

Continuum theory of crystalline defects and mechanical fields

Lecture : Introduction to dislocation theory in linear elasticity and solution methods

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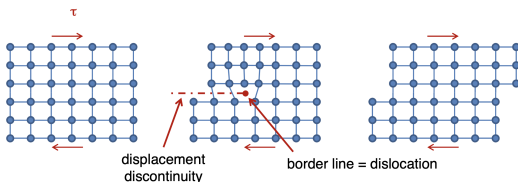
Fondements Théoriques de la Plasticité

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Plasticity foundations: Introduction to dislocations

- Dislocations are responsible for plastic deformation in crystals (e.g. metals, ceramics, rocks..) and understanding their behavior is important in numerous applications (metal forming, aeronautics, semi-conductors ...)
- Crystals are not perfect but contain defects (dislocations ...)

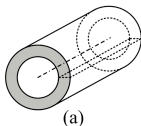


- Dislocations also play an important role in fracture, due to their interactions with cracks (e.g. in ductile materials, a crack tip can nucleate many dislocations shielding and blunting the crack tip).

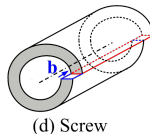
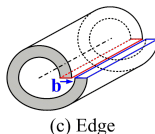
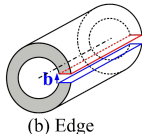
Introduction to dislocations

- Volterra (1907) (Italian Mathematician) mathematically introduced dislocation as crystal line translational defect and rotational defects known as disclinations (see Lecture 3)

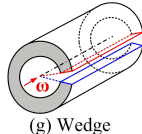
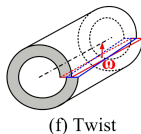
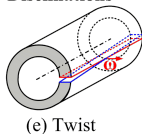
Defect line



Dislocations

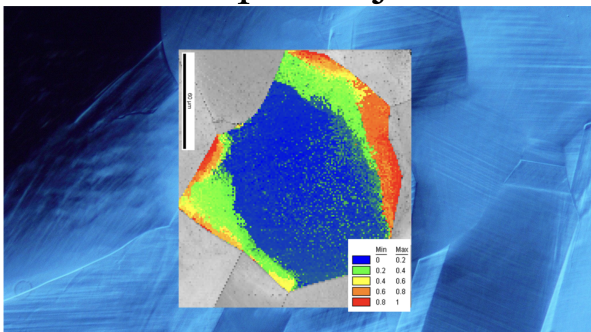


Disclinations



Introduction to dislocations

- Dislocations are at the origin of crystal plasticity



Courbures de
réseau
(GND)
Gradient de
désorientation
aux abords du
joint

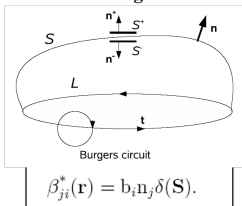
Désorientations intra-granulaires induites par la plasticité cristalline contrainte par les joints de grains (microplasticité sur du Ni polycristallin en traction; grain avec glissement simple prédominant) (Thèse C. Perrin, Univ. Lorraine, LEM3, 2010)

C. Perrin, S. Berbenni, H. Vehoff, M. Berveiller. *Acta Mater.*, 58 :4639–4649, 2010.

Introduction to dislocations

- From Volterra's dislocation to plasticity (slip, yield stress, ...)

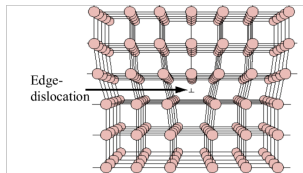
Volterra's single dislocation



V. Volterra's description (Ann. Sci. Ec. Norm. Sup. Paris 24, 401-517, 1907)

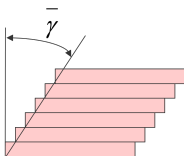
Edge dislocation in a crystal

Burgers vector: $\mathbf{b}$

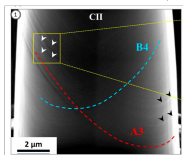


$$\text{bcc: } \mathbf{b} = \frac{1}{2} \langle 111 \rangle, b = \frac{\sqrt{3}}{2} a; \quad \text{fcc: } \mathbf{b} = \frac{1}{2} \langle 110 \rangle, b = \frac{1}{\sqrt{2}} a$$

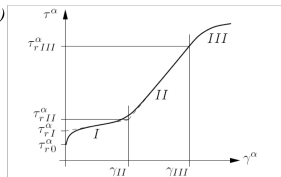
«Discrete to continuum» transition: average
« macroscopic » shear (at the origin of collective
plastic strain in continuum-based plasticity)



Tiba et al., Acta Materialia (2015)

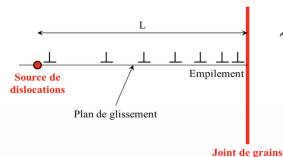
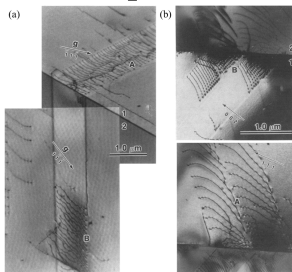


3-stage hardening response in f.c.c.
crystals (oriented for initial single slip)



Introduction to dislocations

Dislocation pile-ups



Micrographies MET d'un acier inoxydable 310 après une déformation montrant la transmission des dislocations du grain 1 au grain 2 au travers du joint de grains. Transmission directe et totale (a) et transmission partielle (b) en créant des dislocations résiduelles au joint de grains. Les systèmes incidents et transmis sont désignés, par A et B dans (a), et inversement dans (b)

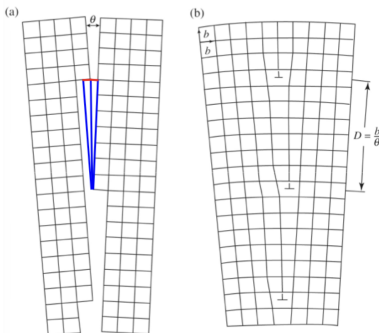
T.C. Lee, I.M. Robertson, H.K. Birnbaum. *Philos. Mag. A*, 62 :131–153, 1990.

Introduction to dislocations

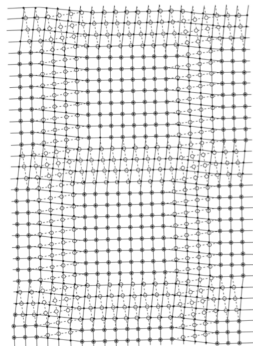
- Grain boundaries as dislocation arrays

Joint de flexion (dislocations coins)

(Ex: 2 grains avec axe de désorientation [001])

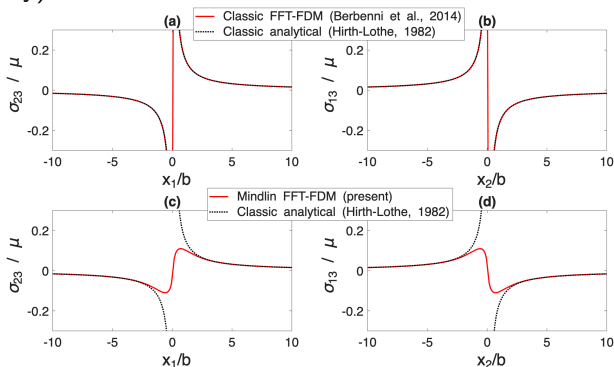


Joint de torsion (dislocations vis)



Introduction to dislocations

- Classic linear elasticity theory and Volterra's dislocation $\Rightarrow$ an infinite stress at dislocation core (singular solution scaling with $1/r$, where r is the distance from the dislocation), while the long range stress is correct $\Rightarrow$ Towards continuum-based method for dislocation core spreading (strain gradient elasticity)



Outline

- 1 Basic equations of the classic linear elasticity
- 2 Elastic Green's function
- 3 Eigenstrain problems: application to dislocation theory in anisotropic and isotropic homogeneous media
- 4 Fourier transform -based solution method in anisotropic media
- 5 Stroh formalism for straight dislocations in anisotropic media

Classic elasticity: Review

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:

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

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

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

- In rectangular Cartesian components:

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

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

$$(\operatorname{curl} \mathbf{A})_{ij} = e_{jkl} A_{il,k} = -(\operatorname{grad} \mathbf{A} : \mathbf{X})_{ij}$$

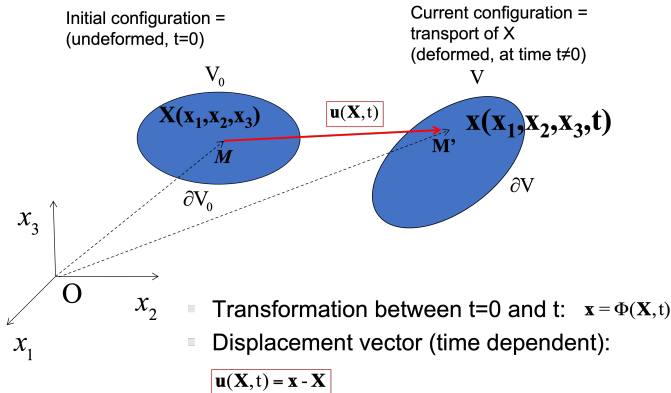
where e_{jkl} is a component of the third-order alternating Levi-Civita tensor and the spatial derivative with respect to a Cartesian coordinate is indicated by a comma followed by the component index.

- 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.

Displacement vector

Definition of displacement vector $\mathbf{u}$ or u_i (index notation):

$$u_i = x_i - X_i \quad (1)$$



Strain and rotation tensors (small deformation)

- In linear elasticity (see e.g. Sadd (2009)), small perturbation hypothesis is used (small deformation)

Strain tensor ε or ε_{ij} (index notation) (change of area):

$$\varepsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}) \quad (2)$$

Rotation tensor ω or ω_{ij} (index notation):

$$\omega_{ij} = \frac{1}{2} (u_{i,j} - u_{j,i}) \quad (3)$$

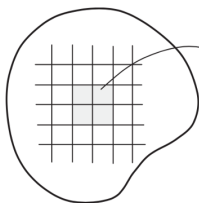
Displacement gradient (distortion) tensor $\mathbf{U} = \nabla \mathbf{u}$ or $U_{ij} = u_{i,j}$ (index notation):

$$U_{ij} = u_{i,j} = \varepsilon_{ij} + \omega_{ij} \quad (4)$$

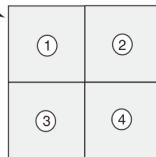
Strain compatibility

Saint-Venant strain compatibility equations for strain (6 relations in 3D, 1 relation in 2D):

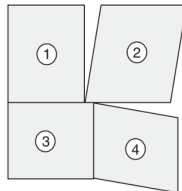
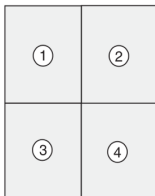
$$\text{Inc}(\boldsymbol{\varepsilon}) = 0 \Leftrightarrow e_{pmk}e_{qnj}\varepsilon_{jk,mn} = 0 \quad (5)$$



(a) Discretized Elastic Solid



(b) Undeformed Configuration



Cauchy stress tensor and balance equations (under static conditions)

Stress tensor σ measures the traction force across an internal surface S inside the body. From Cauchy's rule (tetrahedron):

$$t_i = \sigma_{ij} n_j \quad (6)$$

where t_i is the stress (traction) vector and n_j is the unit surface normal.

Balance of linear momentum (static form) for any applied surface traction T_i^0 , or any applied displacement u_i^0 on the external surface of the body:

$$\sigma_{ji,j} + f_i = 0 \quad (7)$$

where f_i is a body force density vector (proof using Gauss's theorem).

Balance of angular momentum:

$$e_{imn} \sigma_{nm} = 0 \Leftrightarrow \sigma_{ji} = \sigma_{ij} \quad (8)$$

(proof using Gauss's theorem and balance of linear momentum).

Generalized Hooke's law

Stress-strain constitutive law: Generalized Hooke's law

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \quad (9)$$

where C_{ijkl} is the elastic stiffness tensor with minor and major symmetries $C_{ijkl} = C_{ijlk} = C_{jikl} = C_{klij}$.

Inverse of this equation: Strain-Stress constitutive law

$$\varepsilon_{ij} = S_{ijkl}\sigma_{kl} \quad (10)$$

where S_{ijkl} is the elastic compliance tensor with minor and major symmetries with $C_{ijkl}S_{klmn} = \frac{1}{2}(\delta_{im}\delta_{jn} + \delta_{in}\delta_{jm})$.

Isotropic elasticity (with two Lamé moduli: λ and μ : shear modulus)

$$\sigma_{ij} = \lambda\varepsilon_{ll}\delta_{ij} + 2\mu\varepsilon_{ij} \quad (11)$$

Summary of equations for an elastic body (volume V , surface S)

- $t_i = \sigma_{ij}n_j$ (stress vector, stress tensor definition) in V
- $\sigma_{ij,j} + f_i = 0$ (stress equilibrium) in V
- $\sigma_{ij} = \sigma_{ji}$ (symmetry of Cauchy stress tensor) in V
- $\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ (strain/displacement relationship) in V
- $e_{pmk}e_{qnj}\varepsilon_{jk,mn} = 0$ (strain compatibility) in V
- $\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$ (generalized Hooke's law) in V

- $\Rightarrow$ Equilibrium equation in 3D elasticity in terms of displacement (Navier equation):

$$C_{ijkl}u_{k,lj} + f_i = 0 \quad (12)$$

with $\sigma_{ij}n_j = t_i^0$ on S_t (traction boundary condition) and $u_i = u_i^0$ on S_u (displacement boundary condition), with $S = S_t \cup S_u$.

- This is the Navier equation for an anisotropic homogeneous medium (3 unknowns, 3 equations)

Elastic Green's tensor

Green's function method

- Displacement solution $u_k(\mathbf{x}) = G_{km}(\mathbf{x}, \mathbf{x}') F_m(\mathbf{x}')$ in response to a point force $F_m(\mathbf{x}')$ for homogeneous elastic medium:
 $f_i(\mathbf{x}) = \delta_{im} \delta(\mathbf{x} - \mathbf{x}') F_m(\mathbf{x}')$, where δ_{im} is the Kronecker delta tensor and $\delta(\mathbf{x} - \mathbf{x}')$ is the three-dimensional Dirac delta function which is zero everywhere, except at point $\mathbf{x} = \mathbf{x}'$
- From Navier equation (elliptic PDE) and eliminating $F_m(\mathbf{x}')$:

Elastic Green's tensor is defined by:

$$\begin{aligned} C_{ijkl} G_{km,lj}(\mathbf{x}, \mathbf{x}') + \delta_{im} \delta(\mathbf{x} - \mathbf{x}') &= 0 \\ G_{km}(\mathbf{x}, \mathbf{x}') &= 0 \text{ on } S_u \\ C_{ijkl} G_{km,l}(\mathbf{x}, \mathbf{x}') n_j &= 0 \text{ on } S_t \end{aligned} \quad (13)$$

- Symmetry of elastic Green's tensor $\mathbf{G}$:
 $G_{km}(\mathbf{x}, \mathbf{x}') = G_{mk}(\mathbf{x}', \mathbf{x}) = G_{mk}(\mathbf{x}, \mathbf{x}')$ (using Betti's reciprocal theorem).
- Infinite medium (invariance with translation): $G_{km}(\mathbf{x}, \mathbf{x}') = G_{km}(\mathbf{x} - \mathbf{x}')$.

Displacement solution (unbounded infinite medium):

$$u_i(\mathbf{x}) = \int_V G_{ij}(\mathbf{x} - \mathbf{x}') f_j(\mathbf{x}') dV' \quad (14)$$

Calculation of Green's function from Fourier transforms

- The Green's function is calculated with the Fourier Transform. In the Fourier space, let ξ be the Fourier vector of magnitude $\xi = \sqrt{\xi \cdot \xi}$ and components ξ_i in a cartesian coordinate system in a general three-dimensional setting. The complex imaginary number is denoted i and defined as $i = \sqrt{-1}$.

Let $\widetilde{u}_k(\xi)$ be the Fourier transform of the displacement:

$$\widetilde{u}_k(\xi) = \int_V u_k(\mathbf{x}) e^{-i\xi \cdot \mathbf{x}} dV \quad (15)$$

- Conversely, the inverse Fourier transform is defined as:

$$u_k(\mathbf{x}) = \frac{1}{8\pi^3} \int_{V_\xi} \widetilde{u}_k(\xi) e^{+i\xi \cdot \mathbf{x}} dV_\xi$$

- The inverse Fourier transform yields the three-dimensional Dirac delta function as $\delta(\mathbf{x}) = \frac{1}{8\pi^3} \int_{V_\xi} e^{+i\xi \cdot \mathbf{x}} dV_\xi$.

Calculation of Green's from Fourier transforms

- The Fourier transform of Eq. (13) yields:

$$C_{ijkl}\tilde{G}_{km}(\boldsymbol{\xi})\xi_l\xi_j = \delta_{im}$$

The anisotropic elastic acoustic tensor is defined as:

$$K_{ik}(\boldsymbol{\xi}) = C_{ijkl}\xi_l\xi_j \quad (16)$$

- Then, the Green's tensor is given in Fourier space:

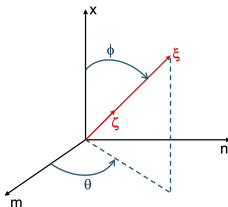
$$\tilde{G}_{ij}(\boldsymbol{\xi}) = \frac{(K(\boldsymbol{\zeta}))_{ik}^{-1}}{\xi^2}$$

where $\boldsymbol{\zeta} = \boldsymbol{\xi}/\xi$.

- The inverse Fourier transform yields:

$$G_{ij}(\mathbf{x}) = \frac{1}{8\pi^3} \int_{V_{\boldsymbol{\xi}}} \frac{(K(\boldsymbol{\zeta}))_{ij}^{-1}}{\xi^2} e^{+i\boldsymbol{\xi}\cdot\mathbf{x}} dV_{\boldsymbol{\xi}}$$

Calculation of Green's from Fourier transforms



- In spherical coordinates, Eq. (22) becomes:

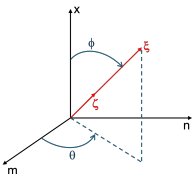
$$G_{ij}(\mathbf{x}) = \frac{1}{8\pi^3} \int_0^{+\infty} \int_0^\pi \int_0^{2\pi} \frac{(K(\boldsymbol{\zeta}))_{ij}^{-1}}{\xi^2} e^{+i\xi x \cos \phi} \xi^2 \sin \phi \, d\theta \, d\phi \, d\xi$$

- Then:

$$G_{ij}(\mathbf{x}) = \frac{1}{8\pi^2} \int_0^\pi \int_0^{2\pi} (K(\boldsymbol{\zeta}))_{ij}^{-1} \delta(x \cos \phi) \sin \phi \, d\theta \, d\phi$$

since $\int_0^{+\infty} e^{+i\xi x \cos \phi} d\xi = \frac{1}{2} \int_{-\infty}^{+\infty} e^{+i\xi x \cos \phi} d\xi = \pi \delta(x \cos \phi)$

Calculation of Green's from Fourier transforms



- Using a transformation of variables $u = \cos \phi$ (then $du = -\sin \phi$) and using the formula: $\delta(au) = \frac{1}{a}\delta(u)$ (with $a = x$) yields:

$$G_{ij}(\mathbf{x}) = \frac{1}{8\pi^2 x} \int_{-1}^1 \int_0^{2\pi} - (K(\zeta))_{ij}^{-1} \delta(u) d\theta du = \frac{1}{8\pi^2 x} \int_{-1}^1 \int_0^{2\pi} (K(\zeta))_{ij}^{-1} \delta(u) d\theta du$$

- Then, using $\int_{-1}^1 f(u)\delta(u) du = f|_{u=0}$ yields $G_{ij}(\mathbf{x}) = \frac{1}{8\pi^2 x} \int_0^{2\pi} (K(\zeta))_{ij}^{-1} \Big|_{u=0} d\theta$

Finally:

$$G_{ij}(\mathbf{x}) = \frac{1}{8\pi^2 x} \int_0^{2\pi} (K(\zeta))_{ij}^{-1} \Big|_{\mathbf{x} \cdot \zeta = 0} d\theta \quad (17)$$

Calculation of Green's from Fourier transforms in isotropic elasticity

- Isotropic elastic stiffness tensor: $C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$
- Acoustic tensor: $K(\zeta)_{ij} = (\lambda + \mu)\zeta_i\zeta_j + \mu\delta_{ij} \Rightarrow$
 $(K(\zeta))_{ij}^{-1} = \frac{1}{\mu} \left(\delta_{ij} - \frac{\lambda + \mu}{\lambda + 2\mu} \zeta_i\zeta_j \right)$
- Using: $\zeta_i = \alpha_i \cos \theta + \beta_i \sin \theta$ in the plane $\mathbf{x} \cdot \zeta = 0$ and $\delta_{ij} = \alpha_i\alpha_j + \beta_i\beta_j + t_it_j$ with $x_i = xt_i$, the analytical integration is straightforward.
- Using $\lambda = \frac{2\mu\nu}{1-2\nu}$ such that: $\frac{\lambda + \mu}{\lambda + 2\mu} = \frac{1}{2(1-\nu)}$, we find:

$$G_{ij}(\mathbf{x}) = \frac{1}{8\pi\mu} \left(\delta_{ij} R_{,kk} - \frac{1}{2(1-\nu)} R_{,ij} \right)$$

Expression of the isotropic elastic Green's tensor:

$$G_{ij}(\mathbf{x}) = \frac{1}{16\pi\mu(1-\nu)R} \left((3-4\nu)\delta_{ij} + \frac{x_ix_j}{R^2} \right) \quad (18)$$

using $R = x = \sqrt{x_ix_i}$; $R_{,i} = \frac{x_i}{R}$; $R_{,kk} = \frac{2}{R}$; $R_{,ij} = \frac{\delta_{ij}}{R} - \frac{x_ix_j}{R^3}$.

Eigenstrains: Application to dislocation theory

Equations for an elastic body with eigenstrains

- Field equations in a body of volume V with eigenstrain field (plastic strain) ε_p or plastic distortion field $\mathbf{U}_p$:

$$\sigma_{ij,j} = 0 \text{ with } \sigma_{ij} = \sigma_{ji}$$

$$\varepsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}) \text{ with } e_{pmk} e_{qnj} \varepsilon_{jk,mn} = 0$$

$$U_{ij} = u_{i,j} = U_{ij}^e + U_{ij}^p$$

$$\sigma_{ij} = C_{ijkl} (\varepsilon_{kl} - \varepsilon_{kl}^p) \text{ with } C_{ijkl} = C_{jikl} = C_{jilk} = C_{klij}$$

⇒ Equilibrium equation in 3D elasticity with eigendistortion (Navier equation):

$$C_{ijkl} u_{k,lj} - C_{ijkl} U_{kl,j}^p = 0 \Leftrightarrow C_{ijkl} u_{k,lj} + f_i^* = 0 \quad (19)$$

with $t_i^0 = 0$ on S_t and $u_i^0 = 0$ on S_u . This is the Navier equation for an anisotropic homogeneous elastic medium with eigenstrains (or eigendistortions) given by fictive body force density $f_i^* = -C_{ijkl} U_{kl,j}^p$.

Solution of eigenstrain problems from Green's function

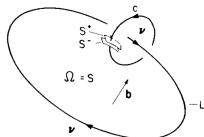
- Displacement solution (unbounded infinite medium):

$$\begin{aligned}
 u_m(\mathbf{x}) &= \int_V G_{mi}(\mathbf{x} - \mathbf{x}') f_i^*(\mathbf{x}') dV' \\
 &= - \int_V G_{mi}(\mathbf{x} - \mathbf{x}') C_{ijkl} U_{kl,j}^p(\mathbf{x}') dV' \\
 &= \int_V G_{mi,j'}(\mathbf{x} - \mathbf{x}') C_{ijkl} U_{kl}^p(\mathbf{x}') dV' \\
 &= - \int_V G_{mi,j}(\mathbf{x} - \mathbf{x}') C_{ijkl} U_{kl}^p(\mathbf{x}') dV'
 \end{aligned}$$

Displacement solution (unbounded infinite medium) (Mura, 1987):

$$u_m(\mathbf{x}) = - \int_V C_{ijkl} G_{mi,j}(\mathbf{x} - \mathbf{x}') U_{kl}^p(\mathbf{x}') dV' \quad (20)$$

Dislocation loop (Volterra)

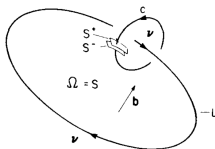


- Let us consider a dislocation loop L in the three-dimensional space formed by a cut in the material over a surface S bounded by L (see Figure). For the sign convention, one has chosen following Mura (1987) the line direction vector $\boldsymbol{\nu}$ and the positive sense of the Burgers circuit C (closed curve encircling the dislocation line) to respect the right-hand rule.
- Now, the displacements are constructed by displacing the upper side of surface S (denoted S^+ by Burgers vector $\mathbf{b}$ with respect to the lower side of surface S (denoted S^-) and then gluing them together.

The Burgers vector $\mathbf{b}$ is defined as such displacement discontinuity:

$$b_i = [u_i] = \oint_C du_i = \oint_C u_{i,j} dx_j \quad (21)$$

Dislocation loop (Volterra)



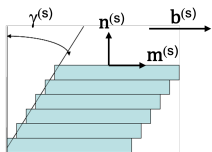
- The plastic distortion denoted U_{ij}^p is caused by the slip b_i of plane S^+ whose normal vector towards plane S^- is n_j . Thus, the expression of the plastic distortion induced by the dislocation loop L for any position vector $\mathbf{x}$ is singular on the surface S (Volterra, 1907)

The expression of U_{ij}^p reads according to Kosevich (1979); Mura (1987):

$$U_{ij}^p(\mathbf{x}) = -b_i n_j \delta(\mathbf{S} - \mathbf{x}), \quad (22)$$

where $\delta(\mathbf{S} - \mathbf{x})$ is a shorthand notation for the one-dimensional Dirac delta function in the direction $\mathbf{n}$, i.e. infinite when $\mathbf{x}$ is on S and zero elsewhere $\delta(\mathbf{S} - \mathbf{x}) \equiv \int_S \delta(\mathbf{x} - \mathbf{x}') dS(\mathbf{x}')$.

From Volterra dislocation to single crystal macroscopic plasticity - Orowan law



- Consider a crystal of volume V with 1 slip system (s)
- Each slip system is defined by 2 unit vectors: $\mathbf{m}^{(s)}$ (glide direction unit vector), $\mathbf{n}^{(s)}$ (unit normal vector to slip plane) where $\mathbf{b}^{(s)} = b\mathbf{m}^{(s)}$ (Burgers vector of dislocations)
- From Volterra loop, $U_{ij}^p(\mathbf{x}) = -b_i^{(s)} n_j^{(s)} \delta(\mathbf{S}^{(s)} - \mathbf{x})$, averaging in the crystal yields: $\overline{U_{ij}^p} = \frac{1}{V} \int_V U_{ij}^p(\mathbf{x}) dV$.
- Then: $\overline{U_{ij}^p} = \overline{\gamma}^{(s)} m_i^{(s)} n_j^{(s)}$, with $\overline{\gamma}^{(s)} = \frac{bS^{(s)}}{V}$ and $S^{(s)} = -\frac{1}{V} \int_V \delta(\mathbf{S}^{(s)} - \mathbf{x}) dV$

Orowan's law:

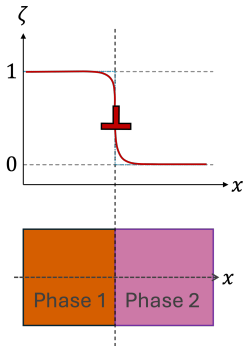
$$\dot{\overline{\gamma}}^{(s)} = \frac{b\dot{S}^{(s)}}{V} = \rho^{(s)} b v^{(s)} \quad (23)$$

Phase field model for dislocations vs. Volterra's description

- Plastic distortion tensor in phase field models for dislocations:

$$U_{ij}^p(\mathbf{x}) = \frac{b\zeta^{(s)}(\mathbf{x})}{d} m_i^{(s)} n_j^{(s)}$$

- Description with platelet inclusion of thickness d with smooth eigenstrain using dislocation phase field $\zeta^{(s)}(\mathbf{x})$ (Figure).



- In the limit $d \rightarrow 0$, Volterra's description is retrieved (see e.g. Rodney, Le Bouar and Finel, Acta Materialia 51, pp. 17–30, 2003).

Volterra equation for displacement field in homogeneous anisotropic media

- Introducing the eigendistorsion of the loop in Eq. (20) yields:

$$u_m(\mathbf{x}) = \int_V C_{ijkl} G_{mi,j}(\mathbf{x} - \mathbf{x}') b_k n_l \delta(\mathbf{S} - \mathbf{x}') dV'$$

- Using: $\int_V \delta(\mathbf{S} - \mathbf{x}') dV' = \int_S dS$ yields:

Volterra equation:

$$u_m(\mathbf{x}) = \int_S C_{ijkl} b_k G_{mi,j}(\mathbf{x} - \mathbf{x}') n_l dS' \quad (24)$$

Mura-Willis equation for stress field in anisotropic media

- The elastic (lattice) distortion tensor $\mathbf{U}_e$ for a Volterra's dislocation loop is given by $U_{mn}^e = u_{m,n} - U_{mn}^p$. Using Eqs. (24) and (22) yields:

$$\begin{aligned} U_{mn}^e(\mathbf{x}) &= \int_S C_{ijkl} b_k G_{mi,jn}(\mathbf{x} - \mathbf{x}') n_l dS' - b_m n_n \delta(\mathbf{S} - \mathbf{x}) \\ &= \int_S C_{ijkl} b_k G_{mi,jn}(\mathbf{x} - \mathbf{x}') n_l dS' - \int_S \delta(\mathbf{x} - \mathbf{x}') b_m n_n dS(\mathbf{x}') \end{aligned}$$

- Using Stokes theorem yields:

$$U_{ij}^e(\mathbf{x}) = \oint_L e_{jnh} C_{pqmn} G_{kp,q}(\mathbf{x} - \mathbf{x}') b_m \nu_h dL' \quad (25)$$

Mura-Willis equation is given from Hooke's law:

$$\sigma_{ij}(\mathbf{x}) = C_{ijkl} \oint_L e_{lnh} C_{pqmn} G_{ip,q}(\mathbf{x} - \mathbf{x}') b_m \nu_l dL'$$

Elastic energy of dislocations

- Self-energy of a dislocation loop and mutual interaction of two dislocation loops: Consider a material with 2 dislocations named A and B creating stress tensors σ_{ij}^A and σ_{ij}^B and elastic strain tensors $\varepsilon_{ij}^{e,A}$ and $\varepsilon_{ij}^{e,B}$
- Superposition principle in linear elasticity yields: $\sigma_{ij} = \sigma_{ij}^A + \sigma_{ij}^B$ and $\varepsilon_{ij}^e = \varepsilon_{ij}^{e,A} + \varepsilon_{ij}^{e,B}$

Elastic strain energy E :

$$E = \frac{1}{2} \int_V \sigma_{ij}(\mathbf{x}) \varepsilon_{ij}^e(\mathbf{x}) dV = E^{S,A} + E^{S,B} + E^I. \quad (26)$$

where $E^{S,A} = \frac{1}{2} \int_V \sigma_{ij}^A(\mathbf{x}) \varepsilon_{ij}^{e,A}(\mathbf{x}) dV$ and $E^{S,B} = \frac{1}{2} \int_V \sigma_{ij}^B(\mathbf{x}) \varepsilon_{ij}^{e,B}(\mathbf{x}) dV$ are self-energies of loops A and B , and E^I is the interaction energy between loops: $E^I = \int_V \sigma_{ij}^A(\mathbf{x}) \varepsilon_{ij}^{e,B}(\mathbf{x}) dV = \int_V \sigma_{ij}^B(\mathbf{x}) \varepsilon_{ij}^{e,A}(\mathbf{x}) dV$ (using $C_{ijkl} = C_{klij}$).

General expression for elastic energy

- Consider no applied traction or displacement from external loading, using the divergence theorem, the elastic energy E writes:

$$E = \frac{1}{2} \int_V \sigma_{ij}(\mathbf{x}) \varepsilon_{ij}^e(\mathbf{x}) dV = -\frac{1}{2} \int_V \sigma_{ij}(\mathbf{x}) U_{ij}^p(\mathbf{x}) dV$$

- Considering a Volterra dislocation loop L with boundary of slip plane S , the plastic distortion induced by slip $\mathbf{b}$ on S reads $U_{ij}^p dV = -b_i n_j dS$ for infinitesimal volume dV .

Final expression for E as surface integral:

$$E = \frac{1}{2} \int_S \sigma_{ij} b_i n_j dS \quad (27)$$

- The general formulation for self-energy of a dislocation loop is obtained by using Eq. (27) together with Mura-Willis equation for the stress field of a dislocation loop, see previous Eq. (34).
- For single screw and edge dislocations, the expressions of self-energy can be found in Hirth and Lothe (1982).

Application to isotropic elasticity

- From the Green's function in homogeneous isotropic elasticity (Eq. 18) together with the Stokes' theorem (see de Wiř (1960) for derivations):

The so-called Burgers formula (good practice exercise):

$$u_m(\mathbf{x}) = -\frac{b_m \Omega}{4\pi} - \frac{1}{4\pi} \oint_L \frac{e_{mlk} b_l dL'_k}{R} - \frac{1}{4\pi} \frac{\lambda + \mu}{\lambda + 2\mu} \left(\oint_L \frac{e_{kni} b_n R_i dL'_k}{R} \right)_{,m} \quad (28)$$

with Ω : solid angle at $\mathbf{x}$ by surface S , $R_i = x_i - x'_i$, $R = \sqrt{R_i R_i}$.

Interaction energy between loops L and L' (Blin (1955)'s formula):

$$E^I = -\frac{\mu}{2\pi} \oint_L \oint_{L'} \frac{e_{ijk} b_i b'_j e_{klm} dL_l dL'_m}{R} + \frac{\mu}{4\pi} \oint_L \oint_{L'} \frac{b_i b'_j dL_i dL'_j}{R} \quad (29)$$

$$+ \frac{\mu}{4\pi} \frac{1}{1 - \nu} \oint_L \oint_{L'} e_{kil} b_i R_{,km} e_{mjn} b'_j dL_l dL'_n$$

Peach-Koehler force on dislocation (driving force)

- Virtual displacement $\delta \mathbf{r}$ of a dislocation loop A of line vector $\boldsymbol{\nu}^A$, such that $\delta \mathbf{r} \cdot \boldsymbol{\nu}^A = 0$. The change of energy is: $\delta E = - \oint_{L_A} \mathbf{f}_i(\mathbf{x}) \delta r_i(\mathbf{x}) dL(\mathbf{x})$,

where $\mathbf{f}$ is a line force (per unit length) on L_A

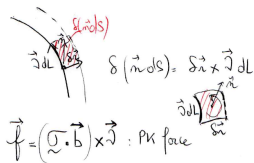
- Suppose only two dislocations A and B , the interaction energy is given by:

$$E^I = \int_V \sigma_{ij}^B(\mathbf{x}) \varepsilon_{ij}^{e,A}(\mathbf{x}) dV = \int_{S_A} \sigma_{ij}^B(\mathbf{x}) n_i^A b_j^A dS(\mathbf{x})$$

- Following the virtual displacement (see figure):

$$\delta(\mathbf{n}^A dS) = \delta \mathbf{r} \times \boldsymbol{\nu}^A dL \text{ and}$$

$$\delta E = \delta E_I = \oint_{L_A} \sigma_{ij}^B(\mathbf{x}) b_j^A e_{imn} \delta r_m(\mathbf{x}) \nu_n^A(\mathbf{x}) dL(\mathbf{x})$$



PK force expression (on dislocation loop A) due to B :

$$f_m(\mathbf{x}) = e_{min} \sigma_{ij}^B(\mathbf{x}) b_j^A \nu_n^A \Leftrightarrow \mathbf{f} = (\boldsymbol{\sigma} \cdot \mathbf{b}) \times \boldsymbol{\nu} \quad (30)$$

- The Peach and Koehler (1950) force is used in DDD codes to make evolve dislocations during plasticity (see M. Fivel's lecture)

Fourier transform (FT) method

Calculation examples

Solution of eigenstrain problems from Fourier transform (FT) method (Mura)

- Navier equation in elasticity with eigendistortion:

$$C_{ijkl}u_{k,lj} - C_{ijkl}U_{kl,j}^p = 0 \Leftrightarrow C_{ijkl}u_{k,lj} + f_i^* = 0 \quad (31)$$

Fourier Transform of Navier equation yields:

$$-C_{ijkl}\xi_l\xi_j\tilde{u}_k(\xi) + i\xi_j C_{ijkl}\tilde{U}_{kl}^p = 0 \Leftrightarrow K_{ik}(\xi)\tilde{u}_k(\xi) = \tilde{f}_i^*(\xi) \quad (32)$$

where $K_{ik}(\xi) = C_{ijkl}\xi_l\xi_j$ is the elastic acoustic tensor associated to anisotropic elastic medium and $\tilde{f}_i^*(\xi) = i\xi_j C_{ijkl}\tilde{U}_{kl}^p$ is the FT of f_i^* .

Displacement solution in Fourier space $\tilde{u}_k(\xi)$ is obtained by inverting the last equation:

$$\tilde{u}_i(\xi) = \tilde{G}_{ij}(\xi)\tilde{f}_j^*(\xi) \quad (33)$$

where $\tilde{G}_{ij}(\xi) = \tilde{K}_{ij}^{-1}(\xi)$ is the Fourier transform of the elastic Green function $G_{ij}(\mathbf{x})$ earlier defined in Eq. (13).

Field solutions in isotropic elasticity

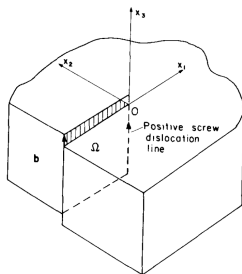
Expressions for isotropic elastic properties:

$$\begin{aligned}\widetilde{G}_{ik}(\boldsymbol{\xi}) &= \frac{1}{\mu} \left(\frac{\delta_{ik}}{\xi^2} - \frac{1}{2(1-\nu)} \frac{\xi_i \xi_k}{\xi^4} \right) \\ \widetilde{f}_j^*(\boldsymbol{\xi}) &= -i2\mu\xi_j \left(\widetilde{U}_{ij}^p(\boldsymbol{\xi}) + \frac{\nu}{1-2\nu} \delta_{ij} \widetilde{U}_{kk}^p(\boldsymbol{\xi}) \right)\end{aligned}\quad (34)$$

Field solutions in isotropic elasticity by inverse FT transforms:

$$\begin{aligned}u_k(\mathbf{x}) &= \frac{-i}{4\pi^3} \int_{V_\xi} \left(\frac{\delta_{ik}\xi_j}{\xi^2} - \frac{1}{2(1-\nu)} \frac{\xi_i \xi_j \xi_k}{\xi^4} \right) \left(\widetilde{U}_{ij}^p(\boldsymbol{\xi}) + \frac{\nu}{1-2\nu} \delta_{ij} \widetilde{U}_{qq}^p(\boldsymbol{\xi}) \right) e^{+i\boldsymbol{\xi} \cdot \mathbf{x}} dV_\xi \\ U_{lk}(\mathbf{x}) &= \frac{1}{4\pi^3} \int_{V_\xi} \left(\frac{\delta_{ik}\xi_j \xi_l}{\xi^2} - \frac{1}{2(1-\nu)} \frac{\xi_i \xi_j \xi_k \xi_l}{\xi^4} \right) \left(\widetilde{U}_{ij}^p(\boldsymbol{\xi}) + \frac{\nu}{1-2\nu} \delta_{ij} \widetilde{U}_{qq}^p(\boldsymbol{\xi}) \right) \\ &\quad \times e^{+i\boldsymbol{\xi} \cdot \mathbf{x}} dV_\xi \\ \varepsilon_{ij}(\mathbf{x}) &= \frac{1}{2} (U_{ij}(\mathbf{x}) + U_{ji}(\mathbf{x})) \\ \sigma_{ij}(\mathbf{x}) &= 2\mu \left(\varepsilon_{ij}(\mathbf{x}) - \varepsilon_{ij}^p(\mathbf{x}) + \frac{\nu}{1-2\nu} \delta_{ij} (\varepsilon_{qq}(\mathbf{x}) - \varepsilon_{qq}^p(\mathbf{x})) \right)\end{aligned}$$

Application 1: Infinite straight screw dislocation



- Non-zero plastic distortion from Eq. (22):
 $U_{32}^p(\mathbf{x}) = b\delta(x_2)H(-x_1)$ where $H(x)$ is the 1D Heaviside function and $\delta(x)$ is the 1D delta Dirac function: good practice exercise, see solutions in Mura (1987)' book.

- Fourier transform: $\widetilde{U_{32}^p}(\boldsymbol{\xi}) = -\frac{b}{(2\pi)^2} \frac{\delta(\xi_3)}{i\xi_1}$

- Displacements (from Eqs. (35)):

$$u_1(\mathbf{x}) = u_2(\mathbf{x}) = 0$$

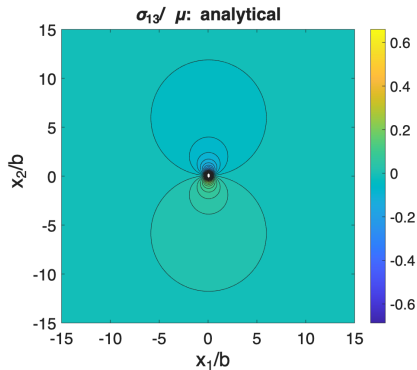
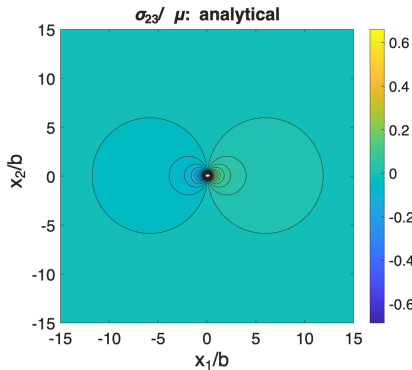
$$u_3(\mathbf{x}) = \frac{b}{2\pi} \tan^{-1}(x_2/x_1) = \frac{b\theta}{2\pi}$$

- Non zero stresses (see Eq. (35)):

$$\sigma_{13}(\mathbf{x}) = -\frac{\mu b}{2\pi} \frac{x_2}{x_1^2 + x_2^2}$$

$$\sigma_{23}(\mathbf{x}) = \frac{\mu b}{2\pi} \frac{x_1}{x_1^2 + x_2^2}$$

Stress results: single screw dislocation (in aluminium)



Application 2: Infinite straight edge dislocation

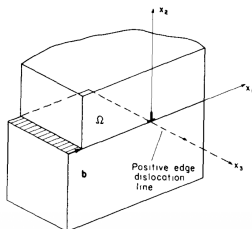
- Non-zero plastic distortion from Eq. (22):
 $U_{12}^p(\mathbf{x}) = b\delta(x_2)H(-x_1)$ (see Mura (1987))

- Fourier transform: $\widetilde{U_{12}^p}(\boldsymbol{\xi}) = -\frac{b}{(2\pi)^2} \frac{\delta(\xi_3)}{i\xi_1}$

- Non-zero displacements (see Eqs. (35)):

$$u_1(\mathbf{x}) = \frac{b}{2\pi} \tan^{-1}(x_2/x_1) + \frac{b}{4\pi(1-\nu)} \frac{x_1 x_2}{x_1^2 + x_2^2}$$

$$u_2(\mathbf{x}) = -\frac{b(1-2\nu)}{8\pi(1-\nu)} \ln(x_1^2 + x_2^2) + \frac{b}{8\pi(1-\nu)} \frac{x_2^2 - x_1^2}{x_1^2 + x_2^2}$$



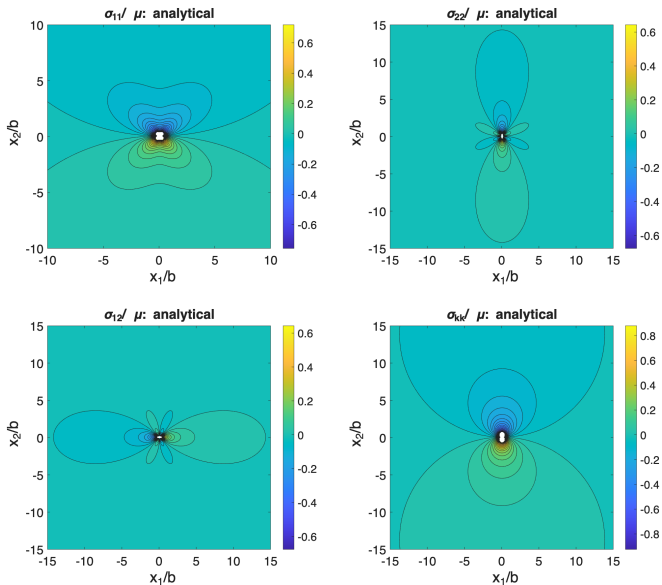
- Non zero stresses (see Eq. (35)) (with $\sigma_{33} = \nu(\sigma_{11} + \sigma_{22})$ in plane strain):

$$\sigma_{11}(\mathbf{x}) = -\frac{\mu b}{2\pi(1-\nu)} \frac{x_2(3x_1^2 + x_2^2)}{(x_1^2 + x_2^2)^2}$$

$$\sigma_{22}(\mathbf{x}) = \frac{\mu b}{2\pi(1-\nu)} \frac{x_2(x_1^2 - x_2^2)}{(x_1^2 + x_2^2)^2}$$

$$\sigma_{12}(\mathbf{x}) = \sigma_{21}(\mathbf{x}) = \frac{\mu b}{2\pi(1-\nu)} \frac{x_1(x_1^2 - x_2^2)}{(x_1^2 + x_2^2)^2}$$

Stress results: single edge dislocation (in aluminium)



Stroh formalism and example

Eshelby-Stroh-Lekhnitskii formalism in anisotropic elasticity: two-dimensional solutions

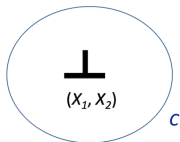
- From equilibrium equation (Navier equation, see Eq. (12) without body force $f_i = 0$): $C_{ijkl}u_{k,lj} = 0$
- Consider displacement vector in 2D: $u_k(x_1, x_2)$ yields:
 $C_{i1\underline{k}1}u_{\underline{k},11} + (C_{i1\underline{k}2} + C_{i2\underline{k}1})u_{\underline{k},11}u_{\underline{k},12} + C_{i2\underline{k}2}u_{\underline{k},22} = 0$ (sum on k)
- Solution in the form of: $u_k = a_k f(z)$ with $z = x_1 + px_2$ then Navier's equation becomes:
 $(C_{i1\underline{k}1} + p(C_{i1\underline{k}2} + C_{i2\underline{k}1}) + p^2 C_{i2\underline{k}2}) a_{\underline{k}} = 0$
- Non-trivial solution (sextic equation in p , 3 pairs of complex conjugates): $\det(C_{i1\underline{k}1} + p(C_{i1\underline{k}2} + C_{i2\underline{k}1}) + p^2 C_{i2\underline{k}2}) = 0$

General displacement solution ((Eshelby et al. (1953), Stroh (1958) and Lekhnitskii (1963), see also: Ting (1996), Hwu (2010)):

$$u_i = 2\text{Re} \sum_{j=1}^3 A_{ij} f_{\underline{j}}(z_{\underline{j}}) \quad (36)$$

where $\mathbf{A}$ is a 3×3 matrix containing eigenvector components $a_{\underline{k}\alpha}$, and $z_{\alpha} = x_1 + p_{\alpha}x_2$ with eigenvalues p_{α}

Application to single straight dislocations in homogeneous anisotropic media



$$u_i = 2\text{Re} \sum_{j=1}^3 \left(A_{ij} f_j(z_j) \right)$$

J.D. Eshelby, *Acta Metall* 1, (1953)

A. N. Stroh, *Philos Mag* 3 (1958)

Z. Suo, *Proc R Soc Lond A* 427 (1990)

- Definition of Burgers vector (see Eq. (21)): $b_i = \oint_C du_i$ where C is the Burgers circuit encircling the dislocation (with line vector $\parallel x_3$).

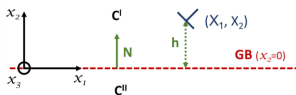
Then, for any position $z_i = x_1 + p_i x_2$ in the plane, the vector function $\mathbf{f}^0$ (for homogeneous medium 0) yields:

$$f_j^0(z_i) = q_j^0 \ln(z_i - s_j) \quad (37)$$

with $s_j = X_1 + p_j X_2$ (dislocation position in the plane) q_j^0 is a complex vector given by:

$$\mathbf{q}^0 = -i \frac{1}{2\pi} \mathbf{B}^T \mathbf{b} \text{ with } B_{ij} = (C_{i2\underline{k}1} + p_j C_{i2\underline{k}2}) A_{\underline{k}j} \quad (38)$$

Application to single straight dislocations in bi-crystals



M.O. Tucker, *Philos Mag* 19 (1969)

V.K. Tewary et al., *J Mater Res.* 4 (1989)

Z. Suo, *Proc R Soc Lond A* 427 (1990)

T.T.C. Ting, *Q J Mech Appl Math* 45 (1996)

Interface condition for perfect bonded interface (displacement and traction continuities) are applied: $u_i^I(x_2 = 0^+) = u_i^{II}(x_2 = 0^-)$ and $\sigma_{i2}^I(x_2 = 0^+) = \sigma_{i2}^{II}(x_2 = 0^-)$

In the case of a bi-crystal ($I + II$), for position $z_j = x_1 + p_j x_2$ in the plane, the vector function $\mathbf{f}$ yields:

$$f_j(z_j) = \begin{cases} f_j^0(z_j) + f_j^I(z_j) & \text{if } x_2 > 0 \\ f_j^{II}(z_j) & \text{if } x_2 < 0 \end{cases}$$

where $f_j^0(z_j)$ is the homogeneous solution.

The expressions for $f_j^I(z_j)$ and $f_j^{II}(z_j)$ are:

$$\begin{aligned} f_j^I(z_j) &= \overline{V_{j\underline{k}}^{I,II}} \overline{f_{\underline{k}}^0(z_j)} \\ f_j^{II}(z_j) &= W_{j\underline{k}}^{I,II} f_{\underline{k}}^0(z_j) \end{aligned} \quad (39)$$

with:

$$\begin{aligned} V^{I,II} &= \left(B^{II} A^{II-1} \overline{A^I} - \overline{B^I} \right)^{-1} \left(B^I - B^{II} A^{II-1} A^I \right) \\ W^{I,II} &= \left(\overline{B^I A^{I-1}} A^{II} - B^{II} \right)^{-1} \left(\overline{B^I A^{I-1}} A^I - B^I \right) \end{aligned}$$

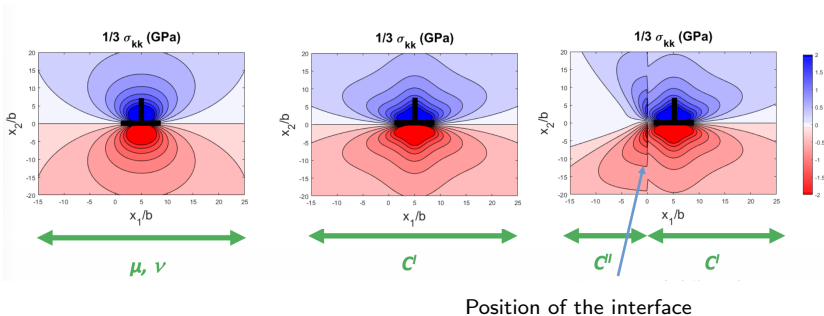
Effect of elastic anisotropy on pressure field in Ag

- Case of silver (Ag) (misorientation of 40 deg. for bicrystal)

Homogeneous iso.

Homogeneous aniso.

Heterogeneous aniso.



- Calculations performed in the PhD thesis of J. Petrazoller (Univ. Lorraine, 2025)
- See also PhD thesis of X. Chen (Univ. Lorraine, 2020) (<https://github.com/AniPlas>).

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