

Multiscale models of metal plasticity

Lecture I: Experimental and continuum thermodynamics basis

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Sixth Summer School in Analysis and
Applied Mathematics

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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



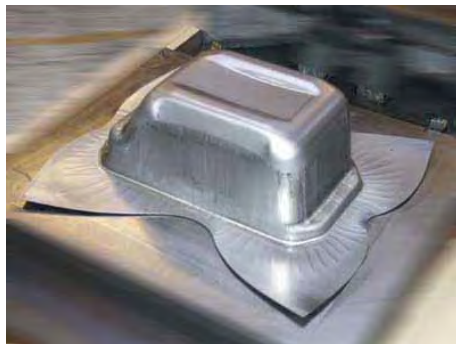
Plasticity applications - Manufacturing



Metal ingot after forging



Lathe cutting metal
from workpiece



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



Cold rolling
of steel



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

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Plasticity applications – Metallic structures



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

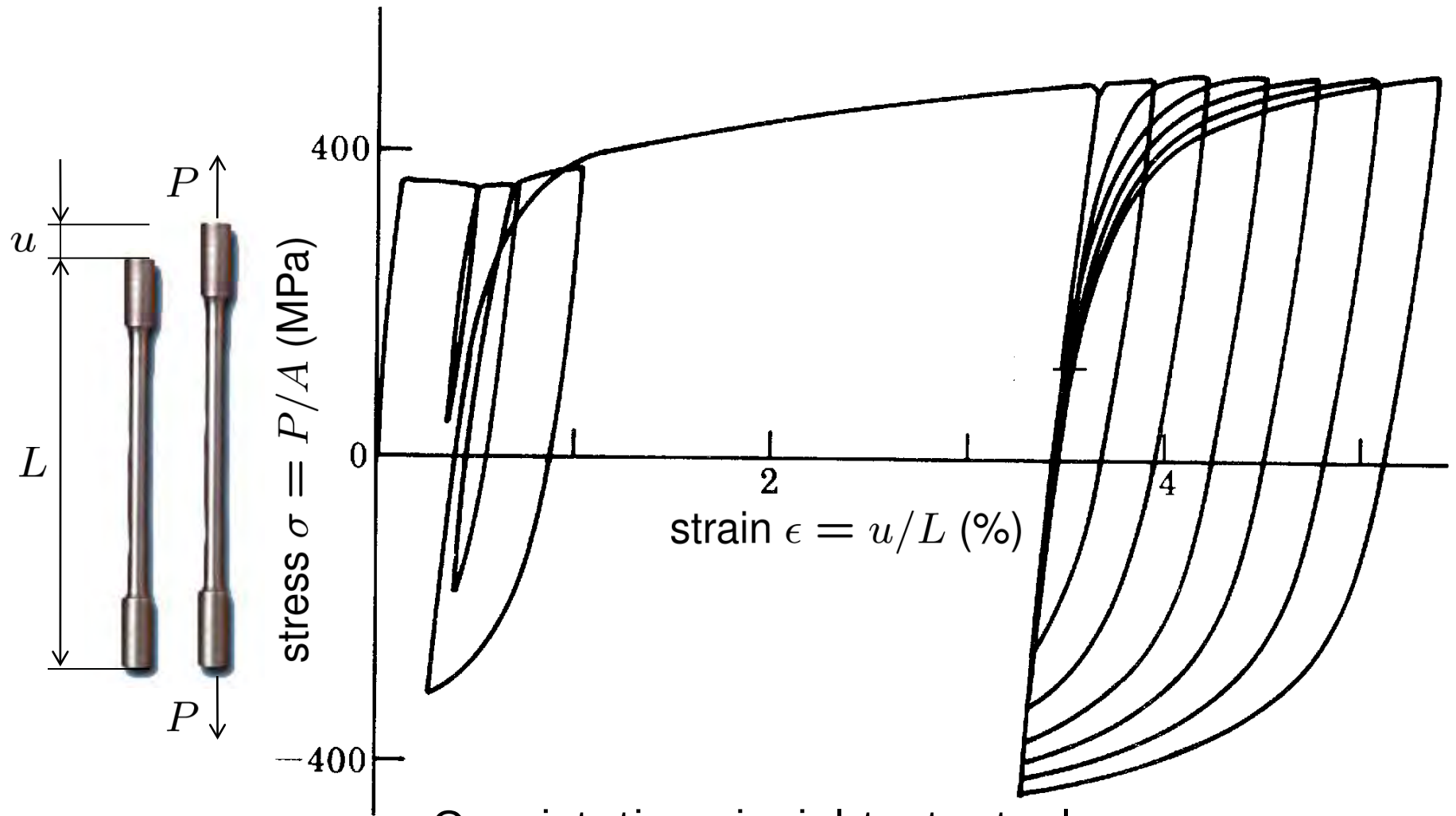
Mid-story collapse,
1995 Kobe earthquake
(EQE Summary Rep., 1995)

Experimental basis of macroscopic 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



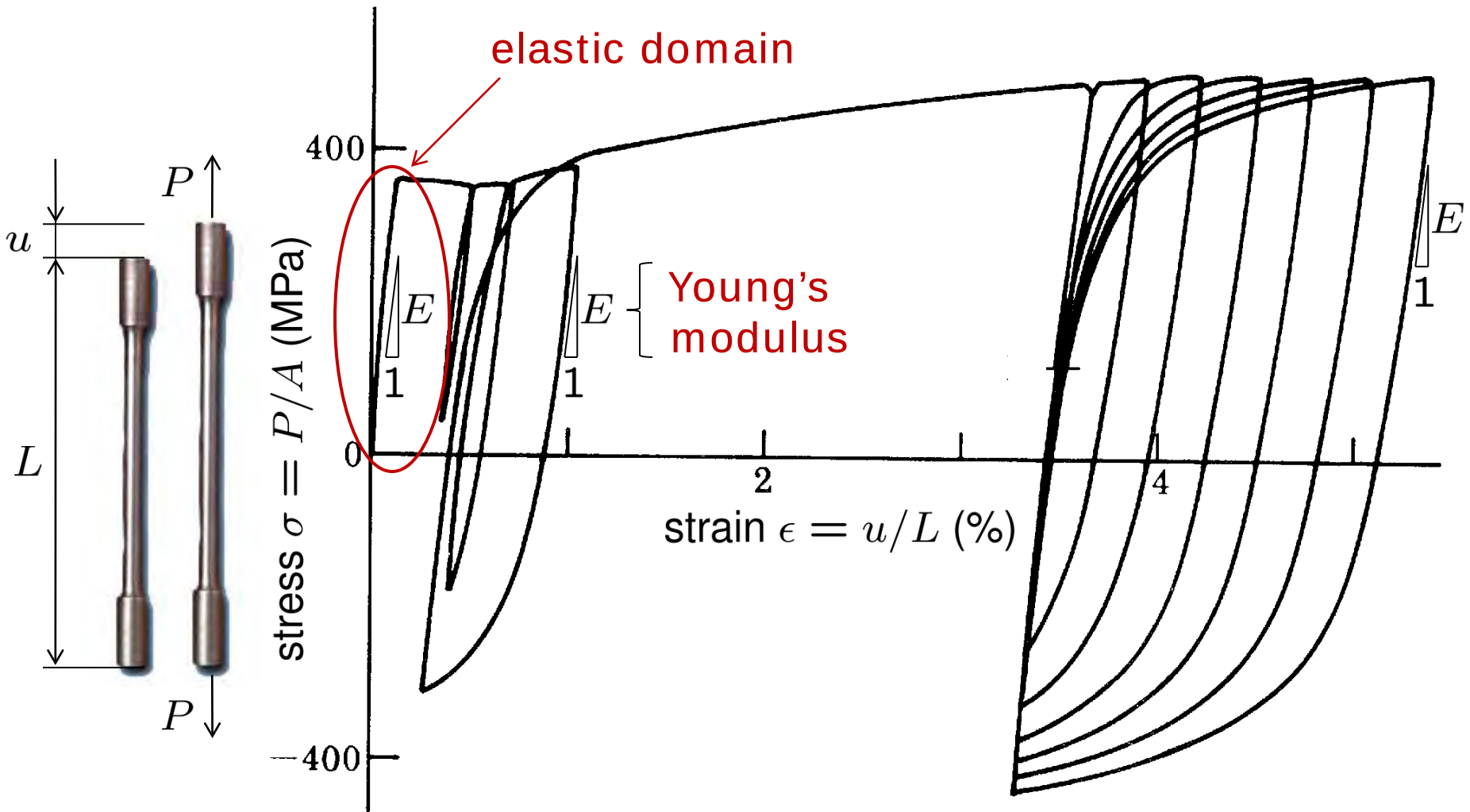
Quasistatic uniaxial test, steel



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

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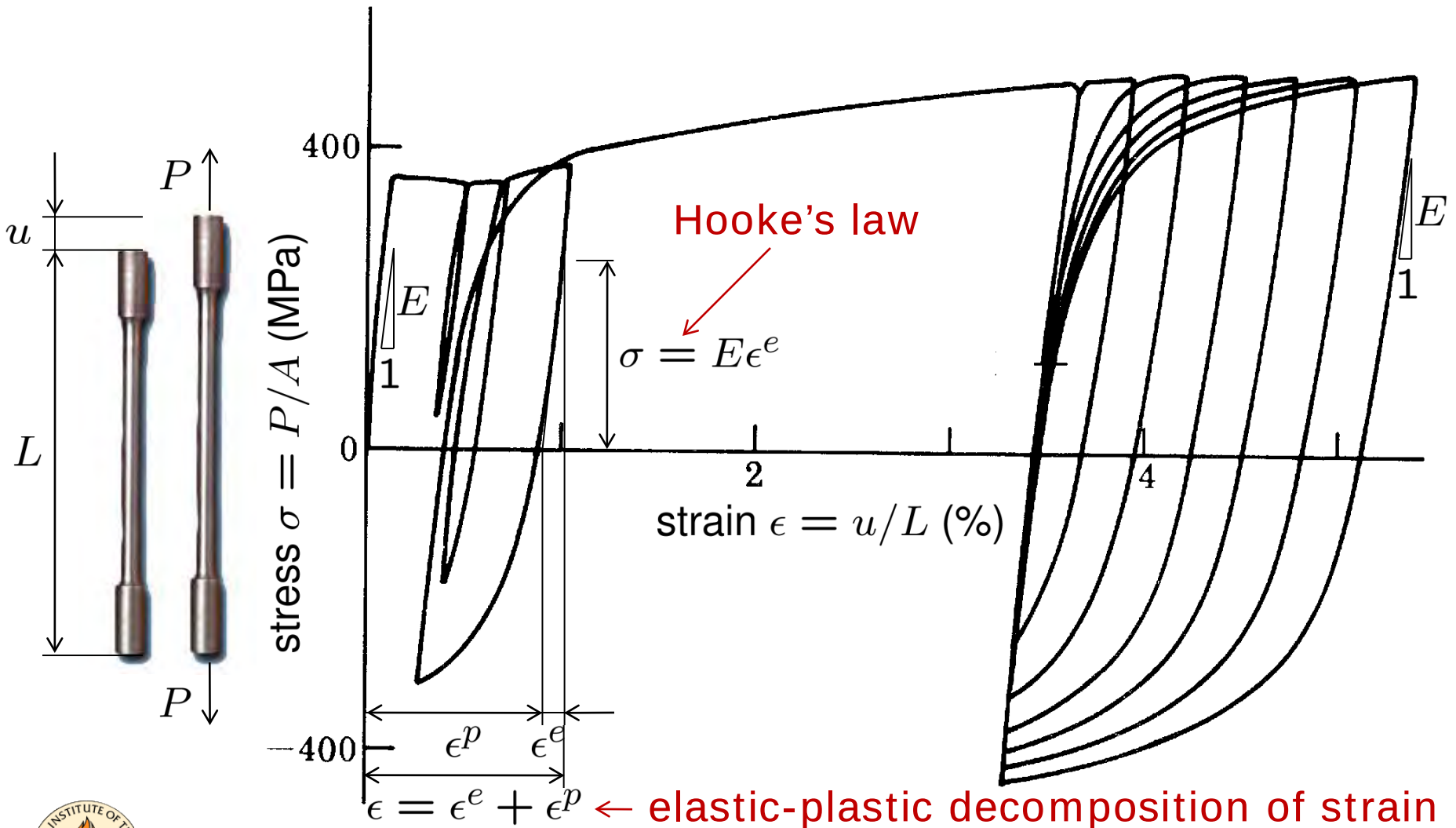
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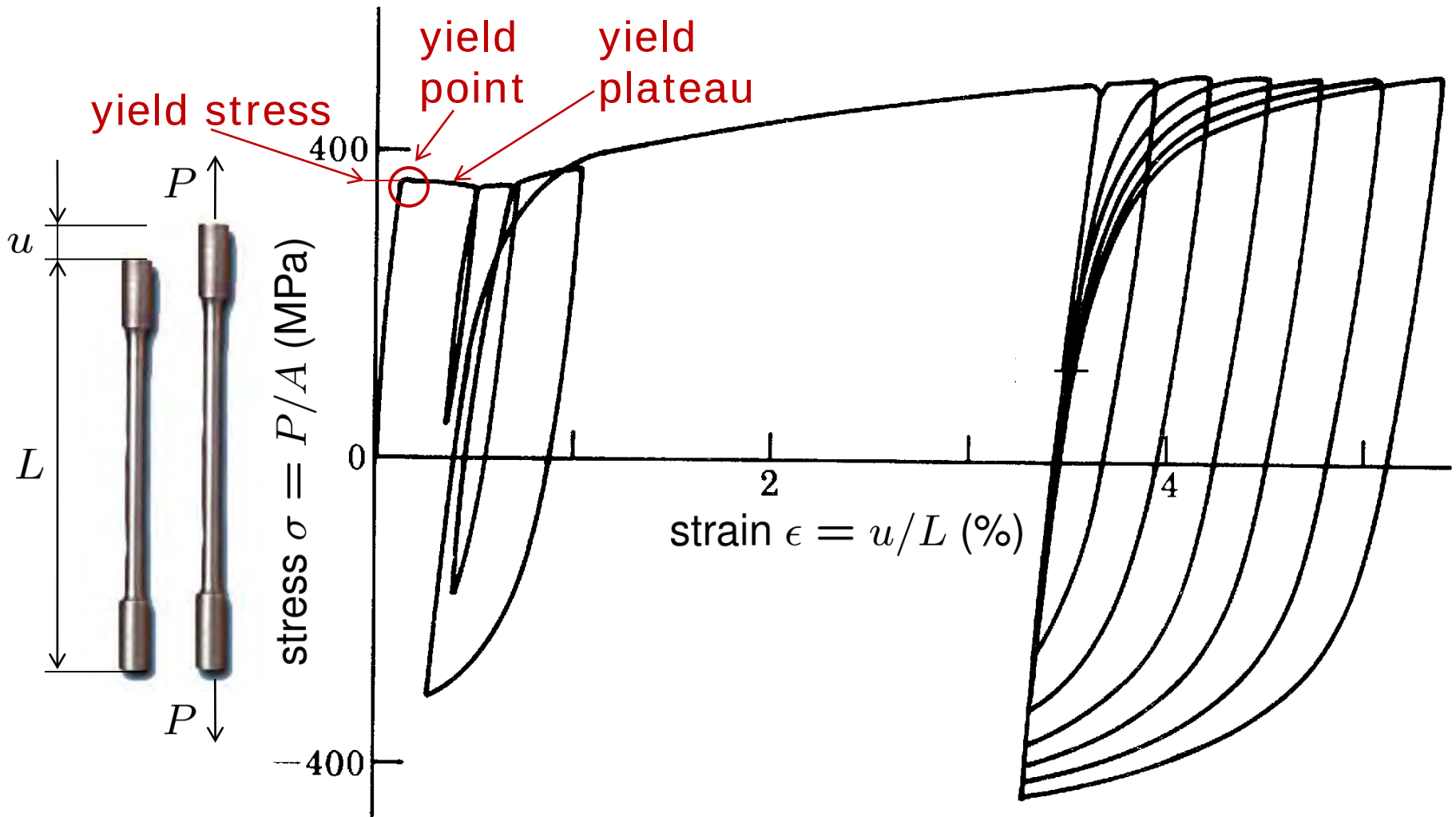
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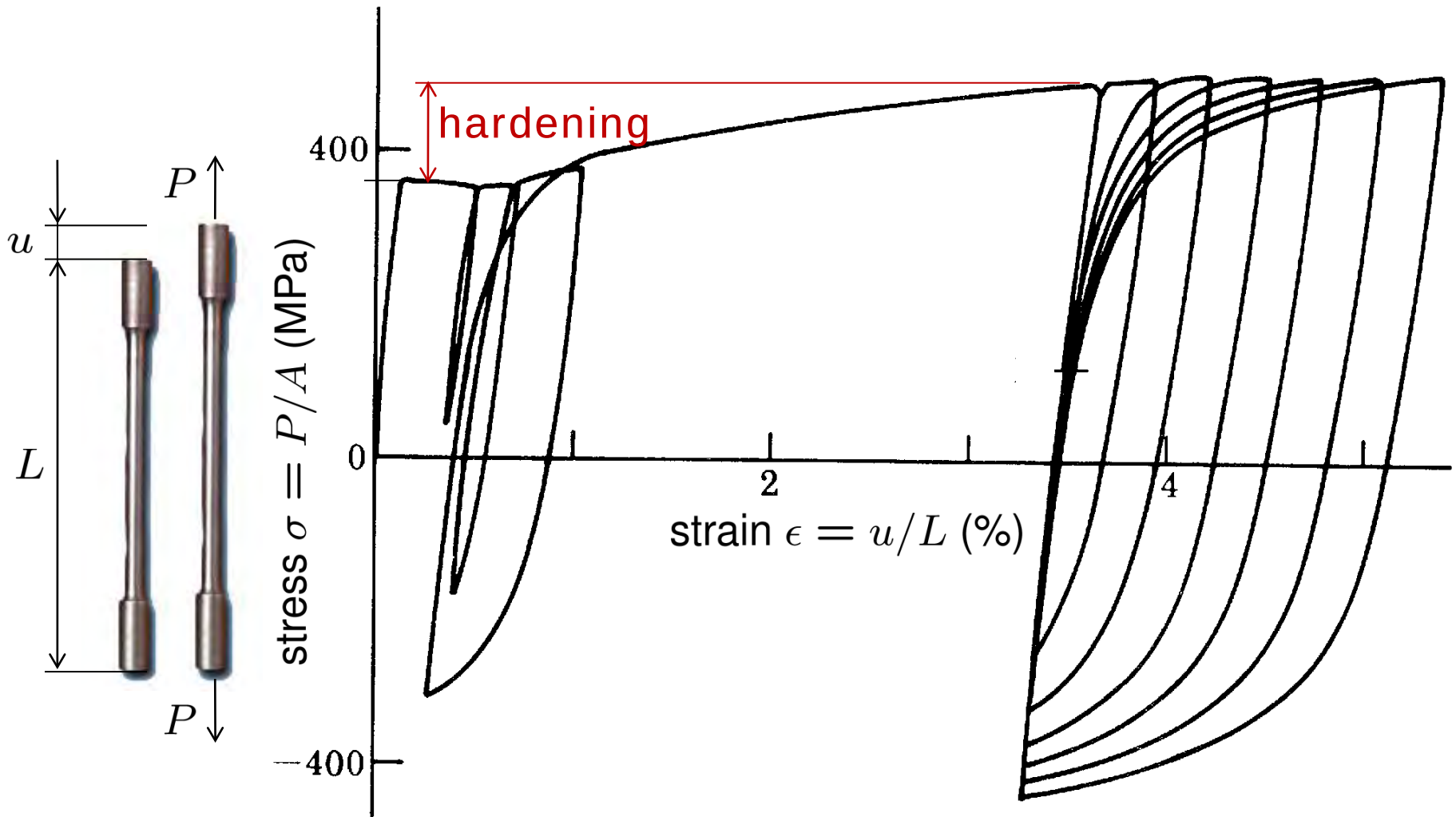
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Proc. Roy. Soc. Lond. A **379**, 439-458 (1982)

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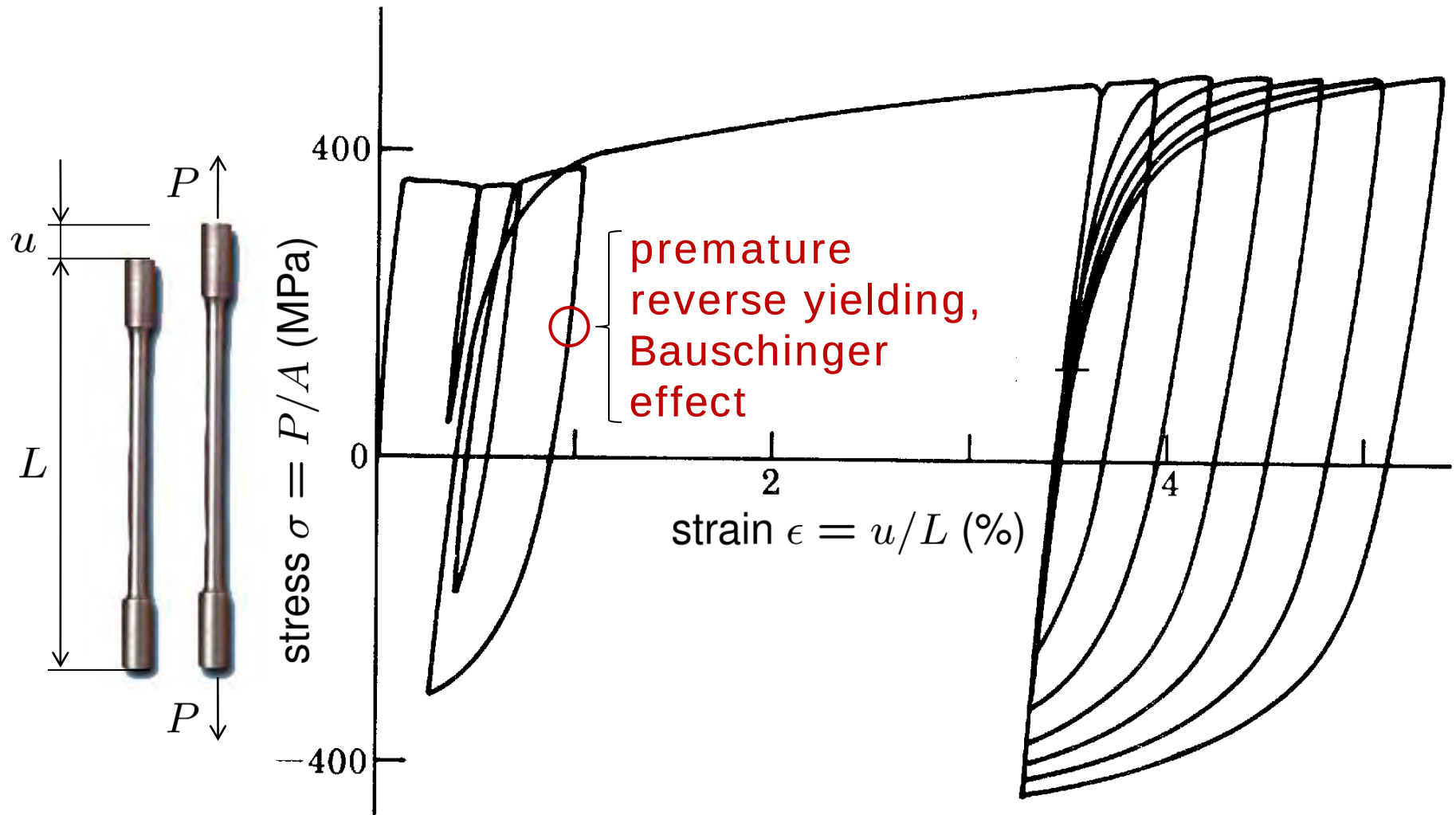
Quasistatic tension-compression test



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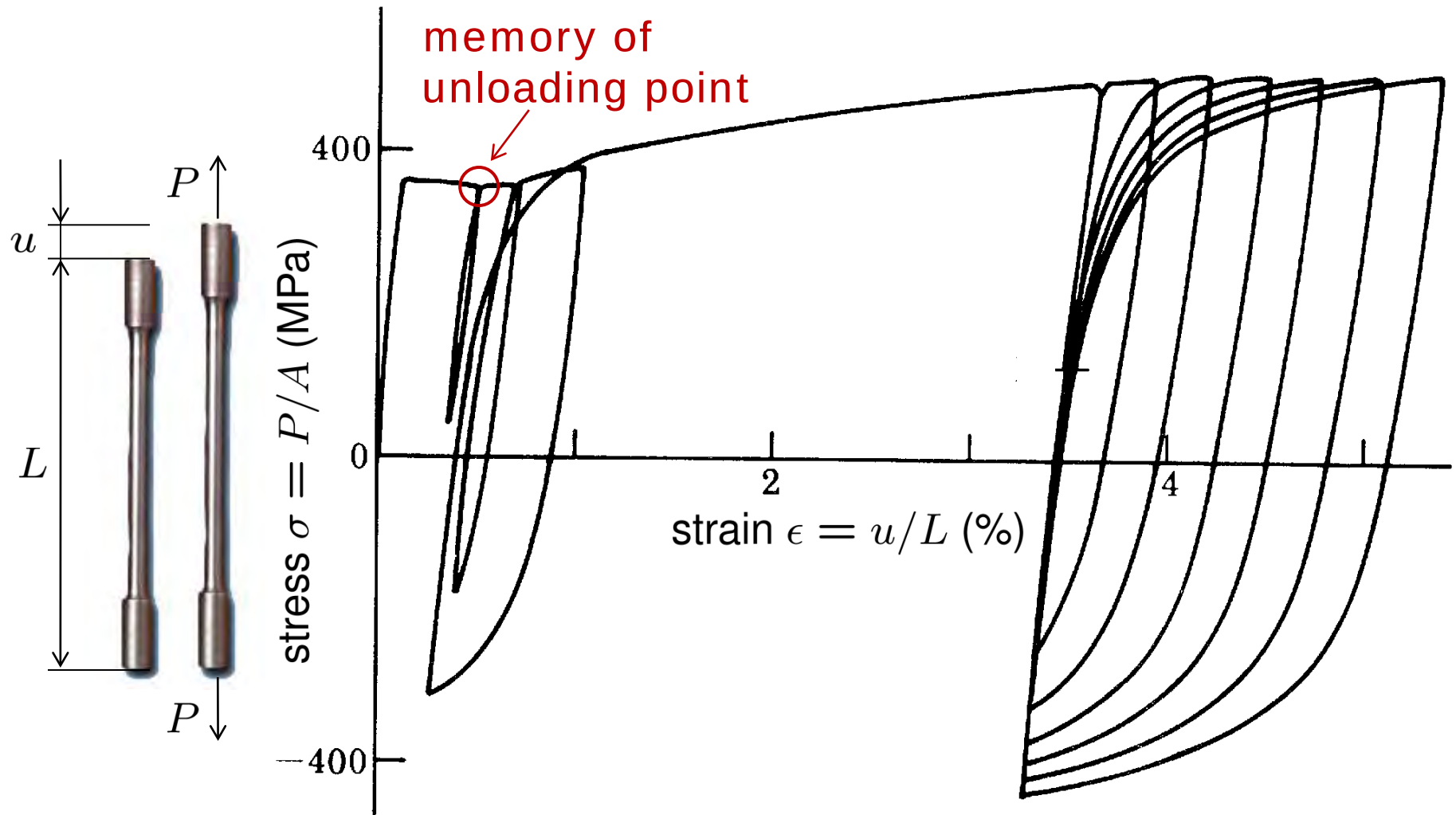
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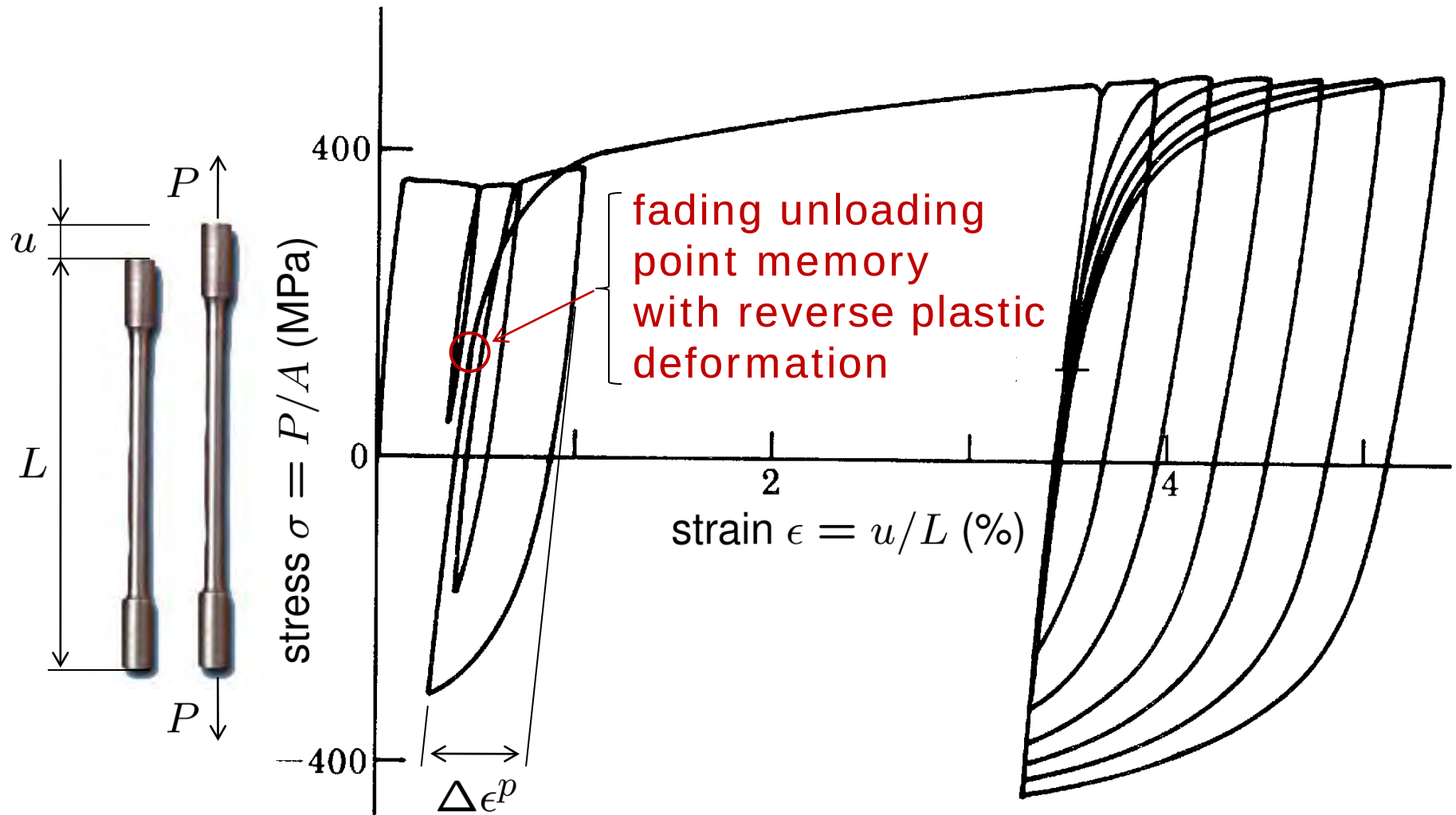
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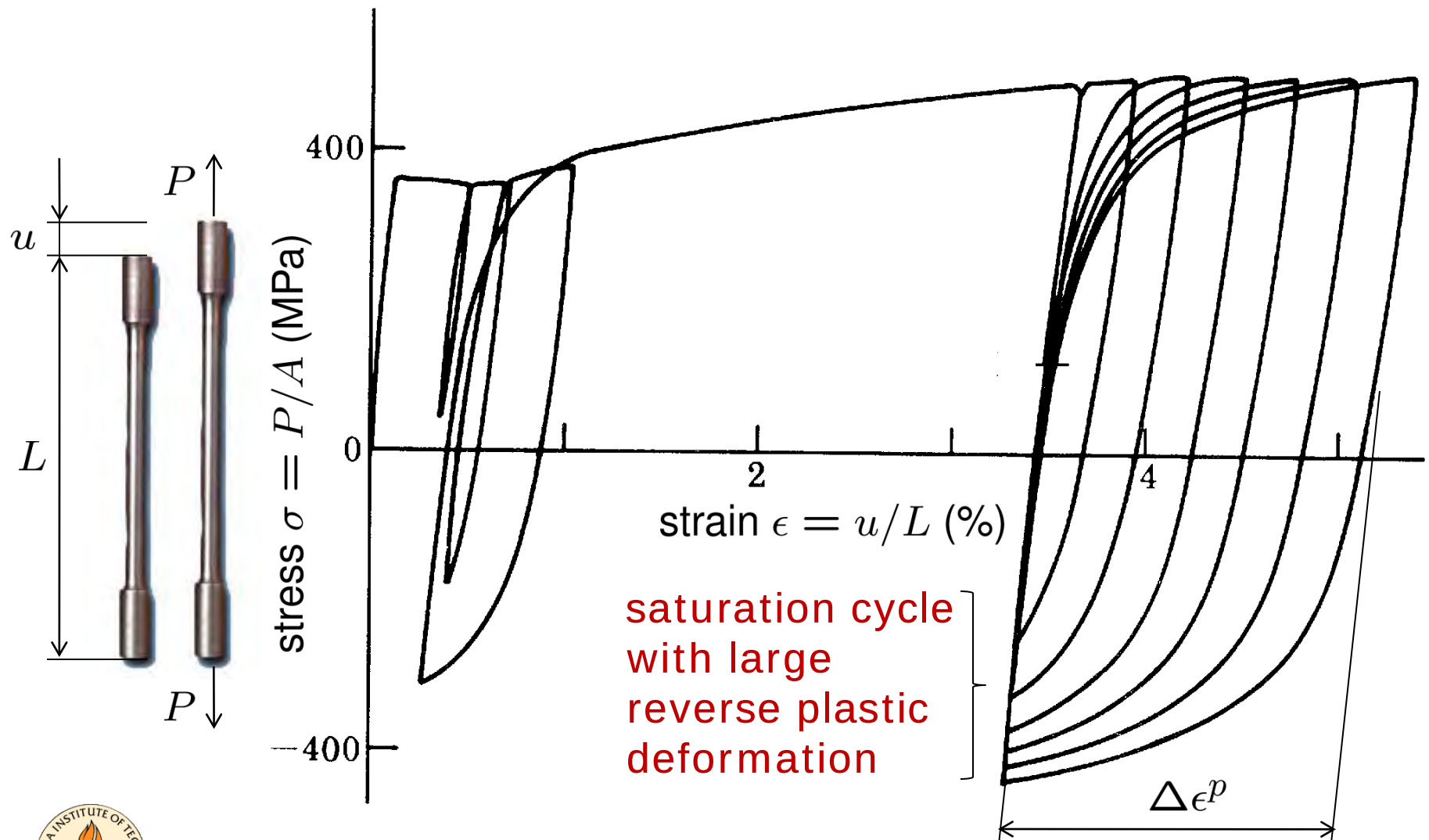
Quasistatic tension-compression test



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

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Quasistatic tension-compression test

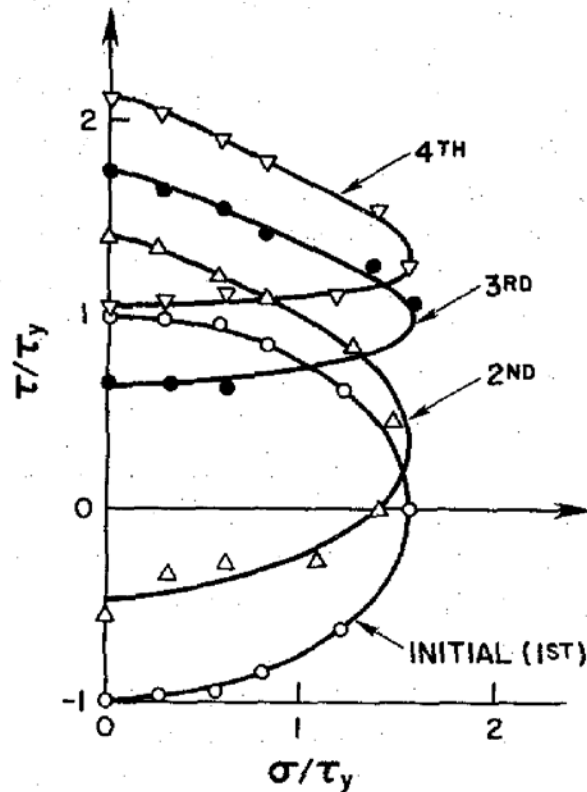


M. Ortiz and E.P. Popov,
Proc. Roy. Soc. Lond. A **379**, 439-458 (1982)

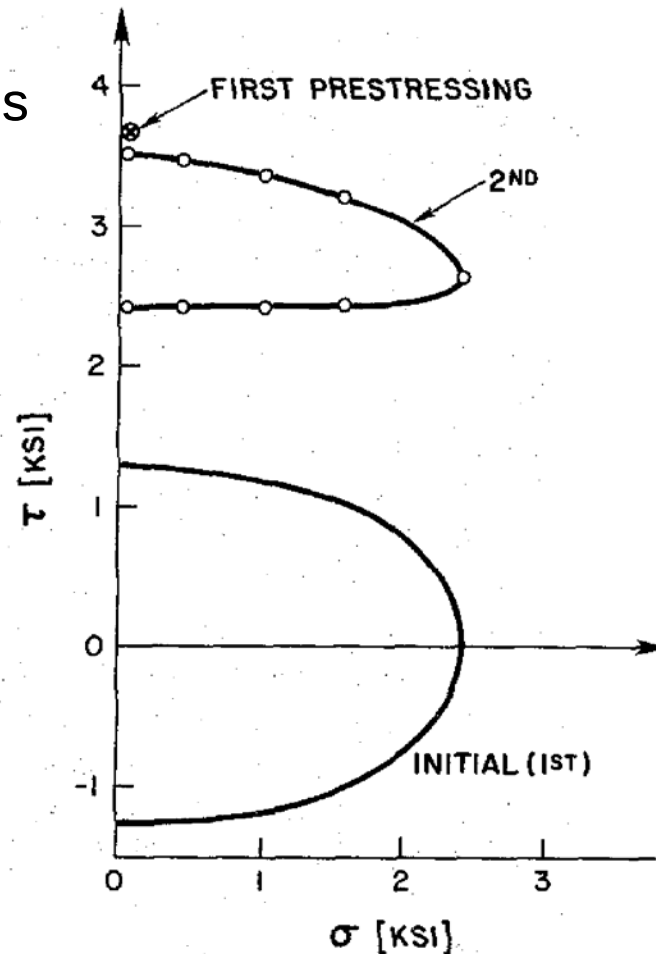
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Multiaxial elastic domain

Quasistatic tension-torsion tests



a) ALUMINUM
AFTER IVEY

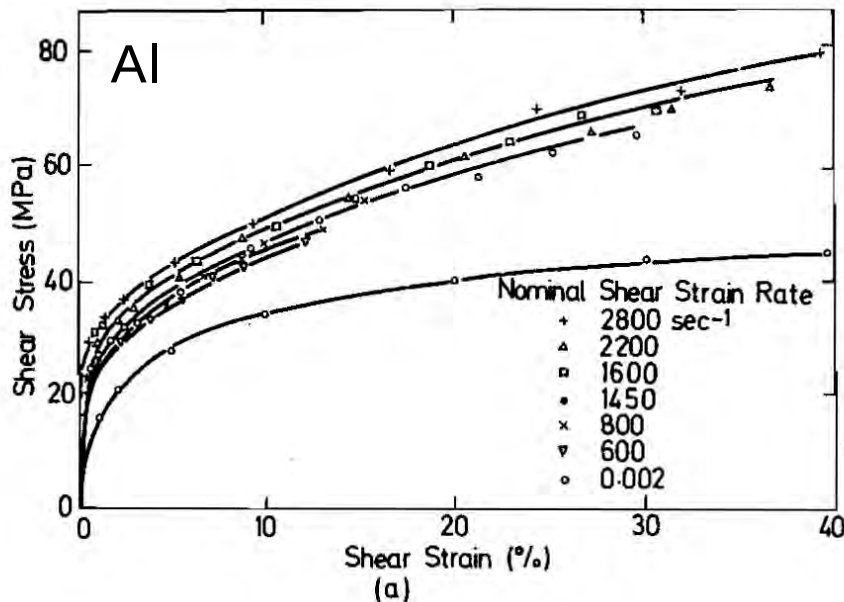


b) ALUMINUM
AFTER PHILLIPS, TANG, AND RICCIUTI

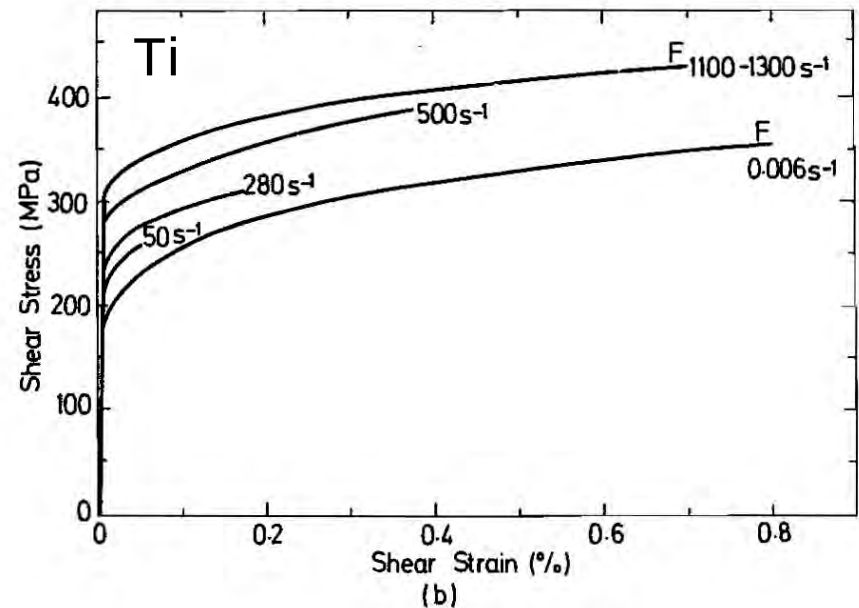


Hardening and strain-rate dependence

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)

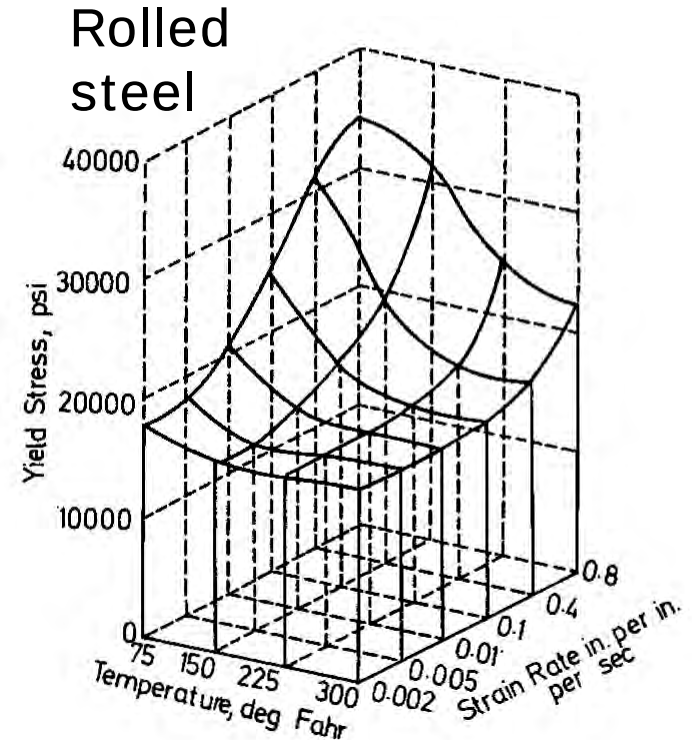
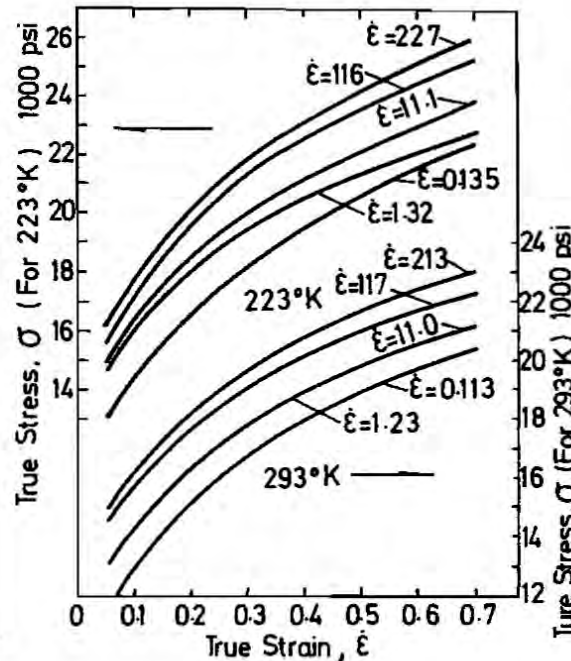
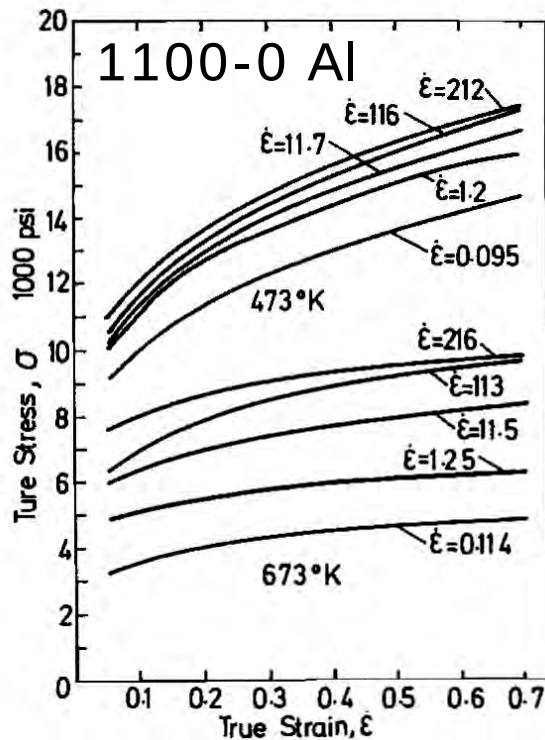


Y. Bai and B. Dodd,
Adiabatic Shear Localization, Pergamon (1992)

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Thermal softening

Servo-hydraulic compression tests



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)

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Dynamic testing



Split-Hopkinson (Kolsky)
pressure bar

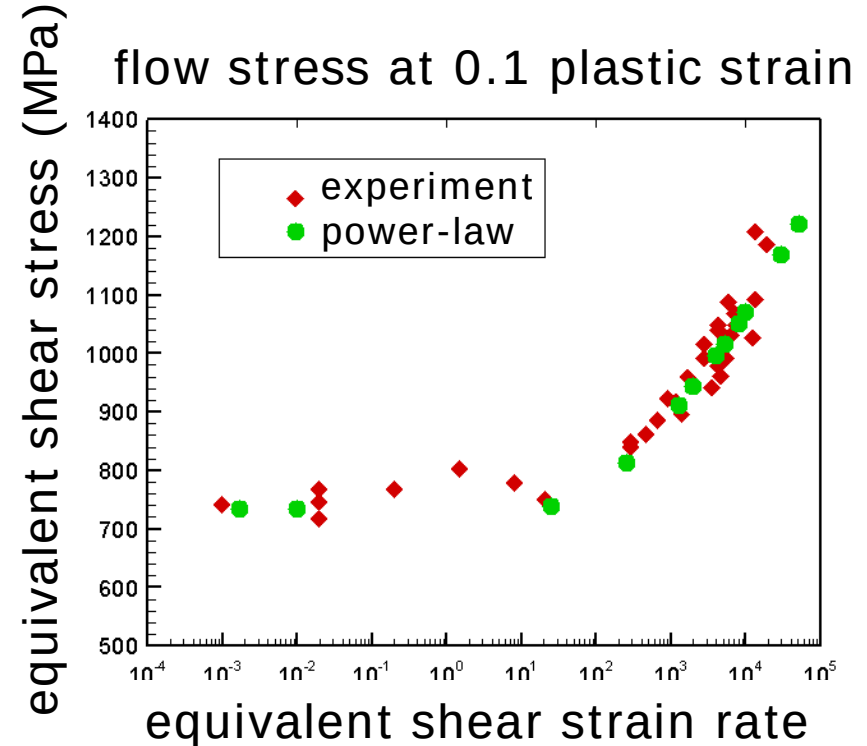
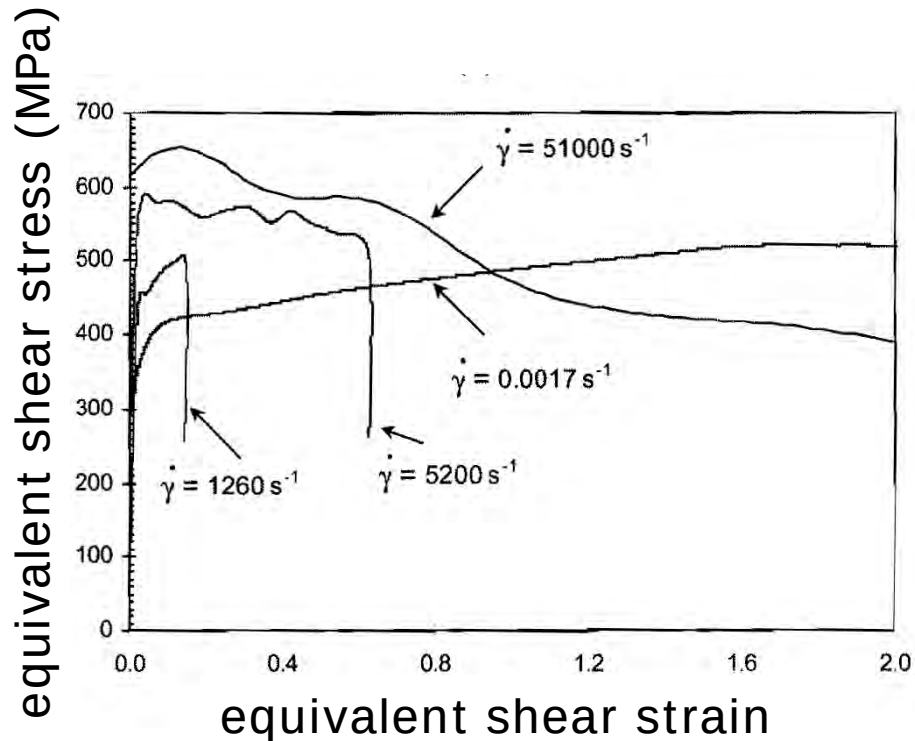
Independent measurements
of stress, strain, temperature
as functions of time



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.

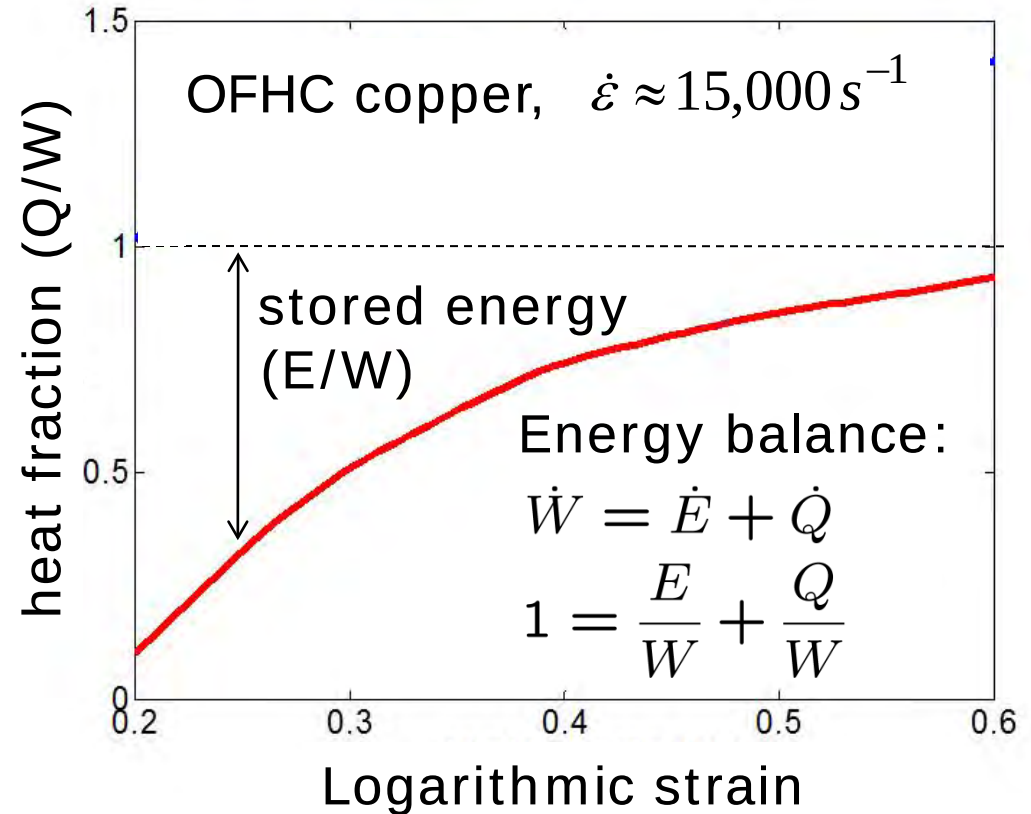
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Energy storage and dissipation



Kolsky (split Hopkinson)
pressure bar



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

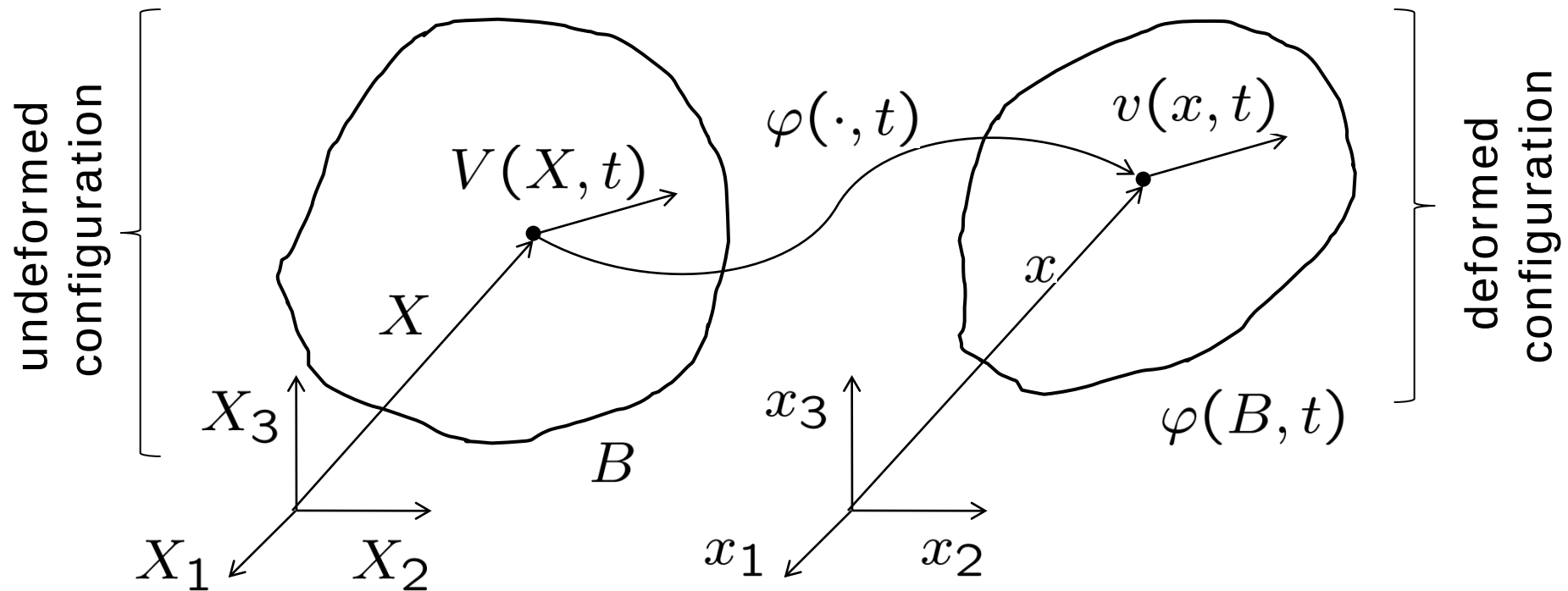


Continuum-thermodynamics framework

- 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



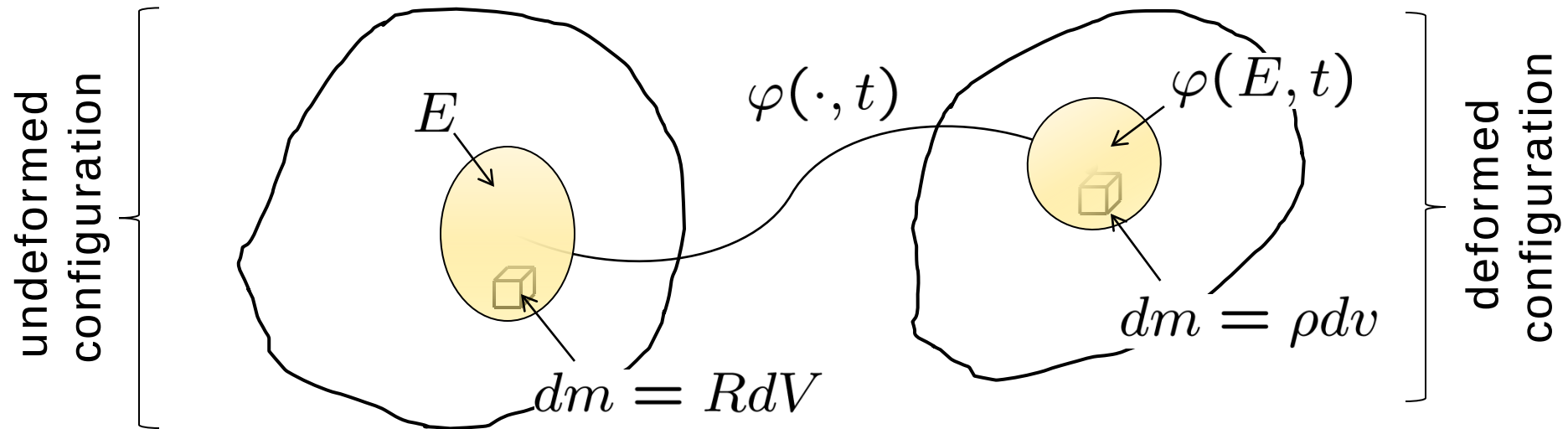
Kinematics for finite deformation



- 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



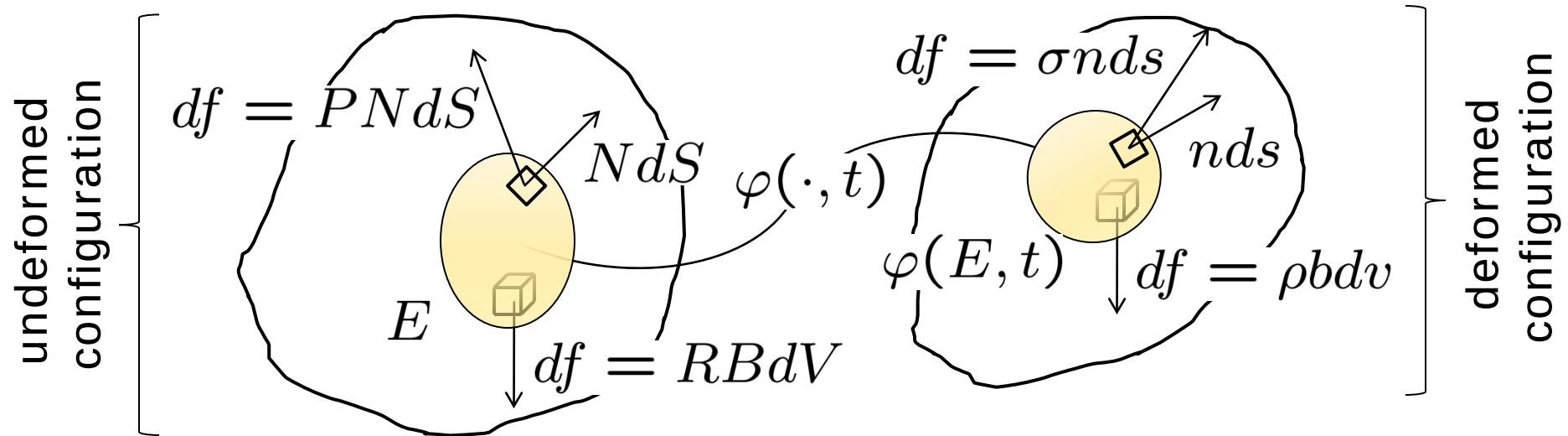
- $R \equiv$ mass density per unit undeformed volume
- $\rho = R/J \equiv$ mass density per unit deformed volume

- Lagrangian: $\frac{d}{dt} \int_E R dV = 0 \Leftrightarrow \dot{R}(X, t) = 0$

- Eulerian: $\frac{d}{dt} \int_{\varphi(E, t)} \rho dv = 0 \Leftrightarrow \dot{\rho} + \rho \nabla \cdot v = 0$



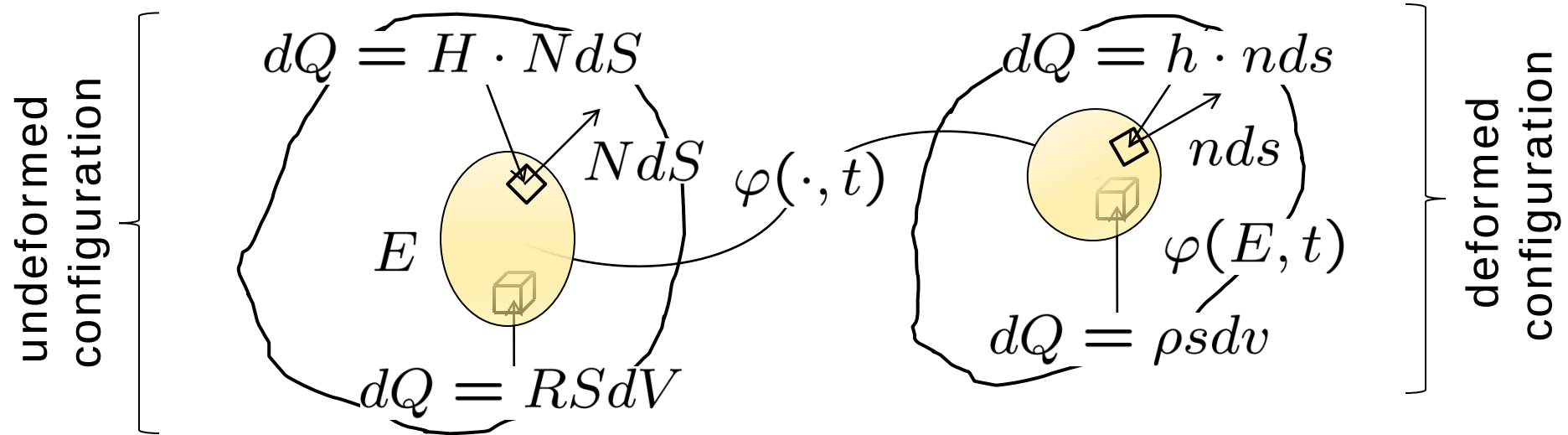
Conservation of linear and angular mom



- $P \equiv$ First Piola-Kirchhoff stress tensor
- $\sigma = J^{-1}PF^T \equiv$ 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: $\rho\dot{v} = \nabla \cdot \sigma + \rho b, \quad \sigma^T = \sigma$



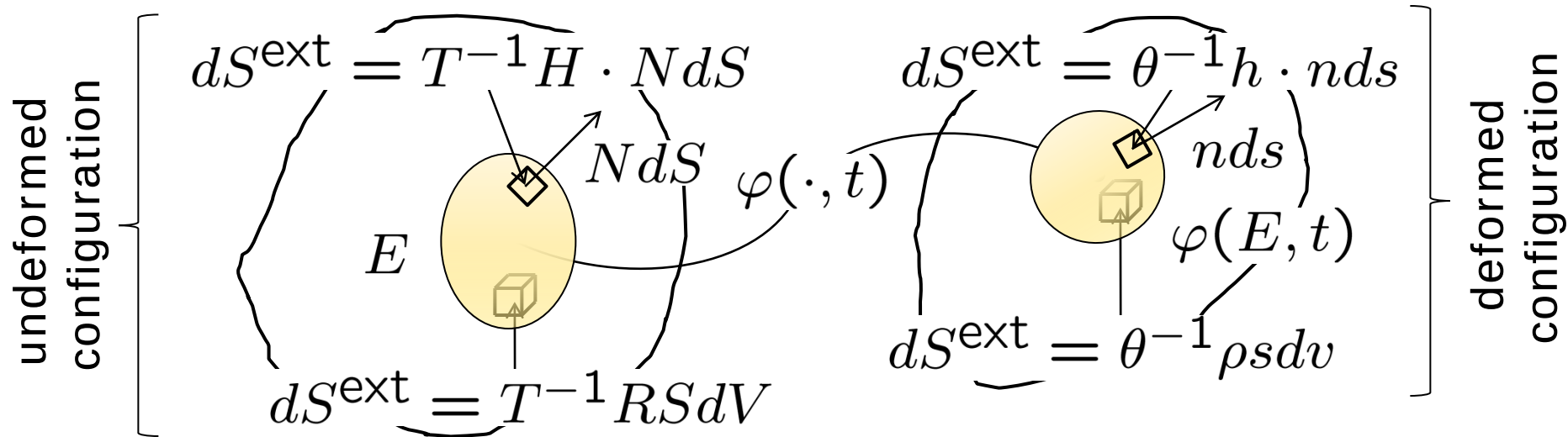
Conservation of energy



- $U \equiv$ Internal energy/unit mass, undeformed conf.
- $u \equiv$ Internal energy/unit mass, deformed conf.
- $H \equiv$ Outward heat flux, undeformed conf.
- $h \equiv$ Outward heat flux, deformed 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, undeformed conf.
- $\theta \equiv$ Absolute temperature, deformed 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,*

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

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



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,

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



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,

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

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

$$\left. \begin{aligned} T &= \frac{\partial U}{\partial N}, \\ \frac{\partial U}{\partial \nabla F} \cdot \nabla \dot{F} &= 0, \dots, & \frac{\partial U}{\partial \ddot{F}} \cdot \ddot{F} &= 0, \dots, \\ \frac{\partial U}{\partial \nabla \dot{N}} \cdot \nabla \dot{N} &= 0, \dots, & \frac{\partial U}{\partial \ddot{N}} \cdot \ddot{N} &= 0, \dots, \end{aligned} \right\}$$



The Coleman-Noll theorem (3 of 3)

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

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

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

q. e. d.

- $\dot{Q}$, P^ν 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: $RA = W^e(F F^{p-1}, T) + W^p(\epsilon^p, T)$
- $W^e(F^e, T) \equiv$ 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:

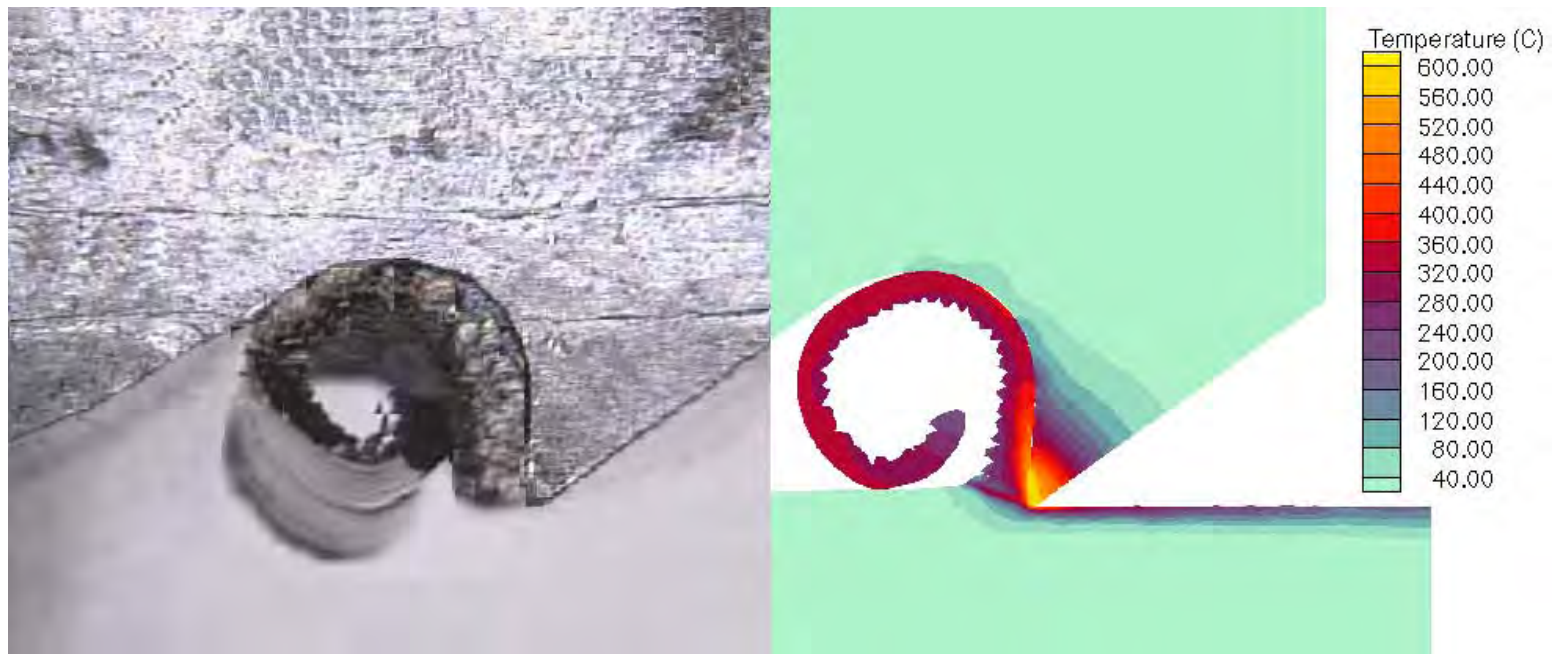
$$\left. \begin{aligned} (\dot{\varphi}(t), \dot{N}(t), \dot{Q}(t)) &\in \operatorname{argmin} G, \quad t \geq 0 \\ (\varphi(0), N(0), Q(0)) &= (\varphi_0, N_0, Q_0) \end{aligned} \right\}$$
- Time-discretized incremental problem, $t_n \rightarrow t_{n+1}$:

$$(\varphi_{n+1}, N_{n+1}, Q_{n+1}) \ni \operatorname{argmin} F_n \equiv \int_B \left[R(\Delta U - T_{n+1} \Delta N) + \Delta t \psi_{n+1} \right] dV$$



Limitations of empirical models

Chip Morphology Validation (Courtesy of Third Wave Systems Inc)



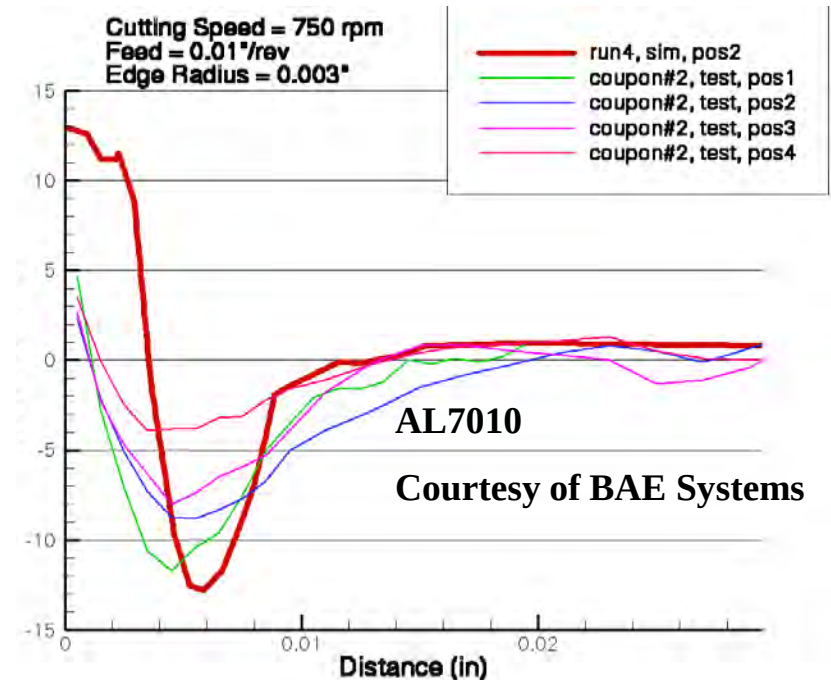
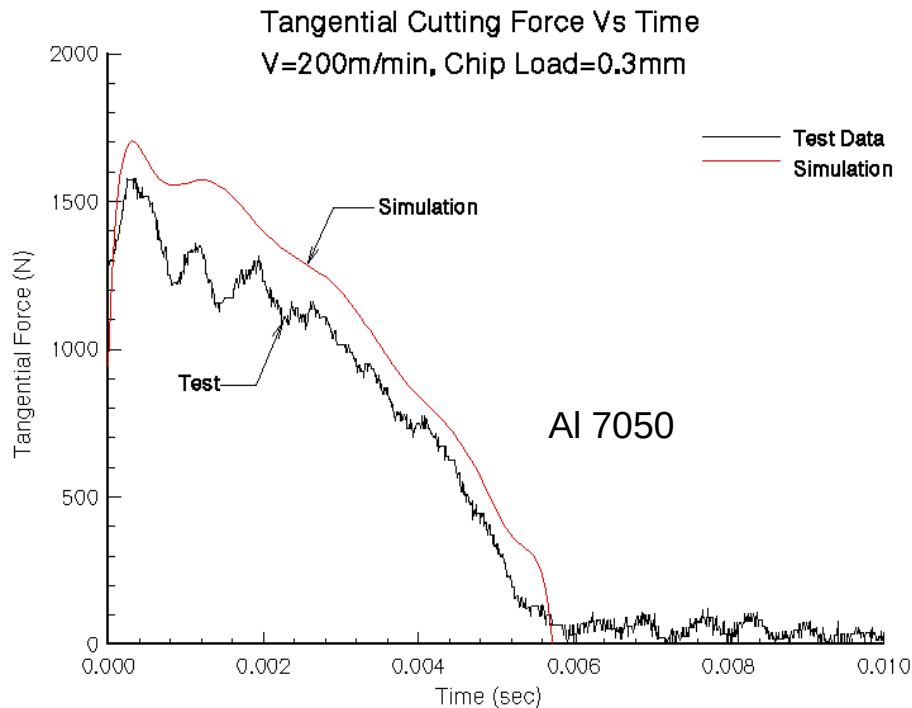
(Courtesy of IWH, Switzerland)

FE simulation



Limitations of empirical models

(Courtesy of Third Wave Systems Inc)



Cutting Force Validation

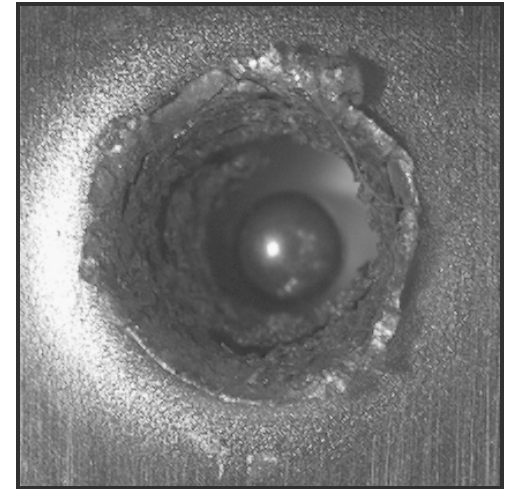
Residual Stress Validation

General trends predicted, but discrepancies remain!

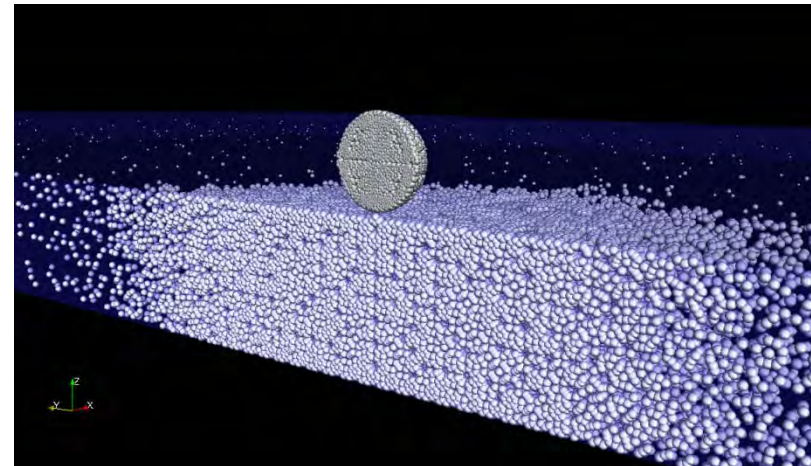


Limitations of empirical models

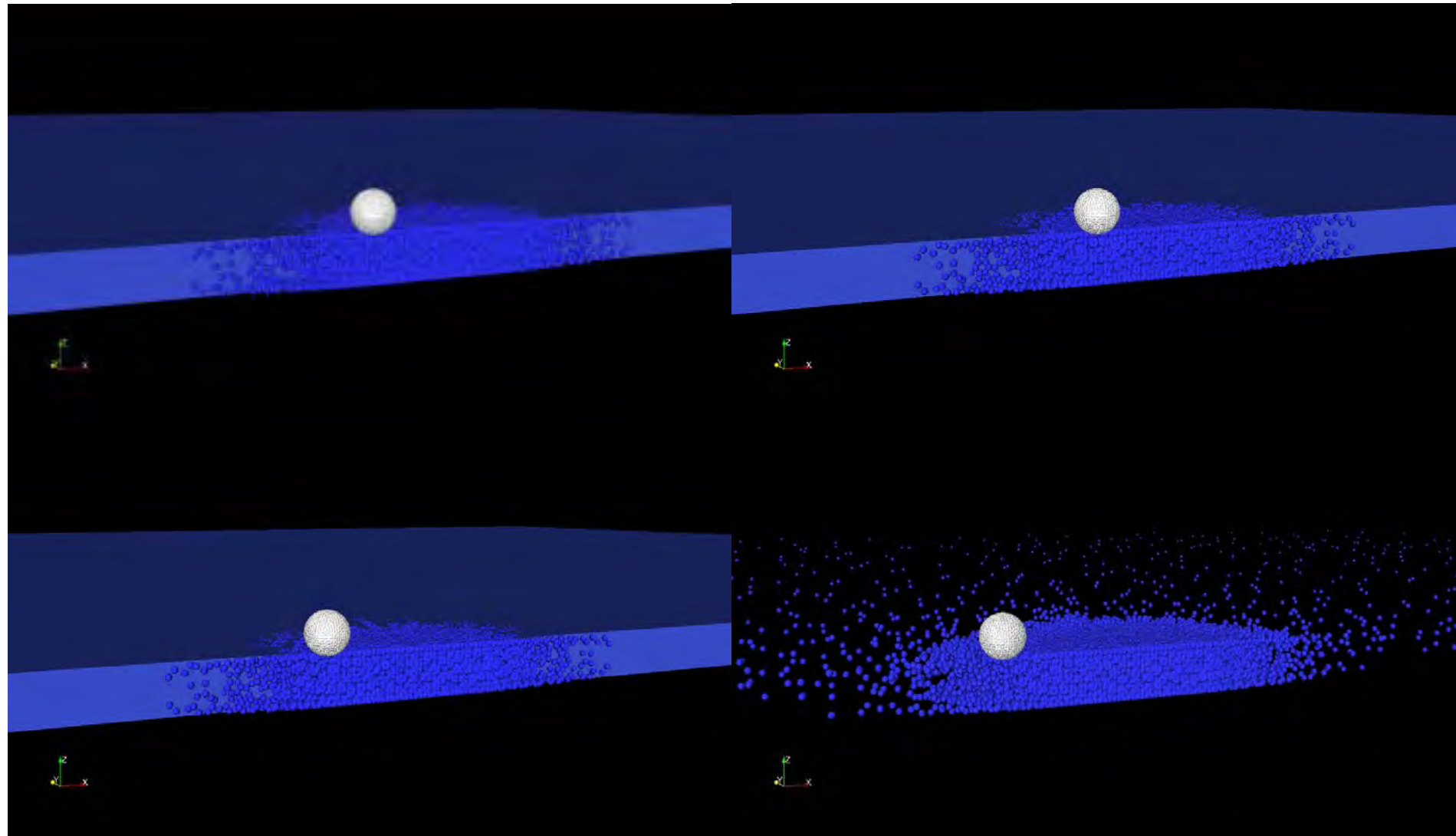
- Target/projectile materials:
 - *Target: Al6061-T6 Plates*
 - *Projectile: 440 C Steel Spheres*
- Experimental facilities: Small Particle Hypervelocity Impact Range (A.J. Rosakis, Caltech)
- Performance measure (output): Perforation area
- Model parameters (inputs):
 - *Plate thickness (62-125 mils)*
 - *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

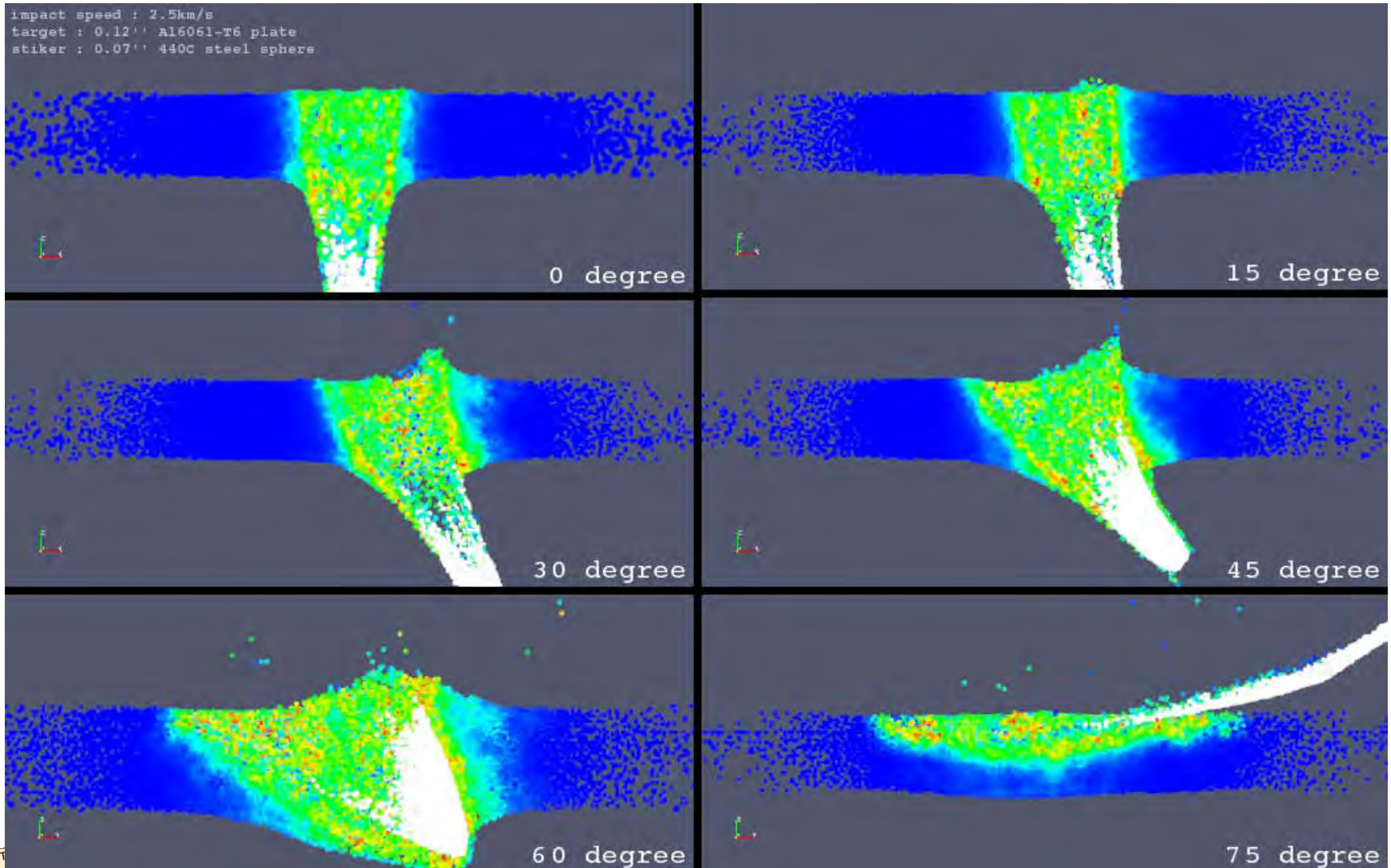


B. Li, F. Habbal and M. Ortiz,
Int. J. Numer. Meth. Eng., **83** (2010) 1541-1579

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OTM – Terminal ballistics

impact speed : 2.5km/s
target : 0.12" Al6061-T6 plate
stiker : 0.07" 440C steel sphere

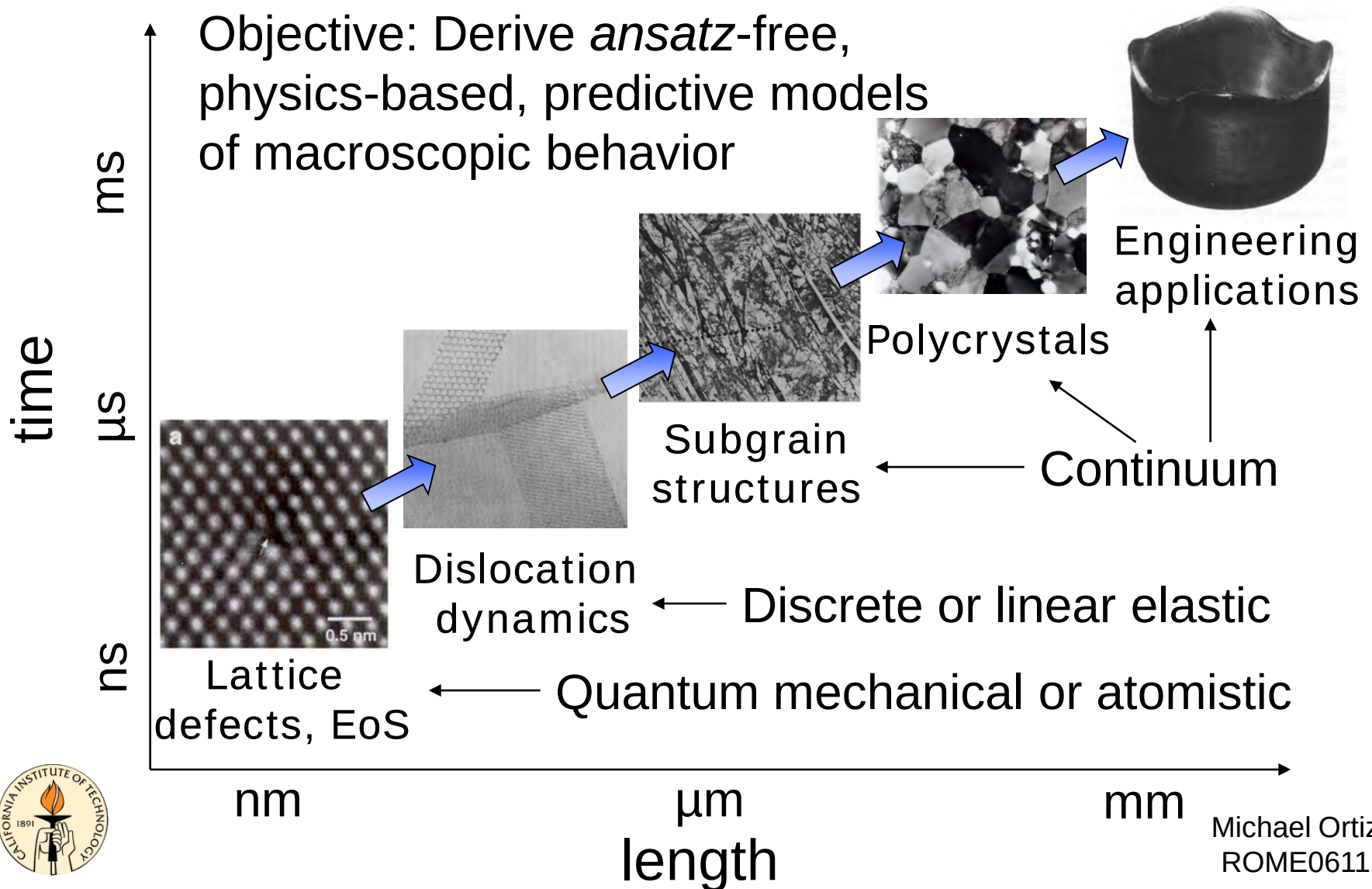


Metal plasticity – Multiscale analysis

- 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



Metal plasticity – Multiscale analysis

