Multiscale models of metal plasticity
Part I: Dislocation dynamics to crystal plasticity

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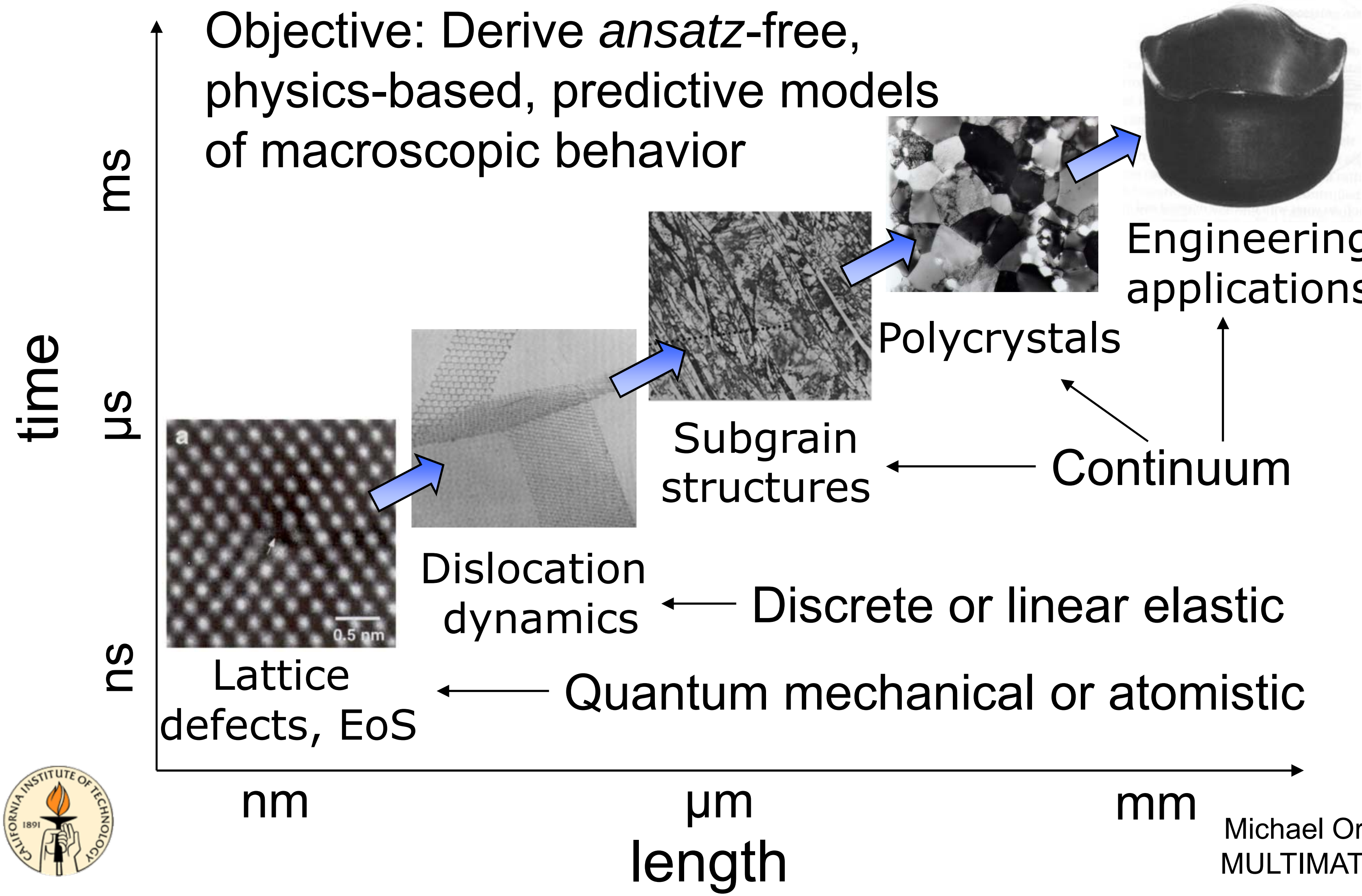
Metal plasticity

- Behavior of polycrystalline metals is too complex to yield to *ad hoc* modeling:
  - *Polycrystalline texture*
  - *Sub-grain microstructures*
  - *Dislocation dynamics*
  - *Atomistic defect cores*
  - *Pressure/temperature/rate dependency*
  - *Scaling and size effects…*
- Alternative paradigm: Multiscale analysis
  - *Derive rigorous models of effective behavior*
  - *Identify underlying microstructural mechanisms*
  - *Develop high-fidelity (but fast!) physics models…*

Metal plasticity – Multiscale analysis



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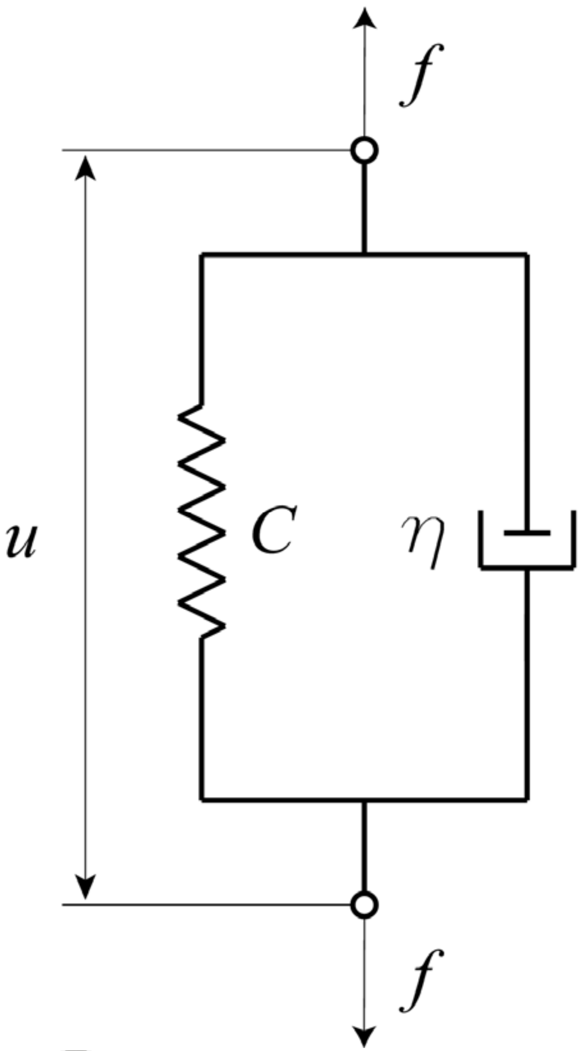
Metal plasticity – Multiscale analysis

- A well-developed body of theory exists for energy minimization problems:
  - *Relaxation*
  - *Γ-convergence*
  - *Optimal scaling*
- This framework suffices for many applications:
  - *Martensitic phase transitions*
  - *Micromagnetics*
  - *Complex polymers*
- However: Plasticity involves dissipation, hysteresis, irreversible behavior
- Need a theoretical framework that extends CoV to dissipative problems…

Classical rate variational problems



- Kelvin solid IV problem:

$$\left.\begin{array}{l} \eta \dot{u}(t) + Cu(t) = f(t) \\ u(0) = u_0 \end{array}\right\}$$

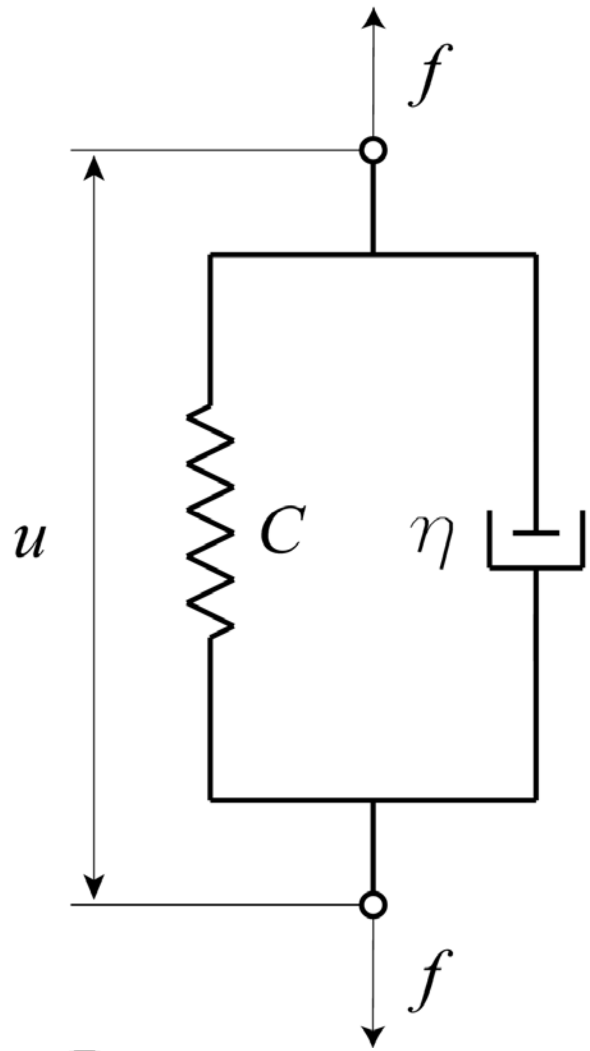
- Potential energy:

$$E(t,u) = \frac{C}{2}u^2 - f(t)u$$

- Dissipation potential: $\Psi(v) = \frac{\eta}{2}v^2$
- Force equilibrium:

$$\partial\Psi(\dot{u}(t)) + DE(t,u(t)) = 0$$

Classical rate variational problems



- Rate potential:

$$G(t,u,v) \equiv \Psi(v) + DE(t,u)\,v$$

- Rate problem: Given t, u,

$$\min_v G(t,u,v)$$

- Euler-Lagrange equations:

$$\partial\Psi(v) + DE(t,u) = 0$$

- IV problem: For $t \in [0,T]$,

$$\left.\begin{array}{l} v(t) \in \operatorname{argmin} G(t,u(t),\cdot) \\ \dot{u}(t) = v(t), \quad u(0) = u_0 \end{array}\right\}$$

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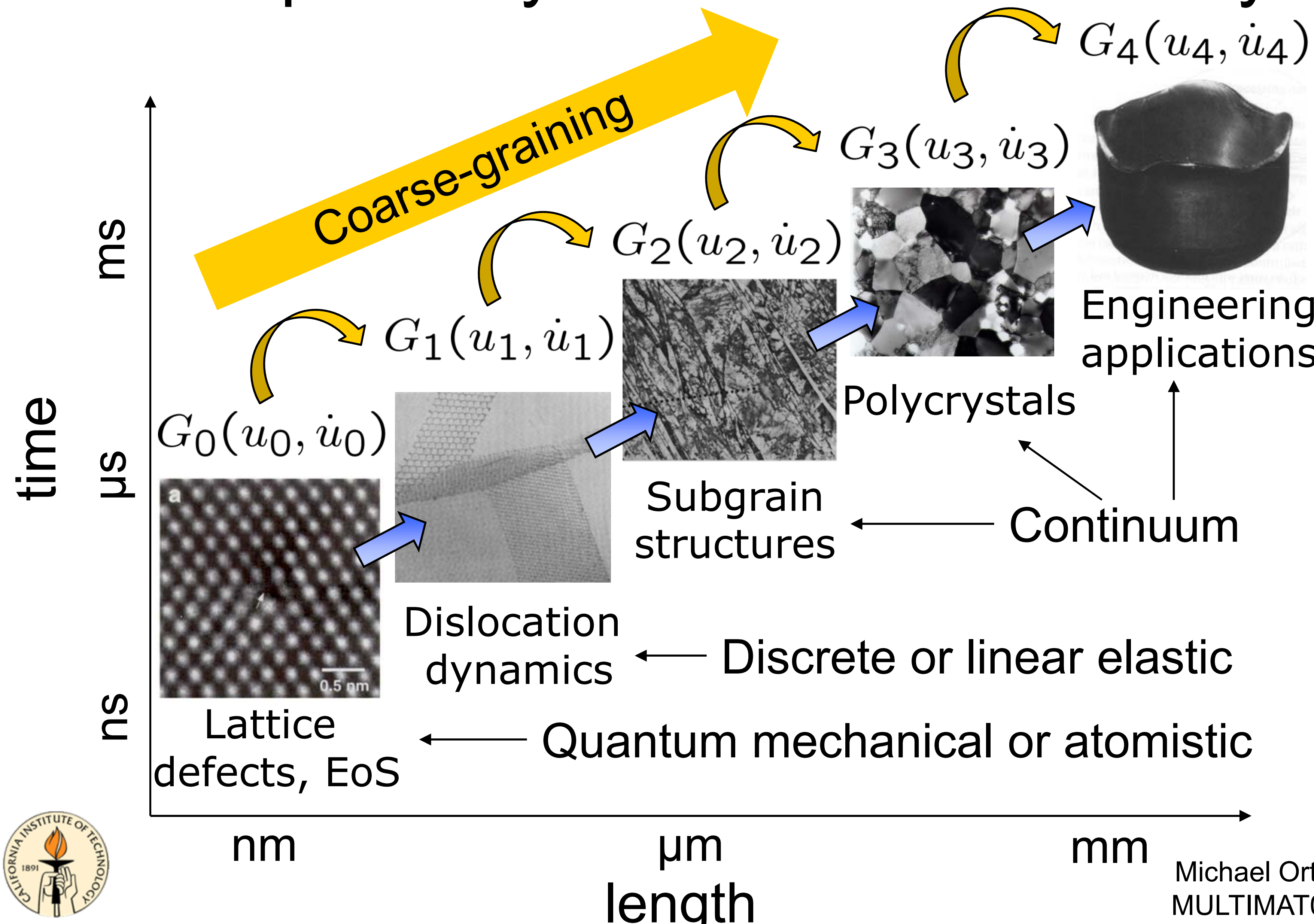
Metal plasticity – Multiscale hierarchy



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Energy-dissipation functionals

- Energy-dissipation functional: For $\epsilon > 0$,

$$F_\epsilon(u) = \int_0^T \mathrm{e}^{-t/\epsilon} G(t, u, \dot{u})\, dt$$

- Minimum principle: $\mathbb{Y} = \{u : [0, T] \to Y\}$,

$$\boxed{\inf_{u \in \mathbb{Y}} F_\epsilon(u)}$$

- Euler-Lagrange eqs., $G(u, \dot{u}) = \Psi(\dot{u}) + DE(u)\dot{u}$,

$$\underline{-\epsilon D^2\Psi(\dot{u})\ddot{u}} + D\Psi(\dot{u}) + DE(t, u) = 0$$

- Relaxation: $$sc^- F_\epsilon(u) \stackrel{?}{=} \underbrace{\int_0^T \mathrm{e}^{-t/\epsilon} \underline{\bar{G}_\epsilon(t, u, \dot{u})\, dt}}_{\text{local?}}$$

- Causal limit: $\epsilon \to 0$?

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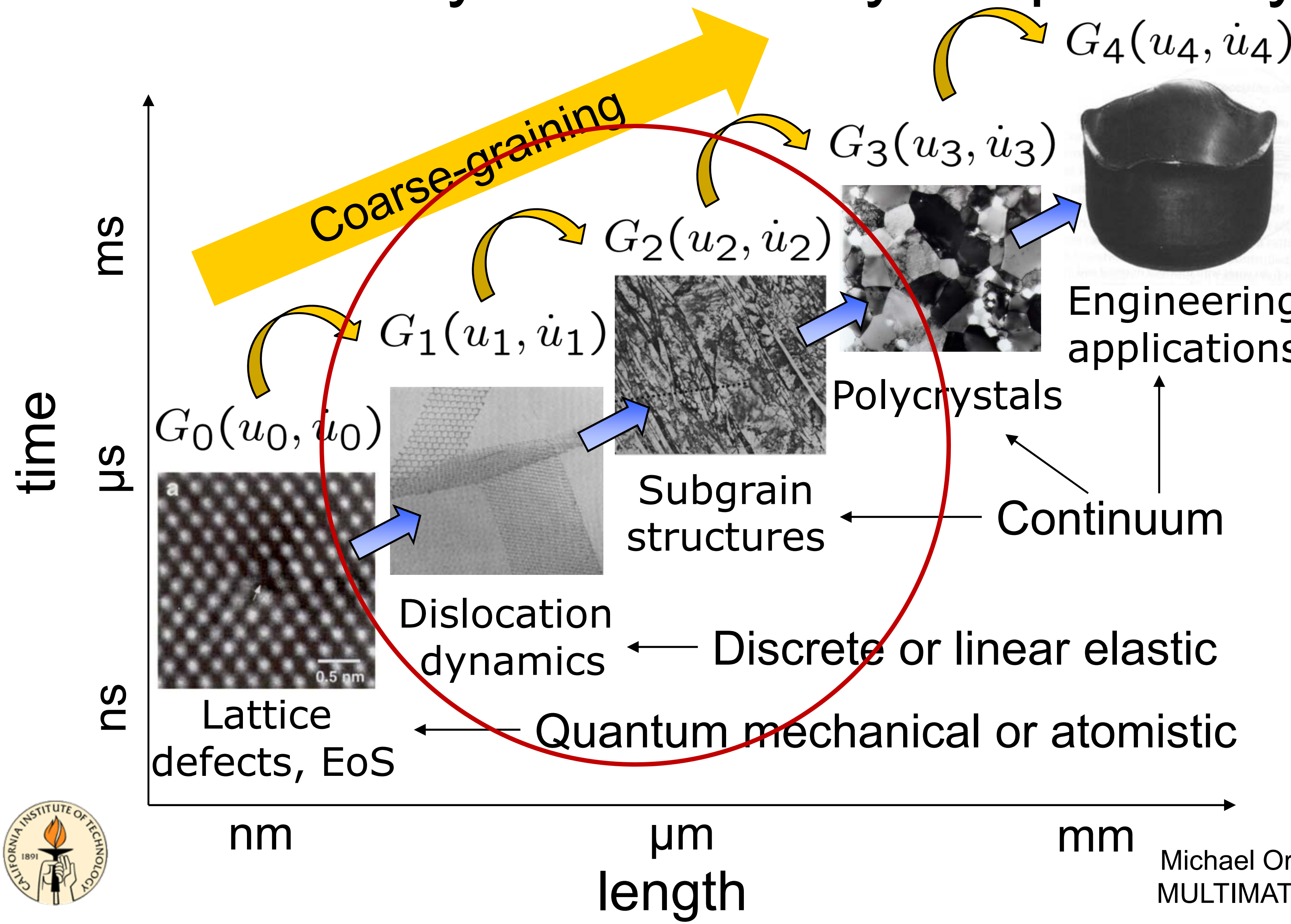
Dislocation dynamics to crystal plasticity



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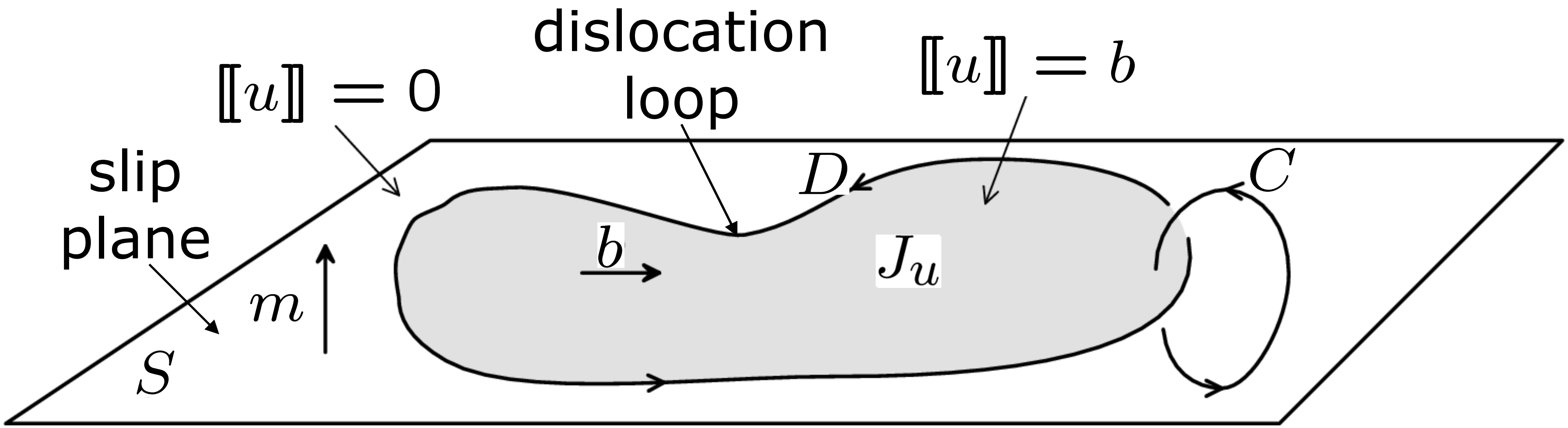
LE dislocations - Kinematics



- Volterra dislocation: $u \in SBV^2(\Omega)$ such that

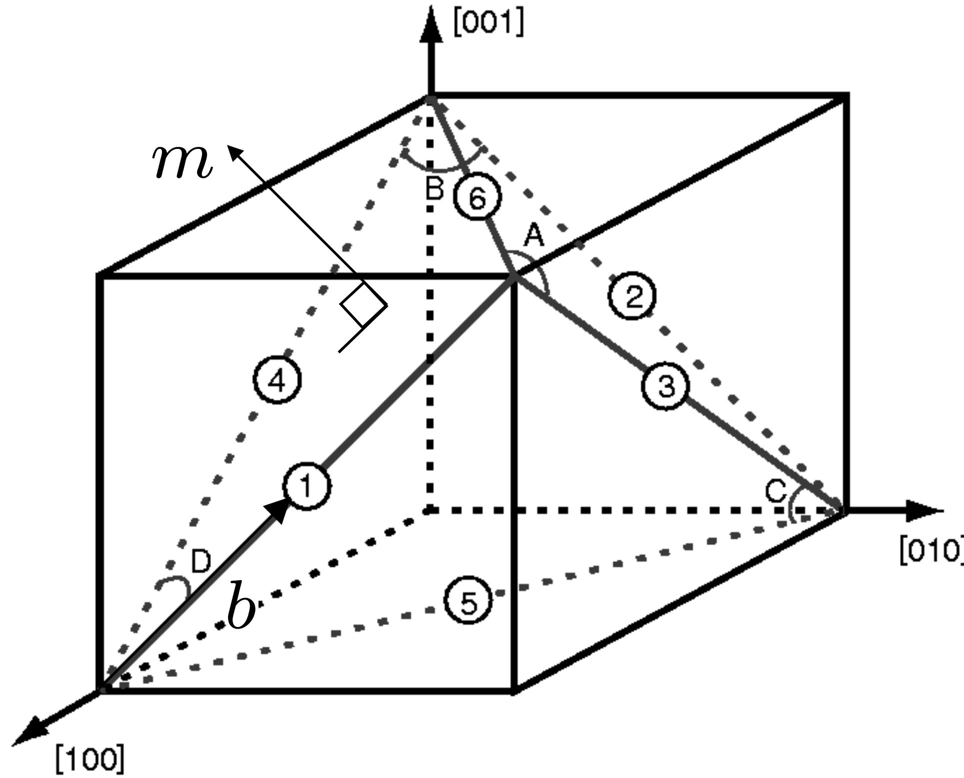
$$Du = \underbrace{\nabla u}_{\text{elastic deformation}} \mathcal{L}^3 + \underbrace{[\![u]\!] \otimes m}_{\text{plastic deformation (currents)}} \mathcal{H}^2 \lfloor J_u \equiv \beta^e + \beta^p$$

elastic deformation plastic deformation (currents)

- Dislocation density: $\alpha = \partial \beta^p$
- Conservation of Burgers vector: $\partial \alpha = \partial^2 \beta^p = 0$

LE dislocations – Constrained theory

- Mobility: $J_u \subset$ {closed-packed planes of lattice}
- Energy: $\beta^p/d=$ lattice-preserving deformation
- Energy: $[\![u]\!]$ in $\text{span}_{\mathbb{Z}}$({shortest translation vectors of lattice}) $\underbrace{*\varphi_\epsilon}$ core-cutoff mollifier



The 12 slip systems of fcc crystals (Schmidt and Boas nomenclature)

$$b \in \mathcal{S}(1,1,0), \quad m \in \mathcal{S}(1,1,1)$$

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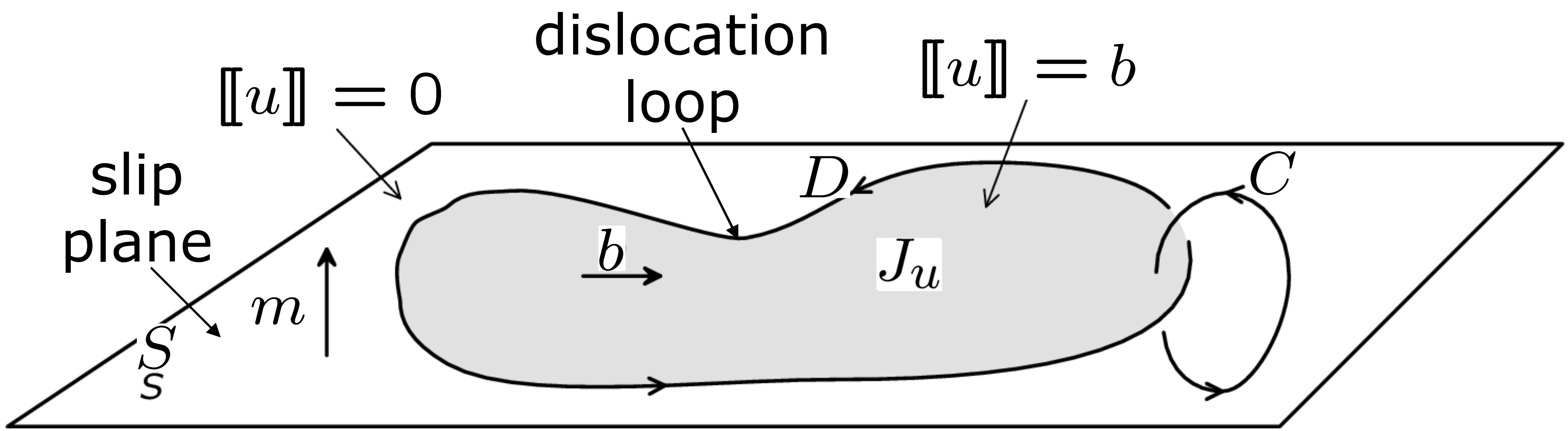
LE dislocations - Kinematics



- Volterra dislocations: $u \in SBV^2(\Omega)$ such that

$$Du = \nabla u \mathcal{L}^3 + [\![u]\!] \otimes m \, \mathcal{H}^2 \lfloor J_u$$

- Energy: $E(u) = \int_\Omega \frac{1}{2} |\epsilon(u)|^2 \, dx,$

where: $\epsilon(u) = \frac{1}{2}(\nabla u + \nabla u^T) \equiv$ elastic strain

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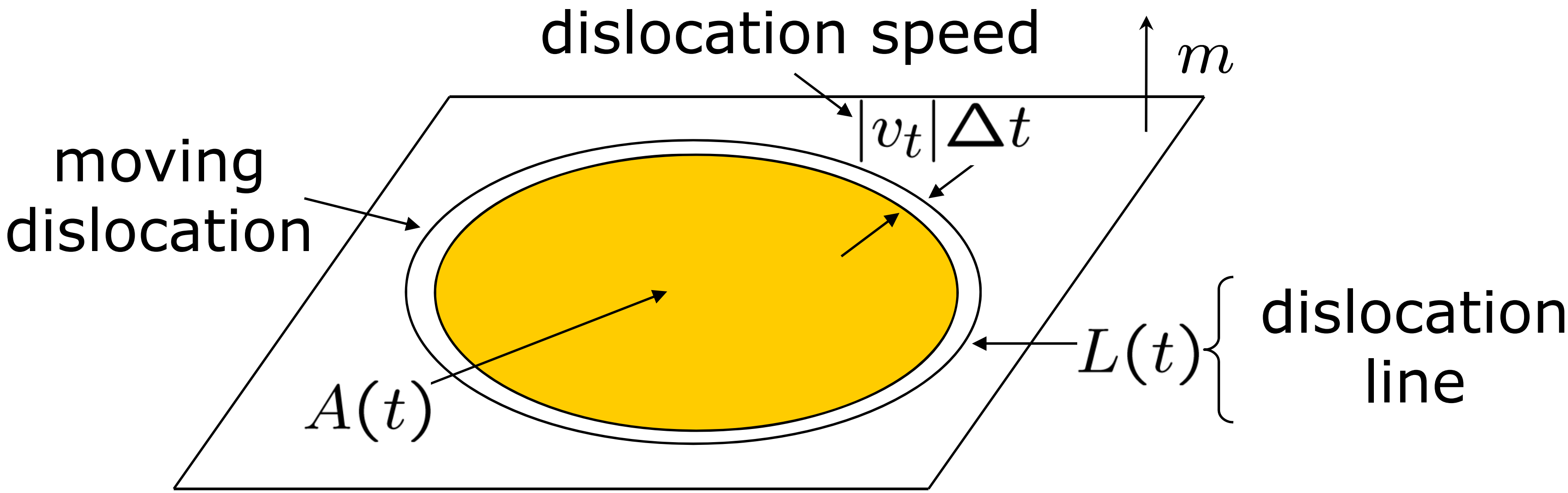
LE dislocations - Dissipation



- Dislocation flux: $\forall \varphi \in C_0^1([0,T]), \forall f \in C_0(\Omega)$,

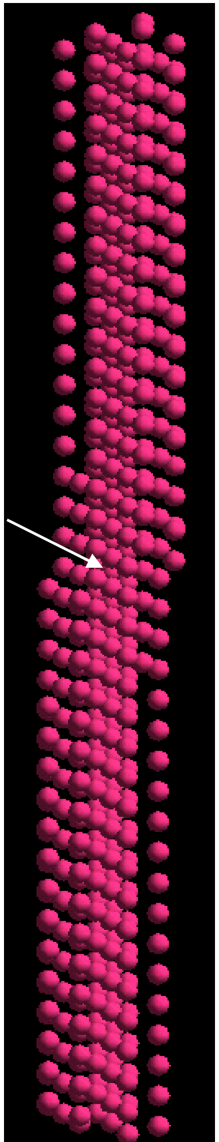
$$\int_0^T \dot{\varphi} \left\{ \int [\![u]\!] \otimes m \, f \, d\mathcal{H}^2 \right\} dt = -\int_0^T \varphi \int_\Omega f d\mu_t(x) dt$$

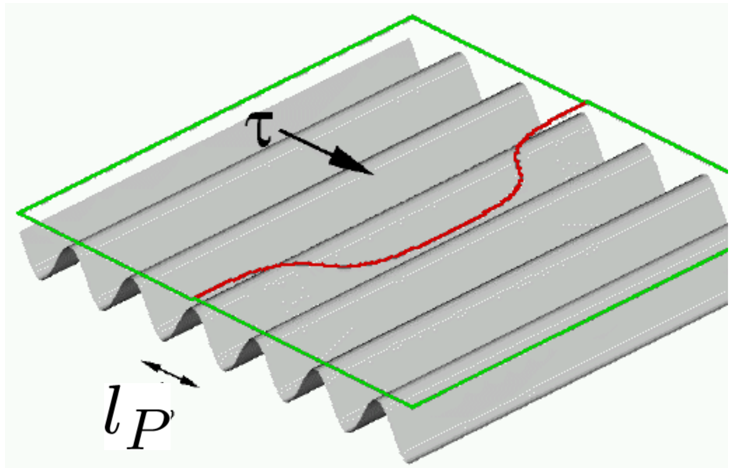
- Dislocation velocity: $\mu_t = -\alpha \times v_t$

- Dissipation: $\Psi(\dot{u}, u) = \int_{J_u} \psi(v_t) \, d\mathcal{H}^2$

LE dislocations – Dissipation

Kink





Stainier, L., Cuitino, A. and Ortiz, M., *JMPS*, **50** (2002) 1511-1554.

- From transition-state theory:

$$\psi(v) = \psi_0 \left(\frac{v}{v_0} \text{asinh} \frac{v}{v_0} - \sqrt{1 + \frac{v^2}{v_0^2}} \right),$$

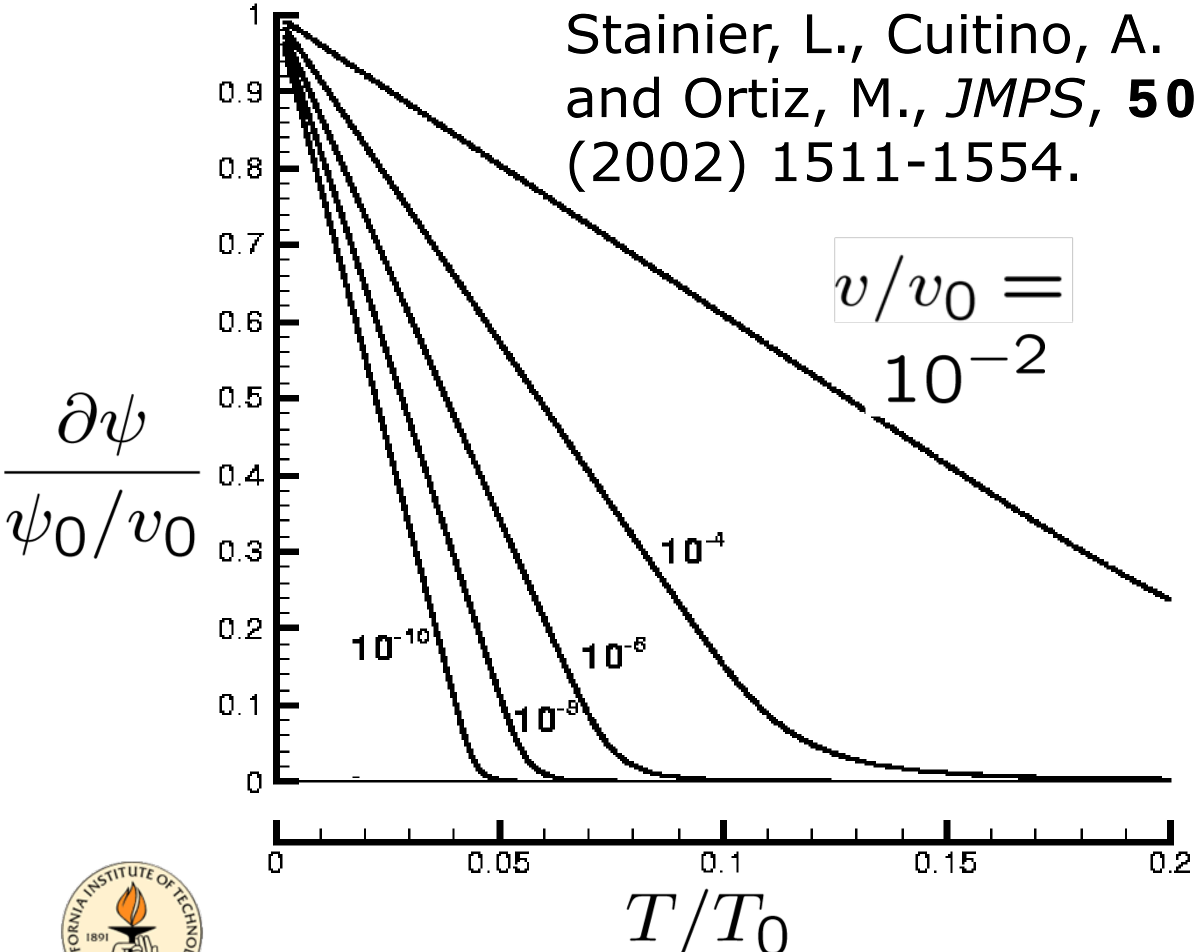
ψ_0, v_0 calculated from atomistic models

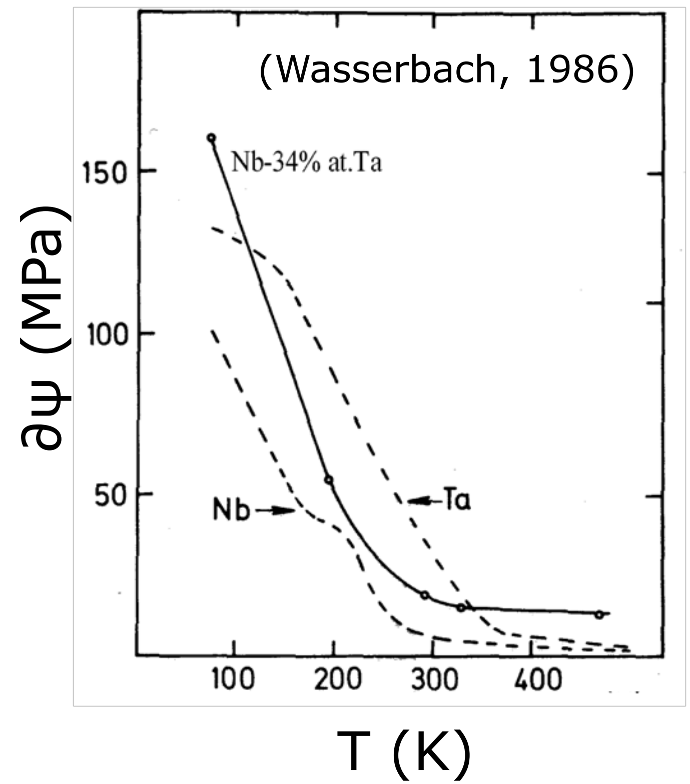
Wang, G. *et al., J. Computer Aided Materials Design*, 2001)

LE dislocations – Dissipation

- Validation of transition-state theory model:

Stainier, L., Cuitino, A. and Ortiz, M., *JMPS*, **50** (2002) 1511-1554.





LE dislocations – Energy-dissipation

- Rate potential: $G(u, \dot{u}) = \Psi(\dot{u}) + DE(u)\dot{u}$
- Energy: $E(u) = \int_\Omega \frac{1}{2} |\epsilon(u)|^2 \, dx$
- Dissipation: $\Psi(\dot{u}, u) = \int_{J_u} \psi(v_t) \, d\mathcal{H}^2$
- Energy-dissipation functional: For $\epsilon > 0$,

$$F_\epsilon(u) = \int_0^T \mathrm{e}^{-t/\epsilon} G(t, u, \dot{u}) \, dt \longrightarrow \text{inf!}$$

- Relaxation: $sc^- F_\epsilon(u)$?
- Causal limit: $\epsilon \to 0$?

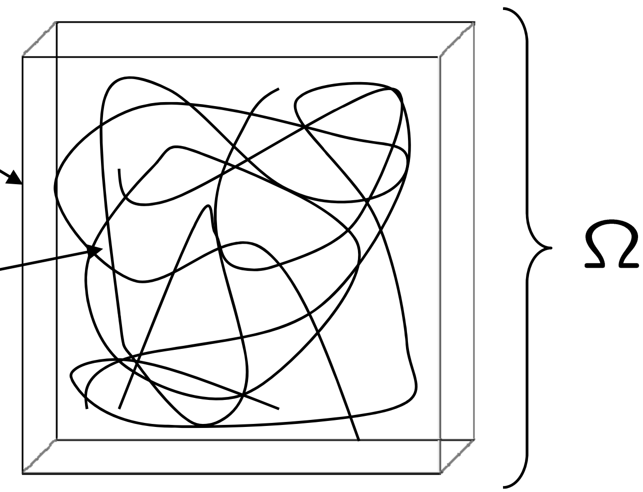
} $\longrightarrow$ Crystal plasticity!

Problems are open!

LE dislocations − Energy models

$u = \bar{\beta}x$ (affine BC)

β^p, α given!



- Average plastic deformation:

$$\bar{\beta}^p = \frac{1}{|\Omega|}\int_{J_u} [\![u]\!] \otimes m \, d\mathcal{H}^2$$

- Elastic energy: $\inf_u \int_{\Omega \setminus S_u} \left(\frac{1}{2}|\epsilon(u)|^2 - \epsilon(u)\cdot\epsilon^p\right) dx$

$$= \underbrace{|\Omega|\left(\frac{1}{2}|\bar{\epsilon}|^2 - \bar{\epsilon}\cdot\bar{\epsilon}^p\right)}_{\text{strain energy}} + \underbrace{E(\alpha)}_{\text{stored energy}}$$

LE dislocations − Energy models

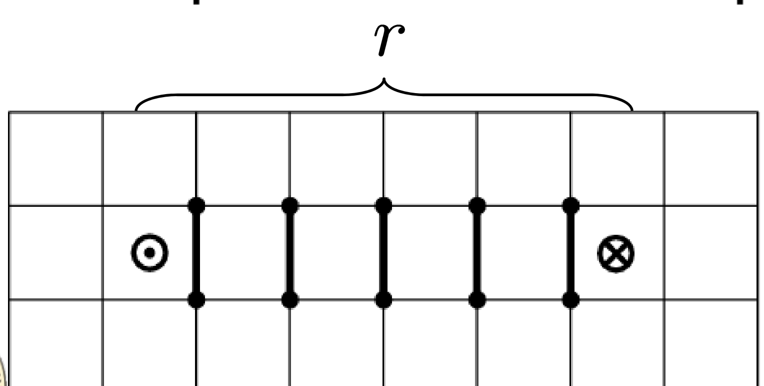
- Stored energy: $E(\alpha) = \int\int \mathrm{tr}[\underbrace{d\alpha^T(x)\Gamma(x,y)d\alpha(y)}_{\text{nonlocal!}}]$

  where: $\Gamma(x,y) =$

  $$\int_\Omega [\nabla G(x,z)\cdot\nabla G(y,z)\, I - \nabla G(x,z)\otimes\nabla G(x,z)]\, dz$$

  and: $G = \Delta^{-1} \equiv$ Green's function of the Laplacian

- Example: Dislocation dipole



$$\longleftarrow \frac{E}{L} \sim \frac{Gb^2}{2\pi}\log\frac{r}{\epsilon} + b\tau r$$

LE dislocations − Energy models

- Conjecture: For sufficiently dilute dislocations,

$$\Gamma - \lim_{h\to\infty} E_h(\alpha) = \underbrace{\int T(\alpha/|\alpha|)d|\alpha|}$$

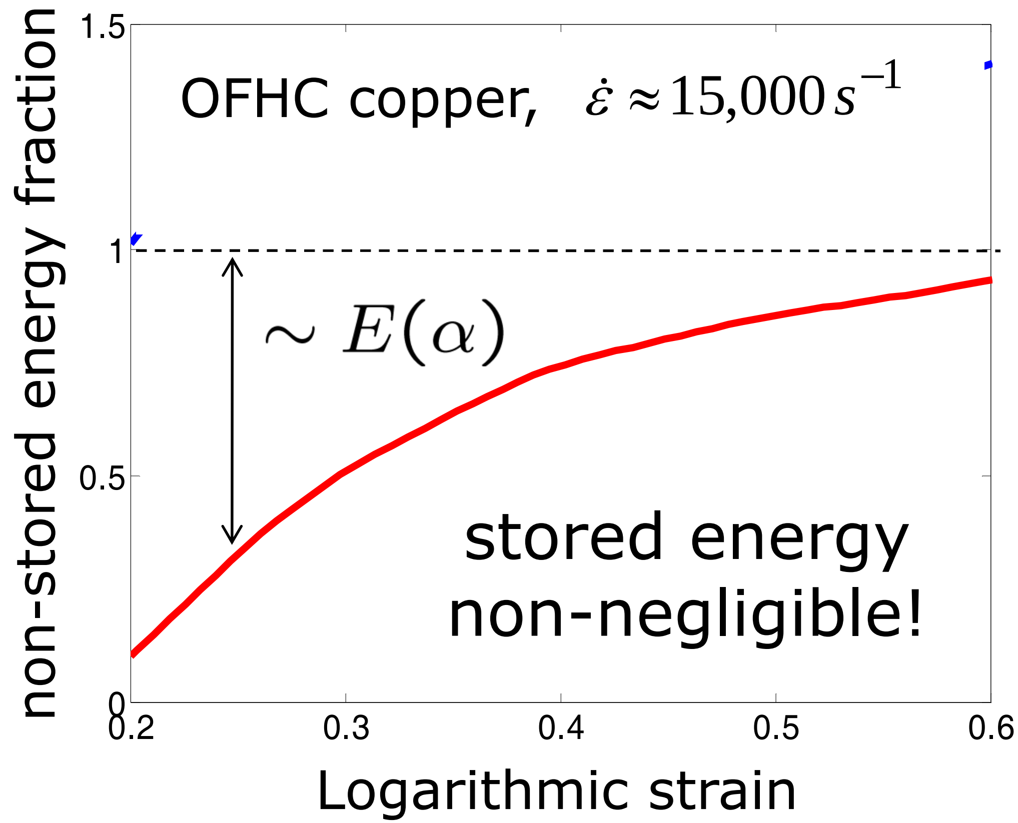
local line tension approximation!

- True in 2D: M. Ponsiglione, *SIAM J. Math. Anal*. **39** (2008) no. 2, 449-469; A. Garroni, G. Leone, M. Ponsiglione, preprint (2008).
- True in 2.5D: Garroni, S. Müller, *SIAM J. Math. Anal*., **36** (2005) no. 6, 1943–1964; S. Cacace, A. Garroni, preprint (2008).

- Frequently used approximation: $E(\alpha) \approx 0$.

LE dislocations – Energy models

Kolsky (split Hopkinson) pressure bar

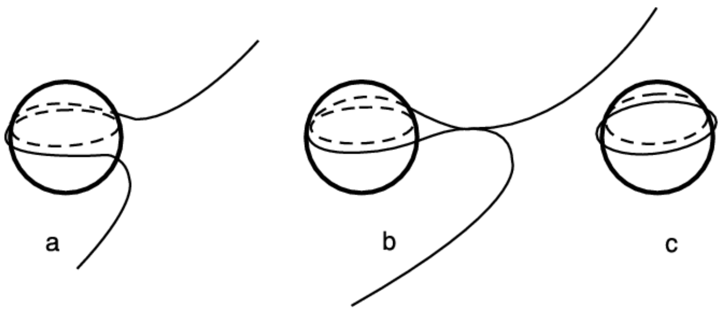


Fraction of total work dissipated as heat

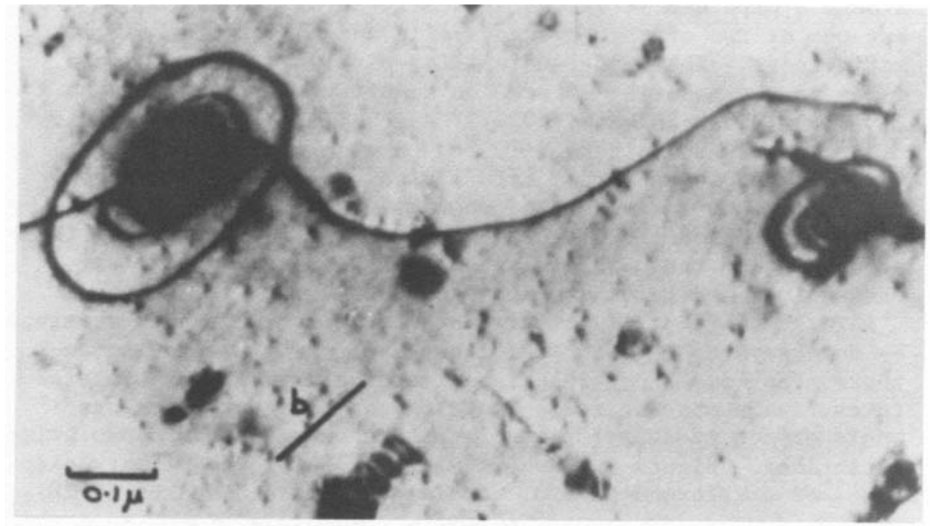
(Rittel, D, Ravichandran, G, Lee, S, *Mechanics of Materials*, **34** (2002) 627-642)

LE dislocations – Dissipation models

- Example: Precipitates.



Impenetrable obstacles

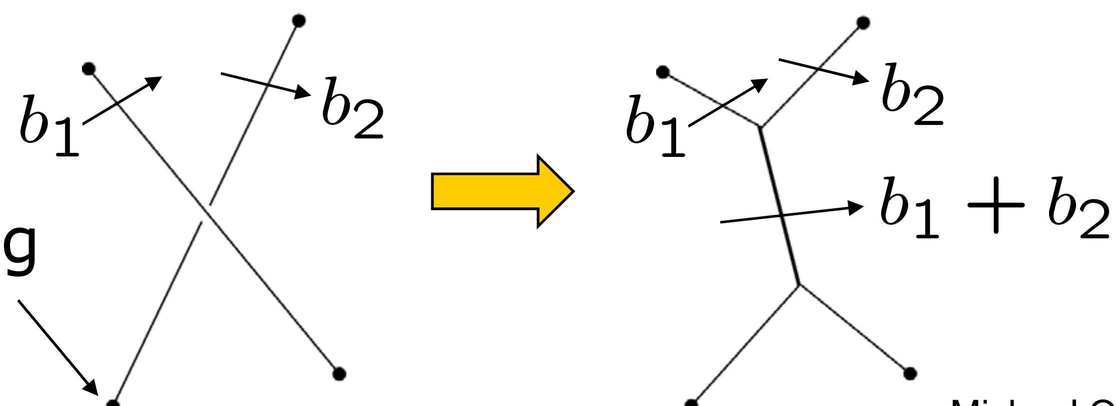


(Humphreys and Hirsch '70)

- Junctions, jogs:

(movie)
(LLNL)

pinning
points



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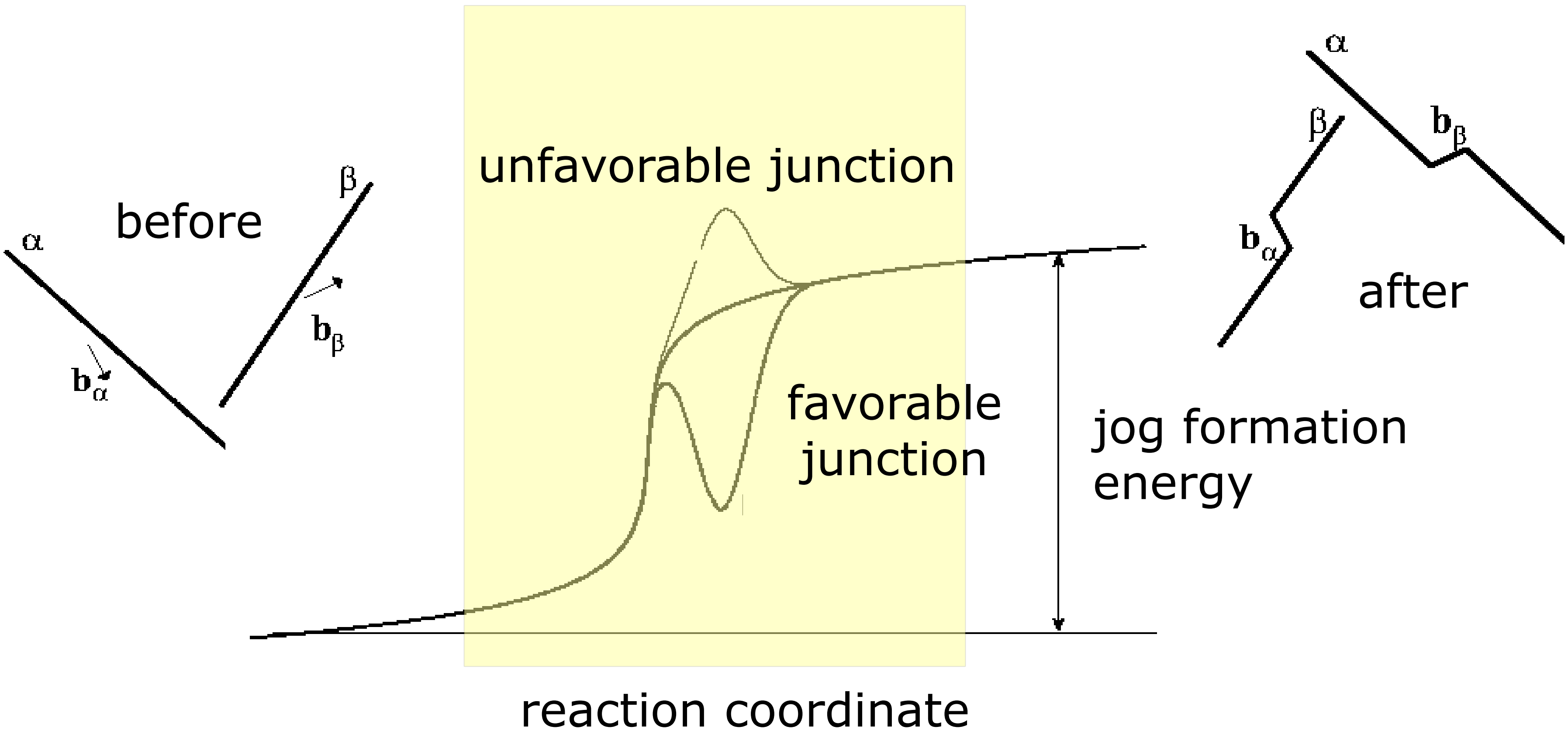
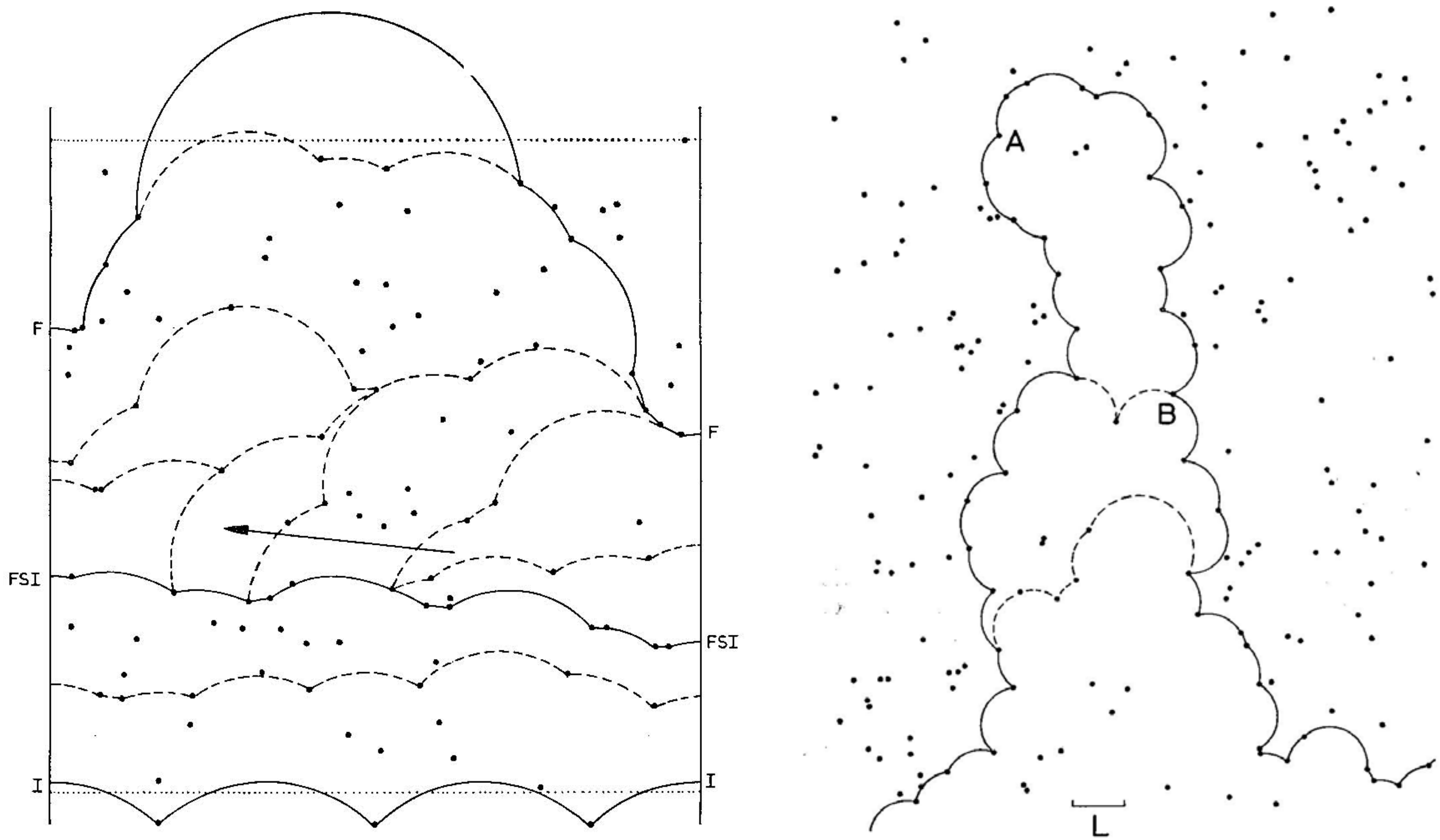
LE dislocations – Dissipation models



Dissipation at junctions and jogs
(Stainier, L., Cuitino, A., Ortiz, M., *JMPS*, **50** (2002) 1511-1554)

LE dislocations – Energy-dissipation models



Dislocation motion through random obstacle array
(Foreman, A.J.E., Makin, M.J., *Phil. Mag.*, **14** (1966) 911)

- Plastic work: $W^p \sim \rho^{1/2}\gamma^{3/2}$, where:

$\rho \equiv$ obstacle density, $\gamma \equiv$ slip strain

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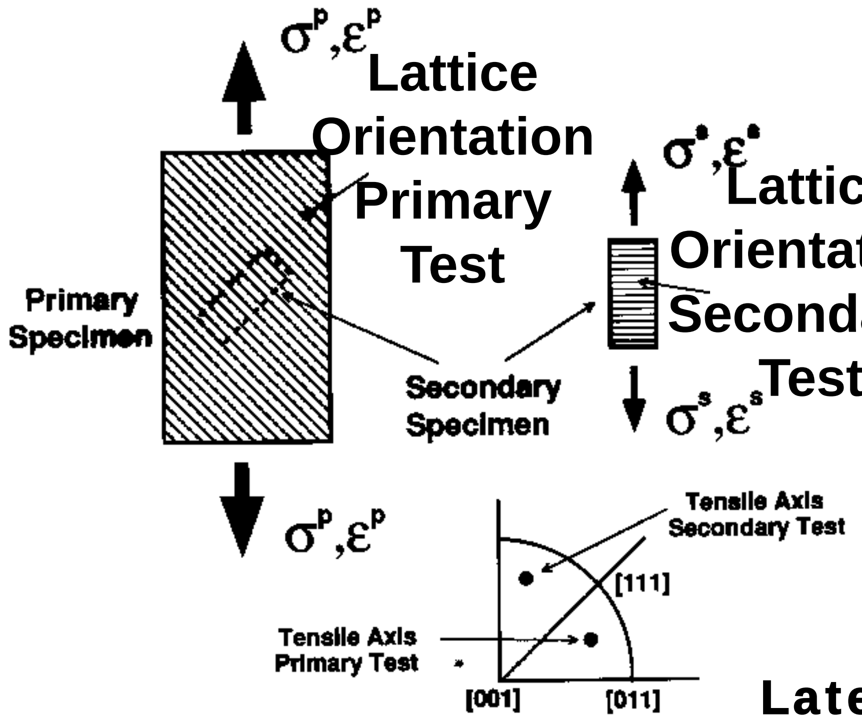
LE dislocations – Energy-dissipation models

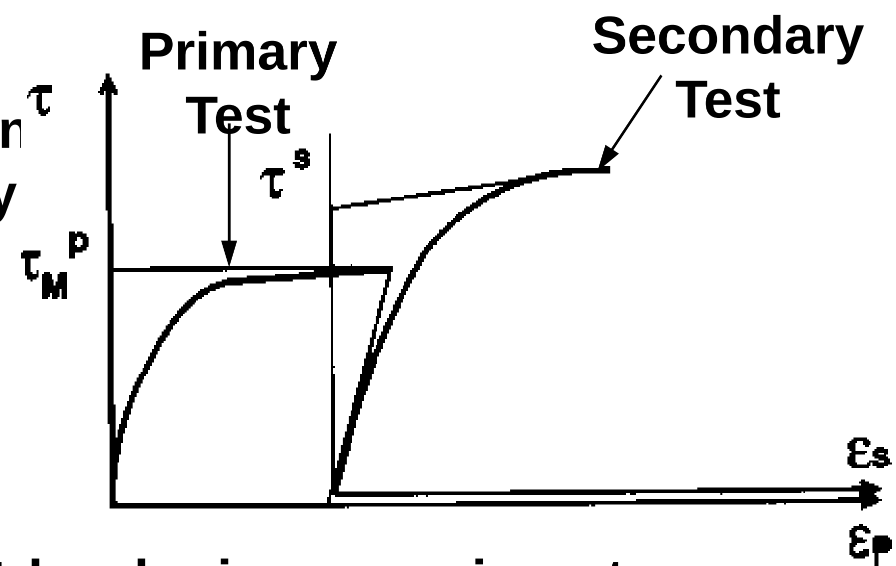
- Forest hardening: Dislocations in secondary systems supply obstacles to the motion of dislocations on primary systems
- Dislocation multiplication: Dislocation density increases as a result of slip activity due to
  - *Activation of fixed sources*
  - *Dynamic sources (cross slip)*
  - *Anihilation*
- Strong latent hardening: High rate of hardening of primary system due to activity on secondary systems

(movie)

(LLNL)

Junctions – Strong latent hardening





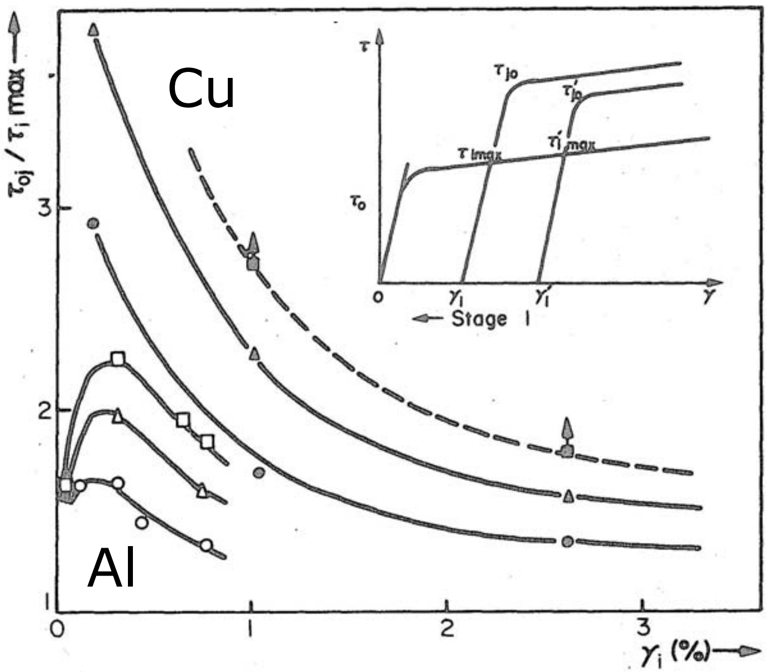
Latent hardening experiments

UF Kocks, *Acta Metallurgica*, **8** (1960) 345

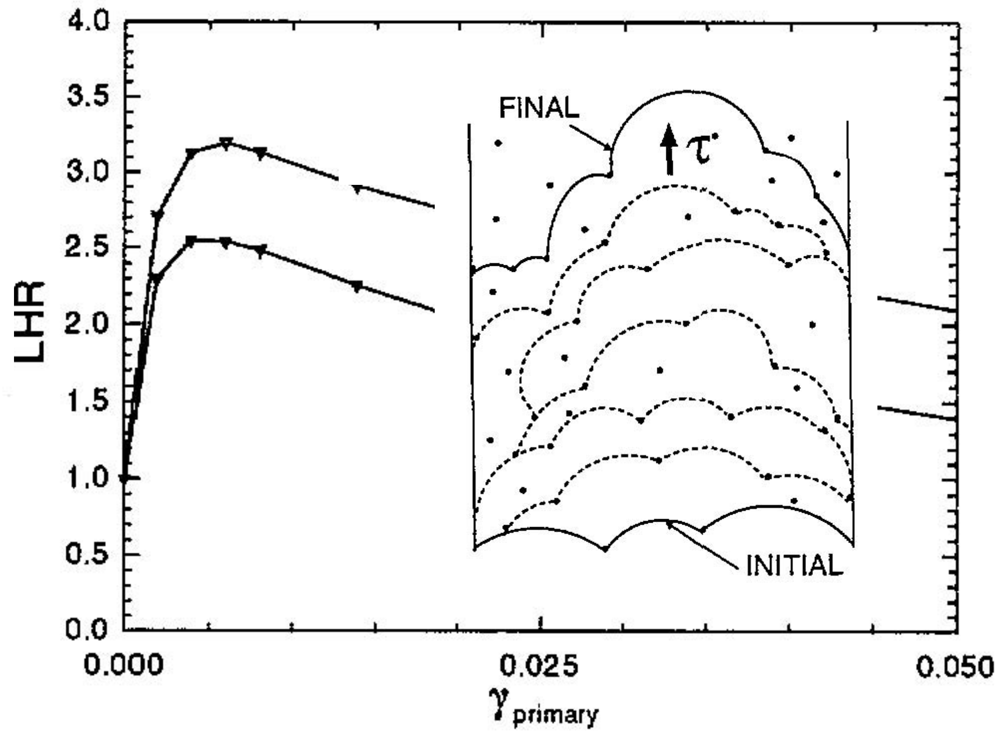
UF Kocks, *Trans. Metall. Soc. AIME*, **230** (1964) 1160

- Strong latent hardening: Crystals much ‘prefer’ to activate a single slip system at each material point, though the active system may vary from point to point

LE dislocations − Energy-dissipation models



Measured latent hardening ratios (Franciosi, P., Berveiller, M., and Zaoui, A., Acta Metall., 28 (1980) 273-283)



Latent hardening ratios predicted from line tension percolation model, multiple slip and dislocation multiplication

(Cuitino, A. and Ortiz, M., *Modelling Simul. Mater. Sci. Engr.*, **1** (1992) 225-263)

Dislocation dynamics to crystal plasticity

- The problem of deriving single crystal plasticity from dislocation dynamics remains open in general
- Mathematical formulation of the problem: Relax dislocation-dynamics energy-dissipation functional, pass to the causal limit
- Many important features of crystal plasticity are understood qualitatively from experiments, microscopy and engineering models
- Most important among those features are:
  - *Crystallographic nature of plastic slip in crystals*
  - *Strong latent hardening under multiple slip*
- These features give rise to microstructure…