Dislocation density tensor

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Plan

1. Statistical theory of dislocations
    - The dislocation density tensor
    - Scalar dislocation densities
2. Continuum crystal plasticity approach
    - Incompatibility and dislocation density tensor
    - Lattice curvature tensor
3. Need for generalized continuum crystal plasticity

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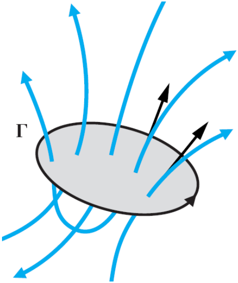
Resulting Burgers vector



Burgers vector

$$\underline{\mathbf{b}}^{s}(\underline{\mathbf{x}})$$

Dislocation line vector

$$\underline{\xi}(\underline{\mathbf{x}})$$

[Kröner, 1969]

Resulting Burgers $\underline{\mathbf{B}}^{s}$ for slip system s for a closed circuit limiting the surface S

$$\begin{aligned} \underline{\mathbf{B}}^{s} &= \left(\int_S \underline{\xi}(\underline{\mathbf{x}}).\underline{\mathbf{n}}\ dS\right) \underline{\mathbf{b}}^{s} \\ &= \int_S \underset{\sim}{\alpha}.\underline{\mathbf{n}}\ dS \end{aligned}$$

where

$$\underset{\sim}{\alpha}(\underline{\mathbf{x}}) = \underline{\mathbf{b}}^{s} \otimes \underline{\xi}(\underline{\mathbf{x}})$$

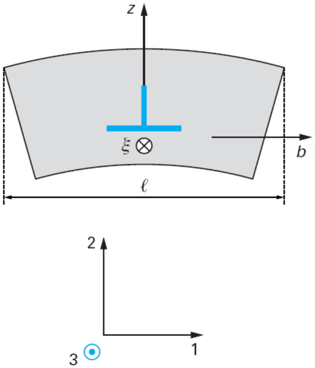
Consider contributions of all systems and **ensemble average** it

$$\underline{\mathbf{B}} = \int_S \underset{\sim}{\alpha}.\underline{\mathbf{n}}\ dS$$

$$\underset{\sim}{\alpha} = \sum_s < \underline{\mathbf{b}}^{s} \otimes \underline{\xi} >$$

Ergodic hypothesis: compute the dislocation density tensor by means of a volume average in DDD simulations

Dislocation density tensor for edge dislocations



n edge dislocations piercing the surface S
convention:

$$\underline{\mathbf{z}} = \frac{\underline{\mathbf{b}}}{b} \times \underline{\boldsymbol{\xi}}$$

Resulting Burgers vector

$$\begin{aligned} \underline{\mathbf{B}} &= nb\,\underline{\mathbf{e}}_1 \\ &= \underset{\sim}{\boldsymbol{\alpha}}.\underline{\mathbf{e}}_3\,S \end{aligned}$$

$$\begin{aligned} \underset{\sim}{\boldsymbol{\alpha}} &= \frac{n}{S}\,\underline{\mathbf{b}} \otimes \underline{\boldsymbol{\xi}} \\ &= -\rho_G\, b\, \underline{\mathbf{e}}_1 \otimes \underline{\mathbf{e}}_3 \end{aligned}$$

$\rho^G = n/S$ is the **density of geometrically necessary dislocations** according to (Ashby, 1970).

$$\begin{bmatrix} 0 & 0 & \alpha_{13} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

out of diagonal component of $\underset{\sim}{\boldsymbol{\alpha}}$

diagonal component α_{33} for **screw dislocations** with $\underline{\mathbf{b}} = b\,\underline{\mathbf{e}}_3$

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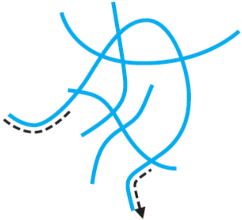
Fourth order and scalar dislocation densities

[Kröner, 1969]



Two–point correlation tensor

$$\underset{\approx}{\alpha}(\underline{\mathbf{x}}\,,\underline{\mathbf{x}}\,') = < \underline{\mathbf{b}}\,(\underline{\mathbf{x}}\,) \otimes \underline{\boldsymbol{\xi}}\,(\underline{\mathbf{x}}\,) \otimes \underline{\mathbf{b}}\,(\underline{\mathbf{x}}\,') \otimes \underline{\boldsymbol{\xi}}\,(\underline{\mathbf{x}}\,') >$$

The invariant quantity

$$\frac{1}{V}\int_V \alpha_{ijij}(\underline{\mathbf{x}}\,,\underline{\mathbf{x}}\,)\,dV = \frac{b^2}{V}\int_V \chi(\underline{\mathbf{x}}\,)\,dV = b^2\,\frac{L}{V} = b^2\rho$$

where L is the total length of dislocation lines inside V and $\chi(\underline{\mathbf{x}}\,)$ equals 1 when there is a dislocation at $\underline{\mathbf{x}}$, 0 otherwise.

ρ is the **scalar dislocation density** traditionally used in physical metallurgy

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Reminder on tensor analysis (1)

The Euclidean space is endowed with an arbitrary coordinate system characterizing the points $M(q^i)$. The basis vectors are defined as

$$\underline{\mathbf{e}}_i = \frac{\partial M}{\partial q^i}$$

The reciprocal basis $(\underline{\mathbf{e}}^i)_{i=1,3}$ of $(\underline{\mathbf{e}}_i)_{i=1,3}$ is the unique triad of vectors such that

$$\underline{\mathbf{e}}^i \cdot \underline{\mathbf{e}}_j = \delta^i_j$$

If a Cartesian orthonormal coordinate system is chosen, then both bases coincide.

Reminder on tensor analysis (2)

The gradient operator for a tensor field $T(\underline{\mathbf{X}})$ of arbitrary rank is then defined as

$$\operatorname{grad} T = T \otimes \boldsymbol{\nabla} := \frac{\partial T}{\partial q^i} \otimes \underline{\mathbf{e}}^{\,i}$$

The gradient operation therefore increases the tensor rank by one.

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$$\mathrm{div}\, T = T \cdot \boldsymbol{\nabla} := \frac{\partial T}{\partial q^i} \cdot \underline{\mathbf{e}}^{\,i}$$

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The divergence operation therefore decreases the tensor rank by one.

The curl operator (or rotational operator) for a tensor field $T(\underline{\mathbf{X}})$ of arbitrary rank is then defined as

$$\mathrm{curl}\, T = T \wedge \boldsymbol{\nabla} := \frac{\partial T}{\partial q^i} \wedge \underline{\mathbf{e}}^{\,i}$$

where the vector product is $\wedge$ $\quad \underline{\mathbf{a}} \wedge \underline{\mathbf{b}} = \epsilon_{ijk} a_j b_k \, \underline{\mathbf{e}}_{\,i} = \underset{\sim}{\underline{\epsilon}} : (\underline{\mathbf{a}} \otimes \underline{\mathbf{b}})$

The component ϵ_{ijk} of the third rank permutation tensor is the signature of the permutation of $(1, 2, 3)$.

The curl operation therefore leaves the tensor rank unchanged.

Reminder on tensor analysis (3)

With respect to a Cartesian orthonormal basis, the previous formula simplify. We give the expressions for a second rank tensor $\underset{\sim}{\mathbf{T}}$

$$\begin{aligned} \operatorname{grad} \underset{\sim}{\mathbf{T}} &= T_{ij,k}\, \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j \otimes \underline{\mathbf{e}}_k \\ \operatorname{div} \underset{\sim}{\mathbf{T}} &= T_{ij,j}\, \underline{\mathbf{e}}_i \end{aligned}$$

We consider then successively the curl of a vector field and of a second rank vector field, in a Cartesian orthonormal coordinate frame

$$\operatorname{curl} \underline{\mathbf{u}} = \frac{\partial \underline{\mathbf{u}}}{\partial X_j} \wedge \underline{\mathbf{e}}_j = u_{i,j}\, \underline{\mathbf{e}}_i \wedge \underline{\mathbf{e}}_j = \epsilon_{kij} u_{i,j}\, \underline{\mathbf{e}}_k$$

$$\operatorname{curl} \underset{\sim}{\mathbf{A}} = \frac{\partial \underset{\sim}{\mathbf{A}}}{\partial x_k} \wedge \underline{\mathbf{e}}_k = A_{ij,k} \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j \wedge \underline{\mathbf{e}}_k = \epsilon_{mjk} A_{ij,k}\, \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_m$$

Reminder on tensor analysis (4)

We also recall the Stokes formula for a vector field for a surface $\mathcal{S}$ with unit normal vector $\underline{\mathbf{n}}$ and oriented closed border line $\mathcal{L}$:

$$\oint_{\mathcal{L}} \underline{\mathbf{u}} \cdot \underline{\mathbf{dl}} = -\int_{\mathcal{S}} (\mathrm{curl}\, \underline{\mathbf{u}}) \cdot \underline{\mathbf{n}}\; ds, \quad \oint_{\mathcal{L}} u_i dl_i = -\epsilon_{kij} \int_{\mathcal{S}} u_{i,j} n_k \, ds$$

Applying the previous formula to $u_j = A_{ij}$ at fixed i leads to the Stokes formula for a tensor field of rank 2:

$$\oint_{\mathcal{L}} \underset{\sim}{\mathbf{A}} \cdot \underline{\mathbf{dl}} = -\int_{\mathcal{S}} (\mathrm{curl}\, \underset{\sim}{\mathbf{A}}) \cdot \underline{\mathbf{n}}\; ds, \quad \oint_{\mathcal{L}} A_{ij} dl_j = -\epsilon_{mjk} \int_{\mathcal{S}} A_{ij,k} n_m \, ds$$

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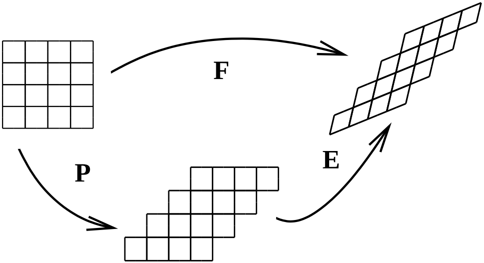
Incompatibility of elastic and plastic deformations



$$\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{E}}.\underset{\sim}{\mathbf{P}}$$

In continuum mechanics, the previous differential operators are used with respect to the initial coordinates $\underline{\mathbf{X}}$ or with respect to the current coordinates $\underline{\mathbf{x}}$ of the material points. In the latter case, the notation $\boldsymbol{\nabla}, \mathrm{grad}, \mathrm{div}$ and curl are used but in the former case we adopt $\boldsymbol{\nabla}_X, \mathrm{Grad}, \mathrm{Div}$ and Curl.

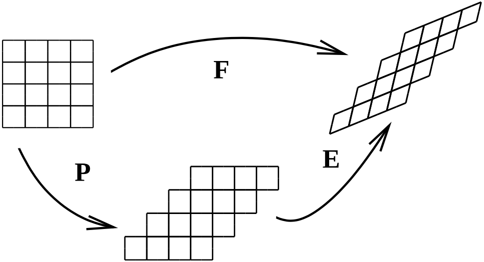
$$\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{1}} + \mathrm{Grad}\,\underline{\mathbf{u}} \quad \Longrightarrow \mathrm{Curl}\,\underset{\sim}{\mathbf{F}} = 0$$

The deformation gradient is a compatible field which derives from the displacement vector field. This is generally not the case for elastic and plastic deformation:

$$\mathrm{Curl}\,\underset{\sim}{\mathbf{E}} \neq 0, \quad \mathrm{Curl}\,\underset{\sim}{\mathbf{P}} \neq 0$$

It may happen incidentally that elastic deformation be compatible for instance when plastic or elastic deformation is homogeneous.

Incompatibility of elastic and plastic deformations



$$\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{E}}.\underset{\sim}{\mathbf{P}}$$

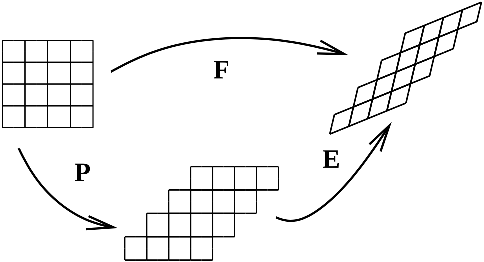
$\underset{\sim}{\mathbf{E}}$ relates the infinitesimal vectors $\underline{\mathbf{d}\zeta}$ and $\underline{\mathbf{dx}}$, where $\underline{\mathbf{d}\zeta}$ results from the cutting and releasing operations from the infinitesimal current lattice vector $\underline{\mathbf{dx}}$

$$\underline{\mathbf{d}\zeta} = \underset{\sim}{\mathbf{E}}^{-1} \cdot \underline{\mathbf{dx}}$$

If S is a smooth surface containing $\underline{\mathbf{x}}$ in the current configuration and bounded by the closed line c, the true Burgers vector is defined as

$$\underline{\mathbf{B}} = \oint_c \underset{\sim}{\mathbf{E}}^{-1}.\underline{\mathbf{dx}}$$

Dislocation density tensor in continuum crystal plasticity



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If S is a smooth surface containing $\underline{\mathbf{x}}$ in the current configuration and bounded by the closed line c, the true Burgers vector is defined as

$$\underline{\mathbf{B}} \;=\; \oint_c \underset{\sim}{\mathbf{E}}^{-1}.\underline{\mathbf{dx}} = -\int_S (\mathrm{curl}\ \underset{\sim}{\mathbf{E}}^{-1}).\underline{\mathbf{n}}\ ds = \int_S \underset{\sim}{\alpha} \cdot \underline{\mathbf{n}}\ ds$$

according to Stokes formula which gives the definition of the true dislocation density tensor

$$\underset{\sim}{\alpha} \;=\; -\mathrm{curl}\ \underset{\sim}{\mathbf{E}}^{-1} \;=\; -\epsilon_{jkl}\ E^{-1}_{ik,l}\ \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j$$

Dislocation density tensor in continuum crystal plasticity

The Burgers vector can also be computed by means of a closed circuit $c_0 \subset \Omega_0$ convected from $c \subset \Omega$:

$$\begin{aligned}\underline{\mathbf{B}} &= \oint_c \underset{\sim}{\mathbf{E}}^{-1} \cdot \underline{\mathbf{dx}} = \oint_{c_0} \underset{\sim}{\mathbf{E}}^{-1} \cdot \underset{\sim}{\mathbf{F}} \cdot \underline{\mathbf{dX}} = \oint_{c_0} \underset{\sim}{\mathbf{P}} \cdot \underline{\mathbf{dX}} \\ &= -\int_{S_0} (\mathrm{Curl}\, \underset{\sim}{\mathbf{P}}) \cdot \underline{\mathbf{dS}} = -\int_S (\mathrm{Curl}\, \underset{\sim}{\mathbf{P}}) \cdot \underset{\sim}{\mathbf{F}}^T \cdot \frac{\underline{\mathbf{ds}}}{J}\end{aligned}$$

Nanson's formula $\underline{\mathbf{ds}} = J \underset{\sim}{\mathbf{F}}^{-T} \cdot \underline{\mathbf{dS}}$ has been used. We obtain the alternative definition of the dislocation density tensor

$$\underset{\sim}{\boldsymbol{\alpha}} = -\mathrm{curl}\, \underset{\sim}{\mathbf{E}}^{-1} = -\frac{1}{J} (\mathrm{Curl}\, \underset{\sim}{\mathbf{P}}) \cdot \underset{\sim}{\mathbf{F}}^T$$

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or equivalently

$$J (\mathrm{curl}\, \underset{\sim}{\mathbf{E}}^{-1}) \cdot \underset{\sim}{\mathbf{E}}^{-T} = (\mathrm{Curl}\, \underset{\sim}{\mathbf{P}}) \cdot \underset{\sim}{\mathbf{P}}^T$$

which is a consequence of $\mathrm{curl}\, \underset{\sim}{\mathbf{F}} = \mathrm{curl}\, (\underset{\sim}{\mathbf{E}} \cdot \underset{\sim}{\mathbf{P}}) = 0$

Dislocation density tensor at small deformation

We introduce the notations

$$\underset{\sim}{\mathbf{H}} = \mathrm{Grad}\,\underline{\mathbf{u}} = \underset{\sim}{\mathbf{H}}^e + \underset{\sim}{\mathbf{H}}^p, \quad \text{with} \quad \underset{\sim}{\mathbf{H}}^e = \underset{\sim}{\boldsymbol{\varepsilon}}^e + \underset{\sim}{\boldsymbol{\omega}}^e, \quad \underset{\sim}{\mathbf{H}}^p = \underset{\sim}{\boldsymbol{\varepsilon}}^p + \underset{\sim}{\boldsymbol{\omega}}^p$$

Within the small perturbation framework

$$\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{1}} + \underset{\sim}{\mathbf{H}} = \underset{\sim}{\mathbf{1}} + \underset{\sim}{\boldsymbol{\varepsilon}}^e + \underset{\sim}{\boldsymbol{\omega}}^e + \underset{\sim}{\boldsymbol{\varepsilon}}^p + \underset{\sim}{\boldsymbol{\omega}}^p \simeq (\underset{\sim}{\mathbf{1}} + \underset{\sim}{\boldsymbol{\varepsilon}}^e + \underset{\sim}{\boldsymbol{\omega}}^e).(\underset{\sim}{\mathbf{1}} + \underset{\sim}{\boldsymbol{\varepsilon}}^p + \underset{\sim}{\boldsymbol{\omega}}^p) \simeq \underset{\sim}{\mathbf{E}}.\underset{\sim}{\mathbf{P}}$$

We have

$$\underset{\sim}{\mathbf{E}} \simeq \underset{\sim}{\mathbf{1}} + \underset{\sim}{\mathbf{H}}^e, \quad \underset{\sim}{\mathbf{P}} \simeq \underset{\sim}{\mathbf{1}} + \underset{\sim}{\mathbf{H}}^p$$

$$\underset{\sim}{\mathbf{E}}^{-1} \simeq \underset{\sim}{\mathbf{1}} - \underset{\sim}{\mathbf{H}}^e$$

so that the dislocation density tensor can be computed as

$$\underset{\sim}{\boldsymbol{\alpha}} \simeq \mathrm{Curl}\,\underset{\sim}{\mathbf{H}}^e = -\mathrm{Curl}\,\underset{\sim}{\mathbf{H}}^p$$

since $\mathrm{Curl}\,\underset{\sim}{\mathbf{H}} = 0$ due to the compatibility of the deformation gradient.

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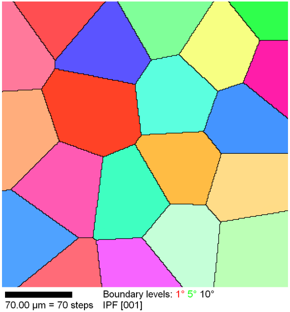
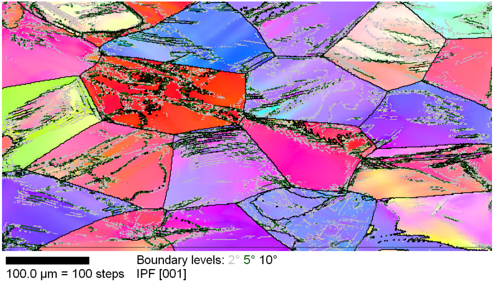
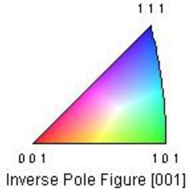
Lattice rotation full field measurement

initial orientations

lattice orientation field after deformation







Dislocation density *vs.* lattice curvature

Experimental techniques like EBSD provide the field of lattice orientation and, consequently, of lattice rotation $\underset{\sim}{\mathbf{R}}^e$ during deformation. Since

$$\underset{\sim}{\boldsymbol{\alpha}} = -\mathrm{curl}\, \underset{\sim}{\mathbf{E}}^{-1} = -\mathrm{curl}\, (\underset{\sim}{\mathbf{U}}^{e-1} \cdot \underset{\sim}{\mathbf{R}}^{eT})$$

the hypothesis of small elastic strain (and in fact of small elastic strain gradient) implies

$$\underset{\sim}{\boldsymbol{\alpha}} \simeq -\mathrm{curl}\, \underset{\sim}{\mathbf{R}}^{eT}$$

If, in addition, elastic rotations are small, we have

$$\underset{\sim}{\boldsymbol{\alpha}} \simeq -\mathrm{curl}\, (\underset{\sim}{\mathbf{1}} - \underset{\sim}{\boldsymbol{\omega}}^e) = \mathrm{curl}\, \underset{\sim}{\boldsymbol{\omega}}^e$$

The small rotation axial vector is defined as

$$\underline{\overset{\times}{\boldsymbol{\omega}}}^e = -\frac{1}{2} \underset{\approx}{\underline{\boldsymbol{\epsilon}}} : \underset{\sim}{\boldsymbol{\omega}}^e, \quad \underset{\sim}{\boldsymbol{\omega}}^e = -\underset{\approx}{\underline{\boldsymbol{\epsilon}}} \cdot \underline{\overset{\times}{\boldsymbol{\omega}}}^e$$

Dislocation density *vs.* lattice curvature

or, in matrix form,

$$[\underset{\sim}{\boldsymbol{\omega}}^e] = \begin{bmatrix} 0 & \omega^e_{12} & -\omega^e_{31} \\ -\omega^e_{12} & 0 & \omega^e_{23} \\ \omega^e_{31} & -\omega^e_{23} & 0 \end{bmatrix} = \begin{bmatrix} 0 & -\overset{\times}{\omega}{}^e_3 & \overset{\times}{\omega}{}^e_2 \\ \overset{\times}{\omega}{}^e_3 & 0 & -\overset{\times}{\omega}{}^e_1 \\ -\overset{\times}{\omega}{}^e_2 & \overset{\times}{\omega}{}^e_1 & 0 \end{bmatrix}$$

The gradient of the lattice rotation field delivers the lattice curvature tensor. In the small deformation context, the gradient of the rotation tensor is represented by the gradient of the axial vector:

$$\underset{\sim}{\boldsymbol{\kappa}} := \mathrm{grad}\, \overset{\times}{\underline{\boldsymbol{\omega}}}{}^e$$

One can establish a direct link between $\mathrm{curl}\, \underset{\sim}{\boldsymbol{\omega}}^e$ and the gradient of the axial vector associated with $\underset{\sim}{\boldsymbol{\omega}}$.

Dislocation density *vs.* lattice curvature

$$
\begin{aligned}
[\mathrm{curl}\, \underset{\sim}{\boldsymbol{\omega}}^{e}] &= \begin{bmatrix} \omega^{e}_{12,3} + \omega^{e}_{31,2} & -\omega^{e}_{31,1} & -\omega^{e}_{12,1} \\ -\omega^{e}_{23,2} & \omega^{e}_{12,3} + \omega^{e}_{23,1} & -\omega^{e}_{12,2} \\ -\omega^{e}_{23,3} & -\omega^{e}_{31,3} & \omega^{e}_{23,1} + \omega^{e}_{31,2} \end{bmatrix} \\
&= \begin{bmatrix} -\overset{\times}{\omega}{}^{e}_{3,3} - \overset{\times}{\omega}{}^{e}_{2,2} & \overset{\times}{\omega}{}^{e}_{2,1} & \overset{\times}{\omega}_{3,1} \\ \overset{\times}{\omega}{}^{e}_{1,2} & -\overset{\times}{\omega}{}^{e}_{3,3} - \overset{\times}{\omega}{}^{e}_{1,1} & \overset{\times}{\omega}{}^{e}_{3,2} \\ \overset{\times}{\omega}{}^{e}_{1,3} & \overset{\times}{\omega}{}^{e}_{2,3} & -\overset{\times}{\omega}{}^{e}_{1,1} - \overset{\times}{\omega}{}^{e}_{2,2} \end{bmatrix}
\end{aligned}
$$

from which it becomes apparent that

$$
\underset{\sim}{\boldsymbol{\alpha}} = \underset{\sim}{\boldsymbol{\kappa}}^{T} - (\mathrm{trace}\, \underset{\sim}{\boldsymbol{\kappa}}) \underset{\sim}{\mathbf{1}}, \quad \underset{\sim}{\boldsymbol{\kappa}} = \underset{\sim}{\boldsymbol{\alpha}}^{T} - \frac{1}{2} (\mathrm{trace}\, \underset{\sim}{\boldsymbol{\alpha}}) \underset{\sim}{\mathbf{1}}
$$

This is a remarkable relation linking, with the context of small elastic strains[1] and rotations, the dislocation density tensor to lattice curvature. It is known as Nye's formula [Nye, 1953].

[1] and in fact of small gradient of elastic strain.

Relating the dislocation density and lattice curvature tensors at finite deformation

$$
\begin{aligned}
\underset{\sim}{\alpha} &= -\mathrm{curl}\ \underset{\sim}{\mathbf{E}}^{-1} = \mathrm{curl}\ \underset{\sim}{\mathbf{U}}^{e-1} . \underset{\sim}{\mathbf{R}}^{T} \\
&= -\left(\epsilon_{jkl}\ \frac{\partial U^{e-1}_{im}}{\partial x_l}\ R_{km}\ +\ U^{e-1}_{im}\ \epsilon_{jkl}\ R^{T}_{mk,L}\ F^{-1}_{Ll} \right)\ \underline{\mathbf{e}}_{\,i} \otimes \underline{\mathbf{e}}_{\,j}
\end{aligned}
$$

The finite lattice curvature tensor is defined as

$$
\underset{\sim}{\mathbf{\Gamma}}\ =\ \frac{1}{2}\ \underset{\approx}{\epsilon} : (\underset{\sim}{\mathbf{R}} . (\underset{\sim}{\mathbf{R}}^{T} \otimes \boldsymbol{\nabla}))
$$

Note that

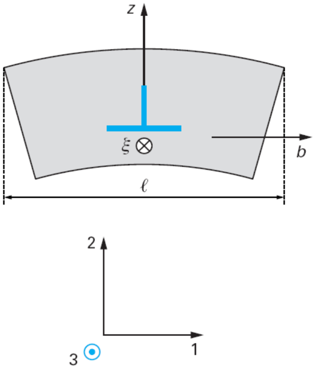
$$
\underset{\sim}{\mathbf{R}} . (\underset{\sim}{\mathbf{R}}^{T} \otimes \boldsymbol{\nabla})\ =\ \underset{\approx}{\epsilon} . \underset{\sim}{\mathbf{\Gamma}}, \quad R^{T}_{mk,l}\ =\ -R^{T}_{mu}\ \epsilon_{ukv}\ \Gamma_{vl}
$$

It follows

$$
\begin{aligned}
\underset{\sim}{\alpha} &= \underset{\sim}{\mathbf{A}}^{el}\ -\ U^{e-1}_{im}\ R^{T}_{mu}\ \epsilon_{klj}\ \epsilon_{kvu}\ \Gamma_{vL}\ F^{-1}_{Ll}\ \underline{\mathbf{e}}_{\,i} \otimes \underline{\mathbf{e}}_{\,j} \\
&= \underset{\sim}{\mathbf{A}}^{el}\ +\ \underset{\sim}{\mathbf{F}}^{e-1} . \left((\underset{\sim}{\mathbf{\Gamma}} . \underset{\sim}{\mathbf{F}}^{-1})^{T}\ -\ \mathrm{Tr}\,(\underset{\sim}{\mathbf{\Gamma}} . \underset{\sim}{\mathbf{F}}^{-1})\ \underset{\sim}{\mathbf{1}} \right)
\end{aligned}
$$

where $\underset{\sim}{\mathbf{A}}^{el}\ =\ \epsilon_{jkl}\ \dfrac{\partial U^{e-1}_{im}}{\partial x_l}\ R_{km}\ \underline{\mathbf{e}}_{\,i} \otimes \underline{\mathbf{e}}_{\,j}$.

Lattice curvature due to edge dislocations



$$\underset{\sim}{\boldsymbol{\alpha}} = -\rho_G b\, \underline{\mathbf{e}}_1 \otimes \underline{\mathbf{e}}_3$$

so that

$$\underset{\sim}{\boldsymbol{\kappa}} = -\rho_G b\, \underline{\mathbf{e}}_3 \otimes \underline{\mathbf{e}}_1$$

the only non–vanishing component is

$$\kappa_{31} = \Phi^e_{3,1}$$

which corresponds to bending with respect to axis 3

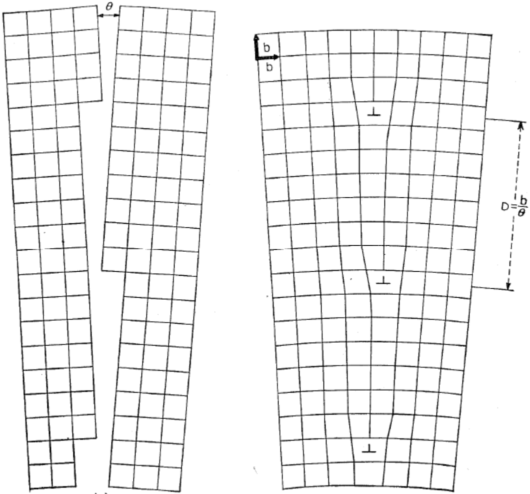
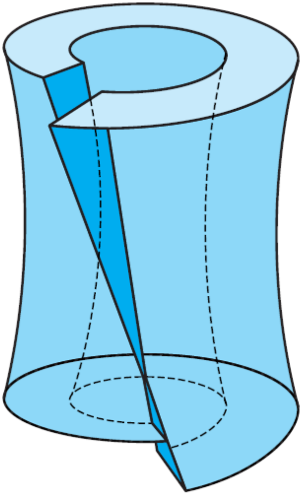


Fig. XI-1. — Joint de grains simple. Le plan de la figure est parallèle à une face du cube et normal à l'axe de rotation relative des deux grains. (*a*) Deux grains ayant un axe quaternaire commun et une différence d'orientation θ. (*b*) Les deux grains sont réunis pour former un bicristal. Cette réunion ne demande qu'une déformation élastique, sauf là où un plan d'atomes se termine sur le joint en une dislocation coin marquée par le symbole ⊥.

Tilt boundary
(Read, 1958)

Lattice torsion due to screw dislocations



[Friedel, 1964]

screw dislocations parallel to $\underline{\mathbf{e}}_3$

$$\underset{\sim}{\alpha} = \rho^G b \, \underline{\mathbf{e}}_3 \otimes \underline{\mathbf{e}}_3$$

$$\underset{\sim}{\kappa} = \underset{\sim}{\alpha}^T - \frac{1}{2}(\mathrm{trace}\, \underset{\sim}{\alpha})\underset{\sim}{\mathbf{1}}$$

$$[\underset{\sim}{\kappa}] = \frac{\rho_G b}{2} \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

torsion with respect to all axes!!!

relaxed Volterra cylinder

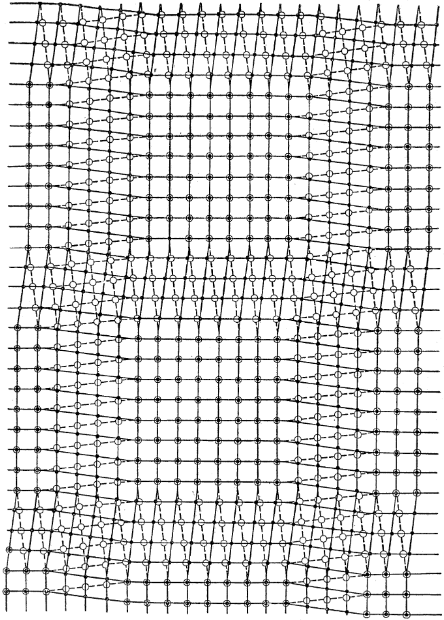


Fig. XII-2. — Joint de torsion pure. Le joint est parallèle du plan de la figure, et les deux grains ont subi une légère rotation relative autour de l'axe quaternaire normal à la figure. Les cercles blancs représentent des atomes juste au-dessus du joint, et les noirs des atomes juste au-dessous. Les grains s'unissent continûment, sauf suivant deux ensembles de dislocations vis qui forment un quadrillage.

Twist boundary

two families of orthogonal screw dislocations

$$\underset{\sim}{\boldsymbol{\alpha}} = -\rho_G b(\underline{\mathbf{e}}_1 \otimes \underline{\mathbf{e}}_1 + \underline{\mathbf{e}}_2 \otimes \underline{\mathbf{e}}_2)$$

$$[\underset{\sim}{\boldsymbol{\kappa}}] = \rho_G b \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

torsion with respect to axis 3

$$\kappa_{33} = \Phi^e_{3,3}$$

(Read, 1958)

Plan

1. Statistical theory of dislocations
   - The dislocation density tensor
   - Scalar dislocation densities
2. Continuum crystal plasticity approach
   - Incompatibility and dislocation density tensor
   - Lattice curvature tensor
3. Need for generalized continuum crystal plasticity

Towards generalized single crystal plasticity

A continuum crystal plasticity model should at least include

- the effect of **scalar dislocation density** ρ_S; this is the case of classical crystal plasticity according to Mandel, Teodosiu, Sidoroff, Asaro which incorporate hardening rules from physical metallurgy
- the effect of **dislocation density tensor**; it is the main ingredient of the continuum theory of dislocations (*closure problem*)
  geometrically necessary dislocation density ρ_G

Combine both! But acknowledge then the fact that the presence of $\underset{\sim}{\alpha}$ in the constitutive equations leads to higher order partial differential equations when inserted in the equilibrium equations. Additional boundary conditions are necessary. Several possibilities:

- since $\underset{\sim}{\alpha}$ is implicitly related to $\underset{\sim}{\mathbf{P}} \otimes \boldsymbol{\nabla}$ and $\underset{\sim}{\mathbf{F}} \otimes \boldsymbol{\nabla}$, consider a strain gradient model or strain gradient plasticity model;
  [Mindlin and Eshel, 1968] [Fleck and Hutchinson, 1997]
- since $\underset{\sim}{\alpha}$ is related to the lattice curvature tensor, raise the lattice rotation to internal degrees of freedom and consider a Cosserat theory.
  [Günther, 1958] [Kröner, 1963] [Mura, T., 1963]

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