

Continuum theory of crystalline defects and mechanical fields

Lecture: Continuum-based theory of dislocations
(Nye, Kröner, Mura, Acharya, ...)

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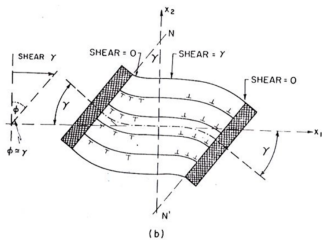
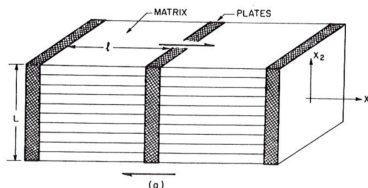
Outline

- 1 Lattice incompatibility and Burgers vector
- 2 Continuum dislocation density tensor (finite strains, small deformation)
- 3 Kröner's stress function "ansatz" for elastic field calculations
- 4 Static FDM method
- 5 Dislocation density transport equation and constitutive equations of evolutive FDM and MFDM
- 6 Examples of case studies in class

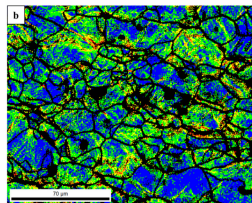
Lattice incompatibility and Burgers vector

Plastic strain gradients and heterogeneities

Geometrically Necessary Dislocations
(GND) (Ashby, 1970)



Measure of GNDs from EBSD
Allain-Bonasso et al. (2012)



GND densities values for 17% tensile deformed sample (a) with 1 value per grain and (b) with details for a smaller part of the map (with 1 value per pixel).

Notations

- In this lecture, we shall use Cartesian (rectangular) coordinates for the presentation of the linear elasticity theory for defects
- A bold symbol denotes a tensor or a vector. Explicit indicial notations using Einstein's summation convention will be used.
- For example: the tensor $\mathbf{A} \cdot \mathbf{B}$, with rectangular Cartesian components $A_{ik}B_{kj}$, results from the dot product of tensors $\mathbf{A}$ and $\mathbf{B}$, and $\mathbf{A} \otimes \mathbf{B}$ is their tensorial product, with components $A_{ij}B_{kl}$. The vector $\mathbf{A} \cdot \mathbf{V}$, with rectangular Cartesian components $A_{ij}V_j$, results from the dot product of tensor $\mathbf{A}$ and vector $\mathbf{V}$. A ":" represents the trace inner product of the two second order tensors $\mathbf{A} : \mathbf{B} = A_{ij}B_{ij}$, in rectangular Cartesian components, or the product of a higher order tensor with a second order tensor, e.g., $\mathbb{A} : \mathbf{B} = A_{ijkl}B_{kl}$.
- The cross product of a second-order tensor $\mathbf{A}$ and a vector $\mathbf{V}$, the **div** and **curl** operations for second-order tensors are defined row by row, in analogy with the vectorial case

Notations

- For any base vector $\mathbf{e}_i$ of the reference frame:

$$(\mathbf{A} \times \mathbf{V})^t \cdot \mathbf{e}_i = (\mathbf{A}^t \cdot \mathbf{e}_i) \times \mathbf{V}$$

$$(\mathbf{div} \mathbf{A})^t \cdot \mathbf{e}_i = \mathbf{div}(\mathbf{A}^t \cdot \mathbf{e}_i)$$

$$(\mathbf{curl} \mathbf{A})^t \cdot \mathbf{e}_i = \mathbf{curl}(\mathbf{A}^t \cdot \mathbf{e}_i).$$

- In rectangular Cartesian components:

$$(\mathbf{A} \times \mathbf{V})_{ij} = e_{jkl} A_{ik} V_l$$

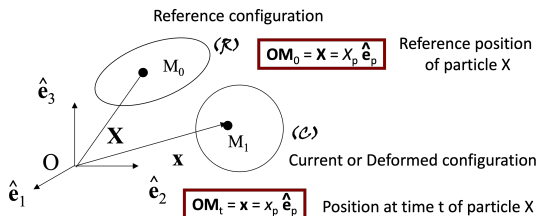
$$(\mathbf{div} \mathbf{A})_i = A_{ij,j}$$

$$(\mathbf{curl} \mathbf{A})_{ij} = (\nabla \times \mathbf{A})_{ij} = e_{jkl} A_{il,k}$$

where e_{jkl} is a component of the third-order alternating Levi-Civita tensor and the spatial derivative with respect to a Cartesian coordinate is indicated by a comma followed by the component index. $\mathbf{I}$ is the second-order unitary tensor with components the Kronecker delta δ_{ij} .

- For any vector or tensor $\mathbf{a}$, $\tilde{\mathbf{a}}(\boldsymbol{\xi})$ denotes the Fourier transform (or FFT) of $\mathbf{a}(\mathbf{x})$, where $\mathbf{x}$ denotes the position vector in real space and $\boldsymbol{\xi}$ denotes the associated Fourier vector.

Large deformation kinematics



- Let (R) be the reference configuration (or initial configuration) of a compact, perfect crystal free of all constraints, and (C) its final (or deformed) configuration, which is compact and continuous.
- The deformed configuration (C) is obtained by applying a continuous, differentiable transformation $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$ with

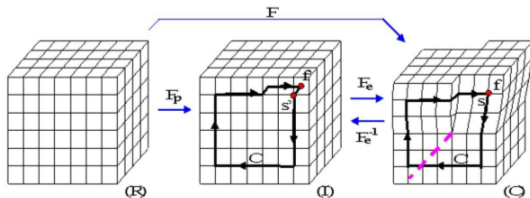
Deformation gradient tensor $\mathbf{F}$ to the reference configuration (R):

$$d\mathbf{x} = \mathbf{F} \cdot d\mathbf{X} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} \cdot \mathbf{X} \quad (1)$$

where the vector $\mathbf{X}$ represents the position in the reference configuration (R) of a point (particle) $\mathbf{x}$ in the final configuration (C).

- The displacement field $\mathbf{u}$ is defined by: $\mathbf{u} = \mathbf{x} - \mathbf{X}$ and $\mathbf{F}$ can write:
 $\mathbf{F} = \mathbf{I} + \mathbf{grad} \mathbf{u} = \mathbf{I} + \mathbf{U}$ ($\mathbf{I}$ is the unit tensor)

Lattice incompatibility



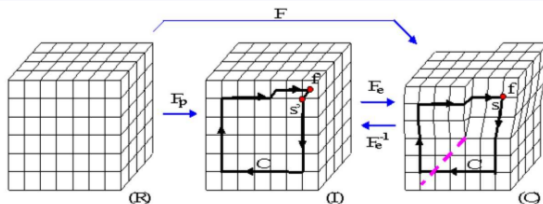
The tensor $\mathbf{F}$ can be decomposed into a plastic component $\mathbf{F}^p$ and an elastic component $\mathbf{F}^e$ (see Kröner (1959); Lee and Liu (1967); Mandel (1972, 1973)):

$$\mathbf{F} = \mathbf{F}^e \cdot \mathbf{F}^p \quad (2)$$

- $\mathbf{F}^p$ represents the plastic component of $\mathbf{F}$. When applied to the reference configuration (R), it leads to a dislocated intermediate configuration (I) in which the Burgers vector $\mathbf{b}$ is introduced as a discontinuity.
- $\mathbf{F}^e$ represents the elastic component of $\mathbf{F}$ that acts on the intermediate configuration (I) to produce the deformed configuration (C). When applied to configuration (I), $\mathbf{F}^e$ restores displacement continuity in configuration (C).
- Conversely, the inverse elastic transformation $\mathbf{F}^{e-1}$ applied to configuration (C) leads to configuration (I), where displacement is discontinuous. $\mathbf{F}^e$ therefore represents an elastic incompatibility that compensates for $\mathbf{F}^p \Rightarrow \mathbf{F}^p, \mathbf{F}^e$ are generally not gradient tensors, unlike $\mathbf{F}$.

Dislocation density tensor

Continuous dislocation density tensor



- Consider the example of a crystal containing a screw dislocation. The closed curve C surrounding the dislocation (represented by the dotted dislocation line) in the deformed configuration (C) represents the Burgers circuit (see Frank (1950) 's definition of Burgers circuit).
- Curve C is conventionally oriented in the direction given by Maxwell's right-hand rule (RH). In the deformed configuration (C), S and F coincide. By applying the inverse elastic distortion $\mathbf{F}^{e-1}$ to (C), the points F and S become the distinct points F' and S' in the intermediate dislocated configuration (I).
- The gap in the closed circuit C , denoted $\mathbf{b}$ and defined according to the "Finish-Start" (FS) convention, is called the true Burgers vector.

Integrating $\mathbf{F}^{e-1}$ along the curve C , from S' to F' , $\mathbf{b}$ is defined as:

$$\mathbf{F}'S' = \mathbf{b} = - \oint_C \mathbf{F}^{e-1} \cdot d\mathbf{x}. \quad (3)$$

Compatibility vs. Lattice Incompatibility

- If $\mathbf{b}$ is zero, $\mathbf{F}^{e-1}$ is the gradient of a vector field, which defines a compatible field:

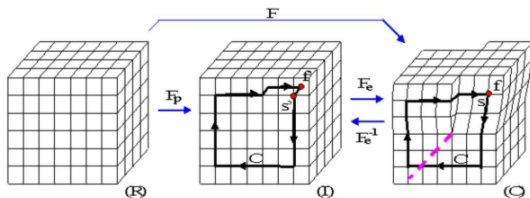
$$\oint \mathbf{F}^{e-1} \cdot d\mathbf{x} = 0 \quad (4)$$

- According to this last equation, the necessary and sufficient condition for $\mathbf{F}^{e-1}$ to be compatible is written in the following form:

$$\mathbf{curl}(\mathbf{F}^{e-1}) = 0 \quad (5)$$

- On the other hand, when $\mathbf{curl}(\mathbf{F}^{e-1}) \neq 0$, $\mathbf{F}_e^{-1}$ is incompatible, and Eq. (6) is the integral incompatibility equation.
- The continuous dislocation density associated with the elastic transformation $\mathbf{F}^{e-1}$ is the Nye dislocation density tensor Nye (1953) α , also known as the excess or polarized dislocation density, or geometrically necessary dislocation density (GNDs), see also Kröner (1958, 1981), Bilby et al. (1955), Ashby (1970).

Continuous dislocation density tensor



- When $\mathbf{b}$ is nonzero, $\mathbf{F}^{e-1}$ is not the gradient of a vector field, which implies lattice incompatibility in the sense that, at a point on the curve C , the lattice displacement takes on distinct values (multi-valued problem)
- If S is a smooth surface, with $\mathbf{n}$ its unit normal, in the current configuration (C) and bounded by the closed line C , the true Burgers vector $\mathbf{b}$ is defined as:

$$\mathbf{b} = - \oint_C \mathbf{F}^{e-1} \cdot d\mathbf{x} = - \int_S \mathbf{curl}(\mathbf{F}^{e-1}) \cdot \mathbf{n} dS = \int_S \boldsymbol{\alpha} \cdot \mathbf{n} dS \quad (6)$$

according to Stokes' theorem, which defines:

The true dislocation density tensor (or Nye tensor) $\boldsymbol{\alpha}$:

$$\boldsymbol{\alpha} = -\mathbf{curl}(\mathbf{F}^{e-1}) = -e_{jkl} F_{il,k}^e \mathbf{e}_i \otimes \mathbf{e}_j \quad (7)$$

Conservation law for the Nye tensor

- From Eq. (7), we have the following mathematical property (from the **div** of the **curl**):

$$\mathbf{div}(\mathbf{curl}(\mathbf{F}^{e-1})) = 0 \quad (8)$$

Therefore, a conservation law follows for α :

$$\mathbf{div} \alpha = 0 \Leftrightarrow \alpha_{ij,j} = 0 \quad (9)$$

- This equation reflects the condition for the closure of a dislocation line in the region occupied by a crystal. In other words, it means that dislocations cannot end inside the medium.

Physical meaning of the dislocation density tensor: screw/edge dislocations

Following Eq. (6), the Burgers vector is given by:

$$\mathbf{b} = \int_S \boldsymbol{\alpha} \cdot \mathbf{n} dS \quad (10)$$

- Then, $\boldsymbol{\alpha}$ can also be written in the following form for a set of dislocations crossing a surface denoted by ΔS (which is not necessarily unit one):

$$\boldsymbol{\alpha} = \mathbf{B} \otimes \boldsymbol{\nu}, \text{ or, in index notation: } \alpha_{ij} = B_i \nu_j, \text{ where } B_i = B \mathbf{e}_i \text{ and } B = \frac{nb}{\Delta S},$$

with n being the number of dislocations of norm b and Burgers vector $\mathbf{b}$ along the direction $\mathbf{e}_i$, crossing the unit normal surface to $\boldsymbol{\nu}$ in the direction $\mathbf{e}_j$:

$$\boldsymbol{\alpha} = \frac{nb}{\Delta S} \mathbf{e}_i \otimes \mathbf{e}_j.$$

- By definition, α_{ij} is a non-symmetric tensor with 9 independent components.
- The diagonal terms represent screw dislocations, since the line vector and the Burgers vector are parallel. The off-diagonal terms represent edge dislocations: the two vectors are orthogonal. There are therefore six types of edge dislocations and three types of screw dislocations.
- In terms of units, the components of α_{ij} are expressed in m of Burgers vectors per m^2 of surface area, i.e. in m^{-1} .

Small deformation assumption

- In a small deformation setting:

$$\mathbf{F} = \mathbf{F}^e \cdot \mathbf{F}^p = \mathbf{I} + \mathbf{U} \simeq \mathbf{I} + \mathbf{U}^e + \mathbf{U}^p \quad (11)$$

where $\mathbf{F}^e \simeq \mathbf{I} + \mathbf{U}^e$, $\mathbf{F}^p \simeq \mathbf{I} + \mathbf{U}^p$ and $\mathbf{F}^{e-1} \simeq \mathbf{I} - \mathbf{U}^e$.

- Small deformation partition of total distortion into elastic distortion $\mathbf{U}^e$ and plastic distortion $\mathbf{U}^p$):

$$\mathbf{U} = \text{grad } \mathbf{u} = \mathbf{U}^e + \mathbf{U}^p \quad (12)$$

The dislocation density tensor α reads:

$$\alpha = \text{curl}(\mathbf{U}^e) = e_{jkl} U_{il,k}^e \mathbf{e}_i \otimes \mathbf{e}_j \text{ or } \alpha = -\text{curl}(\mathbf{U}^p) = -e_{jkl} U_{il,k}^p \mathbf{e}_i \otimes \mathbf{e}_j \quad (13)$$

Small strains and rotations

- In small deformation, the total distortion tensor decomposes into small strain tensor ε and small rotation tensor ω :

$$\begin{aligned}\mathbf{U} &= \mathbf{grad} \mathbf{u} = \varepsilon + \omega \\ \varepsilon &= \frac{1}{2} (\mathbf{grad} \mathbf{u} + (\mathbf{grad} \mathbf{u})^T) \Leftrightarrow \varepsilon = \text{def}(\mathbf{u}) \\ \omega &= \frac{1}{2} (\mathbf{grad} \mathbf{u} - (\mathbf{grad} \mathbf{u})^T)\end{aligned}\quad (14)$$

- Total strain/ rotation partitions into elastic strain (ε^e)/ elastic rotation ((ω^e)) and plastic strain (ε^p)/ plastic rotation ((ω^p)):

$$\begin{aligned}\varepsilon &= \varepsilon^e + \varepsilon^p \\ \omega &= \omega^e + \omega^p\end{aligned}\quad (15)$$

- Thus, the dislocation density tensor α can be decomposed as:

$$\alpha = \mathbf{curl}(\varepsilon^e) + \mathbf{curl}(\omega^e) = (e_{jkl}\varepsilon_{il,k}^e + e_{jkl}\omega_{il,k}^e)\mathbf{e}_i \otimes \mathbf{e}_j \quad (16)$$

Kröner and Nye equations for lattice curvatures

Introducing the axial lattice rotation vector (see Kröner, 1981):

$\Omega^e = \frac{1}{2} e_{mil} \omega_{il}^e \mathbf{e}_m$, with $\omega_{il}^e = e_{ilm} \Omega_m^e$, in Eq. (16) yields (in component form):

$$\begin{aligned}\alpha_{ij} &= e_{mil} e_{jkl} \Omega_{m,k}^e + e_{jkl} \varepsilon_{il,k}^e \\ \alpha_{ij} &= (\delta_{mj} \delta_{ik} - \delta_{mk} \delta_{ij}) \Omega_{m,k}^e + e_{jkl} \varepsilon_{il,k}^e \\ \alpha_{ij} &= \Omega_{j,i}^e - \delta_{ij} \Omega_{k,k}^e + e_{jkl} \varepsilon_{il,k}^e\end{aligned}\quad (17)$$

- Setting $\varepsilon^e = 0$ (no elastic strain) and introducing the Nye's lattice curvature tensor κ , such that $\kappa_{ji} = \Omega_{j,i}^e$:

Nye (1953)'s equations relating curvature and dislocation density are obtained:

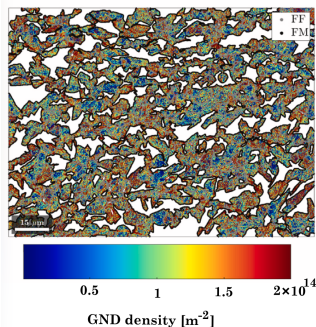
$$\alpha_{ij} = \kappa_{ji} - \delta_{ij} \kappa_{kk} \text{ and } \kappa_{ij} = \alpha_{ji} - \frac{1}{2} \delta_{ij} \alpha_{kk} \quad (18)$$

where the Nye's lattice curvature tensor κ (Nye, 1953) is also known as the contortion tensor (see Kröner, 1981). The first of the last equations is today commonly used in EBSD to experimentally determine the components of α_{ij} (see e.g. Pantleon, 2008).

Measure of Nye tensor from EBSD experimental method and GND densities

$$\alpha = \begin{pmatrix} \text{EBSD image} & \text{EBSD image} & \text{EBSD image} \\ \text{EBSD image} & \text{EBSD image} & \text{EBSD image} \\ \text{EBSD image} & \text{EBSD image} & \text{EBSD image} \end{pmatrix}$$

$$\alpha_{11} - \alpha_{22} = \text{EBSD image}$$



- Nye's (1953) equation used for 2D EBSD:

$$\alpha_{ij} = \kappa_{ji} - \delta_{ij} \kappa_{kk}$$

Pantleon (2008)

$$\kappa_{kl} = \frac{\partial \theta_k}{\partial x_l} \approx \frac{\Delta \theta_k}{\Delta x_l}$$

$$\alpha_{12} = \kappa_{21}$$

$$\alpha_{13} = \kappa_{31}$$

$$\alpha_{21} = \kappa_{12}$$

$$\alpha_{23} = \kappa_{32}$$

$$\alpha_{33} = -\kappa_{11} - \kappa_{22}$$

- Geometrically Necessary Dislocation density $\rho_{GND}^{Nye, 2D}$ (metallurgist view, in m^{-2}) Habibaali et al. (2026) with

$$\rho_{GND}^{Nye, 2D} = \frac{1}{b} \sqrt{\alpha_{12}^2 + \alpha_{13}^2 + \alpha_{21}^2 + \alpha_{23}^2 + \alpha_{33}^2}$$

Kröner's incompatibility tensor (inspired by analogy with magnetostatics)

Total strain compatibility:

$$\begin{aligned} \mathbf{Inc}(\boldsymbol{\varepsilon}) = 0 &\Leftrightarrow -e_{ikm}e_{jln}\varepsilon_{mn,kl} = 0 \\ \text{with } \mathbf{Inc}(\boldsymbol{\varepsilon}) &:= -\mathbf{curl}(\mathbf{curl}\boldsymbol{\varepsilon})^T \end{aligned} \quad (19)$$

- But elastic/plastic strain incompatibility: $\mathbf{Inc}(\boldsymbol{\varepsilon}^e) = -\mathbf{Inc}(\boldsymbol{\varepsilon}^p) \neq 0$

Kröner's incompatibility tensor $\boldsymbol{\eta}$:

$$\mathbf{Inc}(\boldsymbol{\varepsilon}^e) = \boldsymbol{\eta} \Leftrightarrow -e_{ikm}e_{jln}\varepsilon_{mn,kl} = \eta_{ij} \quad (20)$$

Using Eq. (13), the following relationship between $\boldsymbol{\eta}$ and $\boldsymbol{\alpha}$ holds:

$$\boldsymbol{\eta} = -(\mathbf{curl}\boldsymbol{\alpha})^{sym} \Leftrightarrow \eta_{ij} = -\frac{1}{2}(e_{ikl}\alpha_{lj,k} + e_{jkl}\alpha_{li,k}) \quad (21)$$

with divergence free property for $\boldsymbol{\eta}$:

Kröner's incompatibility tensor $\boldsymbol{\eta}$:

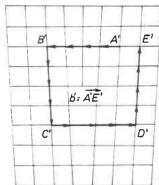
$$\mathbf{div}(\boldsymbol{\eta}) = 0 \Leftrightarrow \eta_{ij,j} = 0 \quad (22)$$

Differential geometric point of view (from Kröner, 1981)

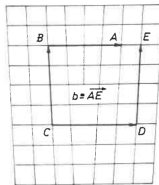
- Frank (1951) defined the dislocation Burgers vector through the Burgers circuit $A'B'C'D'E'$ (see previous definition): the Burgers vector is defined as the closure defect: $\mathbf{b} = \mathbf{A'E'}$ (see figure (a) below with FS/RH rule).
- Let us now express the closure defect $\mathbf{AE}$ (see figure (b) below) with the help of the affine connection Γ_{ml}^h used in differential geometry (assuming Bravais crystal), which describes the change of a vector v^h under parallel displacement.
- Using figure (b), Cartan (1922) transports a vector $\mathbf{CD}$ along the path $\mathbf{CB}$ (from C to B), and then a vector $\mathbf{CB}$ along the path $\mathbf{CD}$ (from C to D).
- Considering the infinitesimal length vectors $\mathbf{CD} = \mathbf{d_1x}(C)$, $\mathbf{BA} = \mathbf{d_1x}(B)$, $\mathbf{CB} = \mathbf{d_2x}(C)$ and $\mathbf{DE} = \mathbf{d_2x}(D)$,
- Law of parallel displacement (transport) of $\mathbf{d_1x}(C)$ along $\mathbf{d_2x}(C)$:

$$d_1x^h(B) = d_1x^h(C) - \Gamma_{ml}^h d_1x^l(C) d_2x^m(C)$$
- Law of parallel displacement (transport) of $\mathbf{d_2x}(C)$ along $\mathbf{d_1x}(C)$:

$$d_2x^h(D) = d_2x^h(C) - \Gamma_{ml}^h d_2x^l(C) d_1x^m(C)$$



(a)



(b)

Identification of dislocation density with Cartan torsion

- Then the closure defect $\mathbf{AE}$ is given by:

$$AE^h = d_1 x^h(C) + d_2 x^h(D) - d_2 x^h(C) - d_1 x^h(B) = -\Gamma_{ml}^h dS^{ml} \quad (23)$$

where $dS^{ml} = e^{mln} dS_n$ is an anti-symmetric surface tensor, which describes the area element enclosed by the four vectors (with e^{mln} the contravariant Levi-Civita tensor and dS_n the classic axial surface vector such that

$$dS_n = \frac{1}{2} e_{nml} dS^{ml})$$

- Taking the anti-symmetric part of Γ_{ml}^h is sufficient since dS^{ml} is anti-symmetric.

the The Cartan's third order torsion tensor denoted $\mathbf{T}$ is defined as:

$$T_{ml}^h = \Gamma_{[ml]}^h = \frac{1}{2} (\Gamma_{ml}^h - \Gamma_{lm}^h) \quad (24)$$

- By expressing an infinitesimal Burgers vector db^k (infinitesimal closure defect) with previously introduced 2nd order dislocation density tensor α (Kröner's definition convention) as: $AE^k = db^k = \alpha^{nk} dS_n = \alpha_{ml}^k dS^{ml}$ with

$$\alpha_{ml}^k = \frac{1}{2} e_{nml} \alpha^{nk} \text{ (or } \alpha^{nk} = e^{nml} \alpha_{ml}^k \text{)}.$$

⇒ The identity between third order dislocation density tensor α_{ml}^k and Cartan's torsion tensor T_{ml}^k is then given by:

$$T_{ml}^k = -\alpha_{ml}^k \quad (25)$$

Kröner's stress function method

Kröner's stress function Ansatz

Kröner's incompatibility tensor η :

$$\text{Inc}(\varepsilon^e) = \eta \quad (26)$$

Second order stress function tensor χ :

$$\sigma = \text{Inc}(\chi) \quad (27)$$

Using generalized Hooke's law $\varepsilon^e = s : \sigma$ with elastic compliance tensor s and Eq. (20) yields:

$$\text{Inc} [s : \text{Inc}(\chi)] = \eta \quad (28)$$

- Since $\text{div curl} = 0$, the balance of linear momentum is automatically satisfied: $\text{div } \sigma = 0$.

Application to isotropic elasticity

- For isotropic elasticity, Kröner (1958) introduced an auxiliary stress potential tensor χ' such that:

$$\begin{aligned}\chi'_{ij} &= \frac{1}{2\mu} \left(\chi_{ij} - \frac{\nu}{1+2\nu} \chi_{kk} \delta_{ij} \right) \\ \chi_{ij} &= 2\mu \left(\chi'_{ij} + \frac{\nu}{1-\nu} \chi'_{kk} \delta_{ij} \right)\end{aligned}\tag{29}$$

In this specific case, the stress potential χ' satisfies:

$$\nabla^4 \chi' = \eta \text{ with } \text{div } \chi' = 0\tag{30}$$

The general solution of Eq. (35) for χ' yields:

$$\chi'_{ij}(\mathbf{x}) = -\frac{1}{8\pi} \int_{\mathbf{V}} |\mathbf{x} - \mathbf{x}'| \eta_{ij}(\mathbf{x}') \, d\mathbf{V}'\tag{31}$$

where $-\frac{1}{8\pi} |\mathbf{x} - \mathbf{x}'|$ is the Green's function (infinite medium) for inhomogeneous bipotential equation $\nabla^4 \chi' = \eta$. Note: $\nabla^4 |\mathbf{x} - \mathbf{x}'| = -8\pi \delta(\mathbf{x} - \mathbf{x}')$.

Application to plane problems - Edge / screw dislocations

- Let us consider a plane problem with straight edge and screw dislocations extended along the x_3 -direction ($\boldsymbol{\nu} = \mathbf{e}_3$ with non zero dislocation densities: $\alpha_{13}(x_1, x_2)$ (edge dislocation) with $\mathbf{b} = b\mathbf{e}_1$), and $\alpha_{33}(x_1, x_2)$ (screw type with $\mathbf{b} = b\mathbf{e}_3$), respectively. Then, Eq. (21) yields the non-zero components of $\boldsymbol{\eta}$: $\eta_{33} = \alpha_{13,2}$ for edge dislocation, $\eta_{13} = \eta_{31} = -\alpha_{33,2}/2$ and $\eta_{23} = \eta_{32} = \alpha_{33,1}/2$.
- Solutions for edge-type dislocation are obtained from:

$$\chi'_{33}(\mathbf{x}) = -\frac{1}{8\pi} \int_V |\mathbf{x} - \mathbf{x}'| \alpha_{13,2'}(\mathbf{x}') dV' \quad (32)$$

- Solutions for screw-type dislocation are obtained from:

$$\begin{aligned} \chi'_{13}(\mathbf{x}) &= \frac{1}{16\pi} \int_V |\mathbf{x} - \mathbf{x}'| \alpha_{33,2'}(\mathbf{x}') dV' \\ \chi'_{23}(\mathbf{x}) &= -\frac{1}{16\pi} \int_V |\mathbf{x} - \mathbf{x}'| \alpha_{33,1'}(\mathbf{x}') dV' \end{aligned} \quad (33)$$

Solutions for single Volterra edge/ screw dislocations

- For single straight Volterra edge and screw dislocations extended along the x_3 -direction $\alpha_{13} = b\delta(x_1)\delta(x_2)$ (edge dislocation) and $\alpha_{33} = b\delta(x_1)\delta(x_2)$ (screw dislocation)
- Solutions for edge dislocation given by Kröner (1958) (after analytical integrations):

$$\chi'_{33} = \frac{b}{8\pi}(\rho^2 \ln \rho)_{,2} \Rightarrow \chi = \chi_{33} = \frac{\mu b}{4\pi(1-\nu)}(\rho^2 \ln \rho)_{,2} \quad (34)$$

$$\sigma_{11} = -\chi_{,22} ; \sigma_{22} = -\chi_{,11} ; \sigma_{12} = \chi_{,12}$$

- Solutions for screw dislocation given by Kröner (1958) (after analytical integrations):

$$\chi'_{13}(x_1, x_2) = -\frac{b}{16\pi}(\rho^2 \ln \rho)_{,2} ; \chi'_{23}(x_1, x_2) = \frac{b}{16\pi}(\rho^2 \ln \rho)_{,1}$$

$$\phi = \chi_{13,2} - \chi_{23,1} = -\frac{\mu b}{8\pi} [(\rho^2 \ln \rho)_{,11} + (\rho^2 \ln \rho)_{,22}] \quad (35)$$

$$\sigma_{23} = -\phi_{,1} ; \sigma_{13} = -\phi_{,2}$$

where $\rho^2 = x_1^2 + x_2^2$.

Static Field Dislocation Mechanics method (Acharya et al.)

Elasto-static field equations

- Consider a continuous crystal of volume V and boundary S containing an excess dislocation distribution represented by the dislocation density tensor α . The goal of this elastostatic problem is to determine the internal stresses caused by the incompatibility of the lattice associated with the presence of α .
- A known stress vector field $\mathbf{t}^d$ is applied at every point on a portion S_t of the boundary S of the volume V . The remaining portion S_u of this surface is subjected at every point to an imposed displacement $\mathbf{u}^d$, then:

$$\begin{aligned}\mathbf{u} &= \mathbf{u}^d \\ \mathbf{t} &= \boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{t}^d.\end{aligned}\tag{36}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor.

- The total distortion of the crystal lattice $\mathbf{U} = \mathbf{grad} \mathbf{u}$ ($\mathbf{u}$ being the displacement vector) is assumed to be integrable (compatible). In small deformation:

$$\mathbf{U} = \mathbf{U}^e + \mathbf{U}^p.\tag{37}$$

Elasto-static field equations

- The only prescribed data in the problem is the tensor α , which is related to the elastic distortion of the lattice $\mathbf{U}^e$ (see previous Equation (13)).
- Assuming generalized Hooke's linear elastic constitutive law for the stress field, we obtain:

$$\boldsymbol{\sigma} = \mathbf{C} : \mathbf{U}^{e, sym} = \mathbf{C} : \boldsymbol{\varepsilon}^e, \quad (38)$$

where $\mathbf{C}$ is the elastic stiffness tensor, with:

$C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij}$. $\boldsymbol{\varepsilon}^e$ represents the elastic strain tensor or the symmetric part of the elastic distortion tensor, and $\boldsymbol{\sigma}$ denotes the Cauchy stress tensor.

- Stress equilibrium equation (without volume and inertia forces) reads:

$$\text{div } \boldsymbol{\sigma} = 0 \quad \text{in } V. \quad (39)$$

Kinematics of static Field Dislocations Mechanics

- Burgers vector $\mathbf{b} = [\mathbf{u}] = \oint_L \mathbf{U}^e \cdot d\mathbf{x}$ (displacement discontinuity) from Volterra (1907) and $\mathbf{U}^e$ is the elastic (lattice) distortion.

Continuum-based dislocation mechanics (Kröner, 1958, 1981):

$$\mathbf{b} = \oint_L \mathbf{U}_e \cdot d\mathbf{x} = \int_S \mathbf{curl} \mathbf{U}^e \cdot \mathbf{n} dS = \int_S \boldsymbol{\alpha} \cdot \mathbf{n} dS. \quad (40)$$

Hence: $\boldsymbol{\alpha} = \mathbf{curl} \mathbf{U}^e$ with $\mathbf{div} \boldsymbol{\alpha} = \mathbf{0}$

- Field Dislocation Mechanics (FDM) theory, see: Acharya (2001); Roy and Acharya (2005); Acharya et al. (2019); Fressengeas (2017)

Stokes-Helmholtz decomposition:

$$\mathbf{U}^e = \mathbf{U}^{e,\perp} + \mathbf{U}^{e,\parallel} = \mathbf{curl} \boldsymbol{\psi} + \nabla \mathbf{w}, \quad (41)$$

- $\mathbf{U}^{e,\parallel}$ belongs to the null-space of the curl operator since $\mathbf{curl} \nabla \mathbf{w} = \mathbf{0}$, while $\mathbf{U}^{e,\perp} = \mathbf{curl} \boldsymbol{\psi}$ satisfies $\mathbf{div} \mathbf{U}^{e,\perp} = \mathbf{0}$ and $\mathbf{U}^{e,\perp} \cdot \mathbf{n} = \mathbf{0}$ on S .

Plastic distortion field

- According to Equation (37), the total strain of the crystal lattice is defined as the sum of the elastic strain $\mathbf{U}^e$ and the plastic strain $\mathbf{U}^p$. The Stokes-Helmholtz decomposition applied to the tensor $\mathbf{U}^p$ is:

$$\mathbf{U}^p = \mathbf{U}^{p,\perp} + \mathbf{U}^{p,\parallel}. \quad (42)$$

- Based on Equations (41) and (42), the gradient vector of the displacement becomes:

$$\mathbf{U} = \nabla \mathbf{u} = \mathbf{U}^{e,\perp} + \mathbf{U}^{p,\perp} + \mathbf{U}^{e,\parallel} + \mathbf{U}^{p,\parallel} \quad (43)$$

- The incompatible parts $\mathbf{U}^{e,\perp}$ and $\mathbf{U}^{p,\perp}$ must cancel out for $\mathbf{U}$ to be a gradient tensor:

$$\mathbf{U}^{e,\perp} + \mathbf{U}^{p,\perp} = 0 \implies \mathbf{U}^{p,\perp} = -\mathbf{U}^{e,\perp} \quad (44)$$

$\Rightarrow$ This relation proves the statement that the incompatibility generated by the plastic transformation is compensated by an elastic incompatibility:

$$\mathbf{U} = \mathbf{U}^{e,\parallel} + \mathbf{U}^{p,\parallel} \implies \mathbf{U}^{p,\parallel} = \nabla \mathbf{z} = \nabla \mathbf{u} - \nabla \mathbf{w} \quad (45)$$

$\Rightarrow$ As shown later (evolutive FDM), compatible plastic strain arises from the compatible slip of dislocations. At the initial state, since we do not know the origin of the dislocation density, we generally set $\mathbf{U}^{p,\parallel} = 0$.

Poisson-type equation for $\mathbf{U}_e^\perp$

Using the Stokes-Helmholtz unique decomposition:

$$\boldsymbol{\alpha} = \mathbf{curl} \mathbf{U}^{e,\perp} \quad (46)$$

- In component form, Equation (46) reads: $\alpha_{ij} = e_{jkl} U_{il,k}^{e,\perp}$
- From $\mathbf{curl} \mathbf{curl} \mathbf{U}^{e,\perp} = \mathbf{grad} \mathbf{div} \mathbf{U}^{e,\perp} - \mathbf{div} \mathbf{grad} \mathbf{U}^{e,\perp}$, taking the curl of Equation (46) and using Equation (41) leads to:

Poisson equation:

$$\Delta \mathbf{U}^{e,\perp} = -\mathbf{curl} \boldsymbol{\alpha} \quad (47)$$

where $\Delta = \nabla \cdot \nabla = \nabla^2$ is the Laplace operator.

- In component form, Eq.(47) reads: $U_{ij,pp}^{e,\perp} = -e_{jkl} \alpha_{il,k}$
- FFT method: $\mathbf{U}^{e,\perp}$ and $\mathbf{w}$ are assumed to be periodic fields (Berbenni et al., 2014; Bertin et al., 2015; Djaka et al., 2017; Berbenni et al., 2020)

Equilibrium equations

The elastostatic field equations (38), (39) and (41) can be formulated as Navier-type partial differential equations in V :

$$\mathbf{div} (\mathbf{C} : \nabla \mathbf{w}) + \mathbf{f}^\perp = 0 \quad (48)$$

with fictive body force density $\mathbf{f}^\perp = \mathbf{div} \mathbf{C} : \mathbf{U}^{e,\perp}$ reflects the lattice incompatibility arising from the presence of polarized dislocations.

- Boundary conditions on S for the solution of the Navier-type equation are given by:

$$\begin{aligned} \mathbf{u} &= \mathbf{u}^d & \text{on } S_u \\ \mathbf{C} : \nabla \mathbf{w} \cdot \mathbf{n} &= \mathbf{t}^d - \mathbf{C} : \mathbf{U}^{e,\perp} \cdot \mathbf{n} & \text{on } S_t. \end{aligned} \quad (49)$$

- These equations form a static standard elasticity problem for the unknown fields $\mathbf{w}$, $\mathbf{U}^{e,\parallel}$, which can therefore be uniquely determined. $\mathbf{f}^\perp$ is determined from solving the Poisson equation (Eq. (47)), once the dislocation density α has been specified.

Equilibrium equations for isotropic homogeneous elastic media with prescribed dislocation density distribution

- In the special case of homogeneous anisotropic elasticity described by the stiffness tensor C_{ijkl} , Navier reduces to:

$$C_{ijkl}w_{k,lj} + C_{ijkl}U_{kl,j}^{e,\perp} = 0. \quad (50)$$

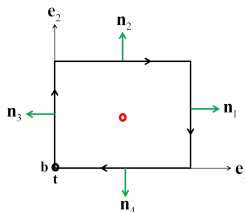
Furthermore, when considering isotropic elasticity, Eq. (50) takes the form:

$$\mu w_{i,kk} + (\lambda + \mu) w_{k,ki} + \lambda U_{kk,i}^{e,\perp} + \mu \left(U_{ik,k}^{e,\perp} + U_{ki,k}^{e,\perp} \right) = 0 \quad (51)$$

where $U_{ij}^{e,\perp}$ is solved from $U_{ij,pp}^{e,\perp} = -e_{jkl}\alpha_{il,k}$.

- These equations will be solved using a fast numerical resolution method by FFT in the case of homogeneous elasticity and heterogeneous heterogeneous elasticity (see Case studies).
- In the following simple examples, we consider the equations for the case of homogeneous isotropic elasticity (Eq. (51)) for straight screw and edge dislocations (to compare with Kröner's method).

Solutions for screw dislocation



- Here, we consider a crystal with a reference frame $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ that is assumed to be infinite in the $\mathbf{e}_3$ direction (see Figure). This crystal contains at its center a screw dislocation with line vector $\nu = \mathbf{e}_3$ and Burgers vector $\mathbf{b} = b\mathbf{e}_3$.
- The only nonzero component of the dislocation density tensor α is $\alpha_{33}(\mathbf{x})$. For this dislocation density, Eq.(47) yields:

$$\begin{aligned} U_{31,11}^{e,\perp} + U_{31,22}^{e,\perp} &= -\alpha_{33,2} \\ U_{32,11}^{e,\perp} + U_{32,22}^{e,\perp} &= \alpha_{33,1} \end{aligned} \quad (52)$$

where $U_{31}^{e,\perp}$ and $U_{32}^{e,\perp}$ are zero at the boundaries with normal vectors $\mathbf{n}_1$ and $\mathbf{n}_3$ for $U_{31}^{e,\perp}$, and $\mathbf{n}_2$ and $\mathbf{n}_4$ for $U_{32}^{e,\perp}$ ($\mathbf{U}^{e,\perp} \cdot \mathbf{n} = 0$ on S).

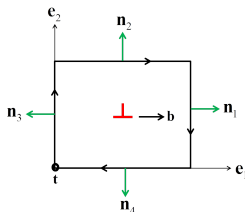
Solutions for screw dislocation

- In the case of a screw dislocation in a homogeneous, linearly elastic, isotropic medium, the only stresses involved are σ_{13} and σ_{23} . Since the vector $\mathbf{w}(w_1, w_2)$, which is the solution to Equation (51), is zero, only the incompatible part of the elastic deformation satisfies the equilibrium equation (51). In this case, the stresses σ_{13} and σ_{23} are given by:

$$\begin{aligned}\sigma_{23} &= \sigma_{32} = \mu U_{32}^{e,\perp} \\ \sigma_{13} &= \sigma_{31} = \mu U_{31}^{e,\perp}\end{aligned}\tag{53}$$

- As an application, we can solve analytically the stresses by the Fourier transform of a single screw dislocation using this method (here as practical exercise on board).

Solutions for edge dislocation



- Here, we consider a crystal with a reference frame $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ that is assumed to be infinite in the $\mathbf{e}_3$ direction (see Figure). This crystal contains at its center an dislocation with line vector $\nu = \mathbf{e}_3$ and Burgers vector $\mathbf{b} = b\mathbf{e}_1$.
- The only nonzero component of the dislocation density tensor α is $\alpha_{13}(\mathbf{x})$. For this dislocation density, Eq.(47) yields:

$$\begin{aligned} U_{11,11}^{e,\perp} + U_{11,22}^{e,\perp} &= -\alpha_{13,2} \\ U_{12,11}^{e,\perp} + U_{12,22}^{e,\perp} &= \alpha_{13,1} \end{aligned} \quad (54)$$

where $U_{11}^{e,\perp}$ and $U_{12}^{e,\perp}$ are zero at the boundaries with normal vectors $\mathbf{n}_1$ and $\mathbf{n}_3$ for $U_{11}^{e,\perp}$, and $\mathbf{n}_2$ and $\mathbf{n}_4$ for $U_{12}^{e,\perp}$ ($\mathbf{U}^{e,\perp} \cdot \mathbf{n} = 0$ on S).

Solutions for edge dislocation

- Assuming that the incompatible parts $U_{11}^{e,\perp}$ and $U_{12}^{e,\perp}$ are known, the compatible parts can now be calculated in the case of homogeneous isotropic behavior using Eq. (51). Thus, we obtain PDE that allow us to calculate the unknown vector $\mathbf{w}(w_1, w_2)$ as in Acharya (2001):

$$\begin{aligned} (\lambda + 2\mu) w_{1,11} + \mu w_{1,22} + (\lambda + \mu) w_{2,12} &= -(\lambda + 2\mu) U_{11,1}^{e,\perp} - \mu U_{12,2}^{e,\perp} \\ \mu w_{2,11} + (\lambda + 2\mu) w_{2,22} + (\lambda + \mu) w_{1,12} &= -\mu U_{12,1}^{e,\perp} - \lambda U_{11,2}^{e,\perp} \end{aligned} \quad (55)$$

- Once w_1 and w_2 are obtained, the four compatible elastic distortions $U_{11}^{e,\parallel}$, $U_{12}^{e,\parallel}$, $U_{21}^{e,\parallel}$, and $U_{22}^{e,\parallel}$ are then derived from $w_{1,1}$, $w_{1,2}$, $w_{2,1}$, and $w_{2,2}$, respectively.
- The (internal) stresses are given by:

$$\begin{aligned} \sigma_{11} &= (\lambda + 2\mu) \left(U_{11}^{e,\parallel} + U_{11}^{e,\perp} \right) + \lambda U_{22}^{e,\parallel} \\ \sigma_{22} &= \lambda \left(U_{11}^{e,\parallel} + U_{11}^{e,\perp} \right) + (\lambda + 2\mu) U_{22}^{e,\parallel} \\ \sigma_{12} &= \mu \left(U_{21}^{e,\parallel} + U_{21}^{e,\parallel} + U_{12}^{e,\perp} \right) \end{aligned} \quad (56)$$

FDM field equations (Acharya et al.)

Burgers vector flux

- We follow Acharya (2001, 2003, 2004, 2011)
- Set of n dislocations with line vector $\boldsymbol{\nu}$ and the same Burgers vector $\mathbf{b}$, such that the dislocation density tensor $\boldsymbol{\alpha} = \mathbf{B} \otimes \boldsymbol{\nu}$ with $B = nb/\Delta S$, the norm of $\mathbf{B}$. These dislocations have an average velocity vector $\mathbf{V}$ (at the adopted resolution scale w.r.t. crystallographic lattice).
- Suppose that these dislocations intersect a closed, oriented curve C , entering it and thus crossing the surface S bounded by C . This creates a Burgers vector flux $\mathbf{f}$ through the differential element $d\mathbf{x}$ tangent to curve C and the rate of Burgers vector through a surface element $d\mathbf{S} = \boldsymbol{\nu} \times d\mathbf{x}$ is: $\mathbf{f} \cdot d\mathbf{x} = \mathbf{B} (\mathbf{V} \cdot d\mathbf{S}) = \mathbf{B} (\mathbf{V} \cdot (\boldsymbol{\nu} \times d\mathbf{x})) = -\mathbf{B} ((\boldsymbol{\nu} \times \mathbf{V}) \cdot d\mathbf{x}) = -(\mathbf{B} \otimes \boldsymbol{\nu}) \times \mathbf{V} \cdot d\mathbf{x}$
- Using a permutation of the mixed product $\mathbf{V} \cdot (\boldsymbol{\nu} \times d\mathbf{x})$ makes it possible to extract $d\mathbf{x}$ and identify the flux tensor $\mathbf{f}$:

$$\mathbf{f} = -(\mathbf{B} \otimes \boldsymbol{\nu}) \times \mathbf{V} = -\boldsymbol{\alpha} \times \mathbf{V} \quad (57)$$

Plastic distortion rate tensor

- Example of application of $\mathbf{f} = -(\mathbf{B} \otimes \boldsymbol{\nu}) \times \mathbf{V}$: Consider a set of edge dislocations with line vector $\boldsymbol{\nu} = \mathbf{e}_1$, Burgers vector $\mathbf{B} = B\mathbf{e}_2$ and velocity vector $\mathbf{V} = V_2\mathbf{e}_2$ in the Cartesian basis $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$, crossing curve C at a point where the tangent vector to C is $\mathbf{e}_3$. Then, it can be checked that $\mathbf{f} \cdot \mathbf{e}_1 = \mathbf{f} \cdot \mathbf{e}_2 = 0$; $\mathbf{f} \cdot \mathbf{e}_3 = -BV_2\mathbf{e}_2$
- Integrated along curve C , the scalar quantity $\mathbf{e}_2 \cdot \mathbf{f} \cdot \mathbf{e}_3 = -\frac{nb}{\Delta S}V_2$ reflects the flux of the Burgers vector across this curve.

The dislocation motion generates the plastic distortion rate tensor:

$$\dot{\mathbf{U}}^p = -\mathbf{f} = \boldsymbol{\alpha} \times \mathbf{V} \quad (58)$$

- This is a tensorial generalization of Orowan's law used in FDM.

Compatible plastic distortion rate tensor

- $\dot{\mathbf{U}}^p$ therefore receives an incompatible contribution from the distribution of excess dislocations $\mathbf{U}^{p,\perp} = -\mathbf{U}^{e,\perp}$ (see Eq. (44)) and a compatible contribution $\dot{\mathbf{U}}^{p,\parallel}$ deriving from dislocation motion (based on the assumption that $\mathbf{U}^p$ receives a compatible contribution from the excess dislocation fluxes Acharya (2001)):

$$\dot{\mathbf{U}}^{p,\parallel} = (\boldsymbol{\alpha} \times \mathbf{V})^{\parallel} \quad (59)$$

- Using the Stokes–Helmholtz decomposition of $\dot{\mathbf{U}}^{p,\parallel}$ is defined as:

$$\dot{\mathbf{U}}^{p,\parallel} = \nabla \dot{\mathbf{z}} \quad (60)$$

Thus, $\dot{\mathbf{U}}^{p,\parallel}$ satisfies the condition:

$$\begin{aligned} \operatorname{div} \dot{\mathbf{U}}^{p,\parallel} &= \operatorname{div} (\boldsymbol{\alpha} \times \mathbf{V}) \\ \dot{\mathbf{U}}^{p,\parallel} \cdot \mathbf{n} &= \operatorname{div} (\boldsymbol{\alpha} \times \mathbf{V}) \cdot \mathbf{n} \text{ on } S \end{aligned} \quad (61)$$

$\Rightarrow$ The compatible plastic strain rate of the dislocations can be determined unambiguously.

Dislocation density transport equation (Burgers vector conservation) - Small strains

- Burgers vector conservation: time derivative of the net Burgers vector in S is equal to the Burgers vector flux through C :

$$\frac{d}{dt} \int_S \boldsymbol{\alpha} \cdot \mathbf{n} dS = \int_C \mathbf{f} \cdot d\mathbf{x}, \quad (62)$$

where $\mathbf{n}$ is the unit normal vector to the surface S .

- According to Stokes' theorem, and considering that the surface S is time-independent:

$$\frac{d}{dt} \int_S \boldsymbol{\alpha} \cdot \mathbf{n} dS = \int_S \frac{d\boldsymbol{\alpha}}{dt} \cdot \mathbf{n} dS = \int_S \mathbf{curl} \mathbf{f} \cdot \mathbf{n} dS \quad (63)$$

Dislocation density transport equation (using Eq. (58):

$$\dot{\boldsymbol{\alpha}} = -\mathbf{curl} \dot{\mathbf{U}}^p = -\mathbf{curl} (\boldsymbol{\alpha} \times \mathbf{V}) \Leftrightarrow \dot{\alpha}_{ij} = -(\alpha_{ij} V_k)_{,k} + (\alpha_{ik} V_j)_{,k} \quad (64)$$

- Boundary conditions should allow for outflow from dislocations. If $\mathbf{n}$ is the outward normal to the boundary S , the dislocation flux is defined by

Dislocation density transport equation (Burgers vector conservation) - Large strains

- Using Nanson's formula (transport of a surface element) in Eq. (63):

$$\mathbf{n}dS = J\mathbf{F}^{-T}\mathbf{N}dS_0 \quad (65)$$

- Velocity gradient tensor:

$$\mathbf{L} = \dot{\mathbf{F}} \cdot \mathbf{F}^{-1} \quad (66)$$

- Continuity equation (conservation of mass):

$$\dot{\rho} + \rho \operatorname{div}(\mathbf{v}) = 0 \quad (67)$$

with $\operatorname{div}(\mathbf{v}) = \operatorname{tr}(\mathbf{L})$

- We can prove the transport equation in finite strain.

Dislocation density transport equation in finite strain:

$$\dot{\boldsymbol{\alpha}} + \operatorname{div}(\mathbf{v})\boldsymbol{\alpha} - \boldsymbol{\alpha} \cdot \mathbf{L}^T = -\operatorname{curl} \dot{\mathbf{U}}^p = -\operatorname{curl}(\boldsymbol{\alpha} \times \mathbf{V}) \quad (68)$$

Dislocation transport: one-dimensional example

- The one-dimensional (1D) version of the transport equation can be derived from Eq. (58) by considering only edge dislocations α_{12} (Djaka et al., 2015). Thus, we have:

$$\dot{\alpha}_{12} = -(\alpha_{12}v_1)_{,1} = -v_0 \frac{\alpha_{12}}{|\alpha_{12}|} (\alpha_{12})_{,1}. \quad (69)$$

- This equation can also be written in the following simplified form:

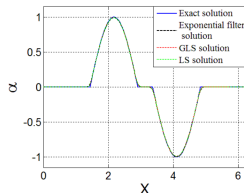
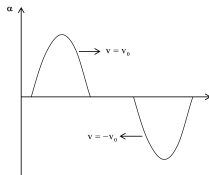
$$\dot{\alpha} = -v_0 \frac{\alpha}{|\alpha|} (\alpha)_{,x} = -v_0 \operatorname{sgn}(\alpha) \alpha_{,x}, \quad (70)$$

with $\alpha_{12} = \alpha$ and the sign function $\operatorname{sgn}(\alpha)$ is defined by:

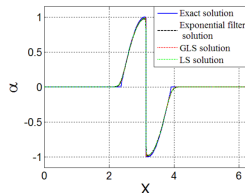
$$\operatorname{sgn}(\alpha) = \begin{cases} 1 & \text{if } \alpha > 0 \\ 0 & \text{if } \alpha = 0 \\ -1 & \text{if } \alpha < 0. \end{cases} \quad (71)$$

- Physical phenomena such as dislocation propagation and annihilation of two dislocations of opposite signs, in particular, two dislocation densities defined opposite signs with a behavior like waves that form a shock.

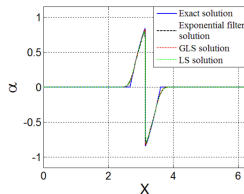
Dislocation transport: one-dimensional example (annihilation)



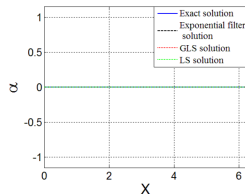
(a)



(b)



(c)



(d)

Thermodynamics: Dissipation

- The plasticity of crystalline materials is an irreversible phenomenon, and dislocations are the physical entities through which this irreversibility manifests
- The constitutive equation for $\mathbf{V}$ is based on the expression of the mechanical dissipation rate D with the requirement to be positive, i.e. $D \geq 0$
- Neglecting inertia effects and body forces, D is considered to be the difference between the power of the applied forces and the derivative of the Helmholtz free deformation energy ψ :

$$D = P_{ext} - \dot{\Phi} = \int_{\partial V} \boldsymbol{\sigma} \cdot \mathbf{n} \cdot \dot{\mathbf{u}} dS - \int_V \dot{\phi} dV \quad (72)$$

where $\mathbf{n}$ is the outward unit normal vector to the boundary surface ∂V .

- In Eq. (72), the time-derivative of the Helmholtz free energy density $\dot{\phi}$ is given by:

$$\dot{\phi} = \frac{\partial \phi}{\partial \boldsymbol{\epsilon}^e} : \dot{\boldsymbol{\epsilon}}^e = \boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}}^e \quad (73)$$

Driving force: FDM-based thermodynamic PK force

- Using the divergence theorem together in Eq. (72) (and the symmetries of elastic stiffness tensor), the dissipation rate D yields:

$$D = \int_V \boldsymbol{\sigma} : \dot{\mathbf{U}}^p dV \geq 0 \quad (74)$$

- Using Eq. (58), the dissipation rate D becomes:

$$D = \int_V \boldsymbol{\sigma} : (\boldsymbol{\alpha} \times \mathbf{V}) dV \geq 0 \quad (75)$$

- The last expression is simplified by rearranging it using Levi-Civita symbol $\mathbf{X}$:

$$D = \int_V \mathbf{X} : (\boldsymbol{\sigma} \cdot \boldsymbol{\alpha}) \cdot \mathbf{V} dV = \int_V \mathbf{F}^\alpha \cdot \mathbf{V} dV \geq 0 \quad (76)$$

$\mathbf{F}^\alpha$ is the Peach-Koehler (PK) thermodynamic driving force for GND motion defined as:

$$\mathbf{F}^\alpha = \mathbf{X} : (\boldsymbol{\sigma} \cdot \boldsymbol{\alpha}) \quad (77)$$

$\Rightarrow \mathbf{F}^\alpha$ is the thermodynamic conjugate of $\mathbf{V}$.

Constitutive equation for thermodynamic PK force

- The definition of the polarized dislocation velocity $\mathbf{V}$ is based on thermodynamic considerations regarding the dissipation rate D , which is positive (Eq. (76)):

$$\mathbf{F}^\alpha \cdot \mathbf{V} \geq 0 \quad (78)$$

- Plastic flow incompressibility due to dislocation glide:

$$\dot{U}_{ii}^p = e_{ikl} \alpha_{ik} V_l = 0 \implies d_l V_l = 0 \text{ where } d_l = e_{mnl} \alpha_{mn} \quad (79)$$

- To satisfy these conditions adequately, the dislocation velocity $\mathbf{V}$ can be defined as follows:

$$\mathbf{V} = \frac{\mathbf{g}}{|\mathbf{g}|} \bar{V} \text{ where } \bar{V} \geq 0, \quad (80)$$

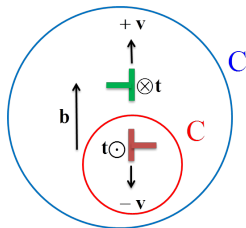
where $\mathbf{g}$ and $\bar{V}$ represent, respectively, the glide force parallel to $\mathbf{V}$ and the average magnitude of the velocity $\mathbf{V}$ of the dislocations.

- The glide force $\mathbf{g}$ is then defined as:

$$\mathbf{g} = \mathbf{F}^\alpha - \left(\mathbf{F}^\alpha \cdot \frac{\mathbf{d}}{|\mathbf{d}|} \right) \frac{\mathbf{d}}{|\mathbf{d}|}, \quad (81)$$

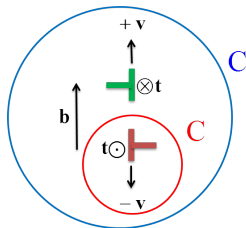
- Finally, $\bar{V}$ is constitutively defined using experimental results.

Phenomenological Mesoscale FDM (PMFDM)



- We follow Acharya and Roy (2006)
- The classification of dislocations into geometrically necessary dislocations (GNDs) (Ashby, 1970) and statistically stored dislocations (SSDs) (zero net Burgers vector) depends heavily on the resolution scale.
- At sufficiently fine resolution scale, all dislocations are GNDs. However, at a sufficiently large (mesoscopic) resolution scale, the presence of SSDs becomes significant. SSDs contribute only to the overall plastic flow and not to long-range internal stresses.
- Figure shows the scale dependence of polarized dislocation densities and the rate of plastic strain.

Coarse graining procedure in PMFDM



- Using an averaging procedure utilized in the study of multiphase flows, Acharya and Roy (2006), they derived the averaged plastic distortion rate at the mesoscale as:

$$\dot{\bar{\mathbf{U}}}^p = \bar{\boldsymbol{\alpha}} \times \bar{\mathbf{V}} + \mathbf{L}^p \quad (82)$$

with plastic distortion rate due to SSDs:

$$\mathbf{L}^p = \overline{(\boldsymbol{\alpha} - \bar{\boldsymbol{\alpha}}) \times \mathbf{V}} = \overline{\boldsymbol{\alpha} \times \mathbf{V}} - \bar{\boldsymbol{\alpha}} \times \bar{\mathbf{V}} \quad (83)$$

and transport equation:

$$\dot{\bar{\boldsymbol{\alpha}}} = -\text{curl} (\bar{\boldsymbol{\alpha}} \times \bar{\mathbf{V}} + \mathbf{L}^p) \quad (84)$$

Field equations of FDM and PMFDM: a summary

- The field equations of FDM (small deformation) are summarized here:

$$\boldsymbol{\alpha} = \text{curl } \mathbf{U}_e^\perp$$

$$\text{div } \mathbf{U}^{e,\perp} = 0$$

$$\text{div } (\nabla \dot{\mathbf{z}}) = \text{div } (\boldsymbol{\alpha} \times \mathbf{V})$$

$$\text{div } [\mathbf{C} : (\nabla(\mathbf{u} - \mathbf{z}) + \mathbf{U}^{e,\perp})] = 0$$

$$\dot{\boldsymbol{\alpha}} = -\text{curl } \dot{\mathbf{U}}^p$$

- Field equations of PMFDM (small deformation) are summarized here:

$$\bar{\boldsymbol{\alpha}} = \text{curl } \bar{\mathbf{U}}_e^\perp$$

$$\text{div } \bar{\mathbf{U}}^{e,\perp} = 0$$

$$\text{div } (\nabla \dot{\bar{\mathbf{z}}}) = \text{div } (\bar{\boldsymbol{\alpha}} \times \bar{\mathbf{V}} + \mathbf{L}^p)$$

$$\text{div } [\mathbf{C} : (\nabla(\bar{\mathbf{u}} - \bar{\mathbf{z}}) + \bar{\mathbf{U}}^{e,\perp})] = 0$$

$$\dot{\bar{\boldsymbol{\alpha}}} = -\text{curl } (\bar{\boldsymbol{\alpha}} \times \bar{\mathbf{V}} + \mathbf{L}^p)$$

References I

- Acharya, A. (2001). A model of crystal plasticity based on the theory of continuously distributed dislocations. *Journal of the Mechanics and Physics of Solids*, 49(4):761–784.
- Acharya, A. (2003). Driving forces and boundary conditions in continuum dislocation mechanics. *Proc. R. Soc. Lond. A*, (June).
- Acharya, A. (2004). Constitutive analysis of finite deformation field dislocation mechanics. *Journal of the Mechanics and Physics of Solids*, 52:301 – 316.
- Acharya, A. (2011). Microcanonical entropy and mesoscale dislocation mechanics and plasticity. *Journal of Elasticity*, 104:23–44.
- Acharya, A., Knops, R., and Sivaloganathan, J. (2019). On the structure of linear dislocation field theory. *Journal of the Mechanics and Physics of Solids*, 130:216–244.
- Acharya, A. and Roy, A. (2006). Size effects and idealized dislocation microstructure at small scales : Predictions of a Phenomenological model of Mesoscopic Field Dislocation Mechanics : Part I. *J. Mech. Phys. Solids*, 54:1687–1710.
- Allain-Bonasso, N., Wagner, F., Berbenni, S., and Field, D. P. (2012). A study of the heterogeneity of plastic deformation in IF steel by EBSD. *Materials Science and Engineering: A*, 548:56–63.

References II

- Ashby, M. (1970). The deformation of plastically non-homogeneous materials. *Philosophical Magazine*, 21:399–424.
- Berbenni, S., Taupin, V., Djaka, K. S., and Fressengeas, C. (2014). A numerical spectral approach for solving elasto-static field dislocation and g-disclination mechanics. *International Journal of Solids and Structures*, 51(23):4157–4175.
- Berbenni, S., Taupin, V., and Lebensohn, R. A. (2020). A fast Fourier transform-based mesoscale field dislocation mechanics study of grain size effects and reversible plasticity in polycrystals. *Journal of the Mechanics and Physics of Solids*, 135:103808.
- Bertin, N., Upadhyay, M. V., Pradelier, C., and Capolungo, L. (2015). A fft-based formulation for efficient mechanical fields computation in isotropic and anisotropic periodic discrete dislocation dynamics. *Modelling and Simulation in Materials Science and Engineering*, 23:065009 (31pp).
- Bilby, B. A., Bullough, R., and Smith, E. (1955). Continuous distributions of dislocations: a new application of the methods of non-Riemannian geometry. *Proc. Roy. Soc. London A*, 231:263–273.
- Djaka, K. S., Taupin, V., Berbenni, S., and Fressengeas, C. (2015). A numerical spectral approach to solve the dislocation density transport equation. *Modelling and Simulation in Materials Science and Engineering*, 23:065008(27pp).

References III

- Djaka, K. S., Villani, A., Taupin, V., Capolungo, L., and Berbenni, S. (2017). Field Dislocation Mechanics for heterogeneous elastic materials: A numerical spectral approach. *Computer Methods in Applied Mechanics and Engineering*, 315:921–942.
- Fressengeas, C. (2017). *Mechanics of Dislocation Fields*. ISTE, Wiley.
- Habibaali, H., Pipard, J.-M., Arlazarov, A., Richeton, T., and Berbenni, S. (2026). Impact of ferrite/martensite interface on nanohardness in a dual-phase steel: A combined experimental and theoretical study. *International Journal of Plasticity*, 204:104753.
- Kröner, E. (1958). *Kontinuumstheorie der Versetzungen und Eigenspannungen*. Collatz L. and Loesch F. (eds.). *Ergebnisse der Angewandte Mathematik* 5, Springer Verlag, Berlin.
- Kröner, E. (1959). Allgemeine kontinuumstheorie der versetzungen und eigenspannungen. *Archive for Rational Mechanics and Analysis*, 4:273–334.
- Kröner, E. (1981). Continuum theory of defects. In *Physics of defects*, pages 215–315. R. Balian et al. (Eds.), Les Houches, Session 35, North Holland, New York.
- Lee, E. H. and Liu, D. T. (1967). Finite strain elastic-plastic theory with application to plane-wave analysis. *Journal of Applied Physics*, 38:19–27.
- Mandel, J. (1972). *Plasticité Classique et Viscoplasticité*. Springer, Wien.

References IV

- Mandel, J. (1973). Équations constitutives et directeurs dans les milieux plastiques et viscoplastiques. *Int. J. Solids Structures*, 9:725–740.
- Nye, J. (1953). Some geometrical relations in dislocated crystals. *Acta Metallurgica*, 1(2):153–162.
- Pantleon, W. (2008). Resolving the geometrically necessary dislocation content by conventional electron backscattering diffraction. *Scripta Materialia*, 58(11):994–997.
- Roy, A. and Acharya, A. (2005). Finite element approximation of field dislocation mechanics. *Journal of the Mechanics and Physics of Solids*, 53(1):143–170.
- Volterra, S. (1907). Sur l'équilibre des corps élastiques multiplement connexes. *Ann. Sci. Ecol. Norm. Sup. III*, 24:401–517.