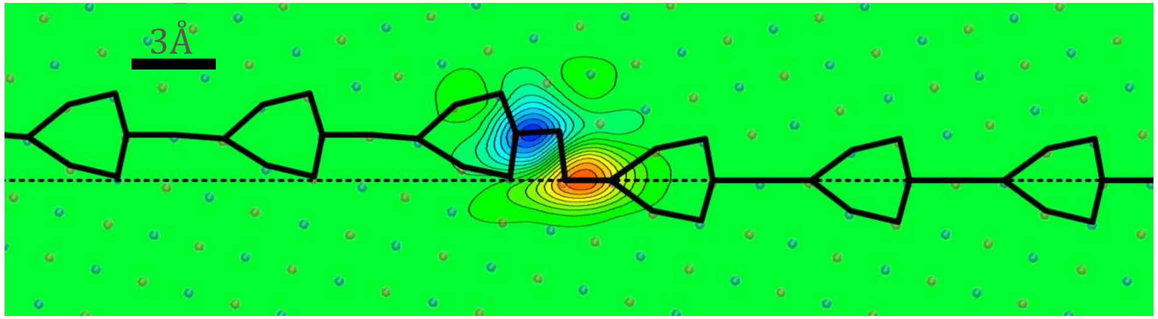
LABORATOIRE D'ÉTUDE DES MICROSTRUCTURES ET DE MÉCANIQUE DES MATÉRIAUX

Challenges in continuous modeling of grain/phase boundaries



Generalized disclination dipole π_{113} in stepped tilt boundary, *X.Y. Sun et al. IJP* ***104****, 134-146 (2018)*

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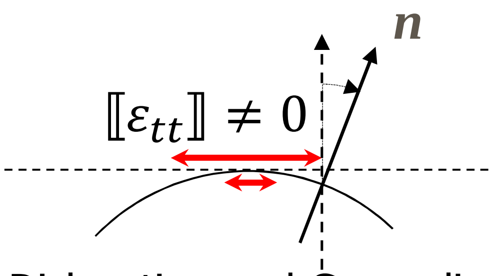
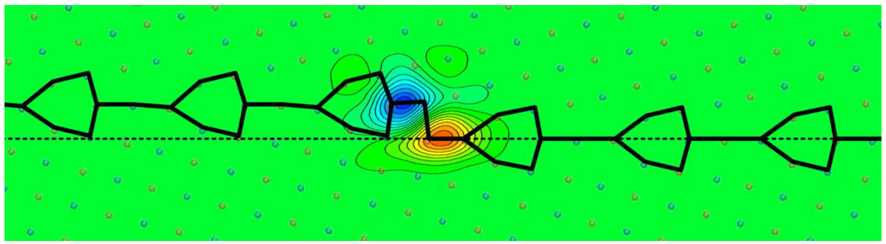
TimeMan, 6 Février 2019

Motivations and modeling tools

- Motivations
  - ✓ Plasticity in nano-structured and slip-system-deprived materials (such as olivine)
  - ✓ Structure/motion of « imperfect » interfaces (with curvature, steps and ledges)
  - ✓ Boundary migration, grain growth, dynamic recrystallization, phase transformation
- Tools for continuous interface modeling at various scales
  - ✓ At microscale-mesoscale: Field Dislocation Mechanics +



  - ✓ At nanoscale: Field Dislocation and Generalized Disclination Mechanics



- Paradigm: converting discontinuities at interfaces into smooth fields

Outline

- Continuous description of interfaces at interatomic scale (FDGDM)
  - ✓ Crystal defect densities (dislocations/disclinations/generalized disclinations)
  - ✓ Elastostatic examples: Twin tips
  - ✓ Dynamic examples: Shear/Compression Coupled Boundary Migration
- Continuous description of interfaces at mesoscopic scale (FDM+)
  - ✓ Burgers vector conservation and tangential continuity of plastic distortion rate
  - ✓ Boundary curvature
- Conclusions
  - ✓ Relevance of continuity at nanoscale
  - ✓ Tangential continuity brings nonlocality to GB description at mesoscale
  - ✓ Spatial coarse graining

Continuous description of interfaces at interatomic scale

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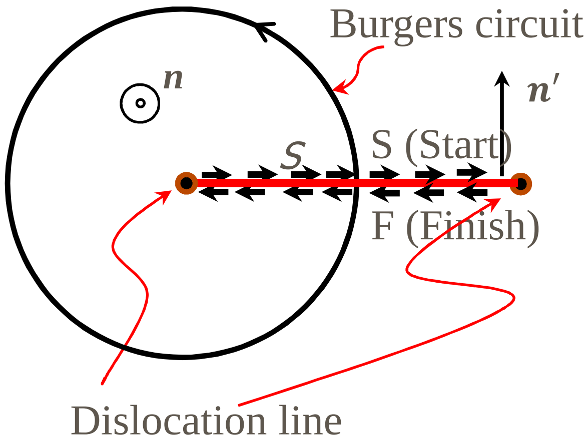
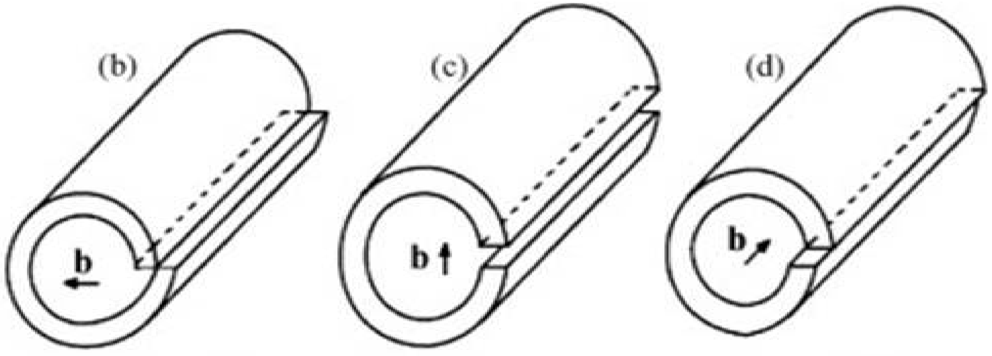
Dislocation densities





V. Volterra, Ann. Sci. Ec. Norm. Sup. III **24**, 401 (1907)

- Discontinuity of elastic translational displacement across a bounded surface

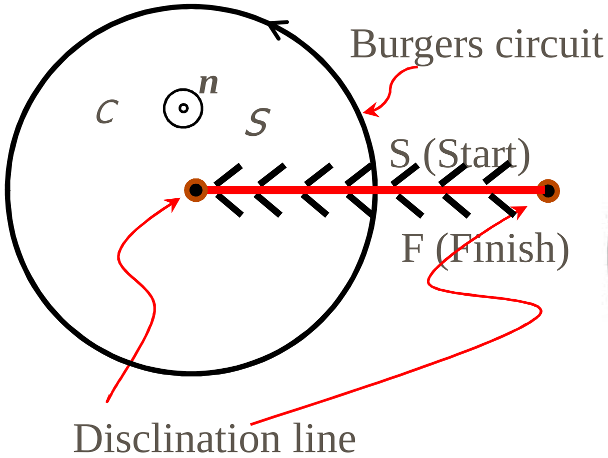
$$\cancel{\boldsymbol{U}_e = \boldsymbol{grad}\,\boldsymbol{u}_e} \Rightarrow [\![\boldsymbol{u}_e]\!] = \boldsymbol{b} = \int_C \boldsymbol{U}_e.\boldsymbol{dx} = \iint_S \boldsymbol{curl}\,\boldsymbol{U}_e.\boldsymbol{n}dS = \iint_S \boldsymbol{\alpha}.\boldsymbol{n}dS \neq 0$$

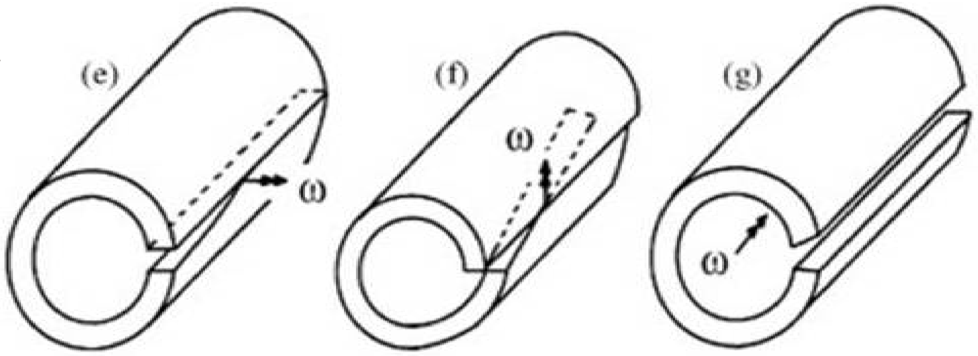
- Incompatibility of the elastic distortion $\boldsymbol{U}_e$ and strain $\boldsymbol{\epsilon}_e$ tensors reflected by Nye's dislocation density tensor $\boldsymbol{\alpha}$: E. Kröner, Erg.Ang.Math. **9**, 1-179 (1958)

$$\boldsymbol{curl}\,\boldsymbol{U}_e = \boldsymbol{curl}\,\boldsymbol{\epsilon}_e + \boldsymbol{curl}\,\boldsymbol{\omega}_e = \boldsymbol{curl}\,\boldsymbol{\epsilon}_e + tr(\boldsymbol{\kappa}_e)\boldsymbol{I} - \boldsymbol{\kappa}_e^t = \boldsymbol{\alpha}$$

- Continuity of elastic rotation tensor, tangential continuity of elastic distortion and strain tensors: $\boldsymbol{\kappa}_e = \boldsymbol{grad}\,\boldsymbol{\omega}_e\ , [\![\boldsymbol{U}_e]\!] \times \boldsymbol{n}' = 0, [\![\boldsymbol{\epsilon}_e]\!] \times \boldsymbol{n}' = 0$

Disclination densities





V. Volterra, Ann. Sci. Ec. Norm. Sup. III **24**, 401 (1907)

- Discontinuity of elastic rotation across a bounded surface

  ~~$\boldsymbol{\kappa}_e = \boldsymbol{grad}\,\boldsymbol{\omega}_e$~~ $\Rightarrow [\![\boldsymbol{\omega}_e]\!] = \boldsymbol{\Omega} = \int_C \boldsymbol{\kappa}_e . \boldsymbol{dx} = \iint_S \boldsymbol{curl}\,\boldsymbol{\kappa}_e . \boldsymbol{n}dS = \iint_S \boldsymbol{\theta} . \boldsymbol{n}dS$

- Incompatibility of the elastic curvature tensor $\boldsymbol{\kappa}_e$ reflected by deWit's disclination density tensor $\boldsymbol{\theta}$:

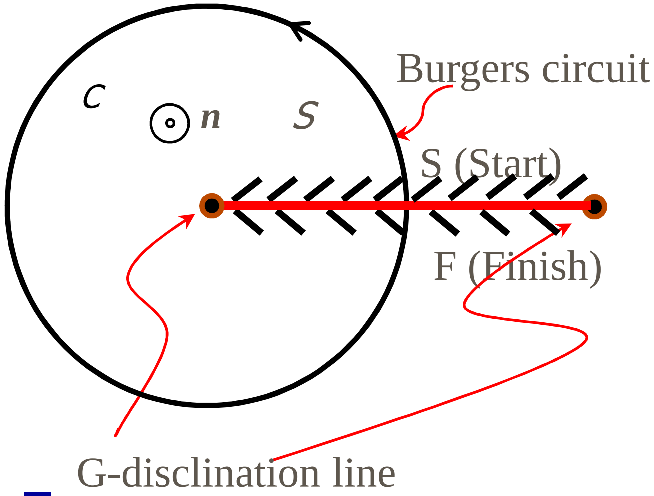
$$\boldsymbol{curl}\,\boldsymbol{\kappa}_e = \boldsymbol{\theta}$$

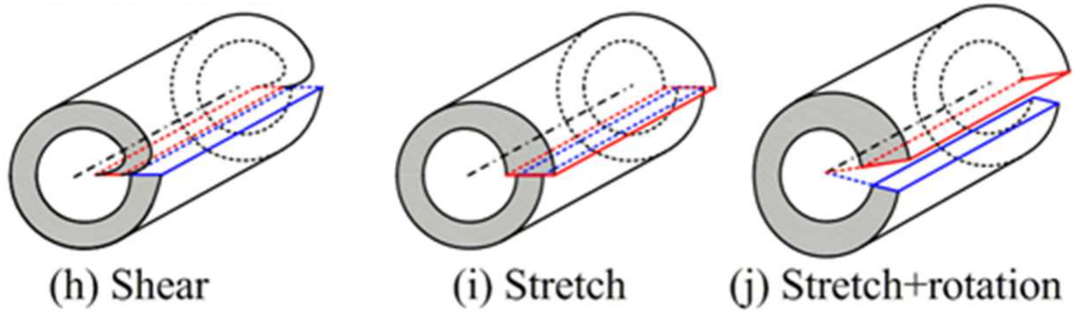
R. deWit, JRNBS-A **5**, 651-680 (1970)

- Tangential continuity of the elastic curvature, distortion and strain tensors $[\![\boldsymbol{U}_e]\!] \times \boldsymbol{n}' = 0,\ [\![\boldsymbol{\varepsilon}_e]\!] \times \boldsymbol{n}' = 0, [\![\boldsymbol{\kappa}_e]\!] \times \boldsymbol{n}' = 0$

C. Fressengeas & B. Beausir, IJSS **156-157**, 210-215 (2019)

Generalized disclination densities





A.Acharya & C. Fressengeas, IJF **174**, 87-94 (2012).

- Discontinuity of elastic distortion across a bounded surface

$$\cancel{\boldsymbol{G}_e = \boldsymbol{grad}\, \boldsymbol{U}_e} \Rightarrow [\![\boldsymbol{U}_e]\!] = \boldsymbol{\Pi} = \int_C \boldsymbol{G}_e.\boldsymbol{dx} = \iint_S \boldsymbol{curl}\, \boldsymbol{G}_e.\boldsymbol{n}dS = \iint_S \boldsymbol{\pi}.\boldsymbol{n}dS$$

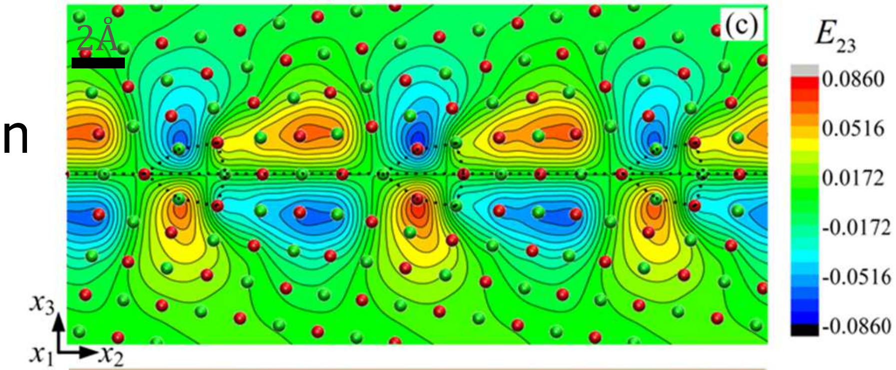
- Incompatibility (non-integrability) of the second-order distortion $\boldsymbol{G}_e$ reflected by the g-disclination density tensor $\boldsymbol{\pi}$:

$$\boxed{\boldsymbol{curl}\, \boldsymbol{G}_e = \boldsymbol{\pi}}$$

Generalized disclination dipoles in straight tilt boundaries

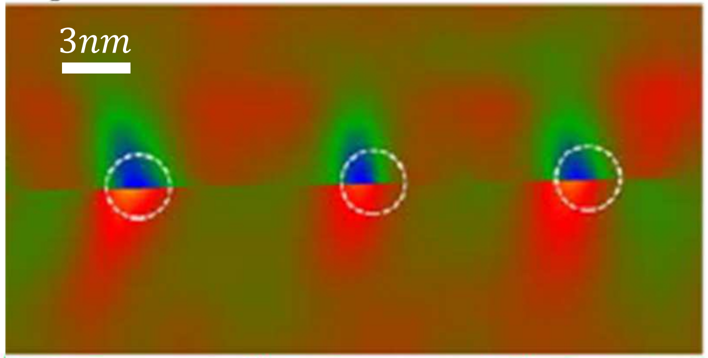
- Shear discontinuity $[\![\varepsilon_{23}]\!]$ accommodated in less than 2 Å in copper $\Sigma 37(610)$ symmetric <100> tilt boundary (18.9°)

X.Y. Sun et al, IJP **77** 75-89 (2016)

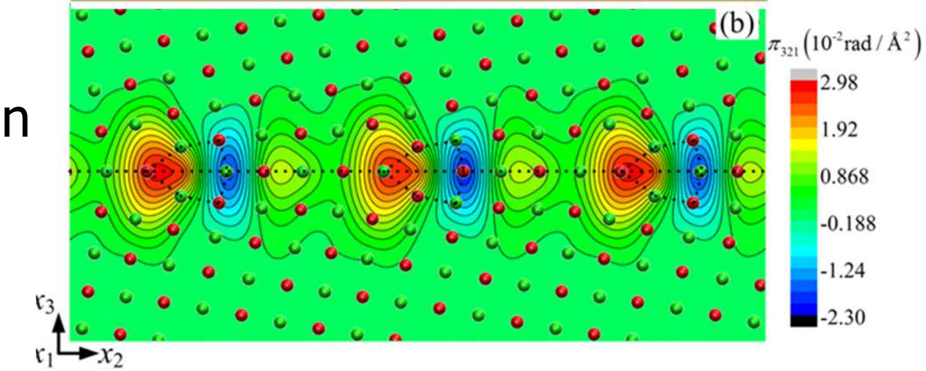


- Shear discontinuity $[\![\varepsilon_{23}]\!]$ in silicon $\Sigma 9$<122> 38.94° tilt boundary from Geometric Phase Analysis

M. Couillard et al, Phil.Mag. (2013)



- G-disclination density field π_{231} reflecting discontinuity of rotation $[\![\omega_{23}]\!]$ and shear strain $[\![\varepsilon_{23}]\!]$ in copper $\Sigma 37(610)$ symmetric <100> tilt boundary (18.9°)

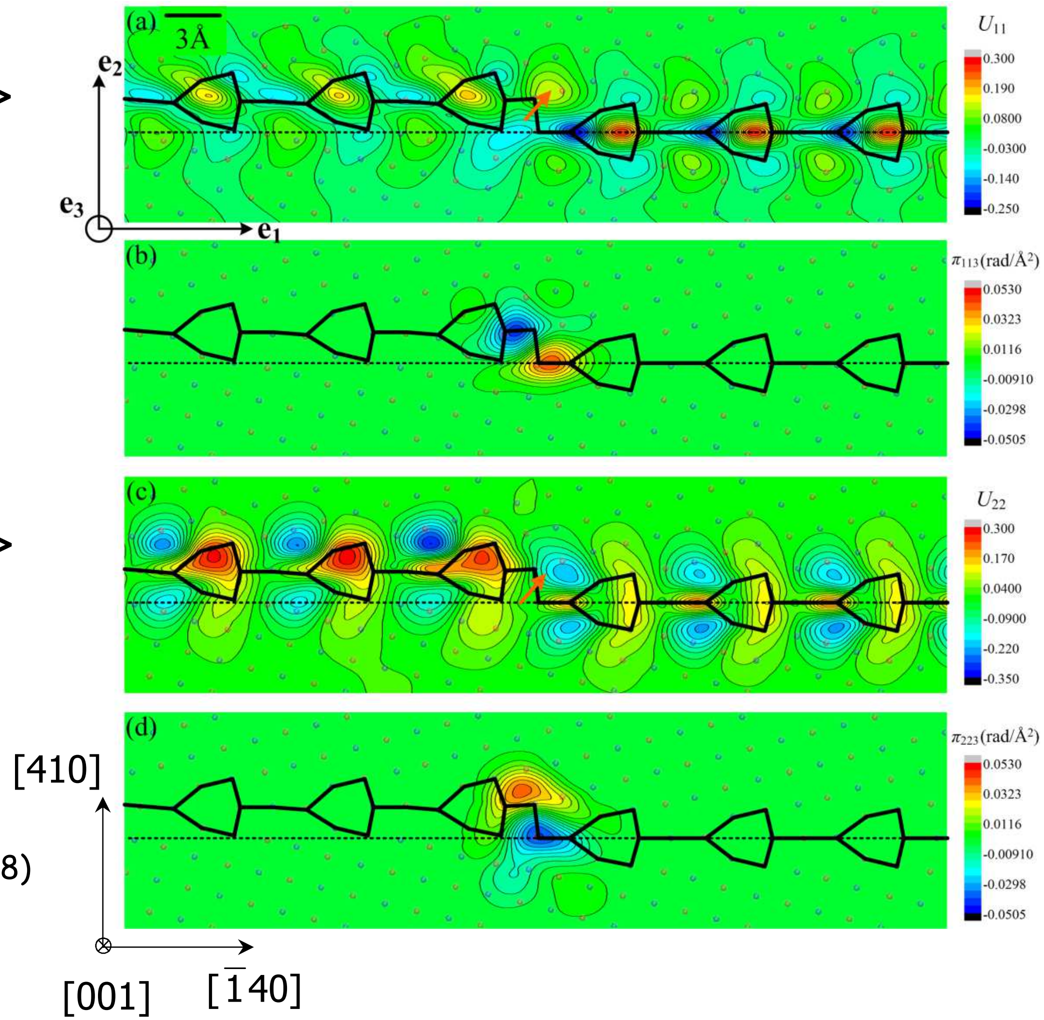


Generalized disclination dipoles in stepped tilt boundaries

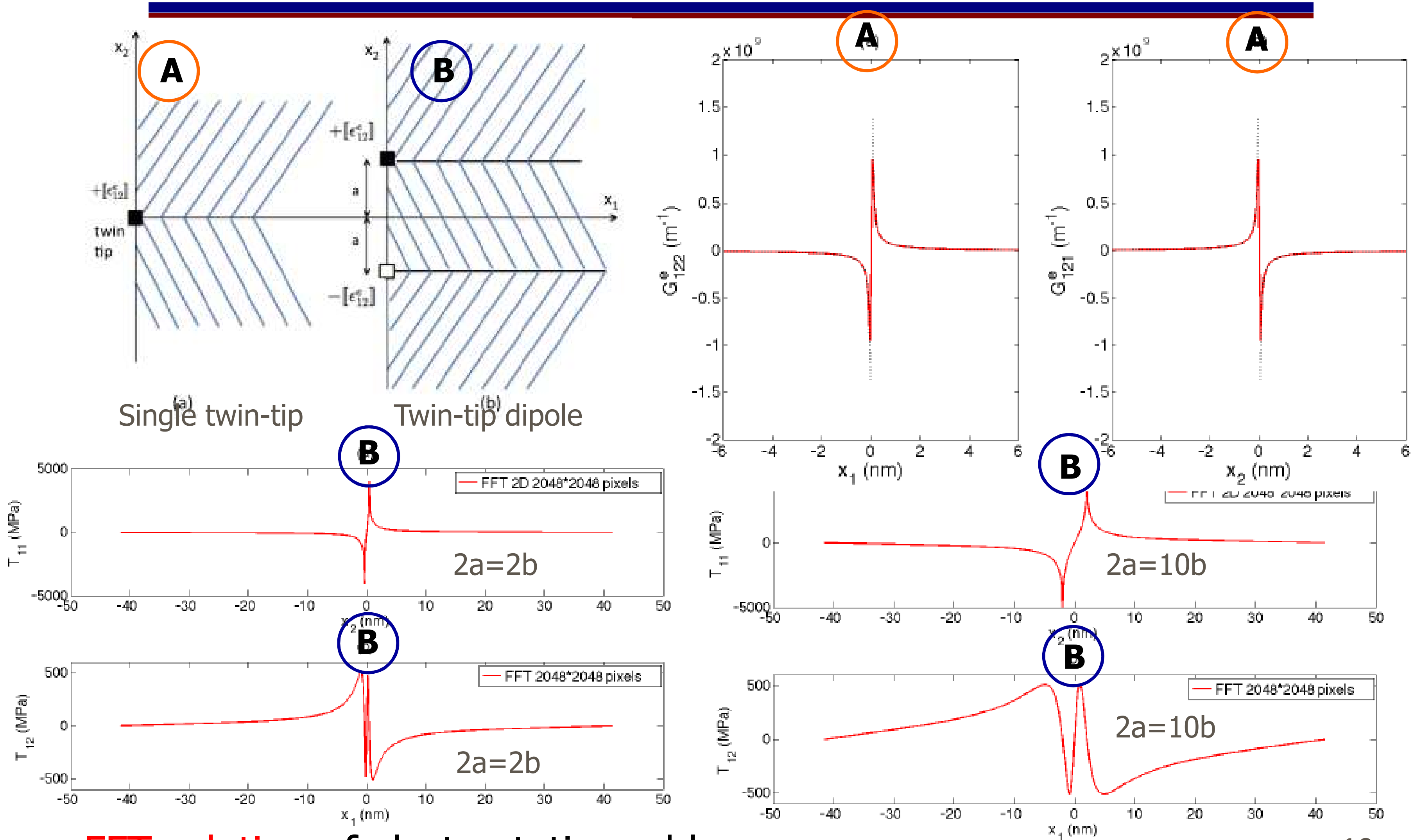
- $[\![\varepsilon_{11}]\!]$ discontinuity in <100> ledge of tilt boundary
  Σ17(410), 28.07°
- π_{113} g-disclination dipole

- $[\![\varepsilon_{22}]\!]$ discontinuity in <100> ledge of tilt boundary
  Σ17(410), 28.07°
- π_{223} g-disclination dipole

X.Y. Sun et al., IJP **104**, 134-146 (2018)

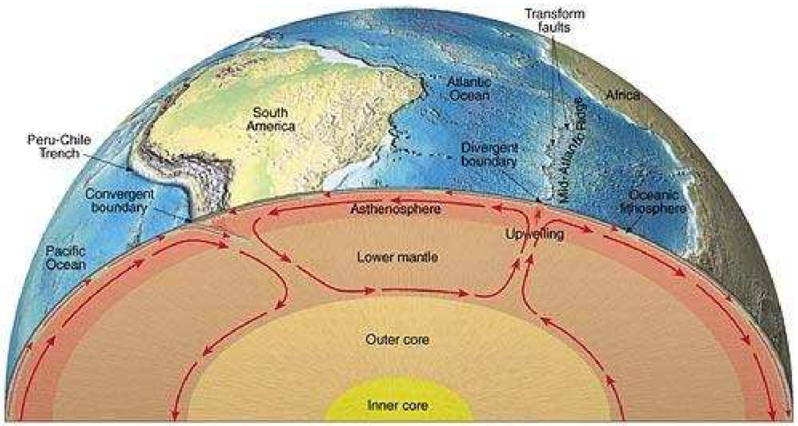


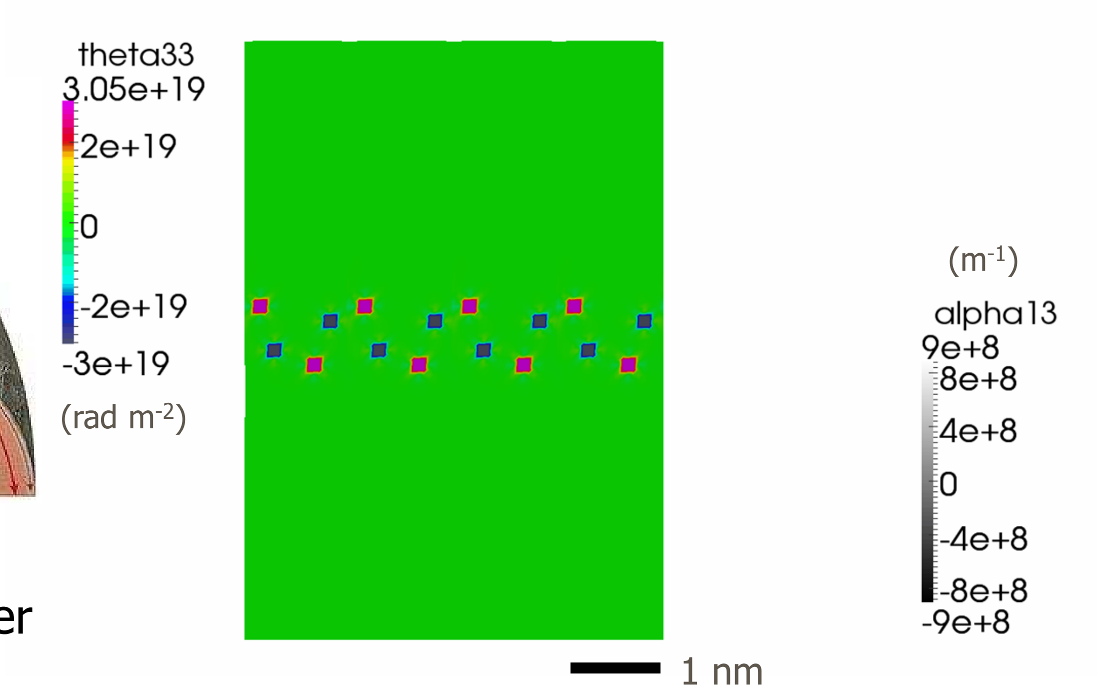
Elasto-static fields of twin-tips



■ FFT solution of elasto-static problem: Berbenni et al, IJSS **51**, 4157-4175 (2014)

Shear Coupled Boundary Migration in olivine





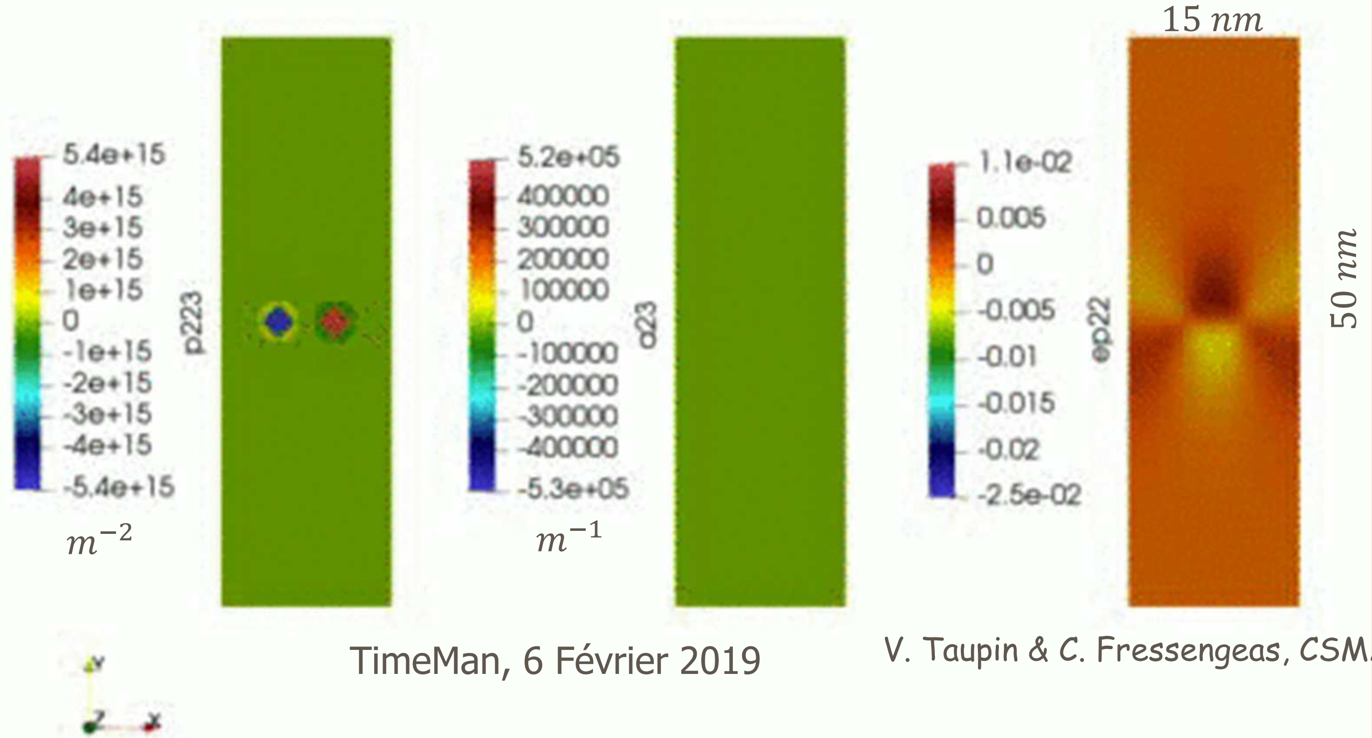
- Olivine $(Mg,Fe)_2SiO_4$: main constituent of the Earth's upper mantle (~70%)
- Orthorombic olivine has only three independent slip systems
- Dislocation glide cannot accommodate mantle's convective motion

- FEM solution of FDDM field equations
- Shear-coupled boundary migration provides an additional deformation mechanism for slip system-deprived olivine

P. Cordier et al., Nature, **507**, 51-56 (2014).

Compression induced boundary migration

- FEM solution of FDGDM field equations
- Migration of π_{223} dipoles generates α_{23} dipoles
- Tangential climb of α_{23} induces normal compression $\dot{U}^p_{22} = \alpha_{23} V_1$
- Normal glide of α_{23} induces shear + rotation $\dot{U}^p_{21} = -\alpha_{23} V_2$



V. Taupin & C. Fressengeas, CSMA 2019

Continuous description of interfaces at mesoscopic scale

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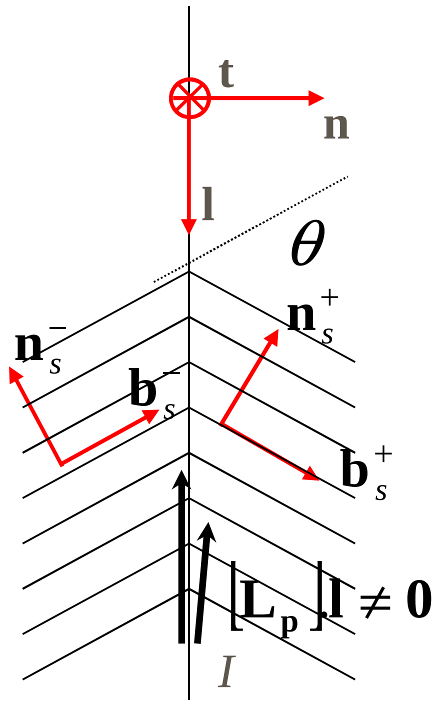
Interfaces in conventional CP: tangential plastic distortion rate discontinuity

- Typical example: symmetric tilt boundary
  - ☞ Discontinuity of the elastic rotation: $[\![\boldsymbol{\omega}_e]\!] = \theta \boldsymbol{n} \times \boldsymbol{l}$
- Tangential discontinuity of plastic distortion rate

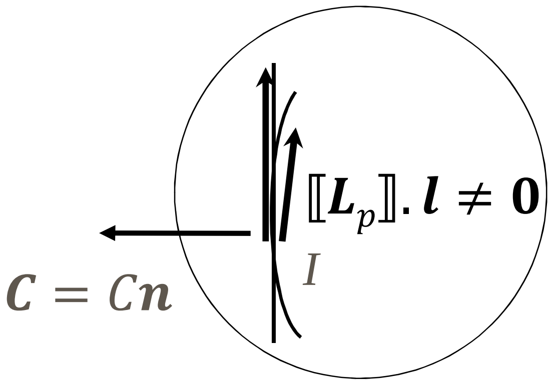
$$\forall \boldsymbol{l} \in I, [\![\boldsymbol{L}_p]\!].\boldsymbol{l} = \left(\sum \dot{\gamma}_s \boldsymbol{b}_s^+ \otimes \boldsymbol{n}_s^+ - \sum \dot{\gamma}_s \boldsymbol{b}_s^- \otimes \boldsymbol{n}_s^- \right).\boldsymbol{l} \neq 0$$

- Any discontinuity $[\![\boldsymbol{L}_p]\!]$ is accepted and (sometimes) accommodated through Frank-Bilby *surface-dislocation* densities in interface



$$\forall \boldsymbol{l} \in I, [\![\boldsymbol{L}_p]\!].\boldsymbol{l} = \dot{\alpha}^{\boldsymbol{S}}(I).\boldsymbol{t} \neq 0$$

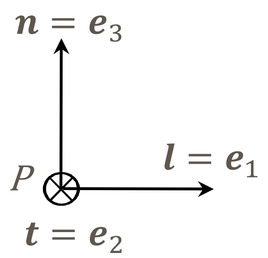
Burgers vector conservation and curvature dynamics



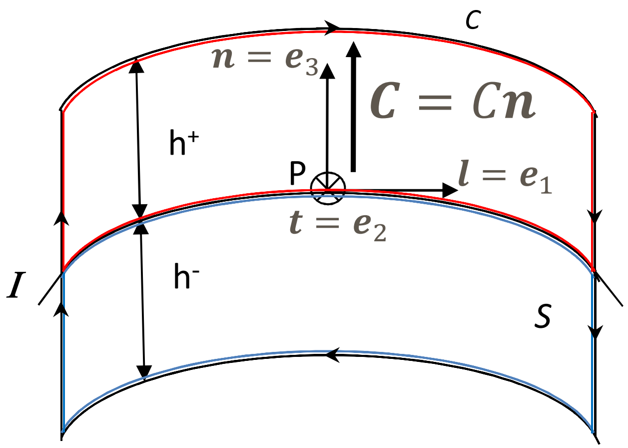
- Ban surface-dislocations $\alpha^S(I)$
- Distribute surface-dislocations in a volumetric layer through tangential continuity of plastic distortion   V. Taupin et al, IJSS **99**, 71-81 (2016)
- Relate tangential plastic distortion rate discontinuity with interface curvature dynamics through GB-mediated plasticity

C. Fressengeas, JMPS **124**, 814-826 (2019)

Continuity constraints on plastic distortion rate on curving interfaces



Darboux directors of curve in I



- Conservation of Burgers vector:

$$\forall l \in I, \dot{\boldsymbol{b}} = \frac{d}{dt}\iint_S \boldsymbol{\alpha}.\boldsymbol{t}dS = -\frac{d}{dt}\int_C \boldsymbol{U}_p.\boldsymbol{l}ds = 0$$

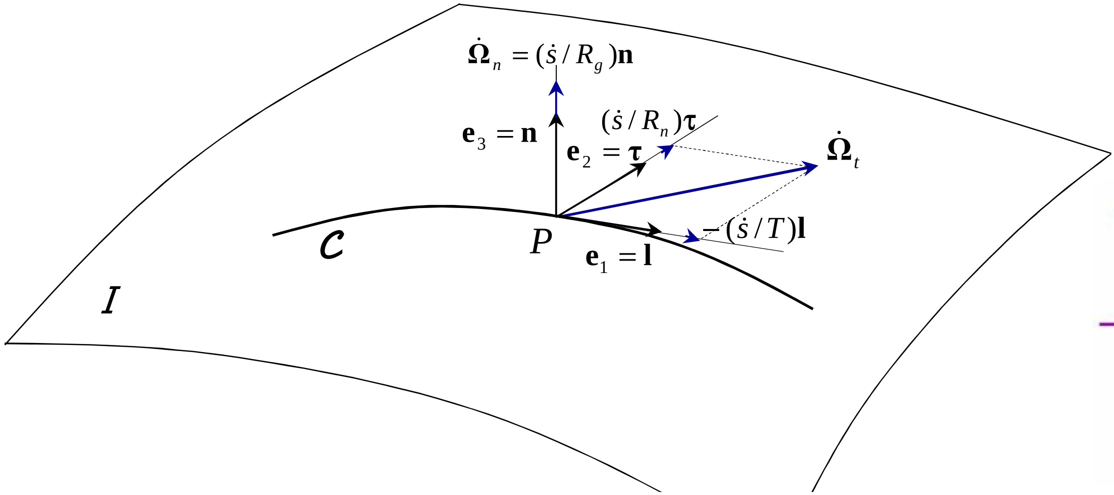
- Allow rotation of interface directors; in the limit $h^+, h^- \to 0, L \to 0$,

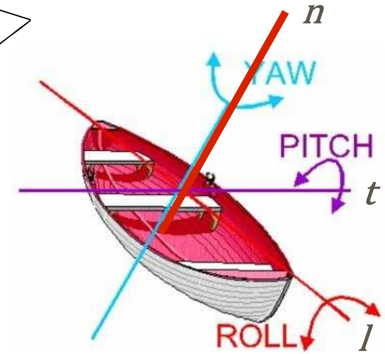
$$\forall \boldsymbol{l} \in I, \left([\![\dot{\boldsymbol{U}}_p]\!] - [\![\boldsymbol{\alpha}]\!] \times \boldsymbol{C}\right).\boldsymbol{l} + [\![\boldsymbol{U}_p]\!].\dot{\boldsymbol{l}} = 0$$

$$\dot{\boldsymbol{l}} = \dot{\boldsymbol{\Omega}} \times \boldsymbol{l},\ \dot{\boldsymbol{\Omega}} = \left(-\frac{\boldsymbol{l}}{T} + \frac{\boldsymbol{t}}{R_n} - \frac{\boldsymbol{n}}{R_g}\right)\dot{s}$$

☞ Darboux' frame rotation components: $1/R_g, 1/R_n, 1/T$, geodesic curvature, normal curvature and geodesic torsion

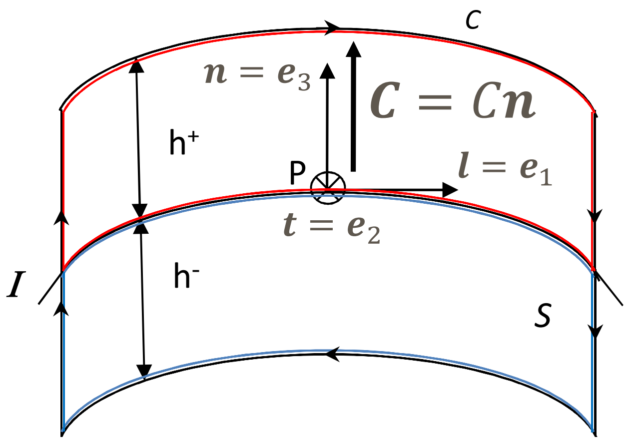
Darboux frame

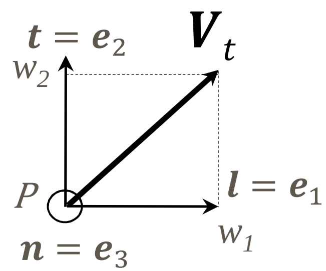




- $\forall i, \dot{\boldsymbol{e}}_i = \dot{\boldsymbol{\Omega}} \times \boldsymbol{e}_i,\ \dot{\boldsymbol{\Omega}} = \left(-\frac{\boldsymbol{l}}{T} + \frac{\boldsymbol{t}}{R_n} - \frac{\boldsymbol{n}}{R_g}\right)\dot{s}$ in rad.s^{-1}: rotation rate of Darboux frame. $1/T$ is the geodesic torsion (roll), $1/R_n$ the normal curvature (pitch),$1/R_g$ the geodesic curvature (yaw).
- Along principal directions $1/T = 0$, normal curvature = principal curvature; geodesic curvature $1/R_g$ not used in the model

Continuity constraints on plastic distortion rate on curving interfaces





- Plastic distortion rate discontinuity in the limit $h^+, h^- \to 0, L \to 0$,

$$\forall \boldsymbol{l} \in I, \left(\left[\!\left[\dot{\boldsymbol{U}}_p\right]\!\right] - [\![\boldsymbol{\alpha}]\!] \times \boldsymbol{C}\right).\boldsymbol{l} + [\![\boldsymbol{U}_p]\!].\dot{\boldsymbol{\Omega}} \times \boldsymbol{l} = 0$$
$$\Leftrightarrow \left([\![\boldsymbol{\alpha}]\!] \times (\boldsymbol{V} - \boldsymbol{C}) + [\![\boldsymbol{U}_p]\!] \times \dot{\boldsymbol{\Omega}}\right) \times \boldsymbol{n} = 0$$
$$\Leftrightarrow [\![\boldsymbol{\alpha}.\boldsymbol{n} \otimes \boldsymbol{V}_t - (V_n - C_n)\boldsymbol{\alpha}_t]\!] + \left[\!\left[\boldsymbol{U}_p\right]\!\right].\boldsymbol{n} \otimes \dot{\boldsymbol{\Omega}}_t = 0$$

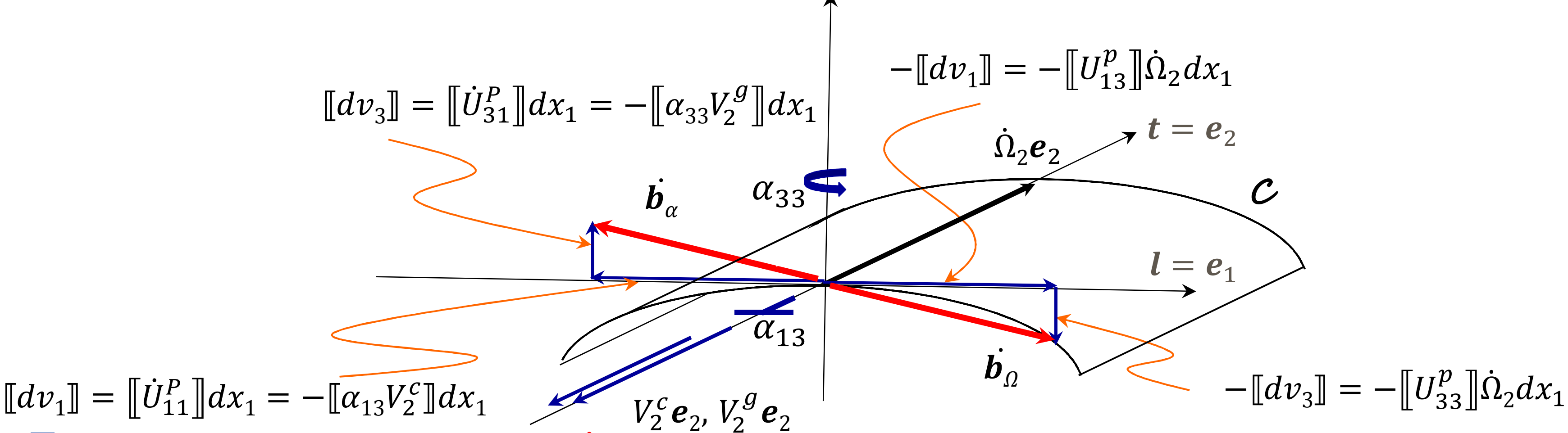
- Interface rotation rate offsets tangential discontinuity of plastic distortion rate

$$\dot{\boldsymbol{\Omega}}_t = -[\![\boldsymbol{\alpha}.\boldsymbol{n} \otimes \boldsymbol{V}_t - (V_n - C_n)\boldsymbol{\alpha}_t]\!]^t.\frac{[\![\boldsymbol{U}_p]\!].\boldsymbol{n}}{([\![\boldsymbol{U}_p]\!].\boldsymbol{n})^2}$$

C. Fressengeas, JMPS **124**, 814-826 (2019)

Cylindrical example

- Principal directions in cylindrical interface (no torsion, only one non-zero principal curvature)



- Interface rotation rate $\dot{\Omega}_2$ offsets discontinuities arising from axial climb V_2^c of α_{13} edges and glide V_2^g of α_{33} screws

$$[\![\dot{U}^p_{11}]\!] = -[\![\alpha_{13}V_2^c]\!] = \dot{\Omega}_2[\![U^p_{13}]\!] \Leftrightarrow \dot{b}_1^\alpha = -\dot{b}_1^\Omega$$
$$[\![\dot{U}^p_{31}]\!] = -[\![\alpha_{33}V_2^g]\!] = \dot{\Omega}_2[\![U^p_{33}]\!] \Leftrightarrow \dot{b}_3^\alpha = -\dot{b}_3^\Omega$$

- Curvature dynamics: $\dot{\Omega}_2 = -[\![\alpha_{33}V_2^g]\!]/[\![U^p_{33}]\!]$

C. Fressengeas, JMPS **124**, 814-826 (2019)

Conclusions

- Continuous modeling of GB elastic structure at nanoscale
  - ✓ Periodic arrays of g-disclination dipoles compose GB core structure
  - ✓ Boundary migration for realistic stress and strain rate fields, numerical efficiency
- At mesoscopic scale, nonlocality is brought to interface modeling by Burgers vector conservation and tangential continuity conditions
- Coarse-graining eased by unique overall structure of the theory
- Related features (not shown here)
  - ✓ Nonlocality, nonlinearity of elasticity in defects cores: V. Taupin et al, JMPS **100**, 62-84 (2017)
  - ✓ Prediction of interface velocity in mesoscopic model: C. Fressengeas, JMPS **124**, 814-826 (2019)
- Potential use for prediction of
  - ✓ Migration of imperfect GBs in both FDM+ and FDGDM
  - ✓ Cracks-extrinsic defects-GB interactions in FDGDM