Discontinuity and Incompatibility

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What kind of problems?

Ultrahigh strain hardening in thin Pd films with nanoscale twins
Schryvers, Pardoen et al.

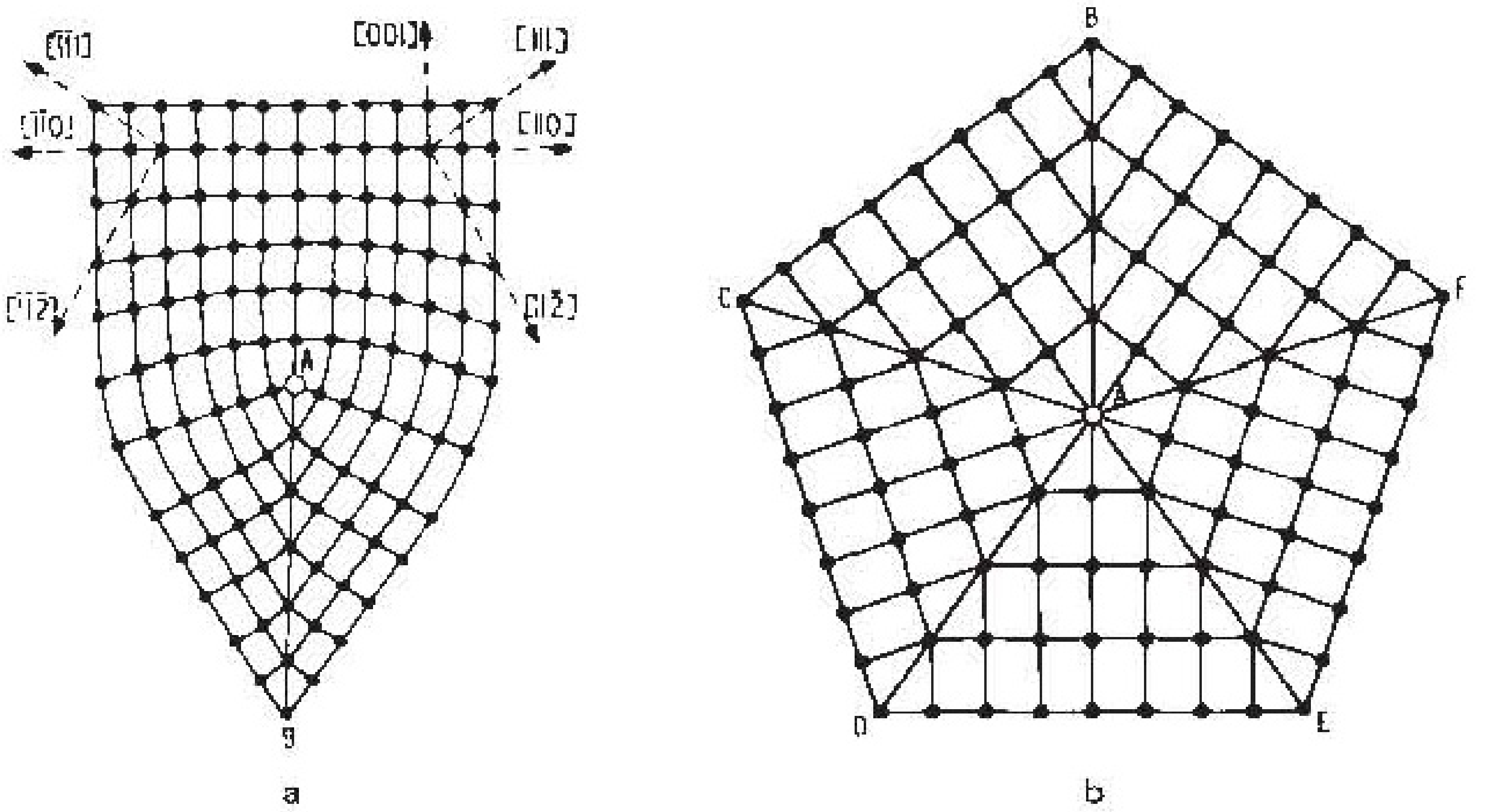


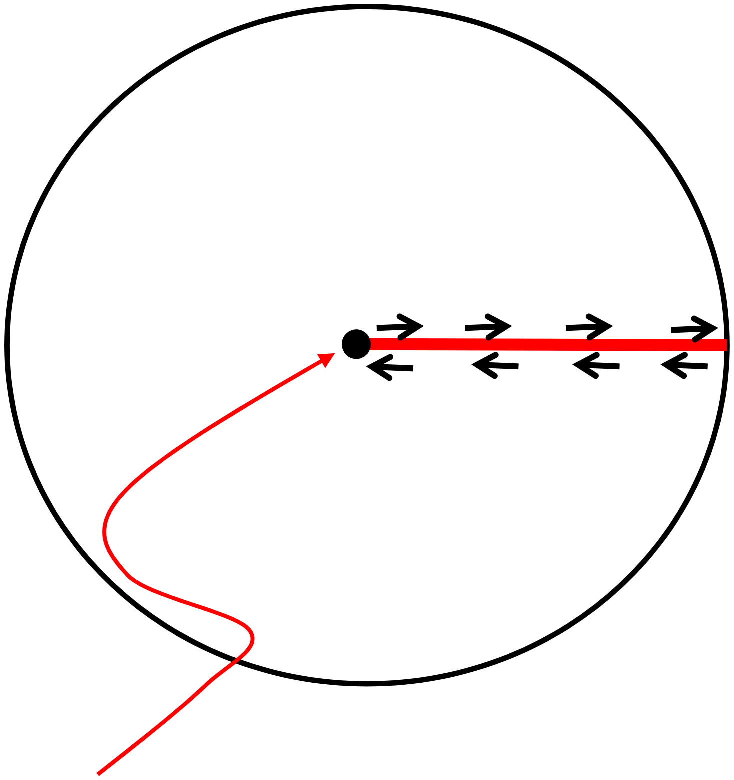
Figure 9 Partial disclinations in fcc crystals. They are edge lines of twin boundaries and pass through the point A. *a*: The 70°32′ partial disclination. *b*: The 7°20′ (= 360° − 5 × 70°32′) partial disclination (star disclination) that borders five twin boundaries. After deWit (39).

from: Kröner and Anthony describing concepts from deWit

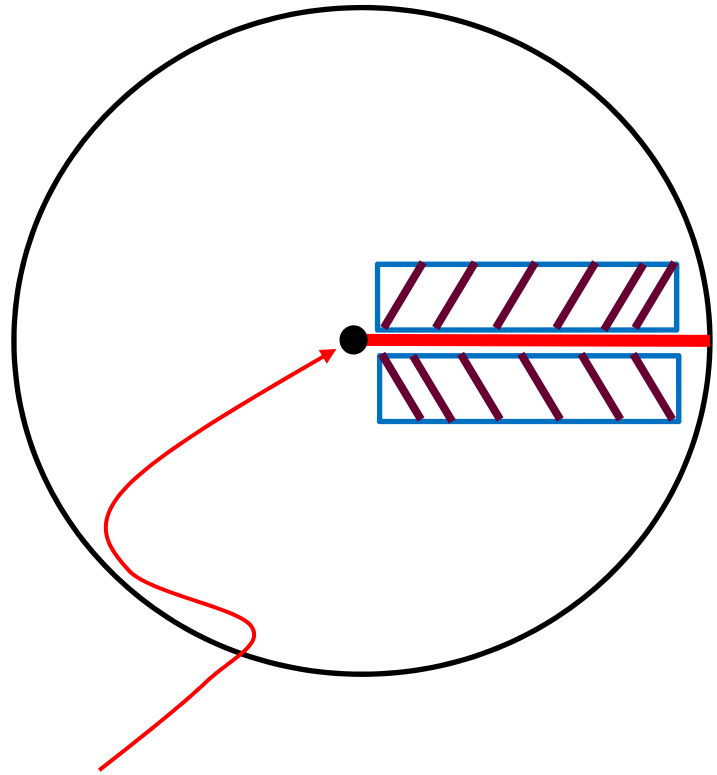
(essentially) complex model - Any prior evidence it should work?

- **Mesoscale Field Dislocation Mechanics (M)FDM**
  - **(** *AA* **– 20/01,03,04,11**; *Roy , AA* **– 05, 06)**
  - **Some Example applications**
    - **Engineering**
      - *Puri, Das, AA* – modeling of Xiang and Vlassak's thin film experiments – **JMPS (2011)**
      - *Mach, Beaudoin, AA* – modeling of inter/intra-grain orientation texture heterogeneities; Winther etc. – **JMPS (2010)**
    - **Physics of Complexity**
      - *Fressengeas, Beaudoin et al.* – dislocation transport + intermittency – **Phys. Rev. B (2009)**
      - *Sethna et al*. – self-organized critical pattern formation – **Phys. Rev Lett., Phys. Rev. B, JMPS – (2006, 2007, 2008, 2010)**
    - **Mathematics**
      - *Tartar, AA* – global existence and uniqueness of FDM system for nonlinear transport – **Bull. of Italian Math. Union – (2011)**
      - *Zhu, Chapman, AA* – Instability of dislocation motion – prediction of heterogeneous slip band microstructures **– (2011)**

Discontinuity within a Discontinuity



Terminating curve of displacement discontinuity = DISLOCATION



Terminating curve of a distortion/ strain discontinuity = G. DISCLINATION

displacement discontinuity surface
= slip ‘boundary’ if identifiable;
stacking fault

distortion discontinuity surface
= phase boundary/grain boundary

Context

- Generalize the work of ***DeWit* (1970)** and collaborators
  - Beyond 'rotational' higher order defects - ***disclinations***
  - Give ***disclinations*** unambiguous physical basis even in materials without any director dofs
  - Finite deformation theory
  - Dynamics (even for quasi-static momentum balances)
  - Theory not constrained to differential geometric constructs (***Kondo, 1950s….; Kröner, Lagoudas, 1992; Clayton, McDowell, Bammann, 2006***)
    - As a result, simpler

Physical Realizations

As terminating curve moves, the slip/phase/grain boundary region
Is ‘drawn out’ or translates

1. Dislocation loops + identifiable slip surfaces, stacking faults

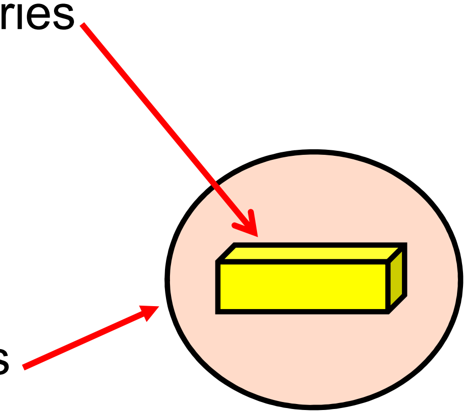
2. G. disclinations + phase boundaries, grain boundaries

3. Finite shear bands

4. ‘Triple’ points terminating phase/grain boundaries

5. Faceted inclusions in phase transforming materials

6. Smooth inclusions in phase transforming materials

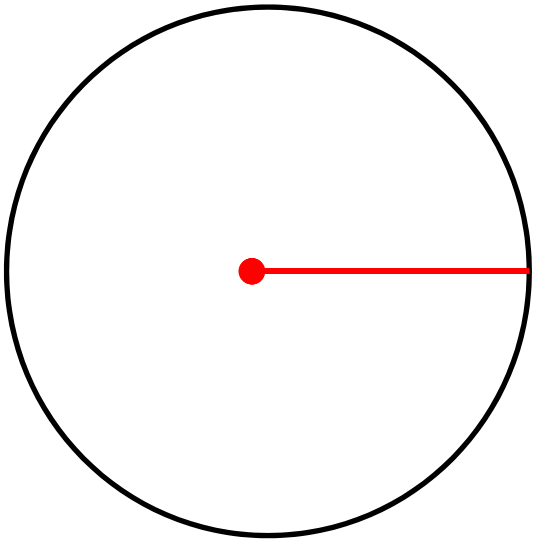


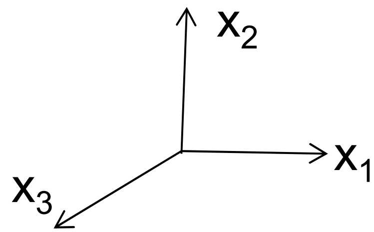
Example Applications

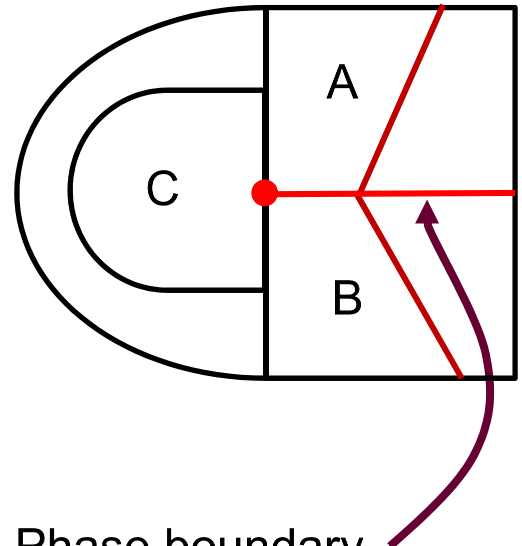
- ***Dynamics*** of
  - Plasticity
  - Phase transformations
  - Coupled plasticity and phase transformations
  - Shear band dynamics in
    - amorphous materials (metallic glasses)
    - Soft active materials
      - **Classical theory + modifications good for inception but do not yield a physically sound basis for post-inception, well-set evolution**
      - **e.g. finite-extent shear bands – almost no theory**
        - **exception – Bigoni et al. – line inclusion models**

Smooth compatible strain/strain gradient fields in punctured domains

Screw dislocation







Phase boundary

$$u_3 = \theta = \arctan\left(\frac{x_2}{x_1}\right)$$

Discontinuous Displacement (even apart from origin)

$$\varepsilon_{13} = -\frac{b}{4\pi}\frac{\sin\theta}{r}$$

$$\varepsilon_{23} = \frac{b}{4\pi}\frac{\cos\theta}{r}$$

Except origin, smooth strain field !!!!

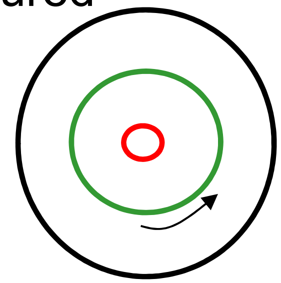
Moral → So, dislocation strain fields are not really the ones from taking a deriv. of the displacement field

For simplicity, consider small defmns.

- **In A and B, uniform strain fields of rank-one connected displ. gradient fields**
- **In C connect A to B smoothly satisfying strain compatibility; can be done (except origin)**
- **Consider smooth strain gradient field except at origin, forgetting disc. on phase boundary**

Mathematical Modeling - Kinematics

- Dump primary *elastic* displacement/distortion fields and work with their incompatible gradients
- Consider irrotational (curl-free) 1,2 distortion fields, say A, in punctured domains



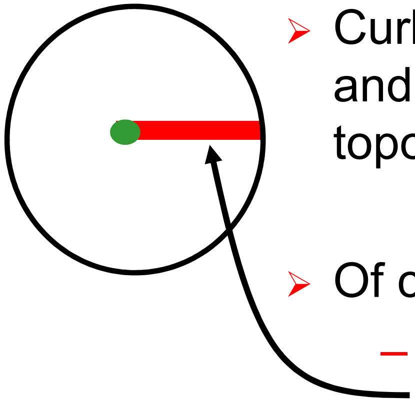
- What is line integral of field along circuits enclosing hole?
  - If l. integral around hole does not vanish, we have field with topological content
- What sort of potential φ (displacement/1-distortion) corresponds to A?
  - i.e. grad φ = A?
- Potential necessarily has to be discontinuous on surfaces
  - Dislocations and g. Disclinations are terminating discontinuities

Kinematics

- Up until here, simpler version of ***Weingarten/Volterra***
  - ***Since do not need to work on symmetric tensors***
  - ***generalized to higher order and works as well for finite deformation***
- Take the continuously distributed defects approach (in principle, applicable to modeling single defects)

  - Make domain simple-connected, fill in hole with field which is not curl-free there.

  - So, A is curl-free outside hole and not curl free inside



    - Curl A has interpretation of line-density (carrying tensorial attributes) and integrated over area patches including its support gives the topological strength of the defect.

    - Of course, now generalize to
      - a whole (fattened) surface, instead of a single hole, being non-curl free - Somigliana
      - the whole body being non-curl free (for instance transition of a crystal to a liquid under extreme shock loading)

Want to make a dynamical theory of

such defect curves and (meta) slipped

regions, taking into account forces,

moments and dissipation

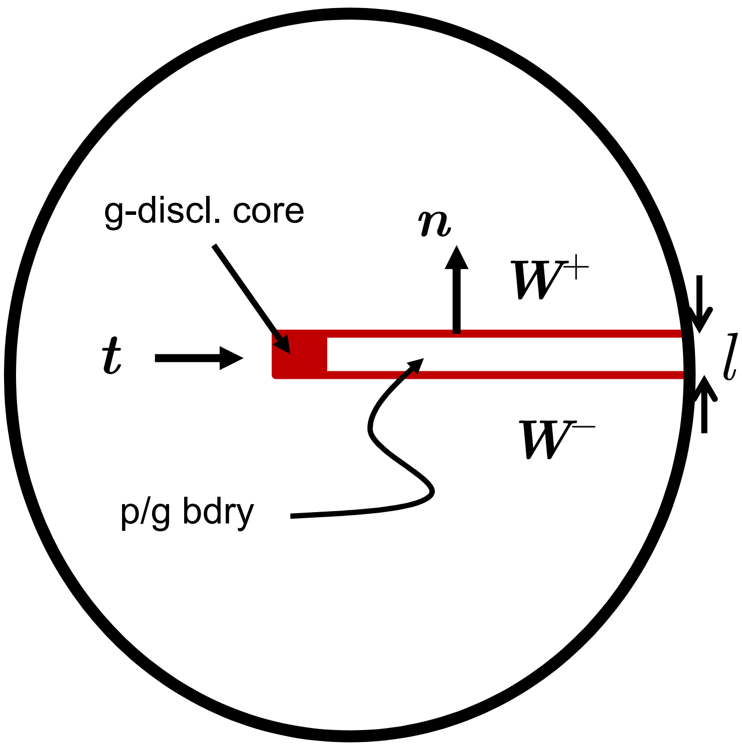
leitmotif – 'when gradients are no longer gradients'

The fundamental kinematical decomposition

All derivatives on current configuration

$\boldsymbol{F} \rightarrow \boldsymbol{F}^e$ = elastic distortion; $\boldsymbol{F}^{e-1} = \boldsymbol{W}$ ielastic 2-distortion $\rightarrow$ 2-tensor

$grad\,\boldsymbol{F}^{e-1} = grad\,\boldsymbol{W} \rightarrow \boldsymbol{Y}$ = ielastic 2-distortion $\rightarrow$ 3-tensor



- Outside layer can make good determination of $\boldsymbol{W}$ and $grad\,\boldsymbol{W}$ from data. Inside layer, cannot tell.
- So, outside layer construct $\boldsymbol{Y} = grad\,\boldsymbol{W}$. Assume field $\boldsymbol{W}$ exists inside layer, but undetermined from coarse measurements.
- **Inside layer**, do obvious interpolation for closest 'gradient'

$$\boldsymbol{Y} = f(t)\left(\boldsymbol{W}^+ - \boldsymbol{W}^- / l\right) \otimes \boldsymbol{n} =: \boldsymbol{S} \quad \text{strip field}$$

$t = \boldsymbol{x} \cdot \boldsymbol{t}$ and f constant in layer outside core and decays to zero inside core

So, $Y_{ij(n)}$ is only non-zero component (any i, j)

$\therefore\; Y_{ij(t)} = 0$ and $Y_{ij(n),t} \neq Y_{ij(t),n}$

- So, in core $curl\,\boldsymbol{Y} \neq \boldsymbol{0}$. Hence, field $\boldsymbol{Y}$ cannot be a gradient.
- **Outside layer**, $\boldsymbol{S} = \boldsymbol{0}$. Hence, $\boldsymbol{Y} = grad\,\boldsymbol{W} + \boldsymbol{S}$ *everywhere.*
- Do Stokes-Helmholtz on $\boldsymbol{S} = \boldsymbol{P} + grad\,\boldsymbol{Z}$.
- Hence, $\boldsymbol{Y} = \boldsymbol{P} + grad(\boldsymbol{W} + \boldsymbol{Z})$.
- Note, $\boldsymbol{P} = -grad\,\boldsymbol{Z}$ outside layer

Kinematical ingredients of model - I

define $curl\, \boldsymbol{Y} = curl\left(\boldsymbol{Y} - grad\, \boldsymbol{W}\right) =: \boldsymbol{\Pi}$ ← ***g. Disclination density***

'Stokes-Helmholtz' of $\boldsymbol{Y} - grad\, \boldsymbol{W} = \boldsymbol{P} + grad\, \boldsymbol{Z}$

Incompatible 2-distortion ($\boldsymbol{P}$)

Compatible 2-distortion ($grad\, \boldsymbol{Z}$)

$$curl\, \boldsymbol{P} = \boldsymbol{\Pi}$$

$$div \boldsymbol{P} = \boldsymbol{0}$$

$$\boldsymbol{P}\boldsymbol{n} = \boldsymbol{0} \text{ on boundary}$$

Kinematical ingredients of model - II

$$\boldsymbol{Y} = \boldsymbol{P} + \underbrace{grad\, \boldsymbol{Z} + grad\, \boldsymbol{W}}$$

Incompatible part of ielastic 2-distortion field - represents Phase/grain boundaries with kinks and corners

Compatible part of ielastic 2-distortion field- represents phase/grain boundaries without kinks and corners

$$grad\, \boldsymbol{A} : \boldsymbol{X} = -curl\, \boldsymbol{A}$$

$$\boldsymbol{P} : \boldsymbol{X} + grad\, \boldsymbol{Z} : \boldsymbol{X} + grad\, \boldsymbol{W} : \boldsymbol{X} = \boldsymbol{Y} : \boldsymbol{X} =: \boldsymbol{\alpha}$$

g. Disclination-induced transformation dislocations

Transformation dislocations

Slip dislocations

Dislocation density

- **It is clear why an infinite g.bdry/incoherent p.bdry can often be represented by slip dislocations**

- **Also clear what of a bdry cannot be so represented**
  - **Symmetric parts; transformation/g. disclination-induced parts**

Topological conservation law for evolution of g.disclination density

$$ {}^{*}\boldsymbol{\Pi} := curl\left(\boldsymbol{W}\left(\boldsymbol{Y} - grad\,\boldsymbol{W}\right)^{2T}\right) \qquad {}^{*}\Pi_{rli} = e_{ijk}\left[W_{lp}\left(Y_{rpk} - W_{rp,k}\right)\right]_{,j} $$

Line density with tensorial attribute

$$ \left(div\boldsymbol{v}\right){}^{*}\boldsymbol{\Pi} + {}^{*}\dot{\boldsymbol{\Pi}} - {}^{*}\boldsymbol{\Pi}\boldsymbol{L}^{T} =: {}^{*}\overset{\circ}{\boldsymbol{\Pi}} = -curl\left({}^{*}\boldsymbol{\Pi}\times\boldsymbol{V}^{\Pi}\right) $$

$$ \Leftrightarrow \overline{\int_{a(t)} {}^{*}\boldsymbol{\Pi}\boldsymbol{n}\,da}^{\bullet} = -\int_{c(t)} {}^{*}\boldsymbol{\Pi}\times\boldsymbol{V}^{\Pi}d\boldsymbol{x} $$

$$ \Rightarrow \boldsymbol{W}\overline{\left(\boldsymbol{Y} - grad\,\boldsymbol{W}\right)^{2T}}^{\bullet} = -\dot{\boldsymbol{W}}\left(\boldsymbol{Y} - grad\,\boldsymbol{W}\right)^{2T} - \boldsymbol{W}\left(\boldsymbol{Y} - grad\,\boldsymbol{W}\right)^{2T}\boldsymbol{L} - \left({}^{*}\boldsymbol{\Pi}\times\boldsymbol{V}^{\Pi}\right) + grad\,\boldsymbol{K} $$

Topological conservation law for evolution of slip dislocation density

$$-curl\,\boldsymbol{W} = grad\,\boldsymbol{W} : \boldsymbol{X} =: \tilde{\boldsymbol{\alpha}} = \boldsymbol{\alpha} - \boldsymbol{P} : \boldsymbol{X} - grad\,\boldsymbol{Z} : \boldsymbol{X}$$

Line density with vectorial attribute

$$\Rightarrow div\,\boldsymbol{\alpha} = div\left(\boldsymbol{P} : \boldsymbol{X} + grad\,\boldsymbol{Z} : \boldsymbol{X}\right)$$

$$\overset{o}{\tilde{\boldsymbol{\alpha}}} = -curl\left(\boldsymbol{\alpha} \times \boldsymbol{V}^{\alpha}\right)$$

$$\Leftrightarrow \dot{\overline{\int_{a(t)} \tilde{\boldsymbol{\alpha}}\,\boldsymbol{n}\,da}} = -\int_{c(t)} \boldsymbol{\alpha} \times \boldsymbol{V}^{\alpha} d\boldsymbol{x}$$

$$\Rightarrow \dot{\boldsymbol{W}} + \boldsymbol{W}\boldsymbol{L} = \boldsymbol{\alpha} \times \boldsymbol{V}^{\alpha}$$

$$W_{ij} = x^{e-1}_{i,j}$$

Only phase transformation with no dislocation plasticity $\boldsymbol{\alpha} \equiv \boldsymbol{0}$

$$Z_{ij} = \zeta_{i,j}$$

Only phase boundaries with no g.disclinations and no dislocations $\boldsymbol{\alpha} \equiv \boldsymbol{0}, \boldsymbol{P} \equiv \boldsymbol{0}$

$$\boldsymbol{P} : \boldsymbol{X} + grad\,\boldsymbol{Z} : \boldsymbol{X} + grad\,\boldsymbol{W} : \boldsymbol{X} = \boldsymbol{\alpha}$$

Thermomechanics

- Two frame-indifferent theories possible
  - ***With*** couple stress $\psi\left(\boldsymbol{W}, \boldsymbol{Y}, {}^{*}\boldsymbol{\Pi}\right)$
  - ***Without*** couple stress $\psi\left(\boldsymbol{W}, \boldsymbol{Y} - grad\,\boldsymbol{W}, {}^{*}\boldsymbol{\Pi}, grad\,\boldsymbol{W} : \boldsymbol{X}\right)$ — $grad\,\boldsymbol{W} : \boldsymbol{X} \leftarrow \tilde{\boldsymbol{\alpha}}$
- Both have objective dissipation → $\left(\quad \right) : \boldsymbol{\Omega} = \boldsymbol{0}$
  - Critical test of kinematic structure of theory
    - In particular, evolution equations
- Theory ***without*** couple stress
  - not clear if regularizes conventional theory in **pure phase-bdry case** (no dislocations/g. disclinations)
  - Definitely works for only dislocation plasticity

Relation with ‘standard’ differential geometric kinematics - I

$$\boldsymbol{W} \text{ invertible };\quad \boldsymbol{d}_\alpha = \boldsymbol{W}\boldsymbol{e}_\alpha$$

$\boldsymbol{e}_\alpha$ is a natural basis for current config.

$$\boldsymbol{d}_{\alpha,\beta} = \bar{\Gamma}^{\mu}_{\alpha\beta}\boldsymbol{d}_\mu$$

$$\Rightarrow \bar{\Gamma}^{\rho}_{\alpha\beta} = \boldsymbol{e}^\rho \cdot \boldsymbol{W}^{-1}\left(\left[\left\{grad\,\boldsymbol{W}\right\}\boldsymbol{e}_\beta\right]\boldsymbol{e}_\alpha + \boldsymbol{W}\boldsymbol{e}_{\alpha,\beta}\right)$$

So, now define as fundamental statement for affine connection:

$$\Gamma^{\rho}_{\alpha\beta} := \bar{\Gamma}^{\rho}_{\alpha\beta} + \underbrace{e^\rho \cdot \boldsymbol{W}^{-1}\left(\left\{\left[\boldsymbol{P} + grad\,\boldsymbol{Z}\right]\boldsymbol{e}_\beta\right\}\boldsymbol{e}_\alpha\right)}_{{}^{*}Q^{\rho}_{\alpha\beta}}$$

Clearly, in this case $\boldsymbol{d}_\alpha$ may not be a basis

Relation with ‘standard’ differential geometric kinematics - II

$$\left(\mathit{\Gamma} = \bar{\mathit{\Gamma}} + {}^{*}Q \right) \qquad R\left(\mathit{\Gamma}\right)^{\alpha}_{\bullet\mu\beta\gamma} := \mathit{\Gamma}^{\alpha}_{\mu\beta,\gamma} - \mathit{\Gamma}^{\alpha}_{\mu\gamma,\beta} + \mathit{\Gamma}^{\alpha}_{\nu\gamma}\mathit{\Gamma}^{\nu}_{\mu\beta} - \mathit{\Gamma}^{\alpha}_{\nu\beta}\mathit{\Gamma}^{\nu}_{\mu\gamma}$$

$$= R\left(\bar{\mathit{\Gamma}}\right)^{\alpha}_{\bullet\mu\beta\gamma} + R\left({}^{*}Q\right)^{\alpha}_{\bullet\mu\beta\gamma} + f\left(\bar{\mathit{\Gamma}}, {}^{*}Q\right)$$

$$\text{invertibility and smoothness of } \boldsymbol{W} \;\Rightarrow\; \boldsymbol{R}\left(\bar{\mathit{\Gamma}}\right) = \boldsymbol{0}$$

$$\therefore\; R\left(\mathit{\Gamma}\right)^{\alpha}_{\bullet\mu\beta\gamma} = R\left({}^{*}Q\right)^{\alpha}_{\bullet\mu\beta\gamma} + \text{huge no. of nonlinear cross-terms}$$

$${}^{*}\boldsymbol{\mathit{\Pi}} \text{ is only a part of } \boldsymbol{R}\left({}^{*}Q\right)$$

$$\rightarrow \left({}^{*}\mathit{\Pi} \cdot X\right)^{\alpha}_{\bullet\mu\beta\gamma} \approx {}^{*}Q^{\alpha}_{\mu\beta,\gamma} - {}^{*}Q^{\alpha}_{\mu\gamma,\beta}$$

Metric affine geometry – Kröner, Lagoudas; Minagawa; Clayton, McDowell, Bammann

$$G_{\gamma\rho}\, {}^{*}Q^{\rho}_{\alpha\beta} \text{ should be skew in } \left(\gamma, \alpha\right)$$

Standard ‘rotational’ disclination density

$$G_{\gamma\rho}\, {}^{*}Q^{\rho}_{\alpha\beta} = \boldsymbol{d}_{\gamma} \cdot \left[\left\{\boldsymbol{P} + grad\, \boldsymbol{Z}\right\}\boldsymbol{e}_{\beta}\right]\boldsymbol{e}_{\alpha} = \boldsymbol{e}_{\gamma} \cdot \left[\boldsymbol{W}^{T}\left\{\boldsymbol{P} + grad\, \boldsymbol{Z}\right\}\boldsymbol{e}_{\beta}\right]\boldsymbol{e}_{\alpha}$$

Our model does not have this symmetry – phase transformations require going beyond Metric Affine Geometry of classical disclinations – but our model is simpler!

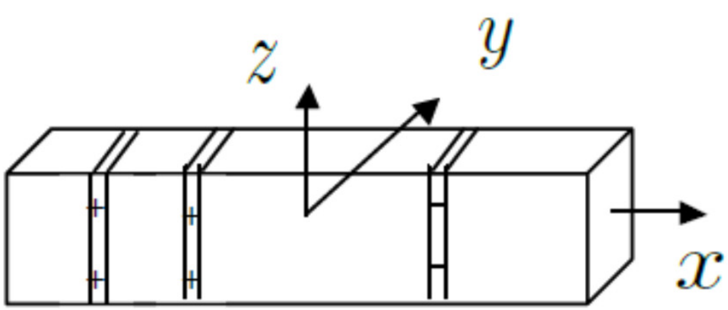
Exact ansatz in FDM

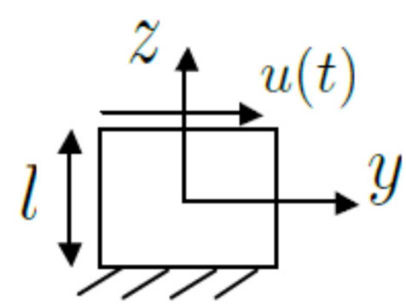
$$\varphi_t^i = \left(\varepsilon \varphi_{xx}^k - \frac{\partial \psi}{\partial \varphi^k}, \varphi_x^k \right) \varphi_x^i \qquad i, k = 1 \text{ to } 4$$

Tartar, AA, 2011
Bull. Italian Math. Union

Scalar equation $\varphi_t = \left(\varphi_x \right)^2 \left(\varepsilon \varphi_{xx} - \frac{\partial \psi}{\partial \varphi} \right)$

AA, JMPS, 2010
Zimmer, Matthies, AA, JMPS, 2010





$$g(t) = \frac{u(t)}{l}$$

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presentations

- ISDMM July 2011
- Plasticity, Jan 2012
- SES, Oct. 2012