Multiscale models of metal plasticity
Lecture IV: Kinetics and work hardening

M. Ortiz

California Institute of Technology

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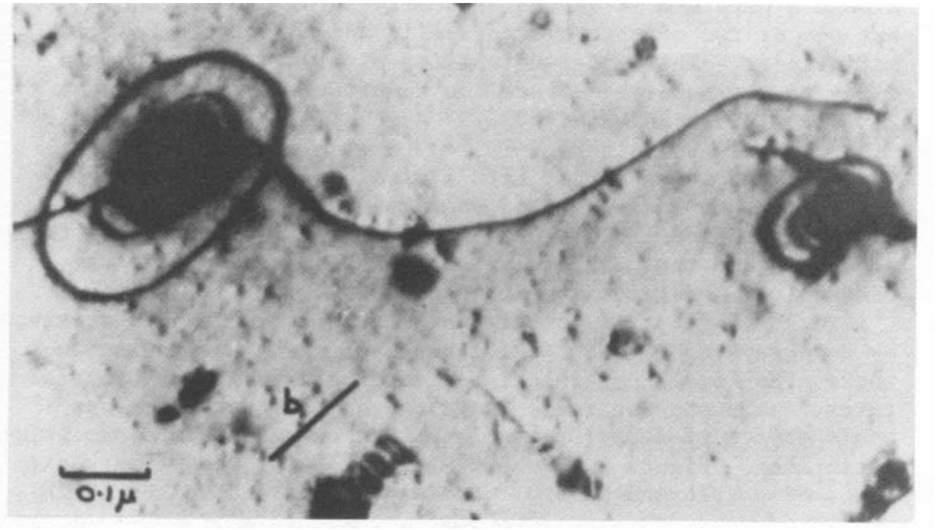
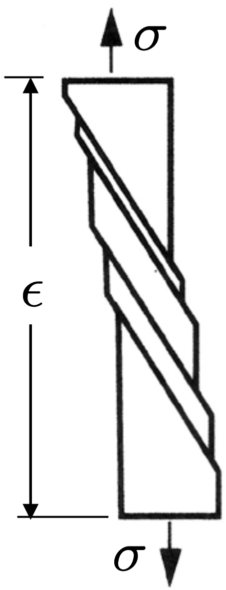
Outline of Lecture #4

- Beyond energy: Kinetics
- Experimental observations, dislocation mobility
- The forest hardening model
- Energy-dissipation functionals
- Phase-field models

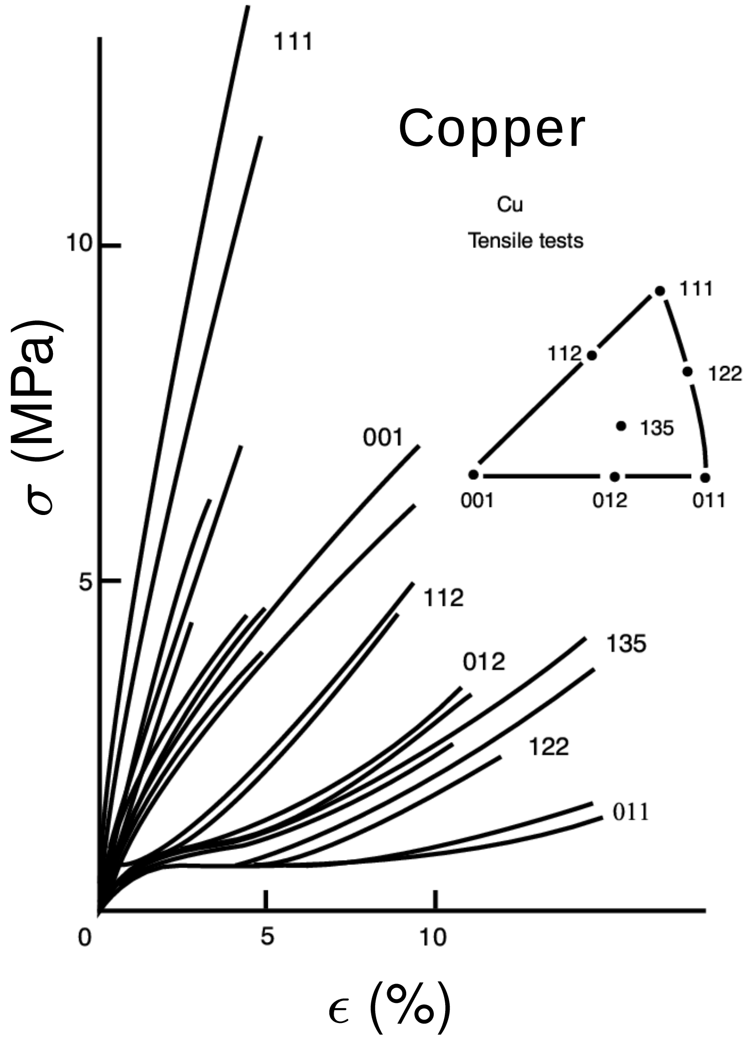


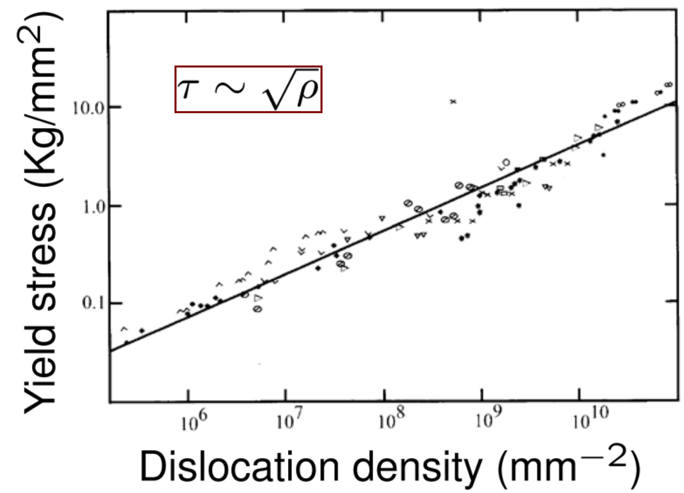
(Humphreys and Hirsch, 1970)

Crystal plasticity – Macroscopic behavior



Uniaxial tension test

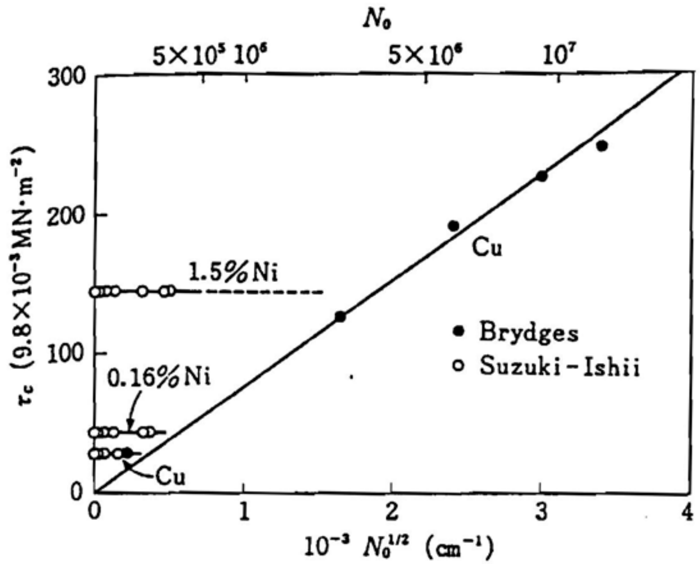


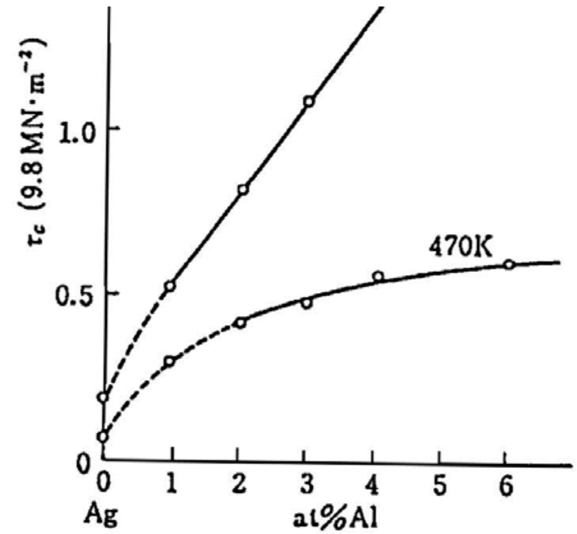


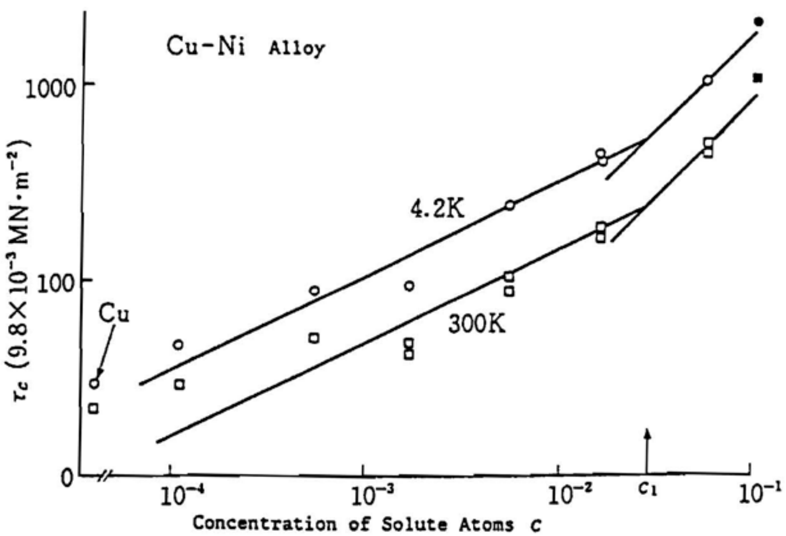
Taylor scaling
(SJ Basinski and ZS Basinski,
Dislocations in Solids,
FRN Nabarro (ed.)
North-Holland, 1979.)

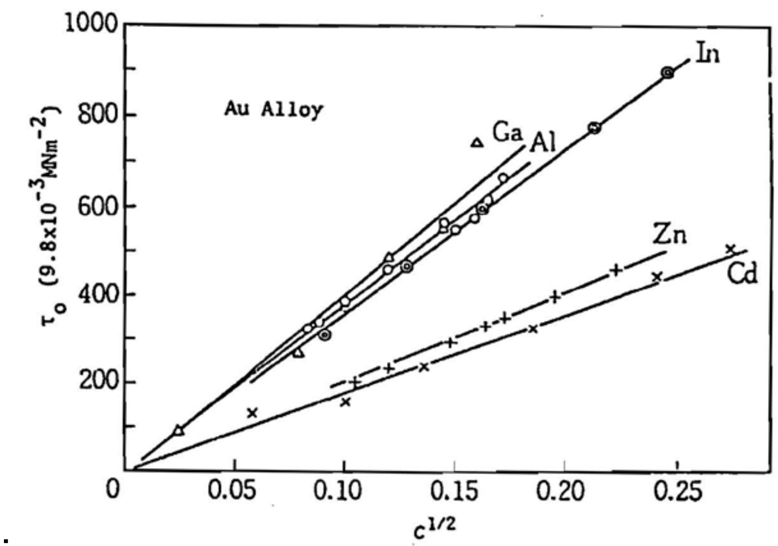
P. Franciosi and A. Zaoui,
Acta Metall., **30** (1982) 2141-2151

Hardening and obstacle density



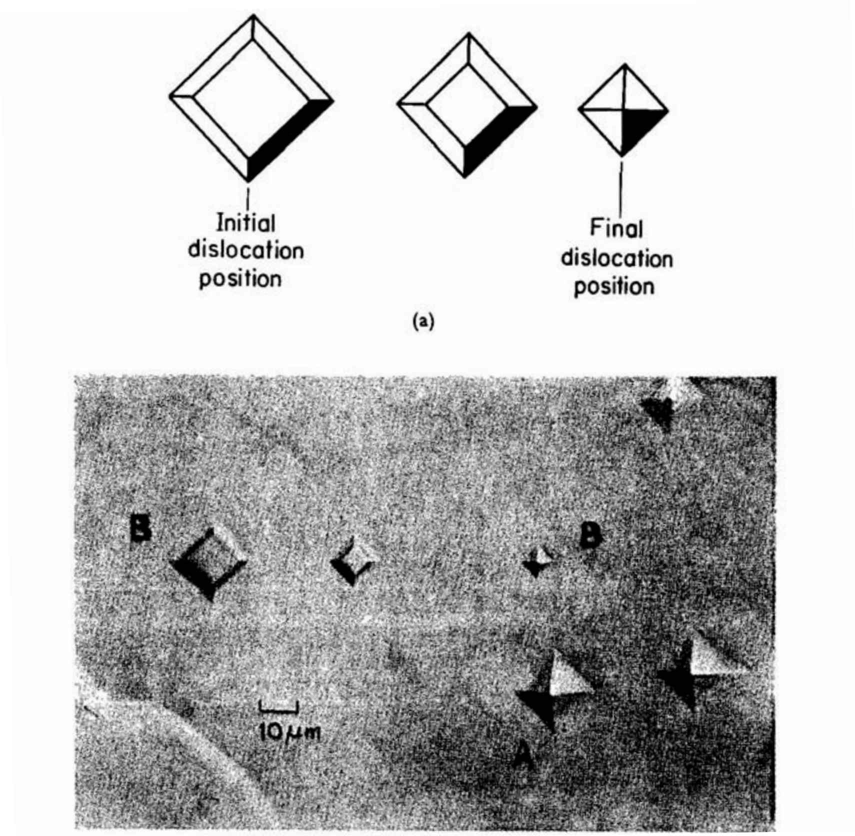




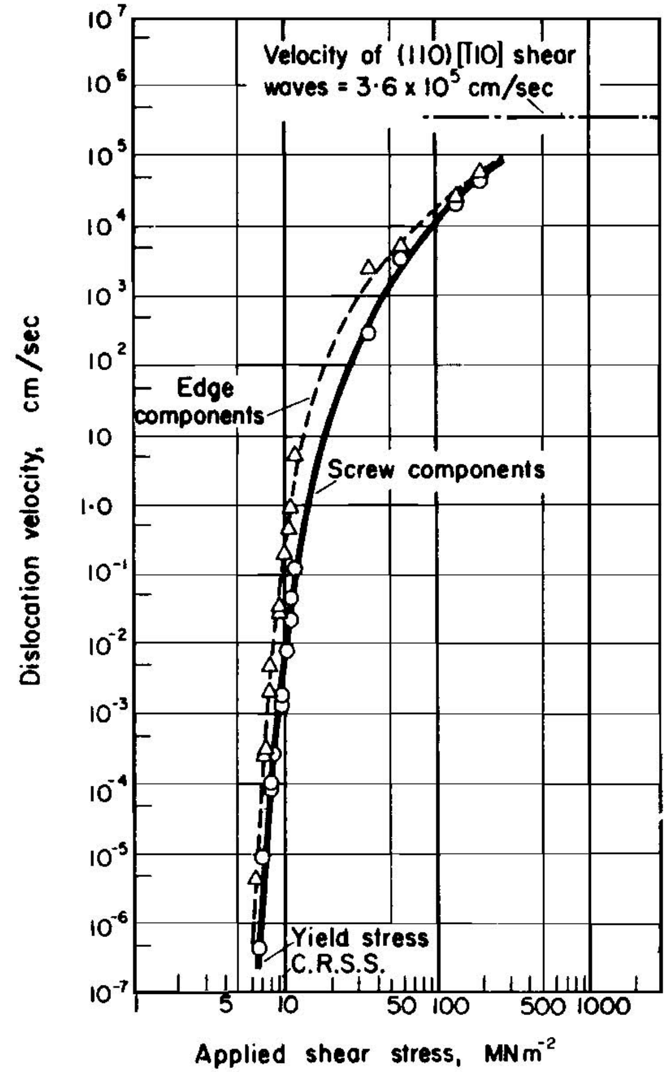


T. Suzuki, S. Takeuchi and H. Yoshinaga,
Dislocation Dynamics and Plasticity, Springer-Verlag, 1985.

Dislocation velocity

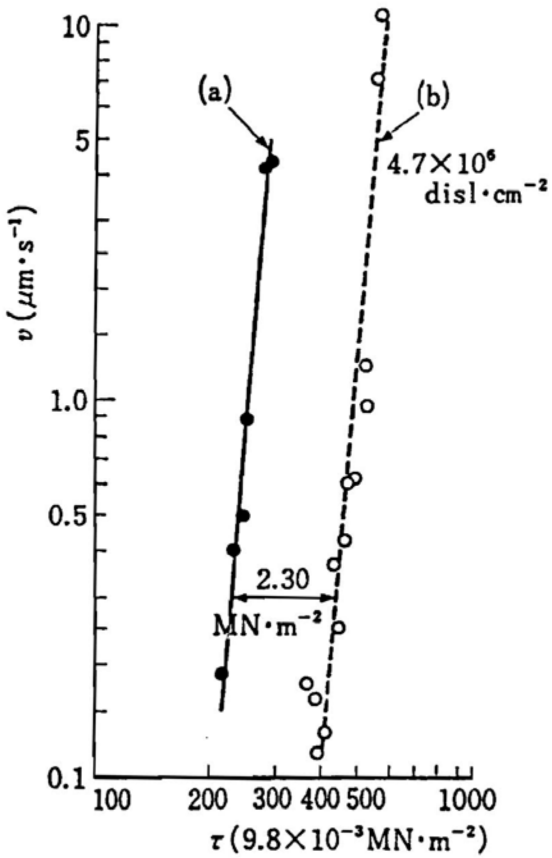


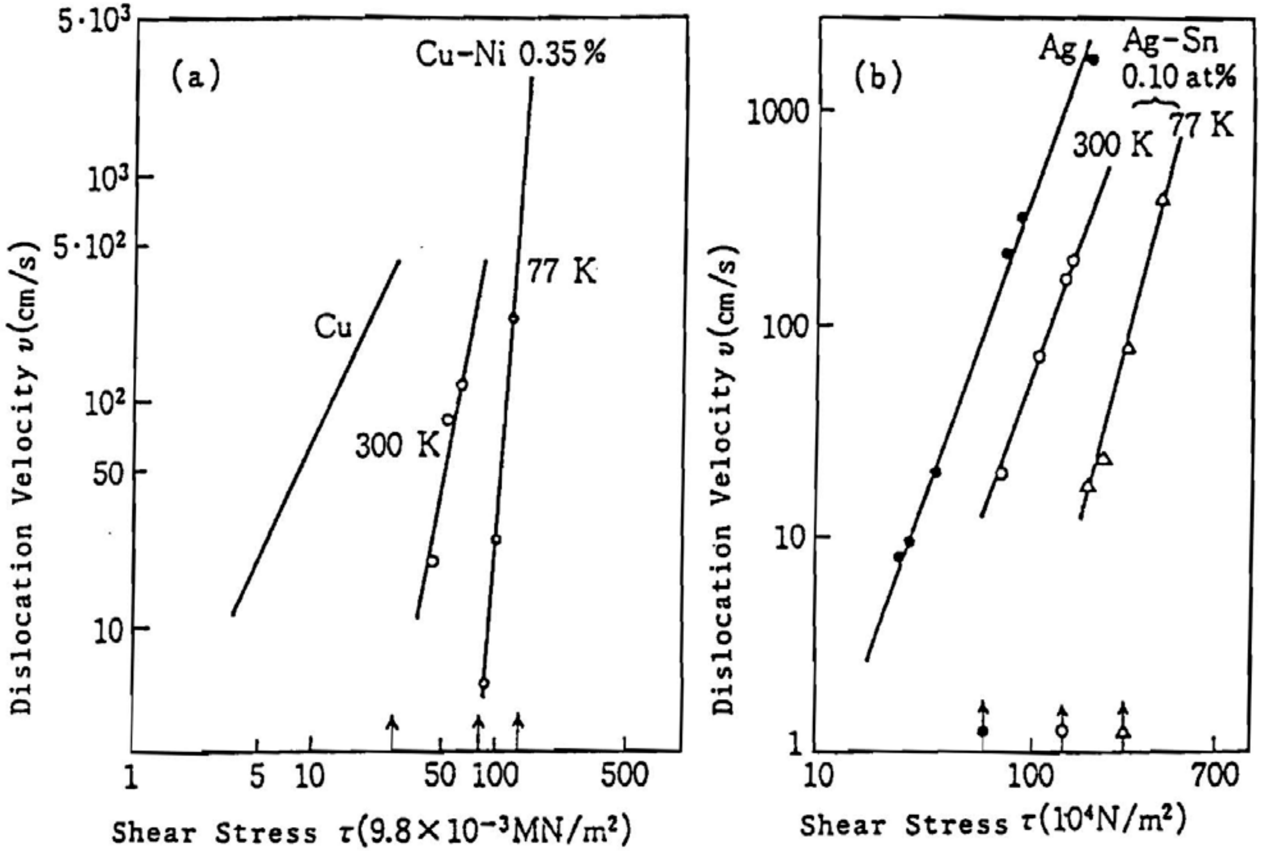
Etch pits on a LiF crystal



T. Suzuki, S. Takeuchi and H. Yoshinaga,
Dislocation Dynamics and Plasticity, Springer-Verlag, 1985.

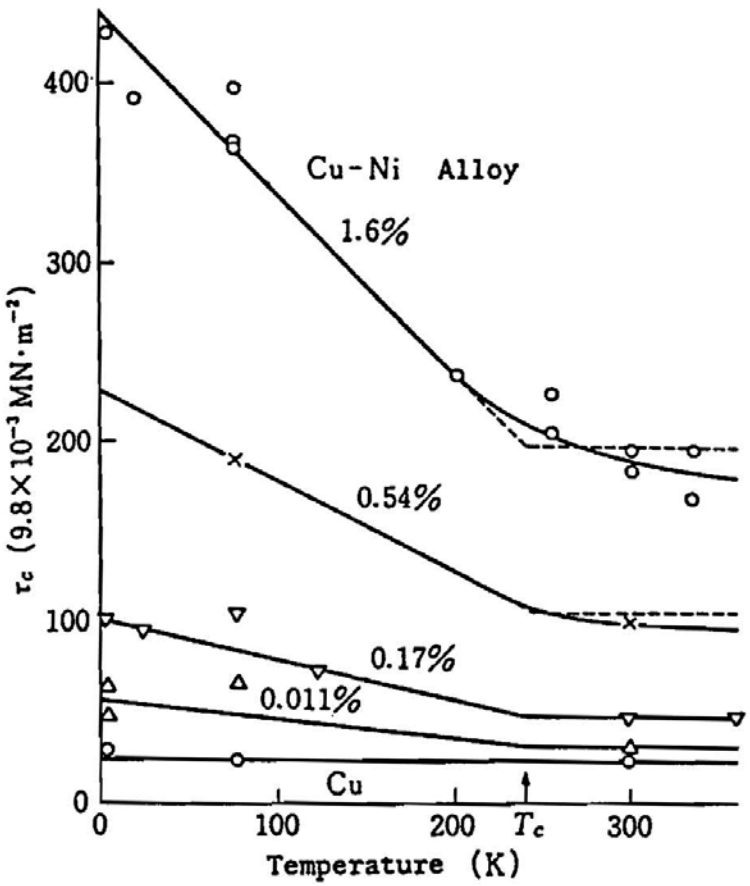
Dislocation velocity

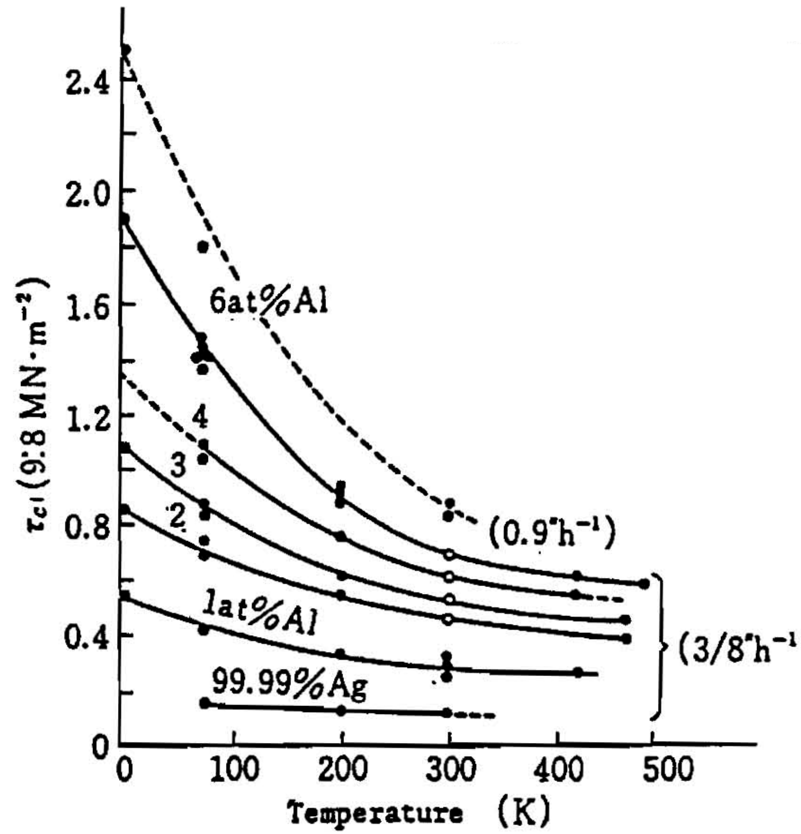




T. Suzuki, S. Takeuchi and H. Yoshinaga,
Dislocation Dynamics and Plasticity, Springer-Verlag, 1985.

Thermal softening

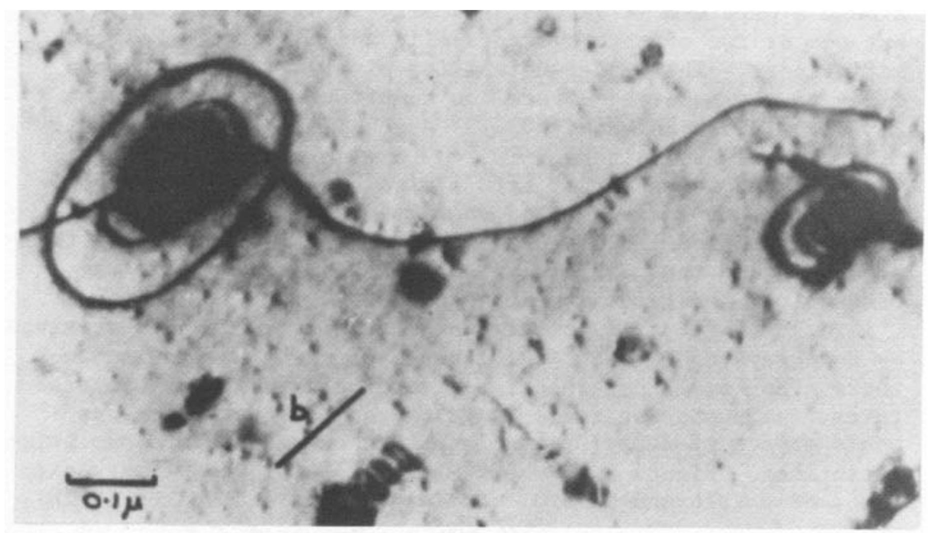




T. Suzuki, S. Takeuchi and H. Yoshinaga, *Dislocation Dynamics and Plasticity*, Springer-Verlag, 1985.

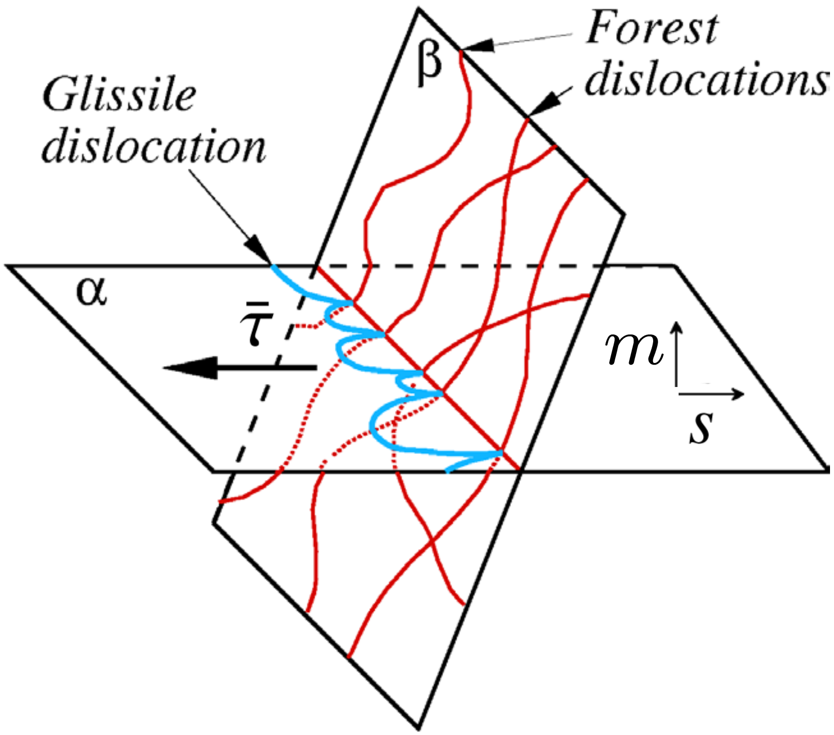
Outline of Lecture #4

- Dislocation motion is governed by kinetics
- Dislocations react with each other irreversibly
- Energy-minimization is not enough to describe dislocation dynamics, hardening
- Need kinetics, time-dependent problems!

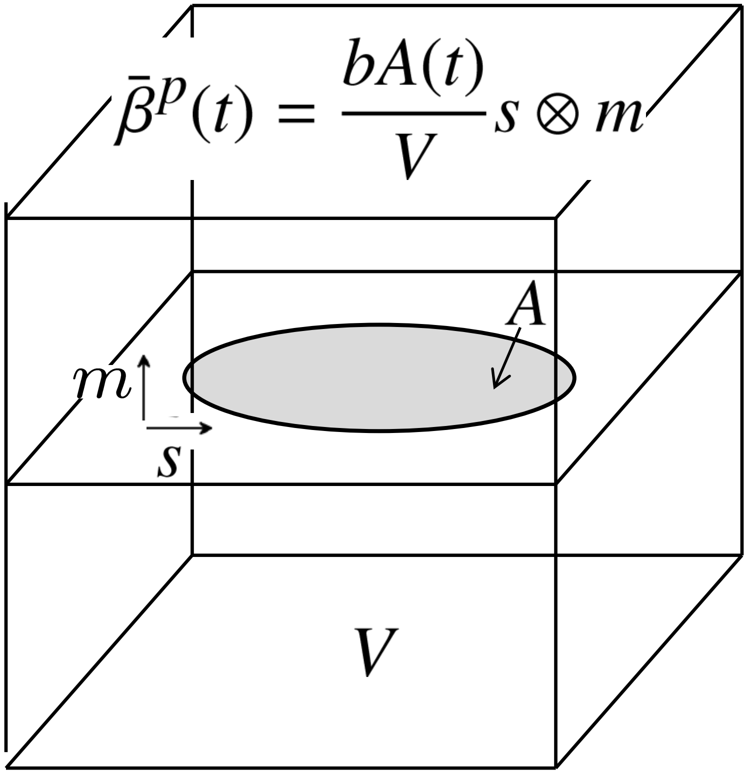


(Humphreys and Hirsch, 1970)

The forest-hardening problem



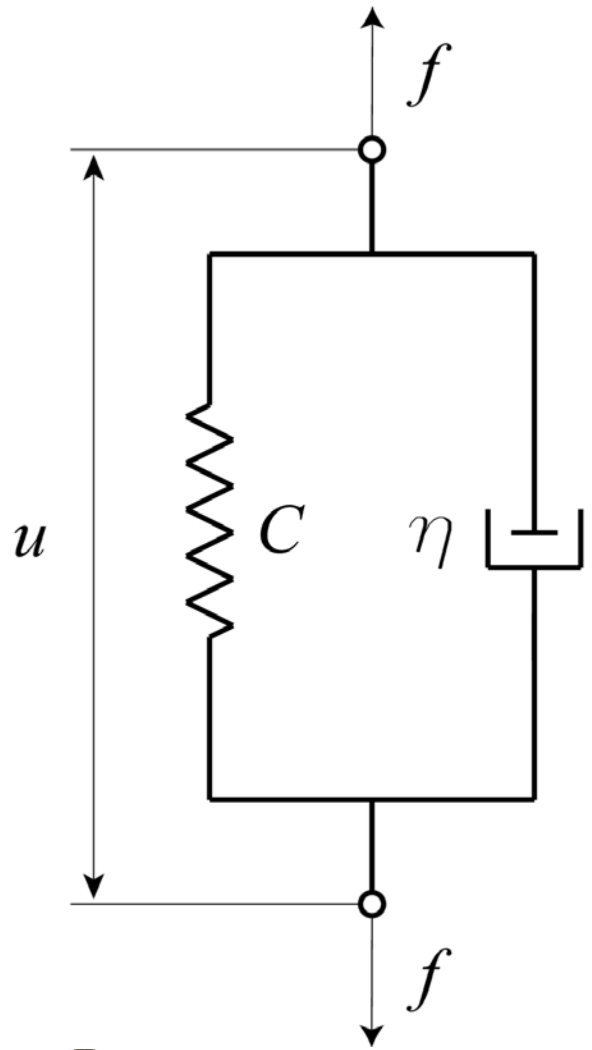
Glissile dislocation moving through forest dislocations



Micro-to-macro transition, single slip

Given: $\bar{\tau}(t) = \bar{\sigma}_{ij}(t) s_i m_j$ ⇒ determine: $\bar{\gamma}(t) = \frac{bA(t)}{V}$

Classical rate variational problems



- Kelvin solid IV problem:

$$\left.\begin{aligned} &\eta \dot{u}(t) + C u(t) = f(t) \\ &u(0) = u_0 \end{aligned}\right\}$$

- Potential energy:

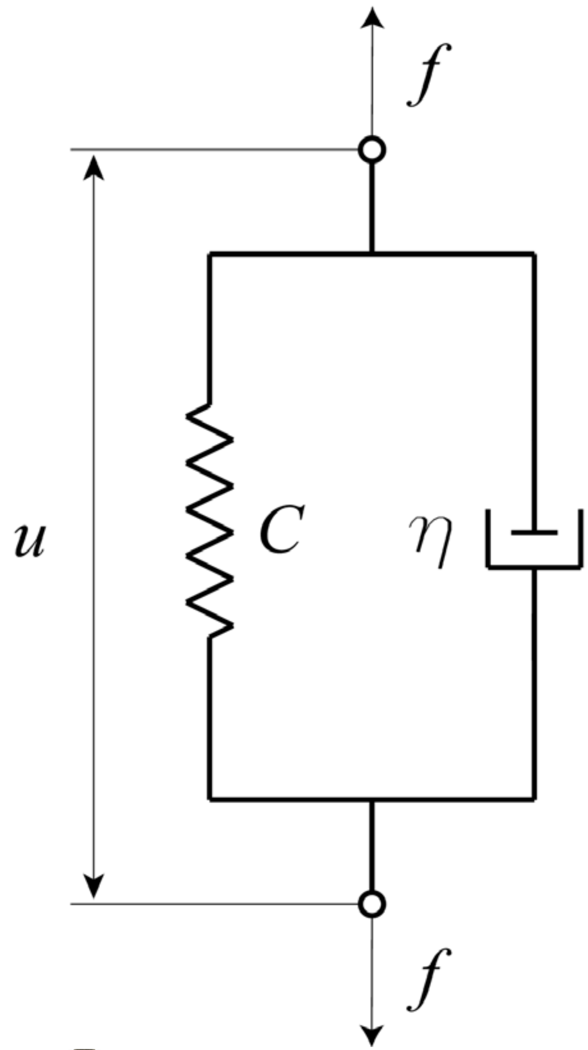
$$E(t,u) = \frac{C}{2} u^2 - f(t) u$$

- 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 $t \in [0,T]$,

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

Forest hardening – External energy

- Energy of LE dislocated crystal, applied stress $\bar{\sigma}_{ij}$:

$$E(u) = \int_{\Omega \setminus J_u} \frac{1}{2} c_{ijkl} u_{i,j} u_{k,l}\, dx + \int_{\partial\Omega} \bar{\sigma}_{ij} n_j u_i \, d\mathcal{H}^2 = E^{\text{int}} + E^{\text{ext}}$$

- Potential of the externally applied stresses:

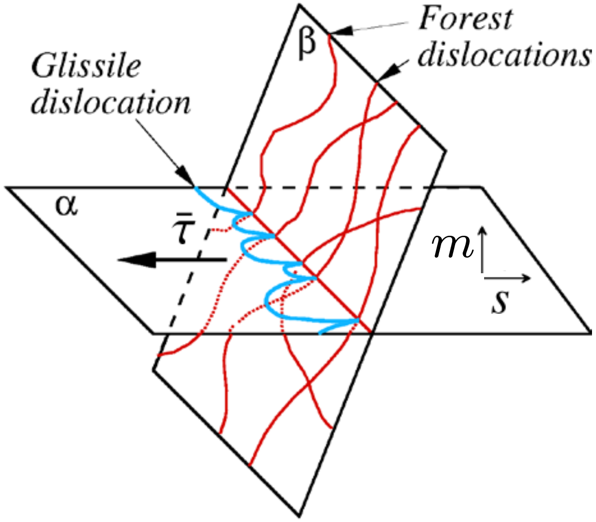
$$E^{\text{ext}} = \int_{\partial\Omega} \bar{\sigma}_{ij} u_i n_j \, d\mathcal{H}^2 = -\bar{\sigma}_{ij} \int_{J_u} [\![u_i]\!] n_j \, d\mathcal{H}^2 = -V \bar{\sigma}_{ij} \bar{\beta}^p_{ij}$$

- Single slip on one single slip plane:

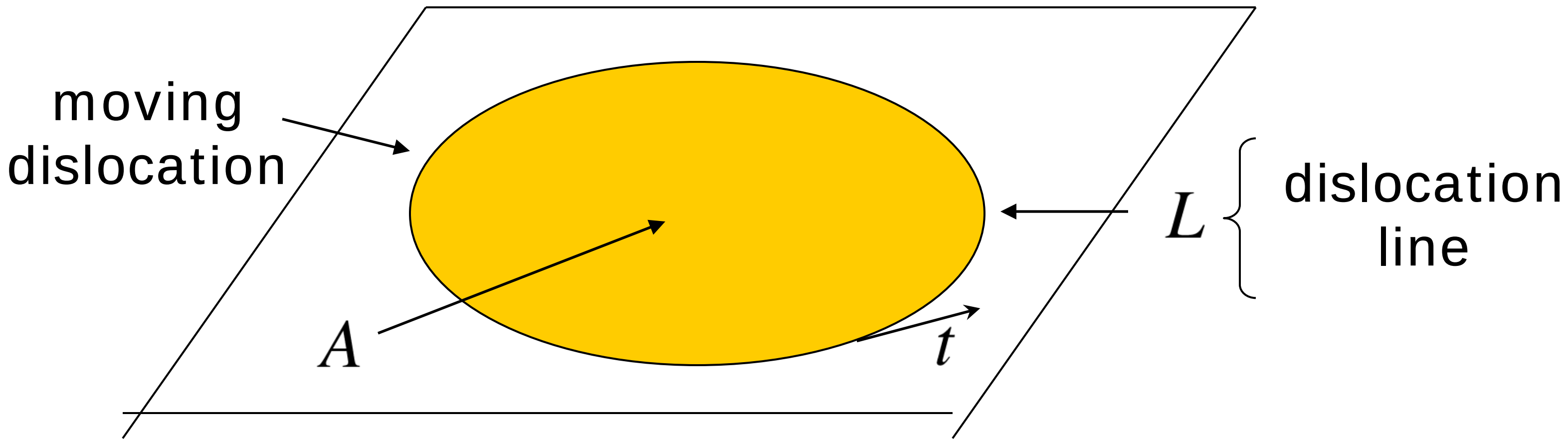
$$E^{\text{ext}} = -V \bar{\sigma}_{ij} \frac{A}{V} b_i m_j = -\bar{\tau}\bar{\gamma}, \quad \text{with:}$$

$\bar{\tau} = \bar{\sigma}_{ij} s_i m_j \equiv$ resolved shear stress

$\bar{\gamma} = \dfrac{bA}{V} \equiv$ macroscopic slip strain



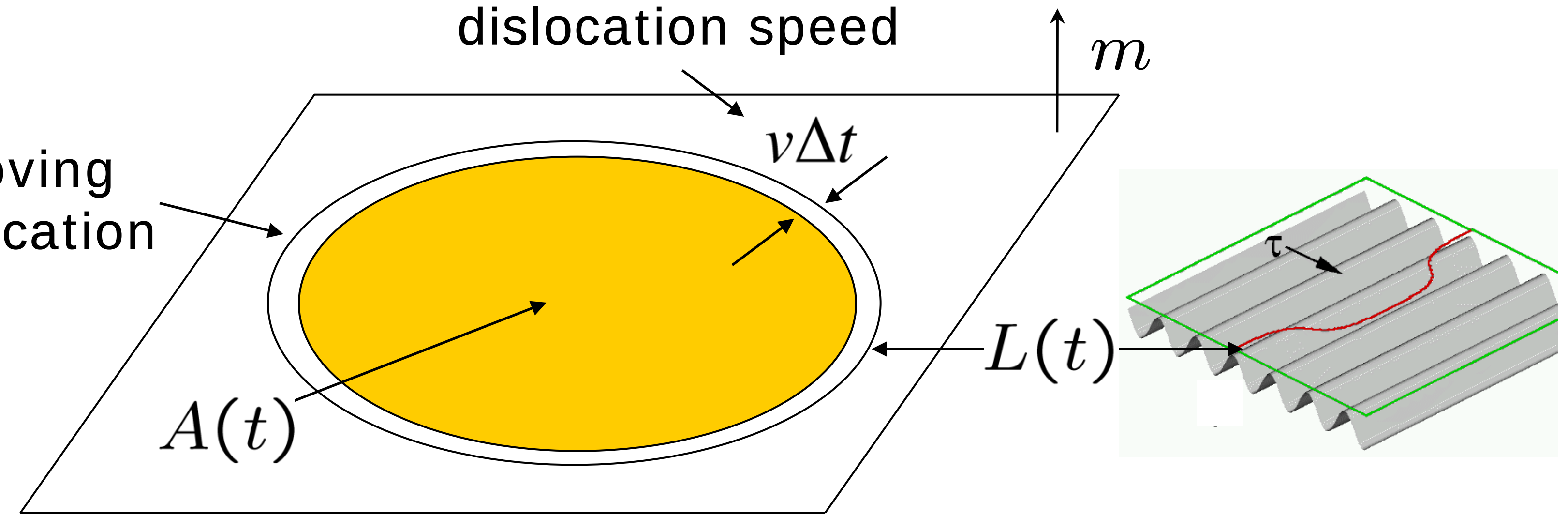
Forest hardening – Stored energy



- Volterra dislocation density: $\alpha = d\beta^p = b \otimes t\mathcal{H}^1 \lfloor L$
- From Mura's formula, general representation: $E^{\text{int}}(\alpha)$
- Dilute limit, line-tension approximation:

$$E^{\text{int}}(\alpha) = \int_L \langle Kb, b\rangle d\mathcal{H}^1$$

Forest hardening – Lattice friction



- Dislocation flux: $\forall \varphi \in C^1_0([0,T]), \forall f \in C_0(\Omega)$,

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

- Dislocation velocity: $\mu = -\alpha \times v$

Peierls stress (lattice friction)

- Dissipation potential: $\Psi^{\text{lat}} = \int_L \tau_c |v|\, d\mathcal{H}^1$

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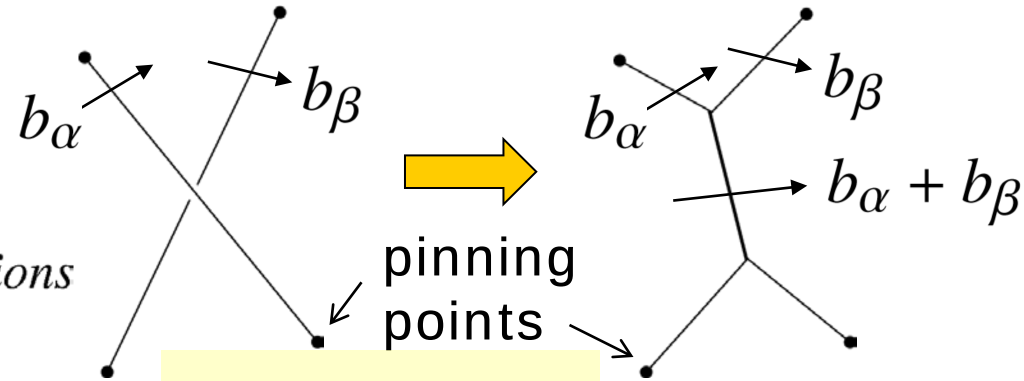
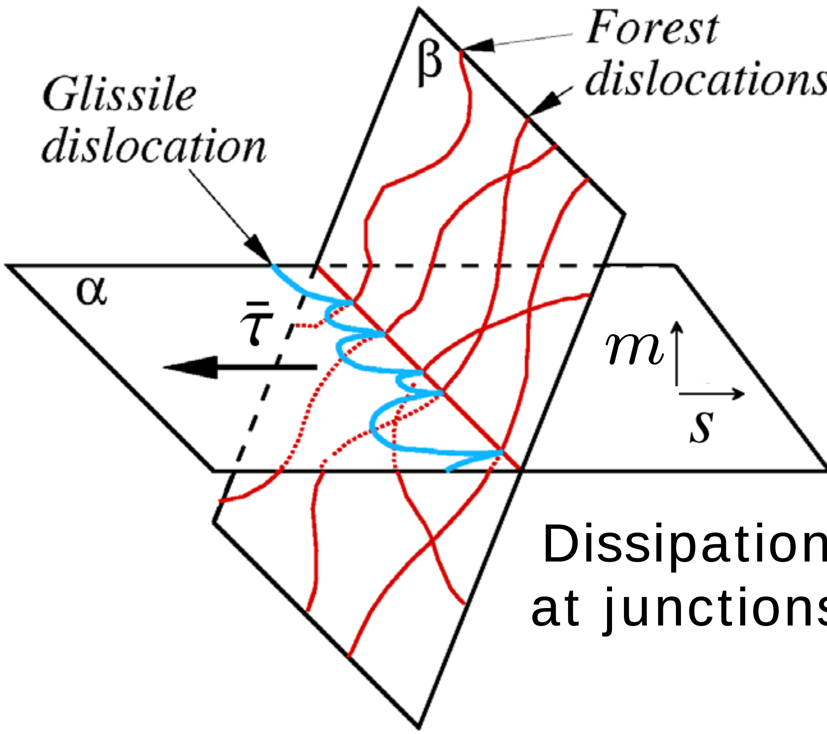
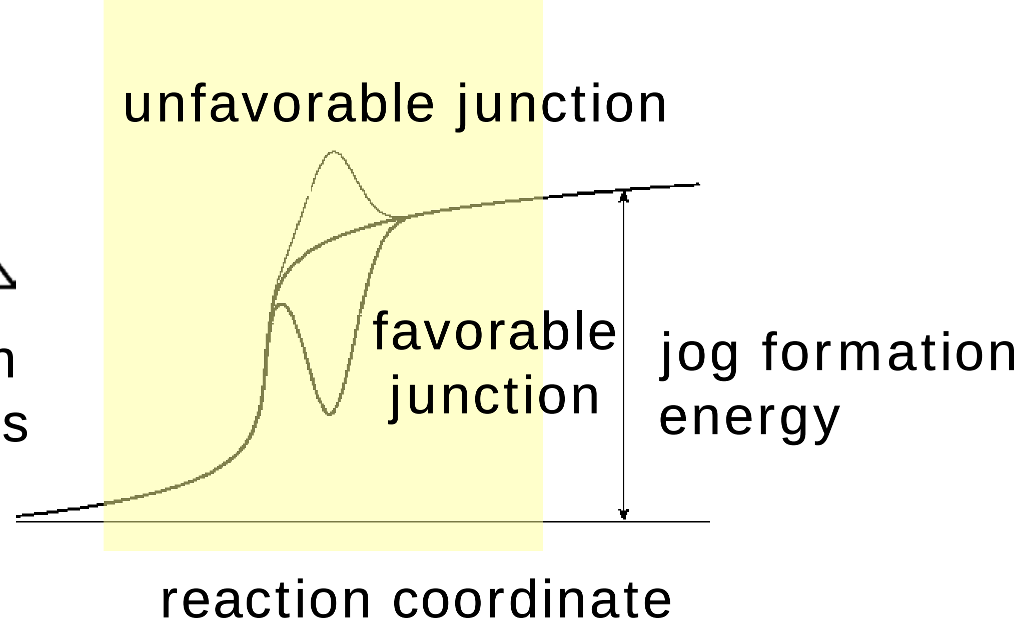
Forest hardening − Dissipation at obstacles

- Junctions, jogs:



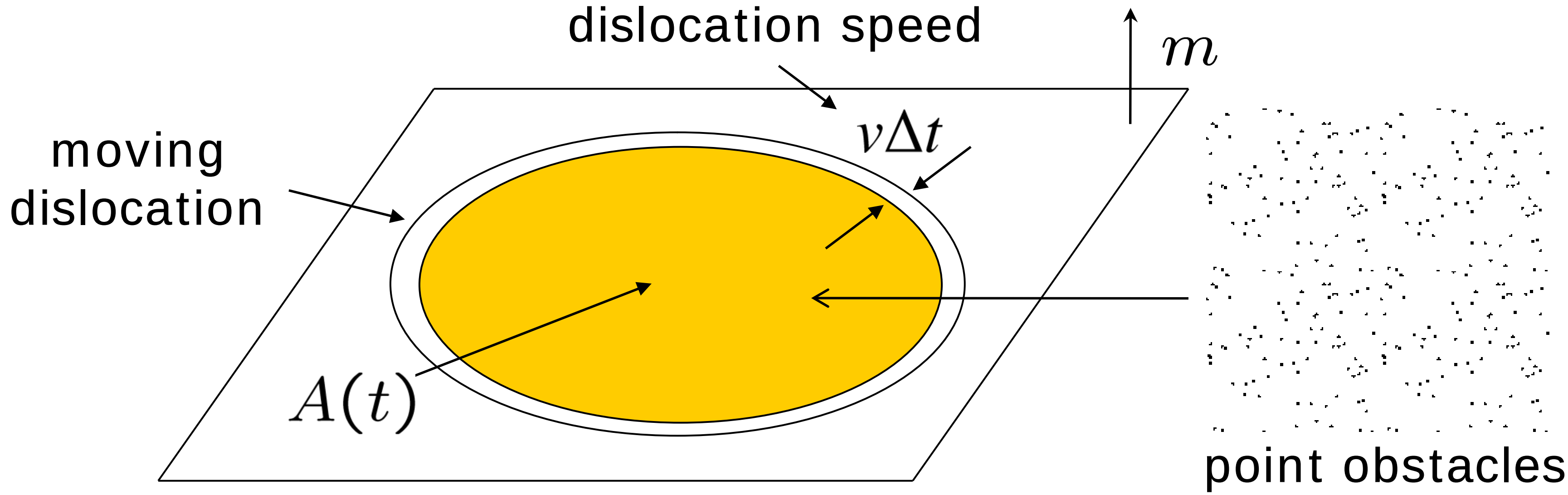


Dissipation
at junctions



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

Forest hardening – Point obstacles



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

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

- Dislocation velocity: $\mu = -\alpha \times \underline{v}$

- Dissipation potential: $\Psi^{\text{obs}} = \sum_{\text{obstacles}} f_c \, |v|$

obstacle strength

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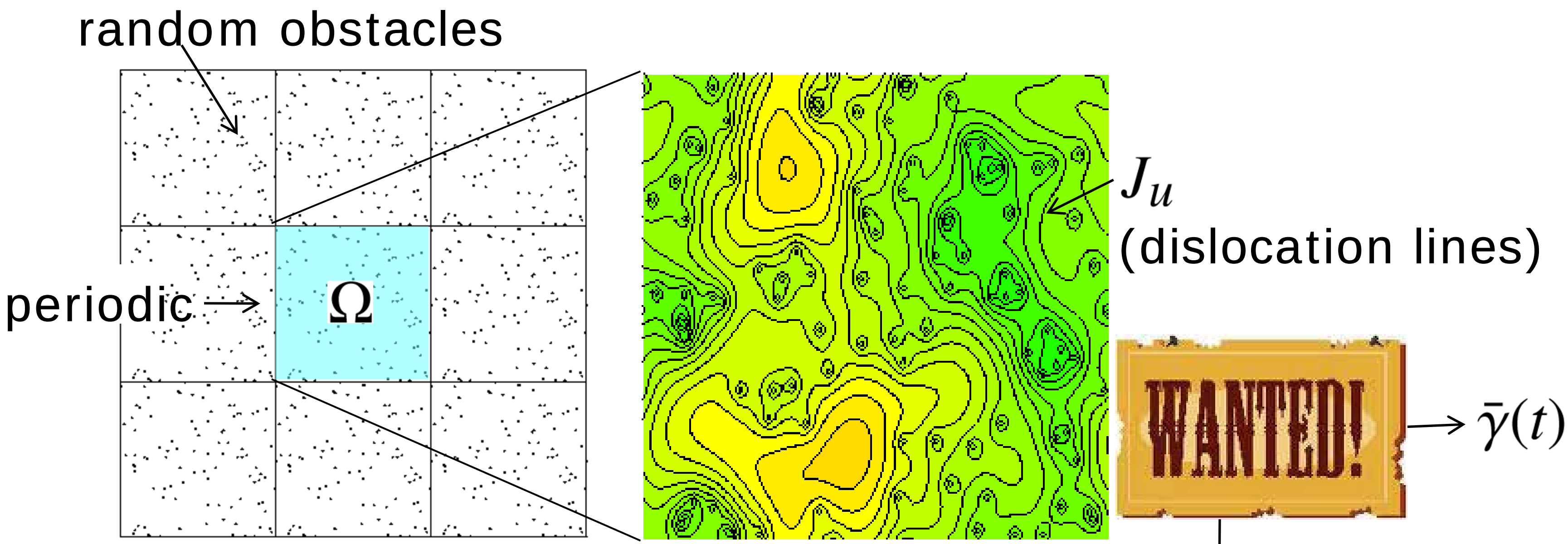
Forest hardening – Summary



- Find: $u : T^2 \times [0,T] \to b\mathbb{Z}$ s. t. $\partial\Psi(u,\dot{u}) + DE(t,u) = 0$
- Energy: $E(u,t) = \int_{J_u} K[\![u]\!]^2 d\mathcal{H}^1 - \bar{\tau}(t) \int_{\Omega} u\, d\mathcal{H}^2$
- Dissipation: $\Psi(u,\dot{u}) = \int_L \tau_c |v|\, d\mathcal{H}^1 + \sum_{\text{obstacles}} f_c\, |v|$

M. Koslowski, A.M.Cuitino and M. Ortiz, *JMPS*, **50** (2002) 2597-2635

Energy-dissipation functionals

- Space of trajectories: $\mathbb{X} = \{u : [0,T] \to X\}$,
- Energy-dissipation functional $F_\epsilon : \mathbb{X} \to \bar{\mathbb{R}}$:

$$F_\epsilon(u) = \underbrace{\int_0^T \mathrm{e}^{-t/\epsilon}}_{\text{“Arrow of time”}} [\underbrace{\Psi(u,\dot{u})}_{\text{Dissipation}} + \underbrace{\frac{1}{\epsilon} E(t,u)}_{\text{Energy}}]\, dt + [\mathrm{e}^{-t/\epsilon} E]_0^T$$

Energy

Dissipation

“Arrow of time”

- Minimum principle: $u \in \operatorname{argmin} F_\epsilon$
- Euler-Lagrange equations (elliptic regularization!):

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

Rate-independent problems

- Energy-dissipation function:

$$F_\epsilon(u) = \int_0^T \mathrm{e}^{-t/\epsilon}[\Psi(u,\dot u) + \frac{1}{\epsilon}E(t,u)]\,dt + [\mathrm{e}^{-t/\epsilon}E]_0^T$$

- Suppose: i) $\Psi(u,\lambda\dot u) = \lambda\Psi(u,\dot u)$, $\forall\lambda \geq 0$; ii) There exists $\mathbb{K} \subset \mathbb{X}$ and a functional $J : \mathbb{X} \to \bar{\mathbb{R}}$ s.t.

$$\Psi(u(t),\dot u(t)) = \frac{d}{dt}J(u(t)), \quad \forall u \in \mathbb{K}$$

- Then (deformation theory):

$$F_\epsilon(u) = \begin{cases} \int_0^T \mathrm{e}^{-t/\epsilon}[J(u) + E(t,u)]\,\frac{dt}{\epsilon} + BC, & \text{if } u \in \mathbb{K}, \\ +\infty, & \text{otherwise}. \end{cases}$$

- Pointwise: $u(t) \in \mathrm{argmin}(J(\cdot)+E(t,\cdot))$, provided $u \in \mathbb{K}$

Forest Hardening – Deformation theory

- Monotonicity:

$$\mathbb{K} = \{u \in \mathbb{X}, \text{ s. t. } u(x,t) \geq 0 \text{ and } u(x,t_2) \geq u(x,t_1),\ t_2 \geq t_1\}$$

- For $u \in \mathbb{K}$ we have $\Psi(u(t), \dot{u}(t)) = \frac{d}{dt} J(u(t))$ with

$$J(u) = \int_\Omega \tau_c u \, d\mathcal{H}^2 + \sum_{\text{obstacles}} f_c \, u$$

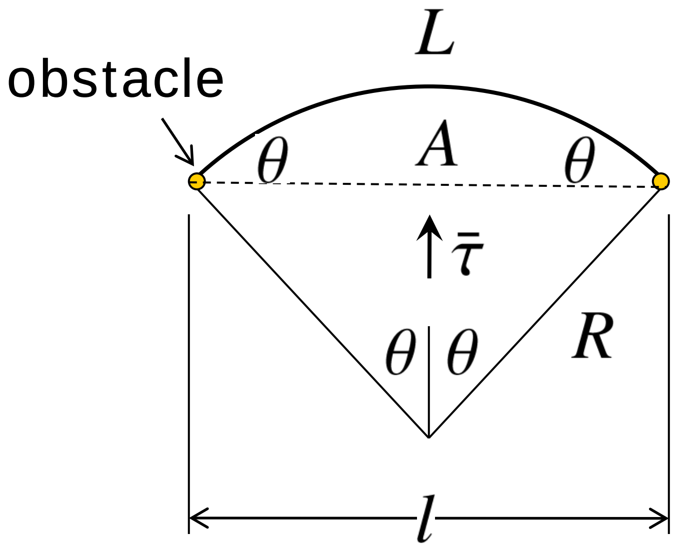
- Deformation-theory minimum principle: Minimize

$$J(u)+E(u,t) = \int_{J_u} K[\![u]\!]^2 d\mathcal{H}^1 - \underbrace{(\bar{\tau}(t)-\tau_c)}_{\text{overstress!}} \int_\Omega u \, d\mathcal{H}^2 + \sum_{\text{obstacles}} f_c u$$

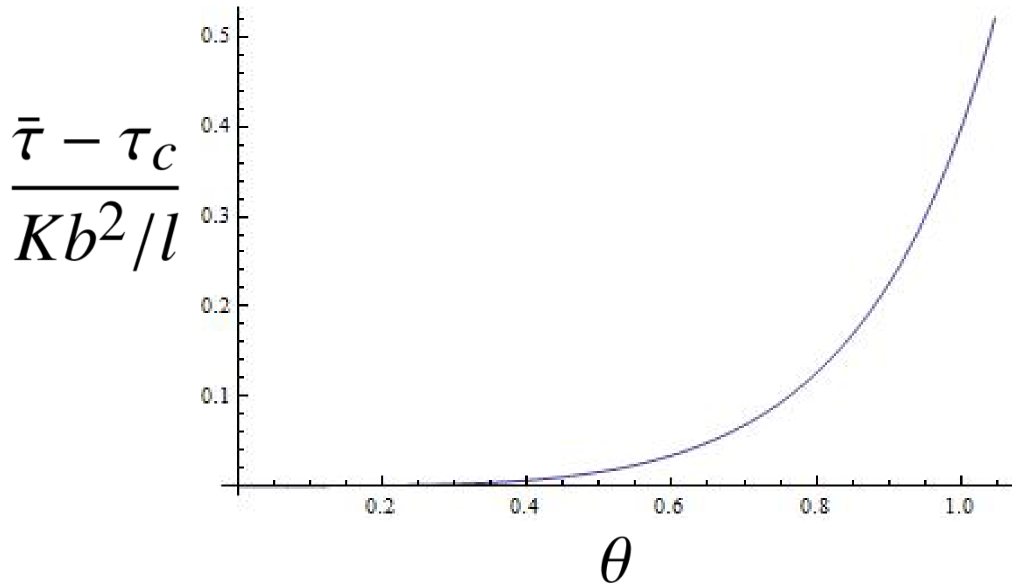
- Minimize pseudo-energy $F = J+E$ pointwise in time!

Forest hardening – Pinning/depinning

- Dislocations move by pinning-depinning at obstacles!



dislocation segment
bowing between obstacles



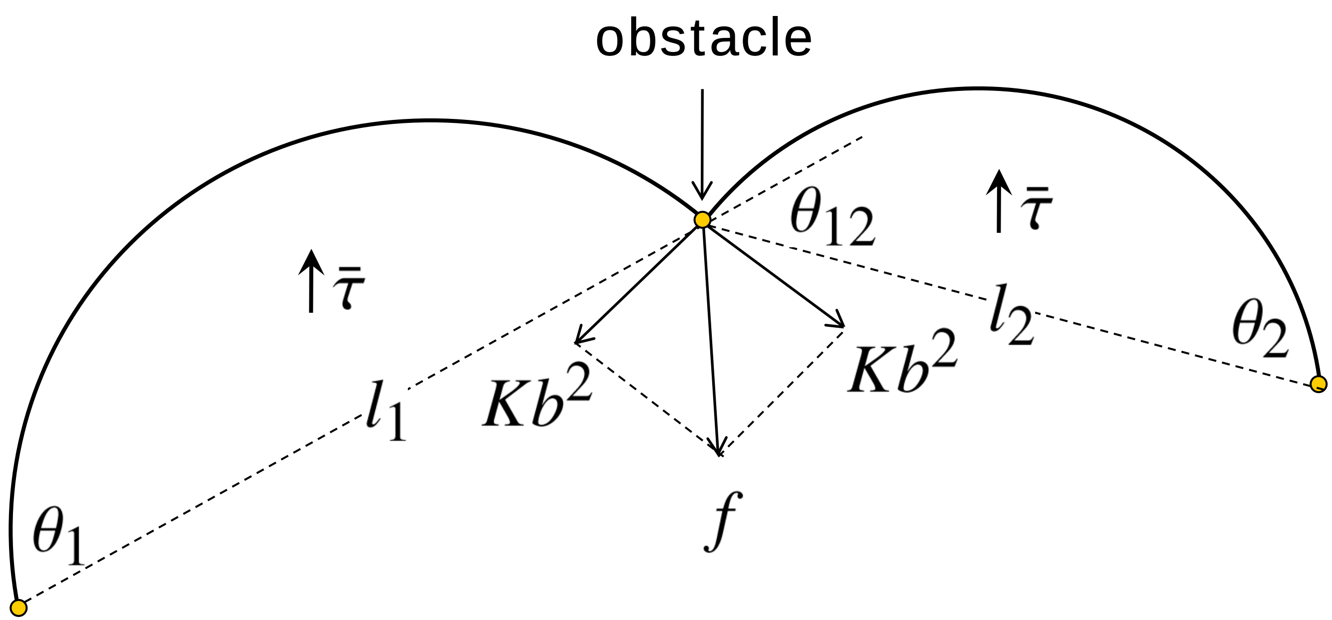
- Deformation-theory energy:

$$F(\theta) = Kb^2 L + (\bar\tau - \tau_c) A$$

- Equilibrium shape:

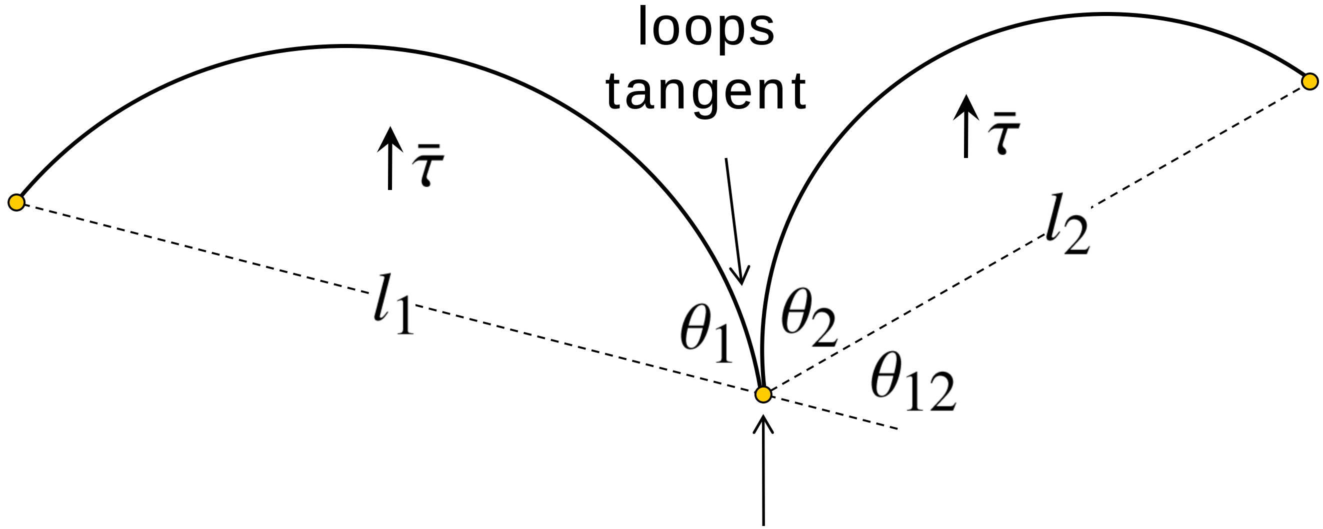
$$\frac{dF(\theta)}{d\theta} = 0 \Rightarrow \theta(\bar\tau, l)$$

Forest hardening – Pinning/depinning



- Obstacle is stable if: $|f(\bar{\tau}, l_1, l_2, \theta_{12})| < f_c$.
- Otherwise, dislocation depins and moves forward.
- Eventually, dislocation gets pinned down and arrests

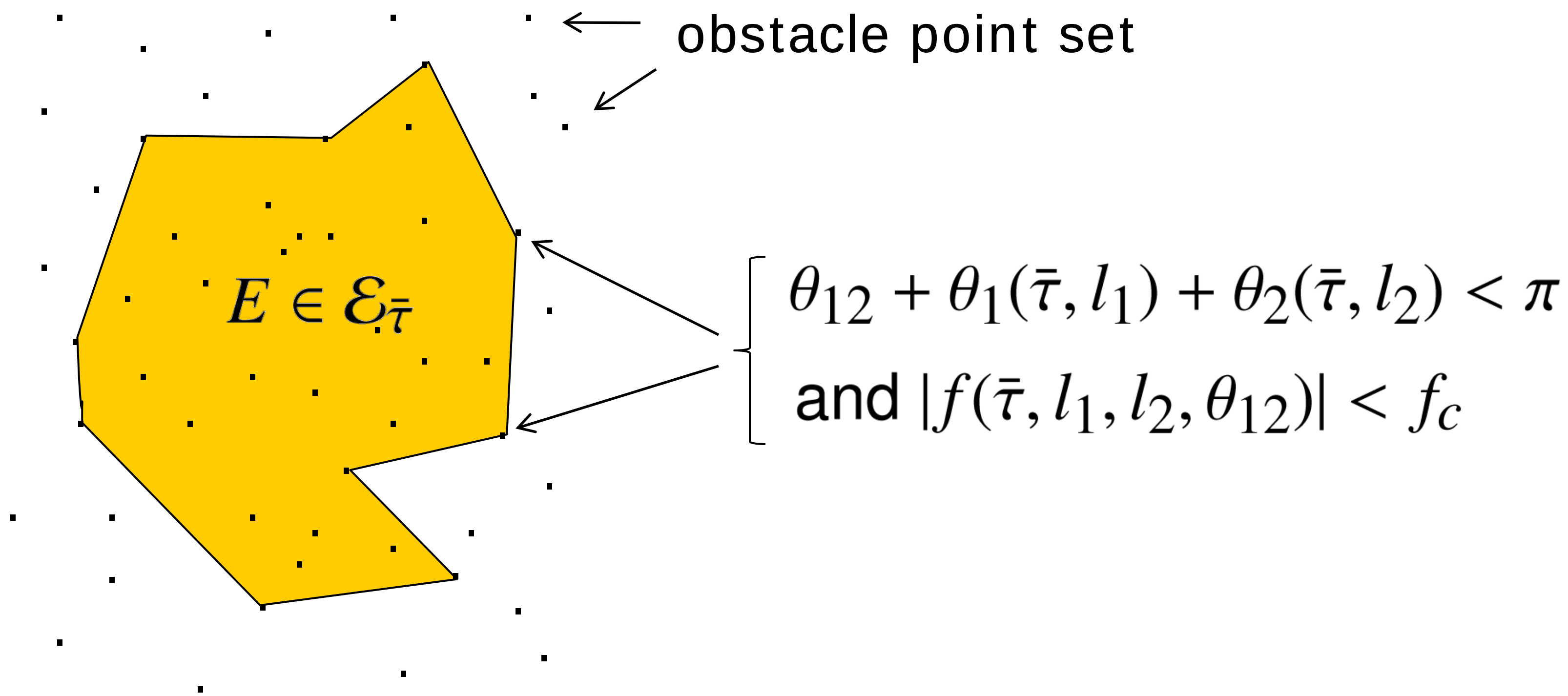
Forest hardening – Pinning/depinning



- Obstacle is stable if $\theta_{12} + \theta_1(\bar{\tau}, l_1) + \theta_2(\bar{\tau}, l_2) < \pi$.
- Otherwise, dislocation depins and moves forward.
- Eventually, dislocation gets pinned down and arrests

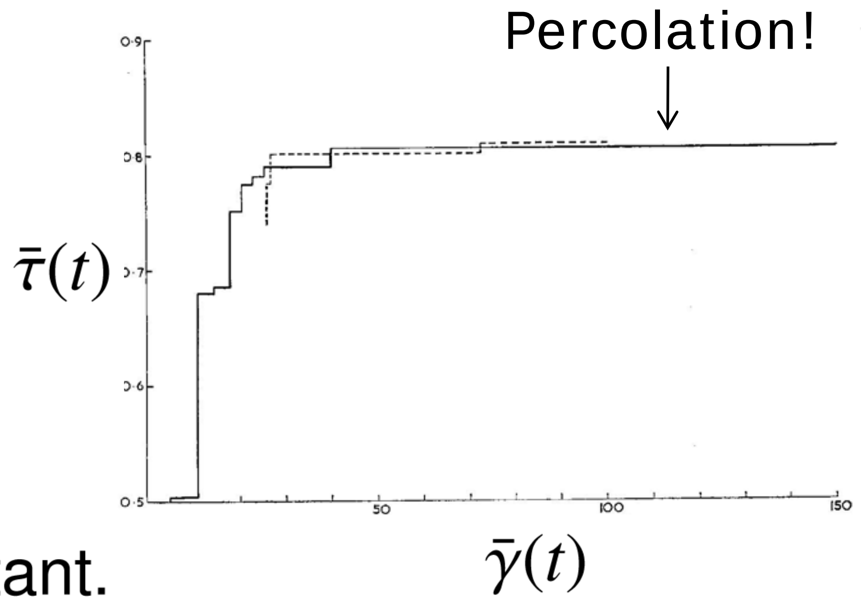
Forest hardening − Single dislocation

- Let $\mathcal{E}_s$ be the set of polygonal domains spanning the obstacle point set such that all vertices are stable for all $\bar{\tau} \le s$.



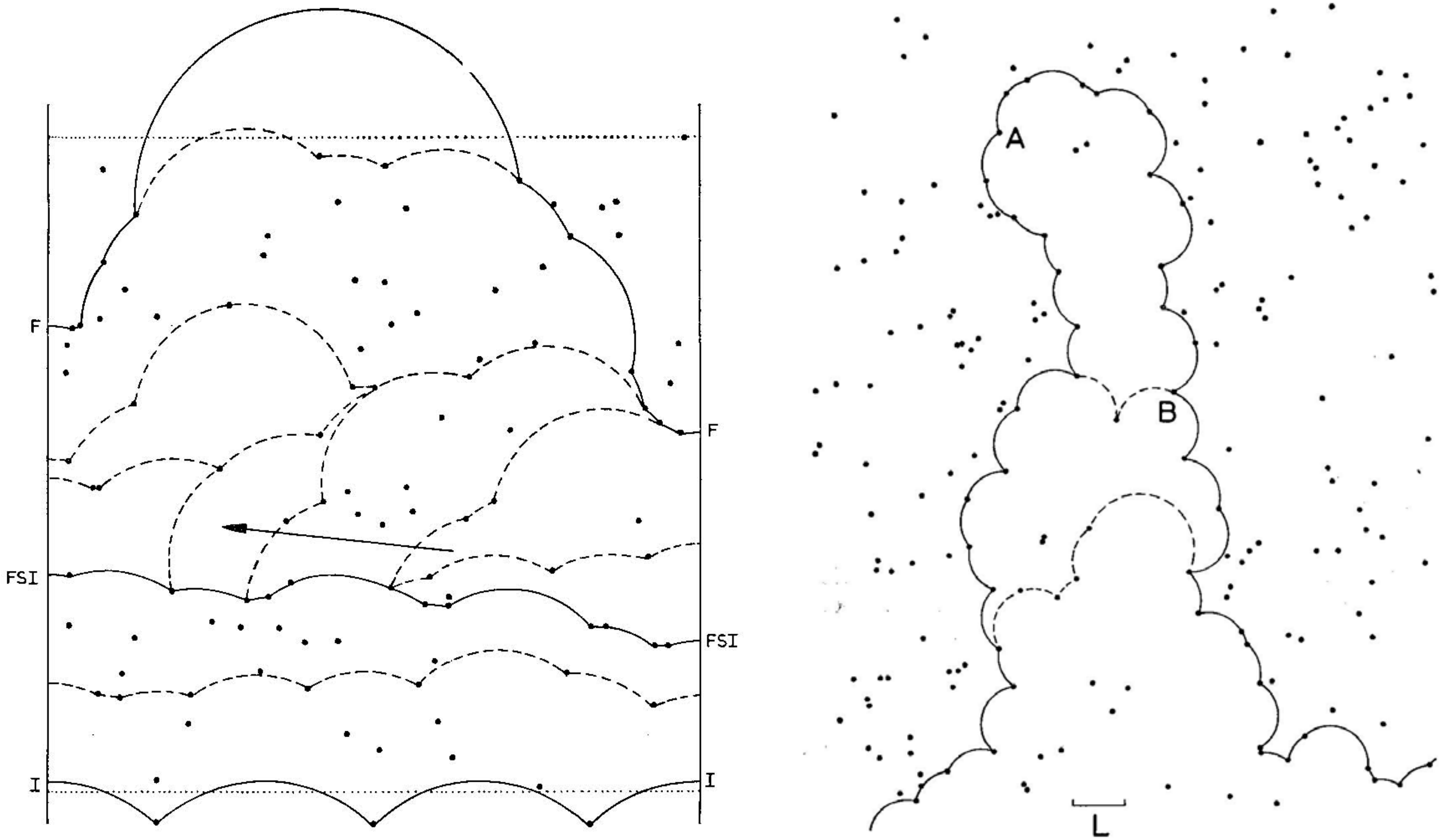
Forest hardening − Single dislocation

- Suppose that $\bar{\tau}(t)$ is increasing, piecewise constant and jumps at times $t_0, t_1, \dots, t_i, \dots$
- Consider a single moving dislocation, $\text{range}(u) = \{0, b\}$.
- Let $u(t_i^-) \to E(t_i^-) \in \mathcal{E}_{\bar{\tau}(t_i^-)}$.
- Then, $u(t_i^+) \to E(t_i^+)$ is the smallest set in $\mathcal{E}_{\bar{\tau}(t_i^+)}$ that contains $E(t_i^-)$.
- Slip strain: $\bar{\gamma}(t) = \dfrac{b|E(t)|}{|\Omega|d}$ increasing, piecewise constant.



A.J.E. Foreman and M.J. Makin, *Phil. Mag.*, **14** (1966) 911.

Forest hardening − Single dislocation



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

- Plastic work: $W^p \sim c^{1/2}\bar{\gamma}^{3/2}$, where:
  $c \equiv$ obstacle density, $\bar{\gamma} \equiv$ slip strain

Michael Ortiz
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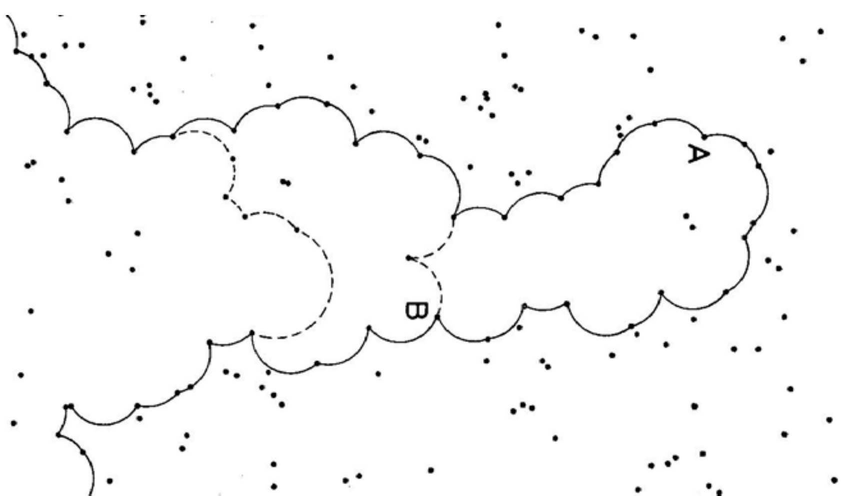
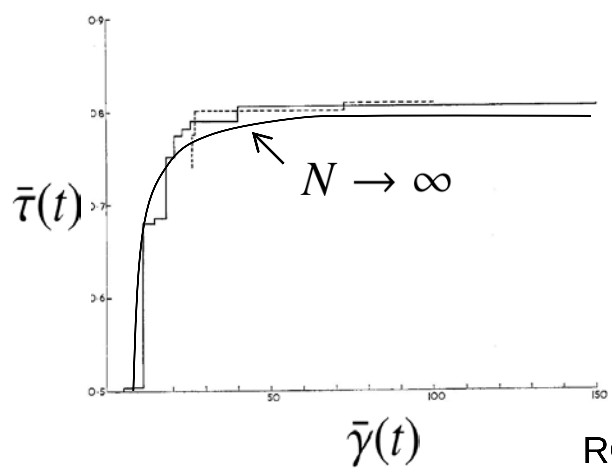
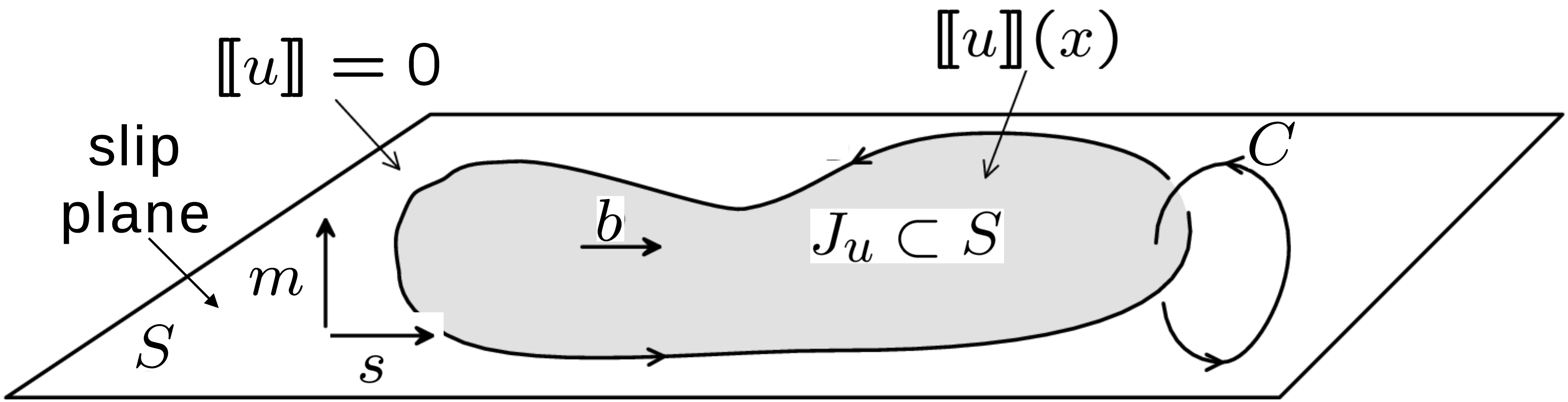
Forest hardening − Summary & outlook

- Model is based on line tension approximation
- Motion by pinning/depinning at obstacles
- Model gives parabolic hardening curve, correct Taylor scaling with obstacle density
- Open mathematical questions:
  - *Limit of infinite number of obstacles (N) at fixed obstacle density, e.g., Poisson distribution of obstacles*
  - *Loading/unloading, hysteresis...*





2½D phase-field model – Assumptions

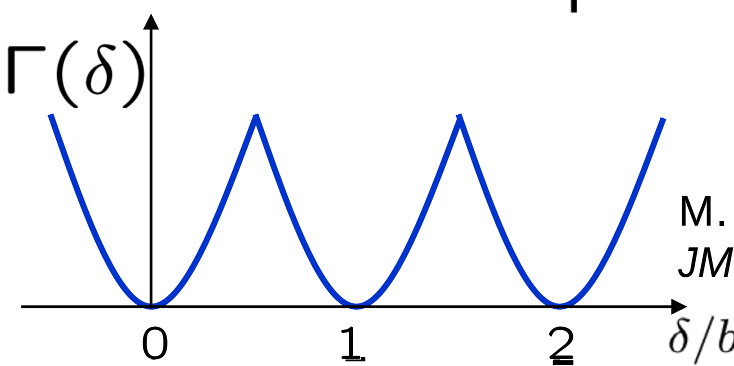


i) Activity on single slip system, single slip plane.

ii) Linear elasticity outside slip plane.

iii) No Peierls potential (translation invariance).

iv) Constrained interplanar potential: With $[\![u]\!] \equiv \delta s$,



$$\Gamma(\delta) = \frac{\mu}{2d}\text{dist}^2(\delta, b\mathbb{Z})$$

M. Koslowski, A.M.Cuitino and M. Ortiz, *JMPS*, **50** (2002) 2597-2635

2½D phase-field model – Energy

- Total energy: With $u \equiv \delta/b$, $E(u) =$

$$\underbrace{\int_{\mathbb{R}^2} \frac{\mu b^2}{2d} \text{dist}^2(u,\mathbb{Z})dx}_{\text{Core energy}} + \underbrace{\frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} \frac{\mu b^2}{4} K|\hat{u}|^2 dk}_{\text{Elastic energy}} - \underbrace{\int_{\mathbb{R}^2} b\tau u dx}_{\text{External}}$$

where $$K = \frac{k_2^2}{\sqrt{k_1^2+k_2^2}} + \frac{1}{1-\nu}\frac{k_1^2}{\sqrt{k_1^2+k_2^2}}$$

- Structure of the energy:

$$E_\epsilon(u) = \frac{1}{2\epsilon}\int_{\mathbb{R}^2} \text{dist}^2(u,\mathbb{Z})dx + |u|^2_{H^{1/2}} + \text{linear term}$$

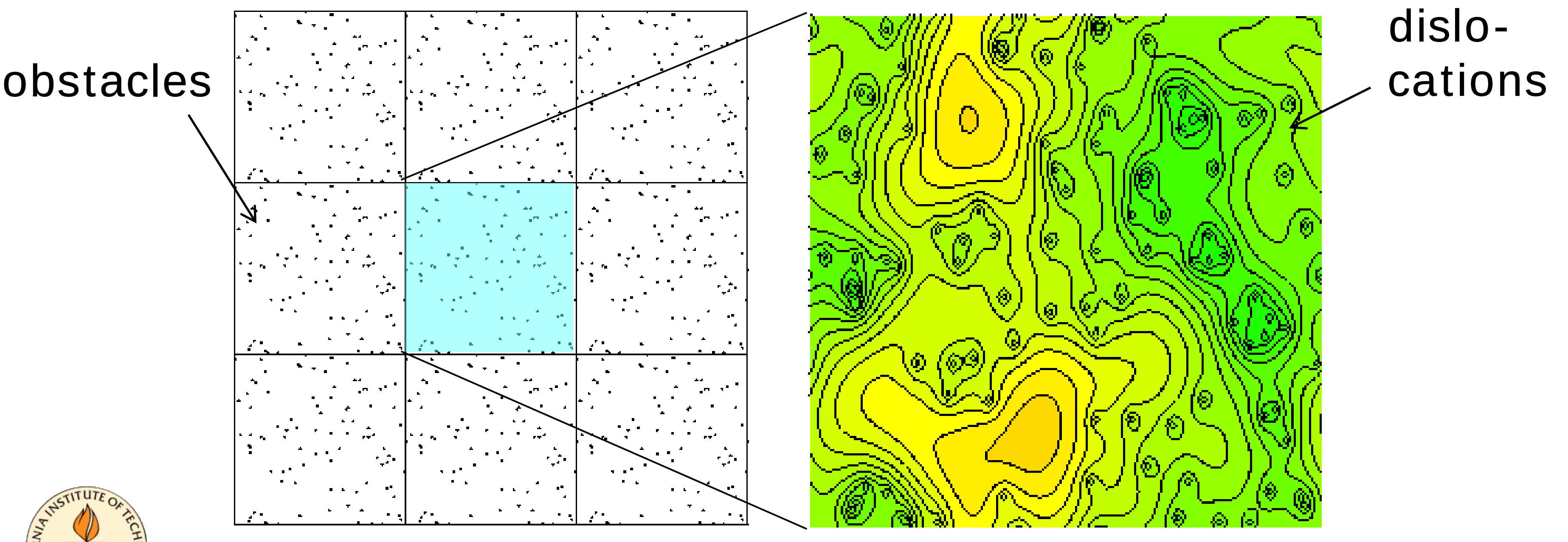
G. Alberti, G. Bouchitté, and P. Seppecher, *C. R. Acad. Sci. Paris Sér I. Math.*, **319** *(1994) 333–338*

A. Garroni and S. Müller, *SIAM J. Math.* Anal., **36** (2005) 1943–1964; *ARMA* **181** (2006) 535–578

2½D phase-field model – Time discretization

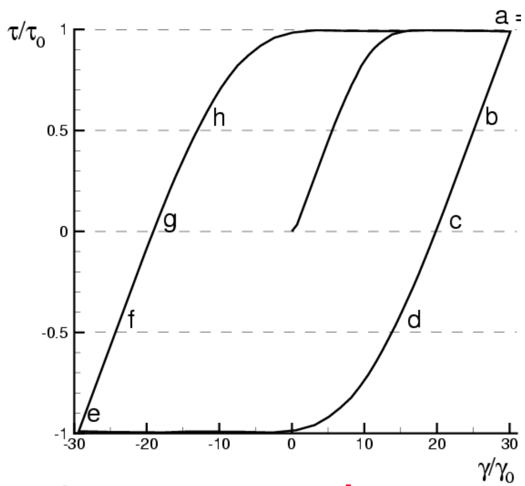
- Time-continuous problem: $\partial\Psi(\dot{u}(t)) + DE(t, u(t)) = 0$
- Time-discrete problem:

$$E(u_{n+1}) - E(u_n) + \Delta t\, \Psi\left(\frac{u_{n+1} - u_n}{\Delta t}\right) \to \inf!$$

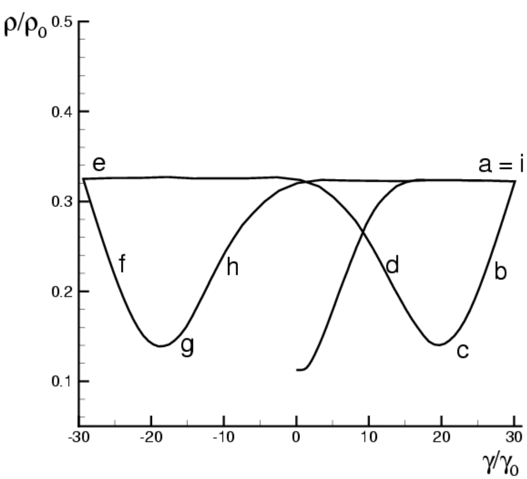


M. Koslowski, A.M.Cuitino and M. Ortiz, *JMPS*, **50** (2002) 2597-2635

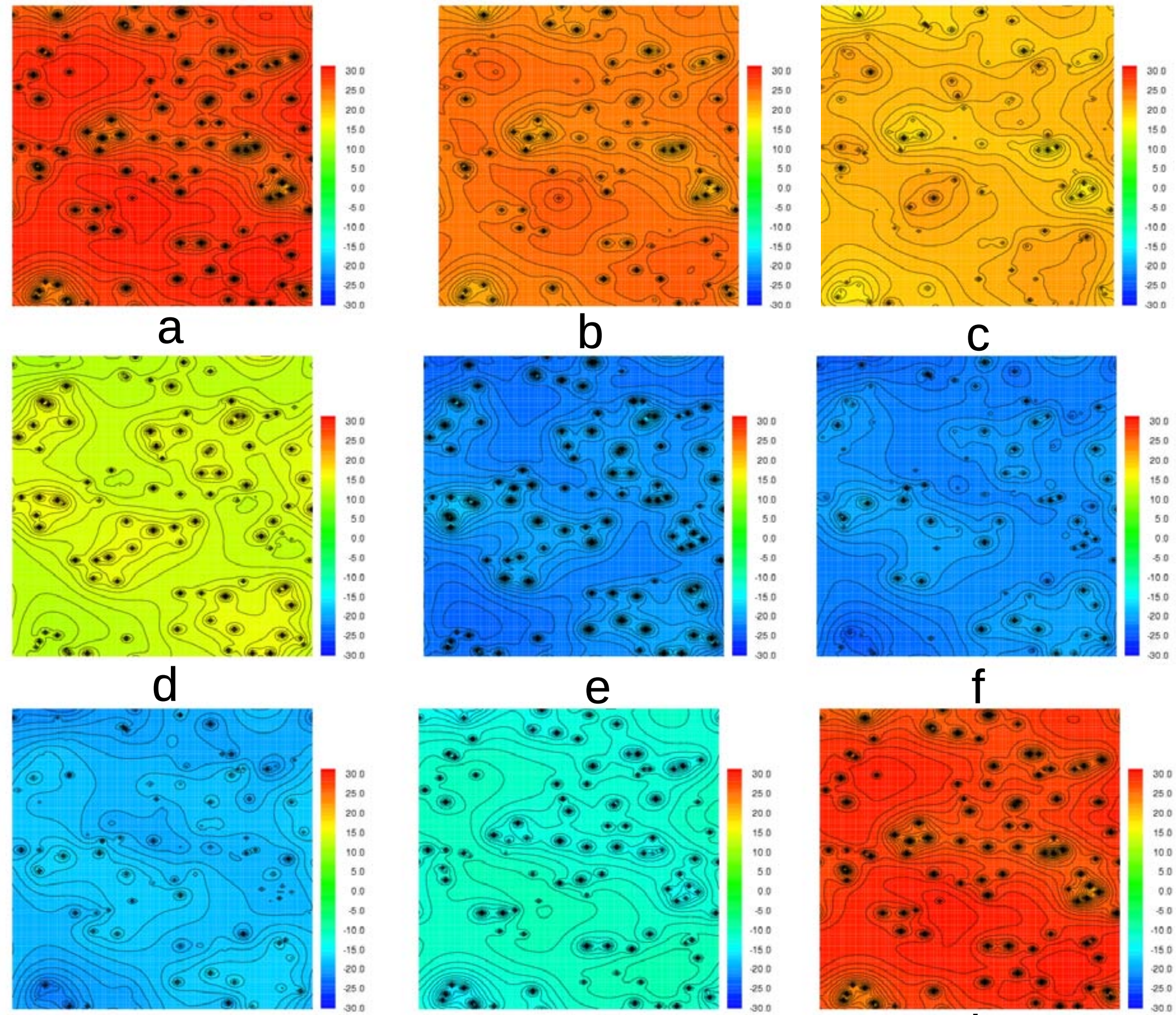
Phase-field dislocation dynamics



Stress-strain curve

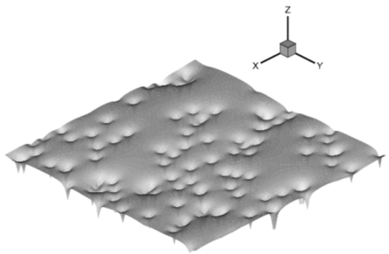


Dislocation density



Michael Ortiz
ROME0611

Return-point and fading memory



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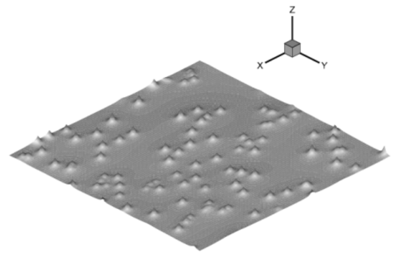

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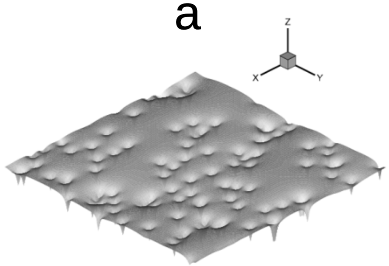

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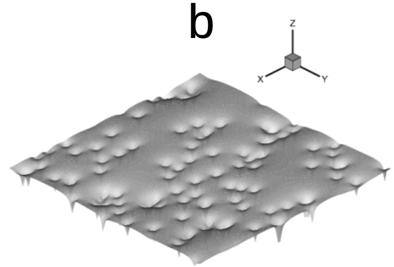

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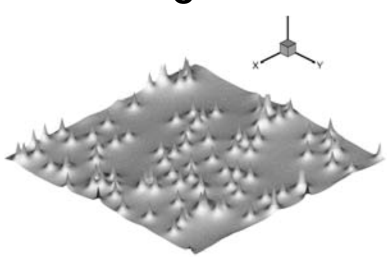

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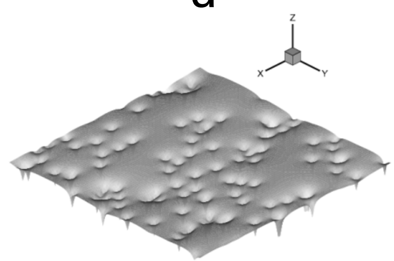
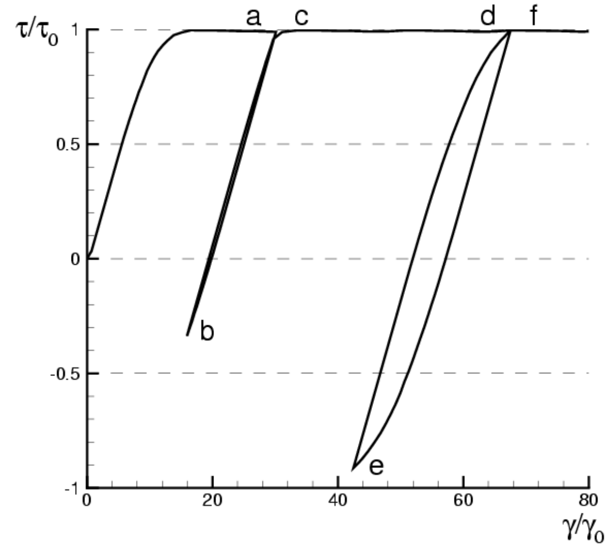


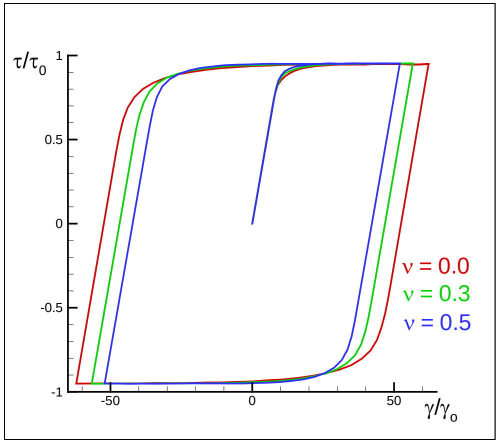
f

Three dimensional view of the evolution of the slip-field, showing the the switching of the cusps.

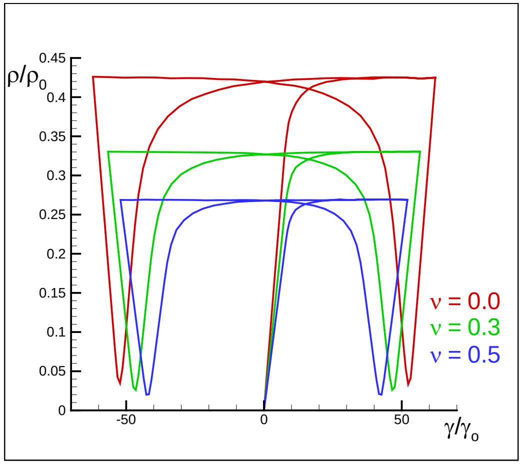


Stress-strain curve.

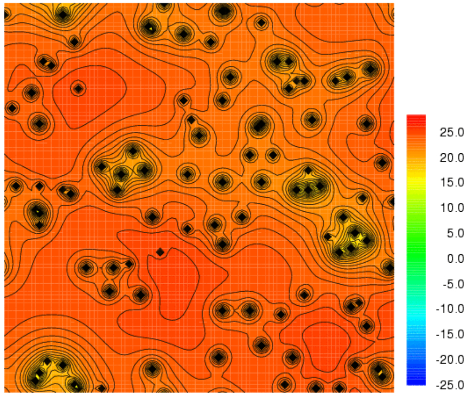
Line-tension anisotropy



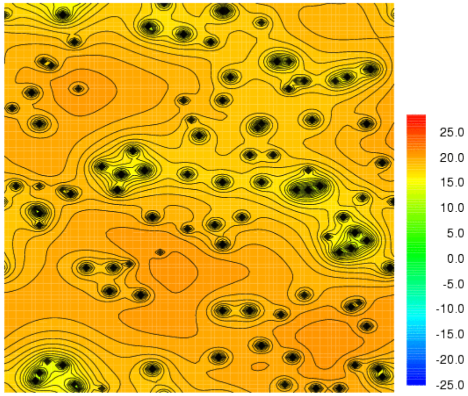
Stress-strain curve.



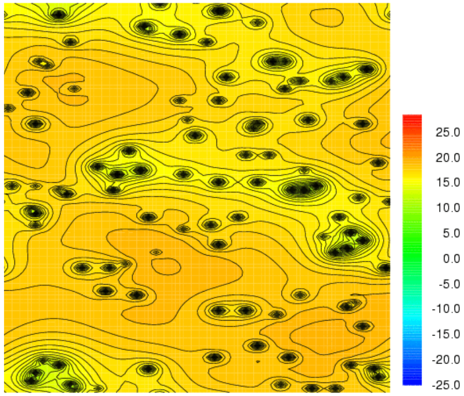
Dislocation density



$\nu = 0.0$



$\nu = 0.3$

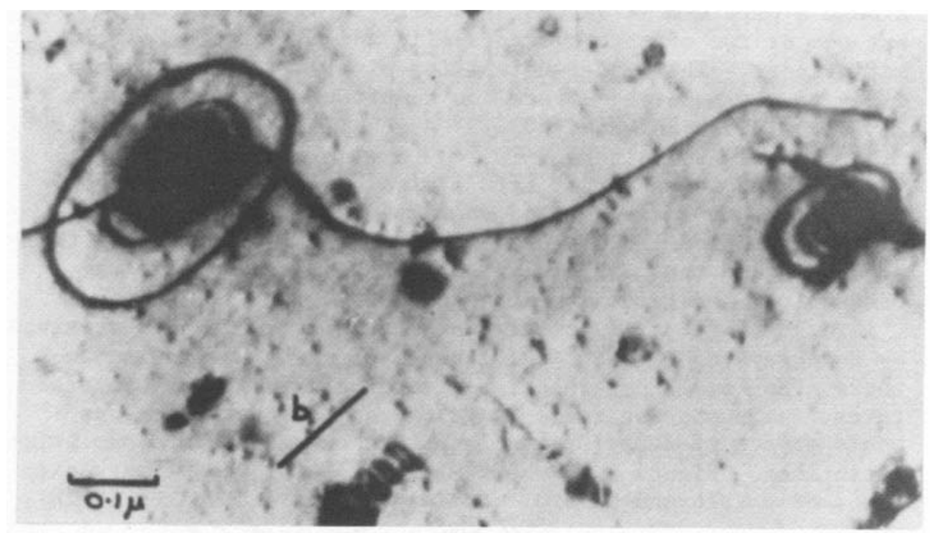


$\nu = 0.5$

b

Summary and outlook

- The forest-hardening model predicts the observed kinetics of hardening in crystals
- A full analytical treatment of the forest-hardening model is still lacking
- Need tools of analysis (similar to CoV) for time dependent evolution problems



(Humphreys and Hirsch, 1970)

Metal plasticity − Multiscale analysis