Dislocation In Large Deformation Framework

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Outline

- Motivation
- Using functional derivation
- Force acting on a dislocation
- Continuum theory of dislocations with large deformation

Dislocation avalanches are like earthquakes on the micron scale

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PD Ispánovity, D Ugi, G Péterffy, M Knapek, S Kalácska, D Tüzes, I. Groma,
Nature communications 13 (1), 1975 (2022)

Large elastic deformation: Lagrangian description

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

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

Rigid body translation:

$$F_{ij} = \frac{\partial x_i}{\partial X_j}$$

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

$$\frac{\delta E}{\delta x_i} = -\partial_j \frac{\delta E}{\delta F_{ij}} = -\partial_j \sigma_{ji}^{1PK} = 0$$

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Rigid body rotation:

$$\epsilon_{ij} = \frac{1}{2}\left(\tilde{F}_{ik}F_{kj} - \delta_{ij}\right)$$

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

$$\frac{\delta E}{\delta x_i} = -\partial_j \frac{\delta E}{\delta F_{ij}} = -\partial_j\left(\frac{\delta E}{\delta\epsilon_{kl}}\frac{d\epsilon_{kl}}{dF_{ij}}\right) = -\partial_j\left(\frac{\delta E}{\delta\epsilon_{kj}}F_{ik}\right) = -\partial_j\left(F_{ik}\sigma^{2PK}_{kj}\right) = 0$$

Plastic deformation

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

The energy depends on only the elastic deformation

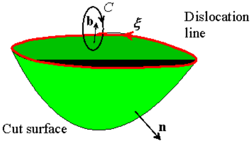
$$\epsilon^{e}_{ij} = \frac{1}{2}\left(F_{mo} F^{-p}_{oi} F_{mp} F^{-p}_{pj} - \delta_{ij}\right) = \frac{1}{2}\left(\tilde{F}^{-p}_{io} C_{op} F^{-p}_{pj} - \delta_{ij}\right)$$

From this

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

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

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



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

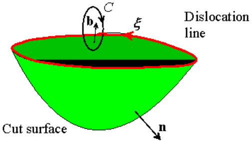
What is F^{-p}_{ij}?

What is the inverse of something containing a Dirac delta?

$$1 + b\delta(x)$$

What is?

$$\frac{1}{1 + b\delta(x)}$$



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

What is F^{-p}_{ij}?
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

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

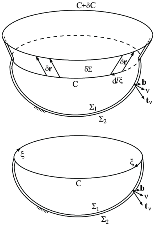
Individual dislocation

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

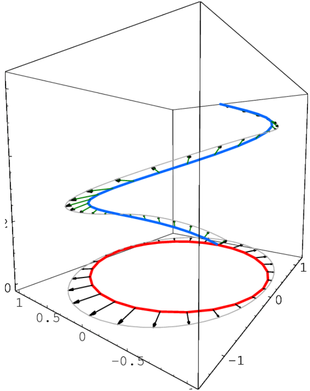
Effective stress

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

Peach Köhler force?



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



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)

$$\begin{aligned} \partial_{\mathrm{t}}\overrightarrow{A} &= \nabla \times (\overrightarrow{v} \times \overrightarrow{A}) = \mathcal{L}_v A \\ & \quad \partial_n(v_n A_l - v_l A_n) \end{aligned}$$

Evolution of the generalized dislocation density tensor

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

Bubnov-Galerkin weighted residual method in Fourier space

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

$$v(\tilde{r},\varphi) \approx v^m(\tilde{r}) + v_1^d(\tilde{r})\cos\varphi + v_2^d(\tilde{r})\sin\varphi$$

$$q'(\tilde{r},\varphi) \approx q(\tilde{r}) + Q_2(\tilde{r})\cos\varphi - Q_1(\tilde{r})\sin\varphi$$

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

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

Plastic potential

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

“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:

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

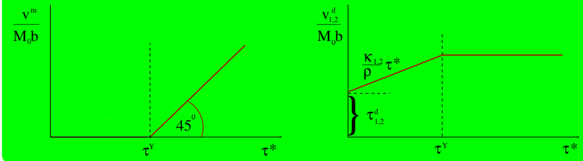
Dynamics

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

$\Downarrow$

τ^*, τ_1^d, τ_2^d

Velocities



Plastic potential

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

Corse grained fields

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

Correlations

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

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

displacement field:

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

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

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

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

P is convex! No LEDS!

No reaction terms!

2D and 3D are practically the same

The instability is "massive"

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

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

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

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

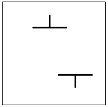
Yield stress

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

FR source$+$ ...

$$\dot{q}^\zeta_S = \sum_\varsigma B_{\zeta,\varsigma}|v^m_\zeta|\rho^\varsigma\rho^\zeta$$

Stochastic term



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

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

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

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)