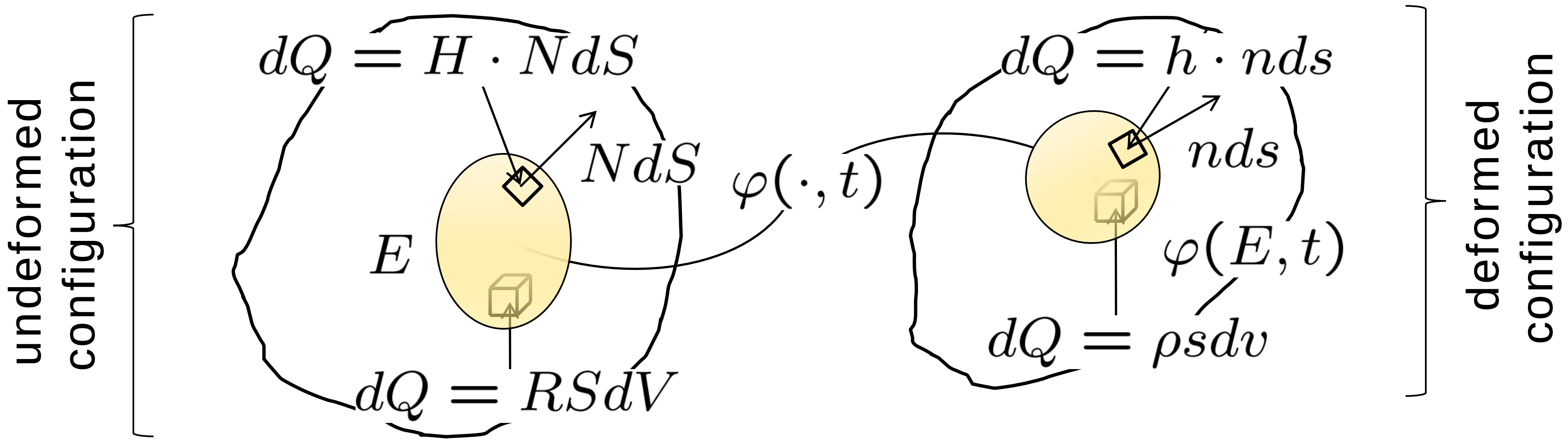
- $R \equiv$ mass density per unit undeformed volume
- $\rho = R/J \equiv$ mass density per unit deformed volume
- Lagrangian: $\frac{d}{dt}\int_E R dV = 0 \Leftrightarrow \dot{R}(X,t) = 0$
- Eulerian: $\frac{d}{dt}\int_{\varphi(E,t)} \rho dv = 0 \Leftrightarrow \dot{\rho} + \rho \nabla \cdot v = 0$

Conservation of linear and angular mom



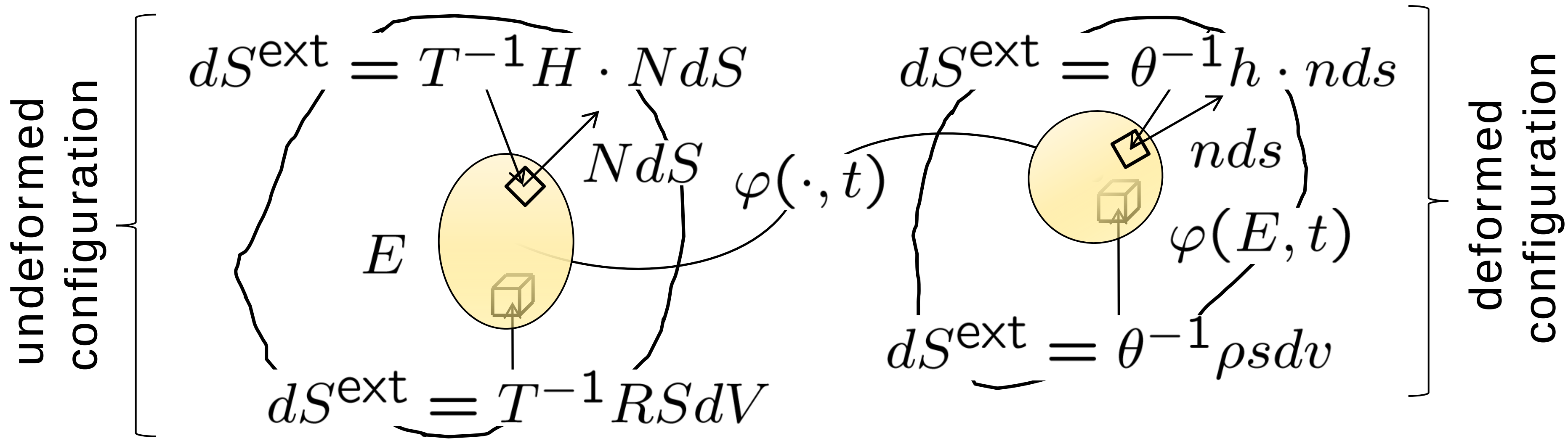
- $P \equiv$ First Piola-Kirchhoff stress tensor
- $\sigma = J^{-1} P F^T \equiv$ Cauchy stress tensor
- $B \equiv$ Body force/unit mass, undeformed conf.
- $b \equiv$ Body force/unit mass, deformed conf.
- Lagrangian: $R\dot{V} = \nabla \cdot P + RB, \quad PF^T = FP^T$
- Eulerian: $\rho\dot{v} = \nabla \cdot \sigma + \rho b, \quad \sigma^T = \sigma$

Conservation of energy



- $U \equiv$ Internal energy/unit mass, undeformed conf.
- $u \equiv$ Internal energy/unit mass, deformed conf.
- $H \equiv$ Outward heat flux, underformed conf.
- $h \equiv$ Outward heat flux, derformed conf.
- Lagrangian: $R\dot{U} = P \cdot \nabla V + RS - \nabla \cdot H$
- Eulerian: $\rho \dot{u} = \sigma \cdot \nabla v + \rho s - \nabla \cdot h$

Second law – Clausius-Duhem inequality



- $N \equiv$ Entropy/unit mass, undeformed conf.
- $\eta \equiv$ Entropy/unit mass, deformed conf.
- $T \equiv$ Absolute temperature, underformed conf.
- $\theta \equiv$ Absolute temperature, derformed conf.
- Lagrangian: $R\dot{N} - \frac{RS}{T} - \nabla \cdot \frac{H}{T} \geq 0$
- Eulerian: $\rho\dot{\eta} - \frac{\rho s}{\theta} - \nabla \cdot \frac{h}{\theta} \geq 0$

The Coleman-Noll theorem

- $Q \equiv$ Internal variable set
- $Y = -R\partial_Q U \equiv$ Conjugate thermodynamic forces
- $P^e = R\partial_F U \equiv$ Equilibrium stresses
- $P^v = P - P^e \equiv$ Viscous stresses

Theorem [Coleman and Noll] *Suppose that a motion satisfies conservation of mass, linear momentum, angular momentum, energy and the Clausius-Duhem inequality. Then,*

i) $U = U(F, N, Q)$; *ii)* $T = \partial_N U(F, N, Q)$;

iii) $P^v \cdot \dot{F} + Y \cdot \dot{Q} - H \cdot \frac{\nabla T}{T} \geq 0$.

The Coleman-Noll theorem (1 of 3)

Sketch of proof: Combine first and second laws,

$$RT\dot{N} - R\dot{U} + P \cdot \dot{F} - H \cdot \frac{\nabla T}{T} \geq 0$$

Assume: $U = U(F, \nabla F, \dots, \dot{F}, \dots, N, \nabla N, \dot{N}, \dots, Q)$. Then,

$$RT\dot{N} - R\Big(\frac{\partial U}{\partial F} \cdot \dot{F} + \frac{\partial U}{\partial \nabla F} \cdot \nabla \dot{F} + \cdots + \frac{\partial U}{\partial \dot{F}} \cdot \ddot{F} + \dots$$
$$\frac{\partial U}{\partial N} \cdot \dot{N} + \frac{\partial U}{\partial \nabla N} \cdot \nabla \dot{N} + \cdots + \frac{\partial U}{\partial \dot{N}} \cdot \ddot{N} + \dots$$
$$\frac{\partial U}{\partial Q} \cdot \dot{Q}\Big) + P \cdot \dot{F} - H \cdot \frac{\nabla T}{T} \geq 0$$

The Coleman-Noll theorem (2 of 3)

Use: $P^v \equiv P - R\partial_F U$, $Y \equiv -R\partial_Q U$ and group terms,

$$R\left(T - \frac{\partial U}{\partial N}\right)\dot{N} - R\left(\frac{\partial U}{\partial \nabla F}\cdot\nabla\dot{F} + \cdots + \frac{\partial U}{\partial \dot{F}}\cdot\ddot{F} + \ldots \right.$$

$$\left.\frac{\partial U}{\partial \nabla N}\cdot\nabla\dot{N} + \cdots + \frac{\partial U}{\partial \dot{N}}\cdot\ddot{N} + \ldots\right) + Y\cdot\dot{Q} + P^v\cdot\dot{F} - H\cdot\frac{\nabla T}{T} \geq 0$$

Since $\nabla\dot{F}, \ldots, \ddot{F}, \ldots, \dot{N}, \nabla\dot{N}, \ldots, \ddot{N}, \ldots$ are arbitrary,

$$\left.\begin{array}{ll} T = \dfrac{\partial U}{\partial N}, & \\ \dfrac{\partial U}{\partial \nabla F}\cdot\nabla\dot{F} = 0, \ldots, & \dfrac{\partial U}{\partial \dot{F}}\cdot\ddot{F} = 0, \ldots, \\ \dfrac{\partial U}{\partial \nabla N}\cdot\nabla\dot{N} = 0, \ldots, & \dfrac{\partial U}{\partial \dot{N}}\cdot\ddot{N} = 0, \ldots, \end{array}\right\}$$

The Coleman-Noll theorem (3 of 3)

Hence, $U = U(F, N, Q)$,

$$\left.\begin{aligned} P &= \frac{\partial U}{\partial N}(F, N, Q) + P^v \\ T &= \frac{\partial U}{\partial N}(F, N, Q) \\ Y &= -\frac{\partial U}{\partial Q}(F, N, Q) \end{aligned}\right\} \text{equilibrium relations}$$

and $\quad Y \cdot \dot{Q} + P^v \cdot \dot{F} - H \cdot \frac{\nabla T}{T} \geq 0 \quad$ (dissipation inequality)

q. e. d.

- $\dot{Q}$, P^v and H not given by the equilibrium relations.
- Need additional (kinetic) constitutive relations.

Onsager's theory of kinetics

- $X = (\dot{Q}, \dot{F}, -\frac{\nabla T}{T}) \equiv$ Thermodynamic forces
- $J = (Y, P^v, H) \equiv$ Thermodynamic fluxes
- Onsager kinetic relations: $J = \partial\psi(X)$
- Dissipation inequality: $X \cdot J = X \cdot \partial\psi(X) \geq 0$
- Assume $0 \in \partial\psi(0) \Rightarrow \psi$ convex!
- Inverse Onsager relations: $X = \partial\psi^*(J)$
- Viscoelasticity: $\dot{Q} = \partial\psi^*(Y)$, $\psi^*(Y)$ strictly convex
- Viscoplasticity: $\psi^*(Y)$ not strictly convex$\Rightarrow$yielding!
- Viscosity law: $P^v = \partial\psi(\dot{F})$, (e. g., Newtonian)
- Heat conduction: $H = \partial\psi(-\frac{\nabla T}{T})$, (e. g., Fourier)

Example: Isotropic von Mises plasticity

- Internal variables: $Q \equiv (F^p, \epsilon^p) \in \mathbb{R}^{n\times n} \times \mathbb{R}$
- $F^p \equiv$ Plastic deformation (upon unloading)
- $\epsilon^p \equiv$ Effective plastic strain (von Mises)
- Free energy: $RA = W^e(FF^{p-1}, T) + W^p(\epsilon^p, T)$
- $W^e(F^e, T) \equiv$ Elastic strain-energy density
- $W^p(\epsilon^p, T) \equiv$ Stored energy $\Rightarrow$ hardening!
- Flow rule, rate-sensitivity:

$$\psi^*(\dot{F}^p, \dot{\epsilon}^p) = \begin{cases} \psi^*(\dot{\epsilon}^p), & \text{if } \dot{\epsilon}^p = |\dot{F}^p F^{p-1}|, \\ +\infty, & \text{otherwise.} \end{cases}$$

- In practice: W^p, $\psi^* \Rightarrow$ power-laws, calibration

Minimum principles – Rate IBVP

- Mixed rate functional: $L(\dot{\varphi}, \dot{N}, \dot{Q}; T) =$

$$\int_B \left[R(\dot{U} - T\dot{N}) + \psi\left(\frac{T\dot{Q}}{\partial_N U}, \frac{T\dot{F}}{\partial_N U}, -\frac{\nabla T}{T}\right) \right] dV$$

- Rate functional: $G(\dot{\varphi}, \dot{N}, \dot{Q}) = \sup_T L(\dot{\varphi}, \dot{N}, \dot{Q}; T)$
- Rate IBVP of coupled thermoviscoplasticity:

$$\left.\begin{array}{l} (\dot{\varphi}(t), \dot{N}(t), \dot{Q}(t)) \in \text{argmin}\, G, \quad t \geq 0 \\ (\varphi(0), N(0), Q(0)) = (\varphi_0, N_0, Q_0) \end{array}\right\}$$

- Time-discretized incremental problem, $t_n \to t_{n+1}$:

$$(\varphi_{n+1}, N_{n+1}, Q_{n+1}) \ni \text{argmin} F_n \equiv$$

$$\int_B \left[R(\Delta U - T_{n+1} \Delta N) + \Delta t \psi_{n+1} \right] dV$$

Q. Yang, L. Stainier and M. Ortiz, *JMPS*, **54** (2006) 401-424

Limitations of empirical models

Chip Morphology Validation

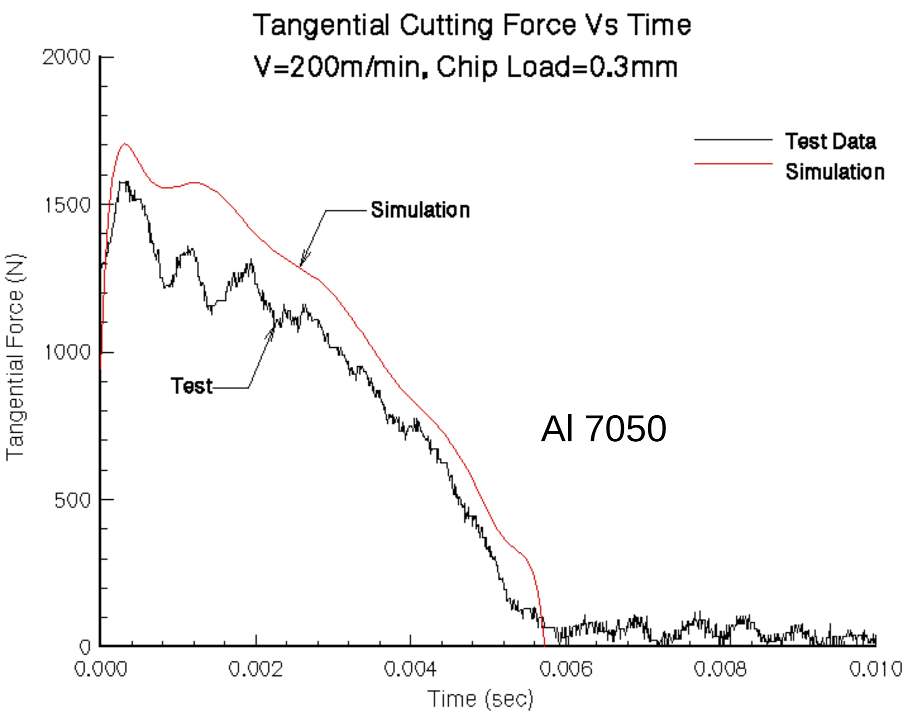
(Courtesy of Third Wave Systems Inc)

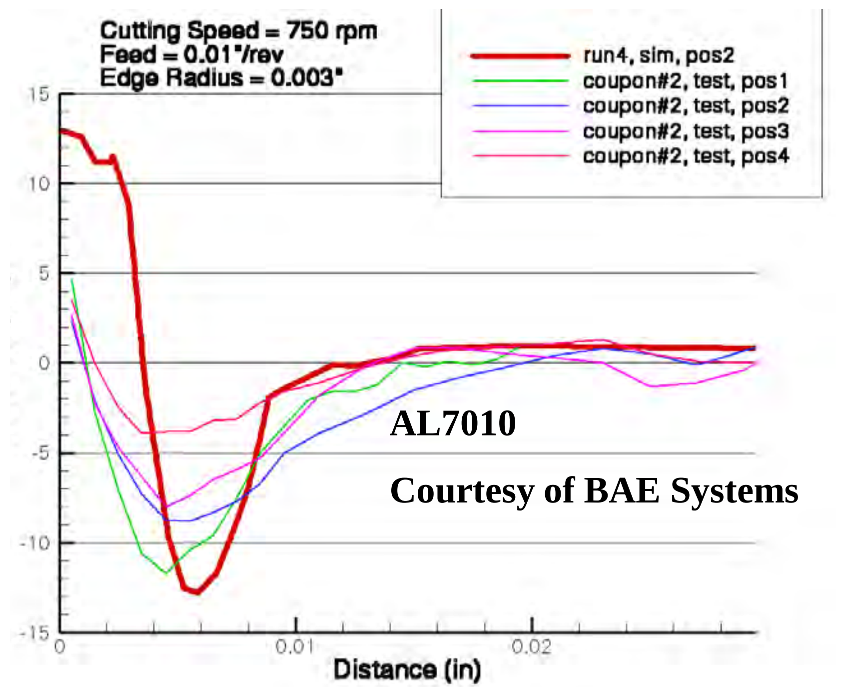
(Courtesy of IWH, Switzerland) FE simulation

T.D. Marusich and M. Ortiz
Int. J. Numer. Meth. Eng., **38** (1995) 3675-3694

Limitations of empirical models

(Courtesy of Third Wave Systems Inc)





Cutting Force Validation

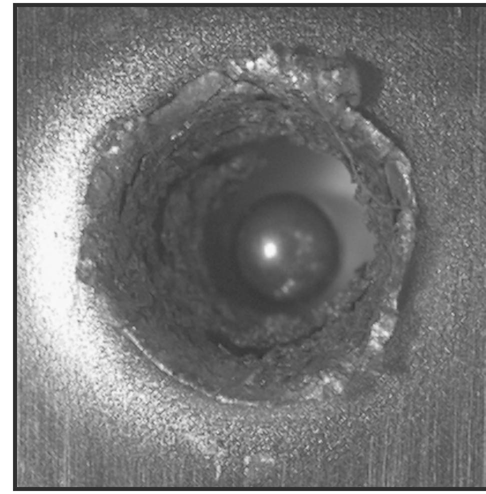
Residual Stress Validation

General trends predicted, but discrepancies remain!

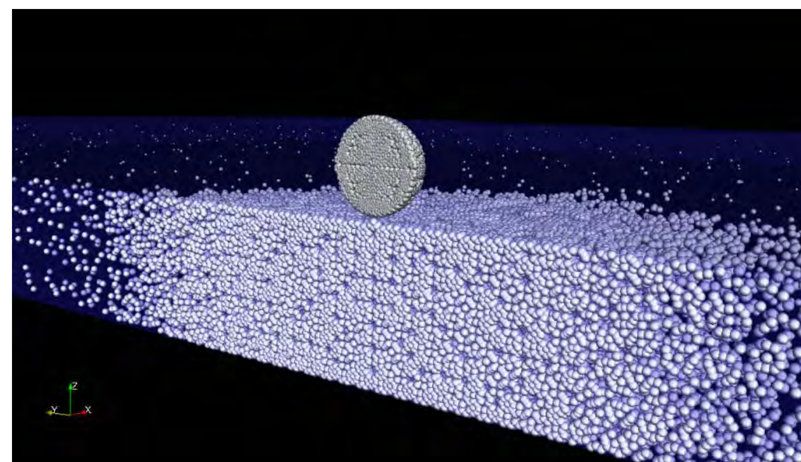
T.D. Marusich and M. Ortiz
Int. J. Numer. Meth. Eng., **38** (1995) 3675-3694

Limitations of empirical models

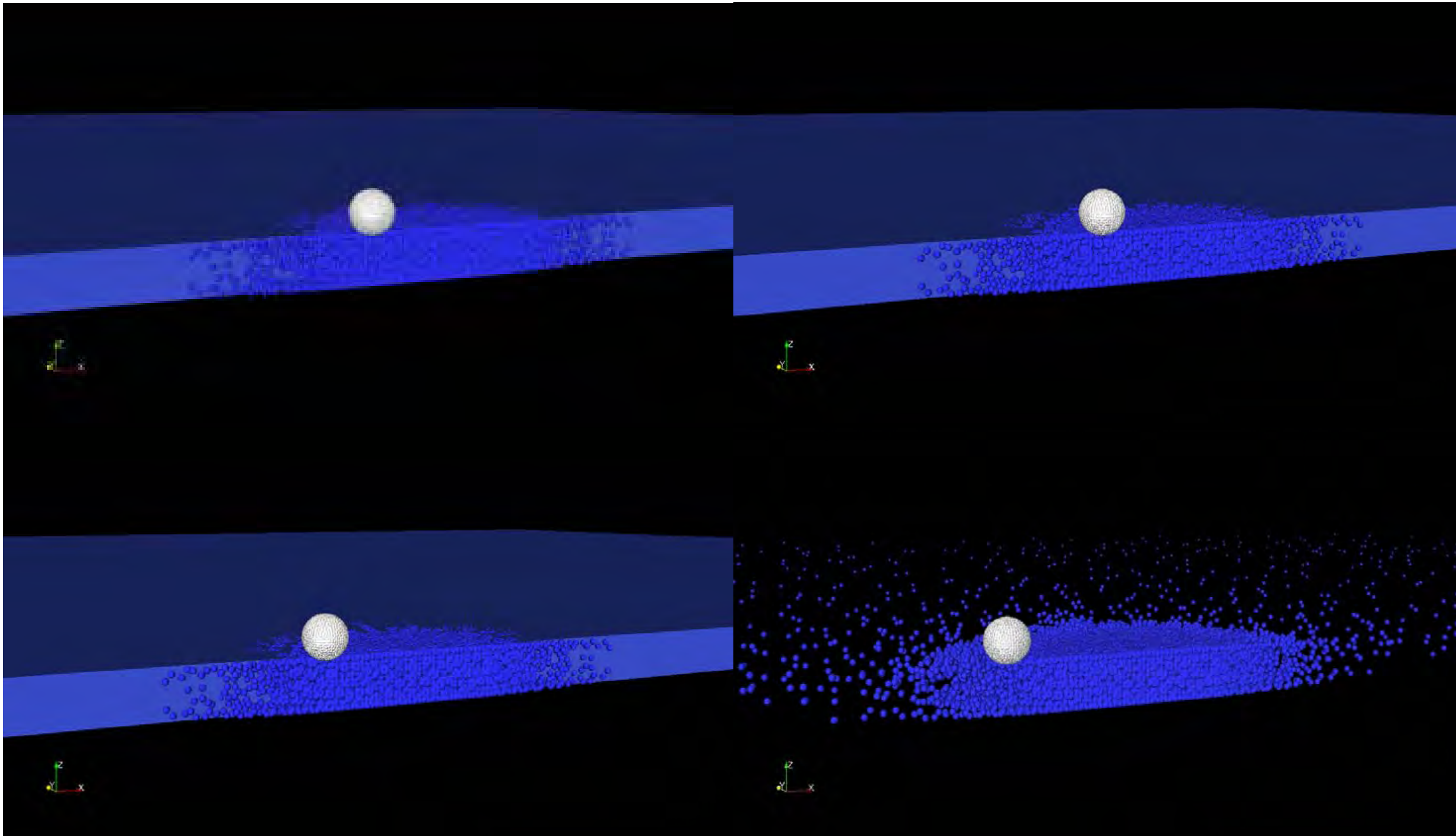
- Target/projectile materials:
  - *Target: Al6061-T6 Plates*
  - *Projectile: 440 C Steel Spheres*
- Experimental facilities: Small Particle Hypervelocity Impact Range (A.J. Rosakis, Caltech)
- Performance measure (output): Perforation area
- Model parameters (inputs):
  - *Plate thickness (62-125 mils)*
  - *Obliquity (0-30 degrees)*
  - *Impact velocity (2-3 km/s)*
- Solver: OTM (Li *et al*., 2010)
- Engineering plasticity models
- Wanted: Maximum modeling error



Steel-on-steel, 2.6 km/s damage zone and impactor

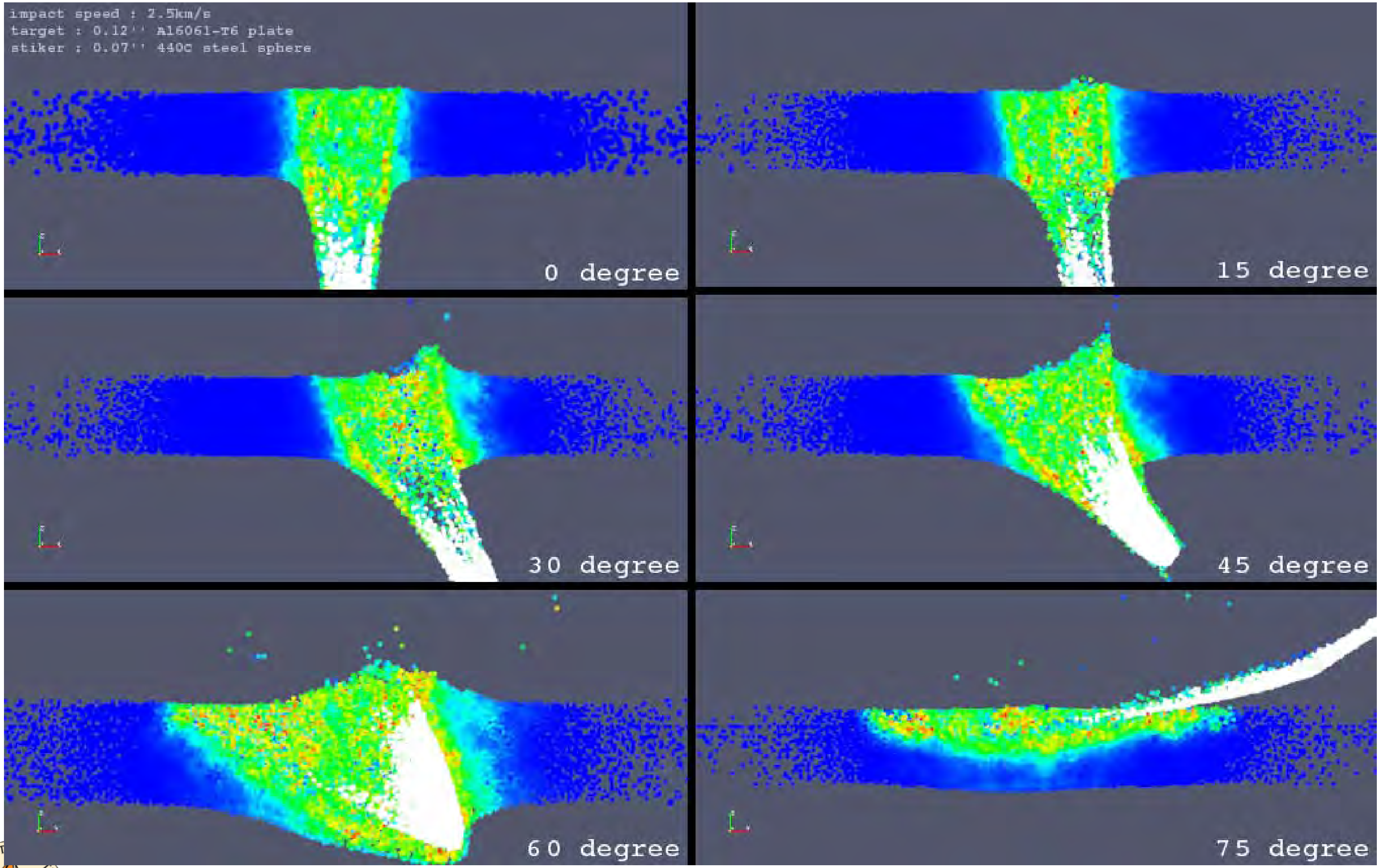


Limitations of empirical models



B. Li, F. Habbal and M. Ortiz,
Int. J. Numer. Meth. Eng., **83** (2010) 1541-1579

OTM – Terminal ballistics

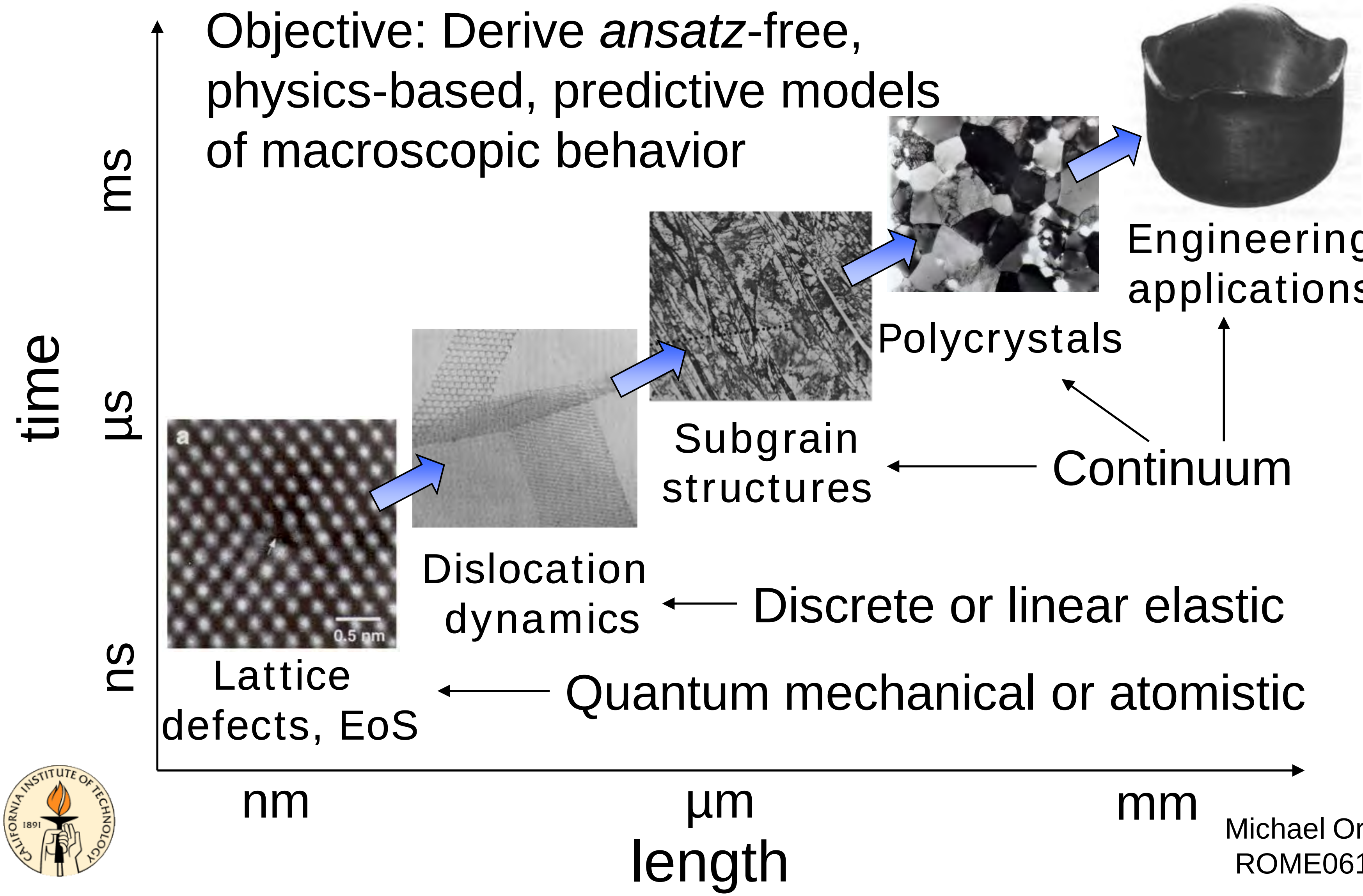


Metal plasticity − Multiscale analysis

- General trend captured by empirical model without *a posteriori* parameter calibration
- However, errors of the order of the order of 20% remain in the calculated perforation area
- Behavior of polycrystalline metals is too complex to yield to *ad hoc* modeling
- Alternative paradigm: Multiscale analysis
  - *Identify underlying microstructural mechanisms*
  - *Derive rigorous models of effective behavior across scales, including kinetics*
  - *Develop high-fidelity (but fast!) physics models...*

Metal plasticity − Multiscale analysis

Objective: Derive *ansatz*-free, physics-based, predictive models of macroscopic behavior



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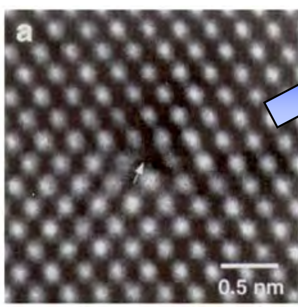
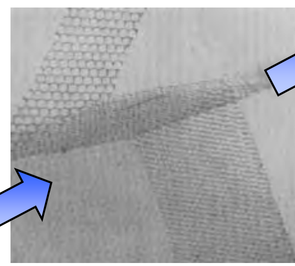
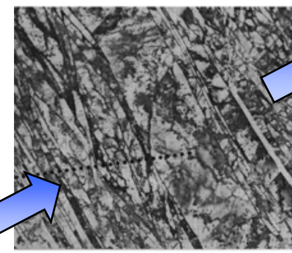


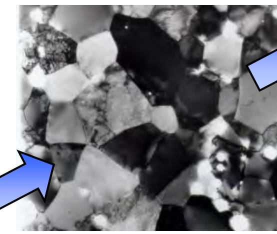
Lattice defects, EoS ← **Lecture #2**: Dislocation energies, the line-tension approximation



Dislocation dynamics ← **Lecture #3**: Dislocation kinetics, the forest-hardening model



Subgrain structures ← **Lecture #4**: Subgrain dislocation structures



Polycrystals

Engineering applications

time: ns, µs, ms

length: nm, µm, mm

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