Current state of the statistical physics-based continuum theory of dislocations
what is next

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April 6, 2025

Outline

- Large deformation
- Kinematical considerations
- Dipole approximations
- Deriving velocity laws
- Generalization to multiple slip
- Stochastic extension
- Summary

Large elastic deformation: Lagrangian description

The state is described by the function $\vec{x}(\vec{X})$
Applying functional derivation

$$-\delta \mathrm{W} = \mathrm{E}[\tilde{\mathrm{x}}(\tilde{\mathrm{X}}) + \delta\tilde{\mathrm{x}}(\tilde{\mathrm{X}})] - \mathrm{E}[\tilde{\mathrm{x}}] = -\int \tilde{\mathrm{f}}(\tilde{\mathrm{x}}(\tilde{\mathrm{X}}))\delta\tilde{\mathrm{x}}(\tilde{\mathrm{X}})\mathrm{d}^3\tilde{\mathrm{X}} = -\int \frac{\delta \mathrm{E}}{\delta \mathrm{x_i}}\delta\tilde{\mathrm{x}}(\tilde{\mathrm{X}})\mathrm{d}^3\tilde{\mathrm{X}} = 0$$

With the notations:

$$\mathrm{F_{ij}} = \frac{\partial \mathrm{x_i}}{\partial \mathrm{X_j}}, \quad \epsilon_{\mathrm{ij}} = \frac{1}{2}\left(\tilde{\mathrm{F}}_{\mathrm{ik}}\mathrm{F_{kj}} - \delta_{\mathrm{ij}}\right)$$

The energy is a functional of ϵ_{ij}, so

$$\frac{\delta \mathrm{E}}{\delta \mathrm{x_i}} = -\partial_{\mathrm{j}}\frac{\delta \mathrm{E}}{\delta \mathrm{F_{ij}}} = -\partial_{\mathrm{j}}\left(\frac{\delta \mathrm{E}}{\delta \epsilon_{\mathrm{kl}}}\frac{\mathrm{d}\epsilon_{\mathrm{kl}}}{\mathrm{dF_{ij}}}\right) = -\partial_{\mathrm{j}}\left(\frac{\delta \mathrm{E}}{\delta \epsilon_{\mathrm{kj}}}\mathrm{F_{ik}}\right) = -\partial_{\mathrm{j}}\left(\mathrm{F_{ik}}\sigma_{\mathrm{kj}}^{\mathrm{2PK}}\right) = 0$$

Plastic deformation

$$F_{ij} = F^{e}_{im} F^{p}_{mj}$$

The energy depends on only the elastic deformation

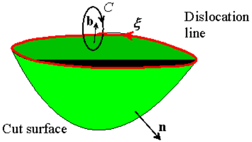
$$\epsilon^{e}_{ij} = \frac{1}{2}\left(F_{mo}F^{-p}_{oi}F_{mp}F^{-p}_{pj} - \delta_{ij}\right) = \frac{1}{2}\left(\tilde{F}^{-p}_{io}C_{op}F^{-p}_{pj} - \delta_{ij}\right)$$

From this

$$-\frac{\delta E}{\delta xi} = \partial_j \frac{\delta E}{\delta F_{ij}} = \partial_j \left[\frac{\delta E}{\delta \epsilon^{e}_{kl}} \frac{d\epsilon^{e}_{kl}}{dF_{ij}}\right] = \partial_j \left[F_{ip} F^{-p}_{pk} \sigma^{2PK}_{kl} F^{-p}_{lj}\right] = \partial_j \left[F_{ip} \sigma^{2PK*}_{pj}\right] = 0$$

Functional derivative with respect to F^{-p}_{ij}

$$E(F^{-p}_{ij} + \delta F^{-p}_{ij}) - E(F^{-p}_{ij}) = \frac{\delta E}{\delta F^{-p}_{ij}} \delta F^{-p}_{ij} = \frac{\delta E}{\delta \epsilon^{e}_{kl}} \frac{d\epsilon^{e}_{kl}}{dF^{-p}_{ij}} \delta F^{-p}_{ij} = \tilde{F}_{ip} F^{e}_{pl} \sigma^{2PK}_{lj} \delta F^{-p}_{ij}$$



$$F^p_{ij} = \delta_{ij} + b_i n_j \delta(\zeta) = \delta_{ij} + \beta^p_{ij}$$

What is F_{ij}^{-p}?

What is the inverse of something containing a Dirac delta?

$$1 + b\delta(x) \approx 1 + \frac{1}{s\sqrt{\pi}} e^{-\frac{x^2}{s^2 b^2}}$$

so

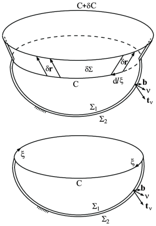
$$(1 + b\delta(x))^{-1} \approx 1 - b\delta(x)$$

$$F^{-p}_{ij} = \delta_{ij} - b_i n_j \delta(\zeta) = \delta_{ij} - \beta^{p}_{ij}$$

Effective stress

$$\sigma^{eff}_{ji} = \tilde{F}_{ip} F^{e}_{pl} \sigma^{2PK}_{lj}$$

Peach Köhler force?



$$\vec{F}_{PK} = (\hat{\sigma}_{eff}\vec{b}) \times \vec{l}$$

Dislocation loops

Loop can be given as $\vec{r}(s)$ but

$$\tilde{\mathrm{r}}(\mathrm{s}) = \tilde{\mathrm{r}}(\mathrm{s}_0) + \frac{\mathrm{d}\tilde{\mathrm{r}}}{\mathrm{ds}}(\mathrm{s}-\mathrm{s}_0) + \frac{1}{2}\frac{\mathrm{d}^2\tilde{\mathrm{r}}}{\mathrm{ds}^2}(\mathrm{s}-\mathrm{s}_0)^2 + ...$$

Probability of the "state" of the dislocation system

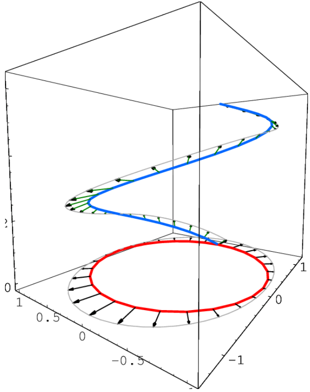
$$\mathrm{p}(\tilde{\mathrm{r}}, \varphi, \mathrm{k}, ..\mathrm{x}_\mathrm{i}..)$$

Variable we work with

$$\rho'(\vec{r}, \varphi) =< \rho > \int p(\vec{r}, \varphi, k, ..x_i..)dk..dx_i..$$

$$k(\vec{r}, \varphi) = \int kp(\vec{r}, \varphi, k, ..x_i..)dk..dx_i..$$

Dislocation loops



Variables $\rho'(\vec{r},\varphi)$, $q'(\vec{r},\varphi) = \rho' k$ and $v(\vec{r},\varphi)$

Evolution of the loops

Quantities:

$$\mathbf{L} = (\cos\varphi, \sin\varphi, \mathrm{k}) = (\tilde{\mathrm{l}}, \mathrm{k})$$
$$\boldsymbol{\alpha}' = \rho'(\mathbf{r}, \varphi)\mathbf{L}(\mathbf{r}, \varphi) \otimes \mathbf{b}$$
$$\mathbf{V}(\tilde{\mathrm{r}}, \varphi) = (\mathrm{v}\sin\varphi, -\mathrm{v}\cos\varphi, -\hat{\mathbf{L}}(\mathrm{v}))$$
$$\hat{\mathbf{L}} = \cos\varphi\partial_{\mathrm{x}} + \sin\varphi\partial_{\mathrm{y}} + \mathrm{k}\partial_{\varphi}$$

Lie derivative (3D)

$$\partial_{\mathrm{t}} \vec{A} = \nabla \times (\vec{v} \times \vec{A}) = \mathcal{L}_v A$$
$$\partial_n(v_n A_l - v_l A_n)$$

Evolution of the generalized dislocation density tensor

$$\partial_{\mathrm{t}} \boldsymbol{\alpha}' = \mathcal{L}_v \boldsymbol{\alpha}'$$
$$\hat{\mathrm{Div}}\, \boldsymbol{\alpha}' = 0$$

Dipole approximation

Bubnov-Galerkin weighted residual method in Fourier space

$$\rho'(\tilde{\mathrm{r}},\varphi) \approx \rho(\tilde{\mathrm{r}}) + 2\kappa_1(\tilde{\mathrm{r}})\cos\varphi + 2\kappa_2(\tilde{\mathrm{r}})\sin\varphi$$

$$\mathrm{v}(\tilde{\mathrm{r}},\varphi) \approx \mathrm{v}^{\mathrm{m}}(\tilde{\mathrm{r}}) + \mathrm{v}_1^{\mathrm{d}}(\tilde{\mathrm{r}})\cos\varphi + \mathrm{v}_2^{\mathrm{d}}(\tilde{\mathrm{r}})\sin\varphi$$

$$\mathrm{q}'(\tilde{\mathrm{r}},\varphi) \approx \mathrm{q}(\tilde{\mathrm{r}}) + \mathrm{Q}_2(\tilde{\mathrm{r}})\cos\varphi - \mathrm{Q}_1(\tilde{\mathrm{r}})\sin\varphi$$

$$\begin{aligned}
\partial_{\mathrm{t}}\rho &= -\partial_x(\rho v_2^d) + \partial_y(\rho v_1^d) + \partial_y(\kappa_1 v^m) - \partial_x(\kappa_2 v^m) \\
&\quad + q v^m + \frac{1}{2}\rho\partial_y v_1^d - \frac{1}{2}\rho\partial_x v_2^d \\
\partial_t\kappa_1 &= \partial_y(\rho v^m + \kappa_1 v_1^d + \kappa_2 v_2^d) \\
\partial_t\kappa_2 &= -\partial_x(\rho v^m + \kappa_1 v_1^d + \kappa_2 v_2^d) \\
\partial_t q &= -\partial_x\left(q v_2^d - v^m Q_1\right) + \partial_y\left(q v_1^d + v^m Q_2\right) \\
&\quad \partial_x\kappa_1 + \partial_y\kappa_2 = 0, \quad \kappa_1 = \partial_y\gamma_{13}, \quad \kappa_2 = -\partial_x\gamma_{13} \\
&\quad Q_1 = \partial_x\rho, \quad Q_2 = \partial_y\rho
\end{aligned}$$

Bubnov-Galerkin weighted residual method in Fourier space

$$\rho'(\tilde{\mathrm{r}},\varphi) \approx \rho(\tilde{\mathrm{r}}) + 2\kappa_1(\tilde{\mathrm{r}})\cos\varphi + 2\kappa_2(\tilde{\mathrm{r}})\sin\varphi$$

$$\mathrm{v}(\tilde{\mathrm{r}},\varphi) \approx \mathrm{v}^{\mathrm{m}}(\tilde{\mathrm{r}}) + \mathrm{v}_1^{\mathrm{d}}(\tilde{\mathrm{r}})\cos\varphi + \mathrm{v}_2^{\mathrm{d}}(\tilde{\mathrm{r}})\sin\varphi$$

$$\mathrm{q}'(\tilde{\mathrm{r}},\varphi) \approx \mathrm{q}(\tilde{\mathrm{r}}) + \mathrm{Q}_2(\tilde{\mathrm{r}})\cos\varphi - \mathrm{Q}_1(\tilde{\mathrm{r}})\sin\varphi$$

$$\begin{aligned}
\partial_t\rho &= -\partial_x(\rho v_2^d) + \partial_y(\rho v_1^d) + \partial_y(\kappa_1 v^m) - \partial_x(\kappa_2 v^m) \\
&\quad + q v^m + \lambda_1(q^2/\rho^3)\rho\partial_y v_1^d - \lambda_2(q^2/\rho^3)\rho\partial_x v_2^d \\
\partial_t\kappa_1 &= \partial_y(\rho v^m + \kappa_1 v_1^d + \kappa_2 v_2^d) \\
\partial_t\kappa_2 &= -\partial_x(\rho v^m + \kappa_1 v_1^d + \kappa_2 v_2^d) \\
\partial_t q &= -\partial_x\left(q v_2^d - v^m Q_1\right) + \partial_y\left(q v_1^d + v^m Q_2\right) \\
&\quad \partial_x\kappa_1 + \partial_y\kappa_2 = 0, \quad \kappa_1 = \partial_y\gamma_{13}, \quad \kappa_2 = -\partial_x\gamma_{13} \\
&\quad Q_1 = \partial_x\rho, \qquad Q_2 = \partial_y\rho
\end{aligned}$$

$$\lambda(\mathrm{x}) = \begin{cases} ax \text{ if } x \to 0 \\ \frac{1}{2} \text{ if } x \to \infty \end{cases}$$

Dipole approximation

$$\rho'(\tilde{\mathrm{r}},\varphi) \approx \rho(\tilde{\mathrm{r}}) + 2\kappa_1(\tilde{\mathrm{r}})\cos\varphi + 2\kappa_2(\tilde{\mathrm{r}})\sin\varphi$$

$$\mathrm{v}(\tilde{\mathrm{r}},\varphi) \approx \mathrm{v}^{\mathrm{m}}(\tilde{\mathrm{r}}) + \mathrm{v}_1^{\mathrm{d}}(\tilde{\mathrm{r}})\cos\varphi + \mathrm{v}_2^{\mathrm{d}}(\tilde{\mathrm{r}})\sin\varphi$$

$$\mathrm{q}'(\tilde{\mathrm{r}},\varphi) \approx \mathrm{q}(\tilde{\mathrm{r}}) + \mathrm{Q}_2(\tilde{\mathrm{r}})\cos\varphi - \mathrm{Q}_1(\tilde{\mathrm{r}})\sin\varphi$$

$$\begin{aligned}
\partial_t \rho &= -\partial_x(\rho v_2^d) + \partial_y(\rho v_1^d) + \partial_y(\kappa_1 v^m) - \partial_x(\kappa_2 v^m) \\
&\quad + q v^m + \lambda_1 \rho \partial_y v_1^d - \lambda_2 \rho \partial_x v_2^d \\
\partial_t \gamma_{13} &= \rho v^m + \kappa_1 v_1^d + \kappa_2 v_2^d \\
\partial_t q &= -\partial_x \left(q v_2^d - v^m Q_1 \right) + \partial_y \left(q v_1^d + v^m Q_2 \right) \\
&\quad \kappa_1 = \partial_y \gamma_{13}, \quad \kappa_2 = -\partial_x \gamma_{13} \\
&\quad Q_1 = \partial_x \rho, \quad Q_2 = \partial_y \rho
\end{aligned}$$

$$\dot{\mathrm{P}}[\rho,\gamma_{13},\kappa_1,\kappa_2,\mathrm{q}] = \int\left[\frac{\delta P}{\delta\rho}\dot{\rho}+\frac{\delta P}{\delta\gamma_{13}}\dot{\gamma}_{13}+\frac{\delta P}{\delta q}\dot{q}\right]dV$$
$$= \int\left[(\ldots.)v^m+(\ldots.)v_1^d+(\ldots.)v_2^d\right]dV<0$$

“Chemical potentials“

$$\mu_\rho=\frac{\delta \mathrm{P}}{\delta\rho},\;\; \mu_\mathrm{q}=\frac{\delta\mathrm{P}}{\delta\mathrm{q}}.$$

Stress like variables

$$\tau^* = \frac{\delta P}{\delta\gamma_{13}}=\tau_{mf}-\partial_y\frac{\delta P}{\delta\kappa_1}+\partial_x\frac{\delta P}{\delta\kappa_2}=\tau_{mf}+\tau_b$$
$$\tau_1^\mathrm{d} = \frac{1}{b\rho}\left[(\partial_y\mu_\rho)\rho+(\partial_y\mu_q)q+\partial_y(\lambda_1\mu_\rho\rho)\right],$$
$$\tau_2^\mathrm{d} = -\frac{1}{b\rho}\left[(\partial_x\mu_\rho)\rho+(\partial_x\mu_q)q+\partial_x(\lambda_2\mu_\rho\rho)\right]$$

Field:

$\rho(\vec{r},t)$, $\kappa_1(\vec{r},t)$, $\kappa_2(\vec{r},t)$, $q(\vec{r},t)$

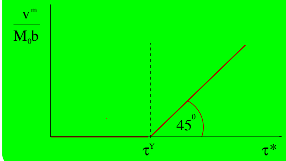
Dynamics

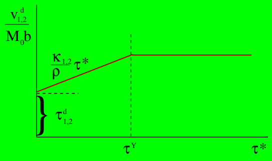
Plastic potential $P[\vec{x},\rho,\kappa_1,\kappa_2,q]$

$\Downarrow$

τ^*, τ_1^d, τ_2^d

Velocities





Plastic potential

$$P[\tilde{x},\rho,\gamma_{13},\kappa_1,\kappa_2,q] = P^{mf}[\rho,\gamma_{13}] + P^{corr}[\rho,\kappa_1,\kappa_2,q]$$

Corse grained fields

$$P^{mf}[\rho,\gamma_{13}]$$

Correlations

$$P^{corr}[\rho,\kappa_1,\kappa_2,q] = \int Gb^2\left[A\rho \ln\left(\frac{\rho}{\rho_0}\right) + \frac{\boldsymbol{\kappa}\cdot\mathbf{D}\cdot\boldsymbol{\kappa}}{2\rho} + \rho\chi\left(\frac{q^2}{\rho^3}\right)\right] dV$$

$$\chi(x) = \begin{cases} ax \text{ if } x << 1 \\ \to 0 \text{ if } x \to \infty \end{cases}$$

displacement field:

$$\frac{\delta P}{\delta x_i} = 0$$

$$\partial_j\left[F_{ip}\sigma^{2PK*}_{pj}\right] = 0$$

Patterning

Main source of instability: $\tau^y = \alpha \mu b \sqrt{\rho}$

Length scale selection: $P^{corr}[\rho, \kappa_{12}, q]$

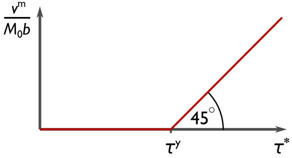
P is convex! No LEDS!

No reaction terms!

2D and 3D are practically the same

The instability is "massive"

Mobility function



$$M\left(\frac{\tau^* - \tau^y}{\tau^y}\right) > 0$$

Strain rate sensitivity

$$M\left(\frac{\tau^* - \tau^y}{\tau^y}\right) = M_0 \left|\frac{\tau^* - \tau^y}{\tau^y}\right|^{\frac{1}{n}-1}$$

Generalization

Monavari and Zaiser (2018)
Annihilation (Kocks-Mecking)

$$\dot{\rho} = B|\dot{\gamma}_{13}|(\sqrt{\rho} - \frac{\rho}{l})$$

$$\dot{\rho}_A = -A|\dot{\gamma}_{13}|\rho \approx -A'|v^m|\rho^2$$

$$\begin{aligned} \partial_t \rho \quad = \quad & -\partial_x(\rho v_2^d) + \partial_y(\rho v_1^d) + \partial_y(\kappa_1 v^m) - \partial_x(\kappa_2 v^m) \\ & + q v^m + \lambda_1 \rho \partial_y v_1^d - \lambda_2 \rho \partial_x v_2^d + \dot{\rho}_A \end{aligned}$$

Annihilation, FR and other sources

q is a conserved quantity

$$\partial_t q = \partial_x \left(-q v_2^d + v^m Q_1\right) + \partial_y \left(q v_1^d + v^m Q_2\right)$$

Extra terms
Annihilation

$$\dot{q}_A = \frac{q}{\rho}\dot{\rho}_A = -Aq|\dot{\gamma}_{13}|$$

FR source+ ...

$$\dot{q}_S = B|v^m|\rho_1\rho$$

Further "local terms" like cross slip, junction formation?

Multiple slip

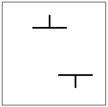
$$\rho^{\zeta}, \quad \kappa^{\zeta}_{1,2}, \quad q^{\zeta} \quad ..$$
$$P(\rho^{\zeta}, ...)$$

Yield stress

$$\tau^{Y}_{\zeta} = \sqrt{\sum_{\varsigma} h_{\zeta,\varsigma}\rho_{\varsigma}} = \alpha(\rho_1/\rho_{\zeta}, ...)Gb\sqrt{\rho_{\zeta}}$$

FR source+ ...

$$\dot{q}^{\zeta}_{S} = \sum_{\varsigma} B_{\zeta,\varsigma}|v^{m}_{\zeta}|\rho^{\varsigma}\rho^{\zeta}$$



τ^Y is an independent variable

Deterministic case

$$\partial_t \tau^Y = -\alpha G b \frac{1}{\sqrt{\rho}} \partial_t \rho = -(\alpha G b)^2 \frac{1}{\tau^Y} \partial_t \rho$$

Stochastic case

$$\partial_t \tau^Y = -(\alpha G b)^2 \frac{1}{\tau^Y} \partial_t \rho + \delta(\vec{X}, t)$$

$$< \delta(\vec{X}, t) \delta(\vec{X}', t') > = ????$$

Determining the parameters

Averaging for the *yz* plane

$$\tau_{ext} - \alpha\mu b\sqrt{\rho} = \frac{\mu b}{2\pi(1-\nu)\rho} D_{22}\partial_1\kappa_2$$

$$\alpha\sqrt{\rho}\kappa_2 = A^*\partial_1\rho$$

Combining the two

$$\tau_{ext}\left(\sqrt{\rho}\right)^2 - \alpha\mu b\left(\sqrt{\rho}\right)^3 = \frac{\mu b\alpha}{2\pi(1-\nu)} A^* D_{22}\partial_1\partial_1\sqrt{\rho}$$

Introducing $\xi(x) = \sqrt{\rho}$

$$\partial_1\left\{\frac{\tau_{ext}}{3}\xi^3 - \frac{\alpha\mu b}{4}\xi^4\right\} = \partial_1 \frac{\mu b\alpha}{2\pi(1-\nu)} \frac{A^* D_{22}}{2} \left(\partial_1\xi\right)^2$$

This follows that

$$e = \frac{\mu b \alpha}{2\pi(1-\nu)} \frac{A^* D_{22}}{2} (\partial_1 \xi)^2 - \left\{ \frac{\tau_{ext}}{3} \xi^3 - \frac{\alpha \mu b}{4} \xi^4 \right\}$$

is "conserved".

$$\partial_1 \xi = \pm \frac{1}{C} \sqrt{e - \phi(\xi)}$$

where

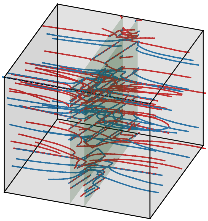
$$\phi(\xi) = -\frac{\tau_{ext}}{3} \xi^3 + \frac{\alpha \mu b}{4} \xi^4$$

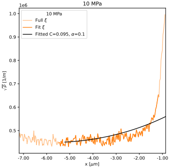
$$C^2 = \frac{\mu b \alpha}{2\pi(1-\nu)} \frac{A^* D_{22}}{2}, \quad e = \phi\left(\sqrt{\rho(x=-L/2)}\right)$$

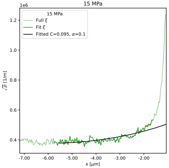
$$\frac{1}{C} \int_{\xi(-L/2)}^{\xi(x)} \frac{1}{\sqrt{e + \frac{\tau_{ext}}{3} \xi^3 - \frac{\alpha \mu b}{4} \xi^4}} d\xi = x + L/2$$

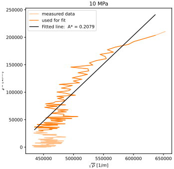
$$\int_{x0}^{x} \kappa dx = \frac{A^*}{\alpha} (\xi(x) - \xi(x_0))$$

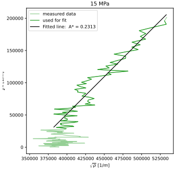
DDD with a wall











Summary

- 3D continuum theory obtained on a systematic manner
- DDD verification (doable)
- Parameter determination (doable)
- Incorporating local events (junction formation, cross slip, ...) (?)
- Adding random aspects (doable)

Details in:
István Groma, Péter Dusán Ispánovity, Thomas Hochrainer, **Dynamics of curved dislocation ensembles**, Physical Review B, 103, 174101, (2021)