Le Centre Francophone en Mathématique a été organisé à Bucarest pour une periode de 4 ans a partir du 1-er Janvier 2017,
par l'Agence Universitaire de la Francophonie et l'Institut de Mathématique Simion Stoilow de l'Académie Roumaine
en parteneriat avec la Faculté de Mathématique et Informatique de l'Université de Bucarest et le GDRI ECO-Math.

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Modélisation par champs des phases de la déformations des cristaux

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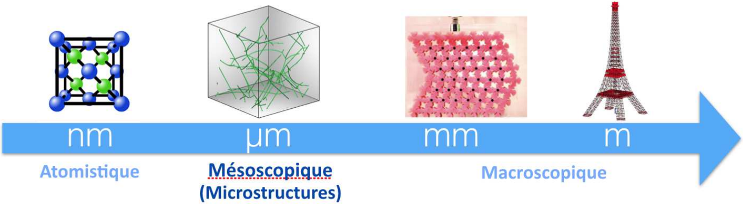
Phase field method is based on the Ginzburg-Landau theory of phase transitions. In this theory, a continuous function, so-called order parameter, has been introduced to describe the equilibrium thermo-dynamical properties of a system that undergoes a phase transition. In this course, we will apply this theory to describe solid-to-solid phase transformations, as observed in martensitic materials, where crystallographic relation between different solid phases has to be taken into account in order to reproduce properly the elastic interactions. Secondly, we will present a theory that goes beyond the classical Landau theory in order to study the coupling between phase transition and plasticity using GL(2,Z) group symmetry.

Retour

Plan: Introduction to continuum mechanics

- Motivation
- Review of linear algebra
- Lagrangian description of deformation
- Eulerian description of deformation (Ionescu)
- Strain
- Small strain approximation
- Continuum Theory of Crystalline Solids
- Plasticity and Dislocations

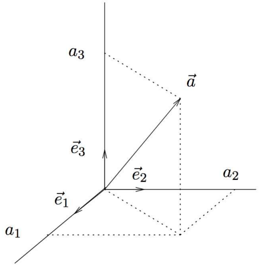
Scale of continuum mechanics



- In classical continuum mechanics, the world is idealized as a three dimensional Euclidean space
- A point in space is identified by a unique set of three real numbers (x_1, x_2, x_3)
- A Euclidean space is endowed with a metric, which defines the distance between points: $d = \sqrt{x_i x_i}$
- Matter is idealized as a continuum, which has two properties: (i) it is infinitely divisible (you can subdivide some region of the solid as many times as you wish); and (ii) it is locally homogeneous

Vector and Matrices

- vector: $\boldsymbol{a} = (a_1, a_2, a_3)$
- inner product : $\boldsymbol{a} \cdot \boldsymbol{b} = a_1 b_1 + a_2 b_2 + a_3 b_3$
- Einstein summation on repeated indices: $\boldsymbol{a} \cdot \ \boldsymbol{b} = \sum_{i=1}^{3} a_i b_i = a_i b_i$
- Matrix representation: $\boldsymbol{a} = a_1 \boldsymbol{e}_1 + a_2 \boldsymbol{e}_2 + a_3 \boldsymbol{e}_3 = \sum_i a_i \boldsymbol{e}_i = a_i \boldsymbol{e}_i$
- Components: $a_i = \boldsymbol{a}.\boldsymbol{e}_i$

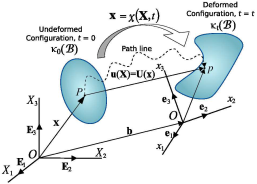


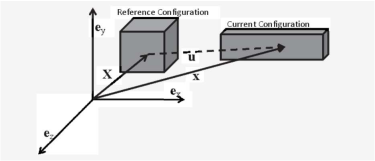
Matrices

- In any fixed rectangular cartesian coordinates a matrix defines a linear transformation
- $A_{m,n} = \begin{pmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,n} \\ A_{2,1} & A_{2,2} & \cdots & A_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m,1} & A_{m,2} & \cdots & A_{m,n} \end{pmatrix}$
- matrix-vector product $\boldsymbol{b} = \boldsymbol{Aa} \Longrightarrow b_i = A_{ij} a_j$
- tensorial product
  $\boldsymbol{a} \otimes \boldsymbol{b} : \quad (\boldsymbol{a} \otimes \boldsymbol{b})\boldsymbol{c} = (\boldsymbol{b} \cdot \boldsymbol{c})\boldsymbol{a}, \quad \forall \boldsymbol{c}, \quad (\boldsymbol{a} \otimes \boldsymbol{b})_{ij} = a_i b_j$
- matrix inner product $\boldsymbol{A} : \boldsymbol{B} = A_{ij} B_{ij}$
- matrix product $\boldsymbol{AB} = \boldsymbol{C} \Longrightarrow C_{ij} = A_{ik} B_{kj}$
- We can also represent a second order tensor as: $\mathbf{A} = A_{ij} \mathbf{e}_i \otimes \mathbf{e}_j$
- Tranpose: switch rows and columns
- Tranpose: $(\boldsymbol{A} \cdot \boldsymbol{B})^T = \boldsymbol{B}^T . \boldsymbol{A}^T$
- Trace: $\sum_i A_{ii} = A_{ii}$

Continuum kinematics

- Lagrangian description of deformation $\mathbf{x}(\mathbf{X}) = \mathbf{X} + \mathbf{u}(\mathbf{X})$
- **Material coordinates:** $\mathbf{X} = (X_1, X_2, X_3)$
- $\boldsymbol{u}(\boldsymbol{X})$ **is the displacement vector**
- **Deformation:** $\boldsymbol{x}(\boldsymbol{X}) = (x_1(\boldsymbol{X}), x_2(\boldsymbol{X}), x_3(\boldsymbol{X}))$





Continuum kinematics

- Example of homogenous deformation: $x_1 = \frac{1}{\sqrt{2}}X_1 - \sqrt{1}X_2 + 3$, $x_2 = \frac{1}{\sqrt{2}}X_1 + \sqrt{1}X_2 + 3$, $x_3 = X_3$

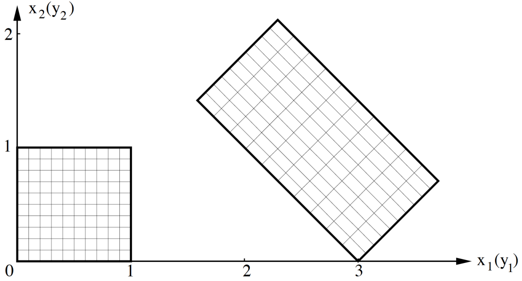


Figure 2.2: Example of a homogeneous deformation. The reference configuration on the left deforms to the deformed configuration on the right under the deformation described in Eq. (2.15).

Continuum kinematics

- Example of inhomogenous deformation:
  $x_1 = X_1 + 0.1\sin(2\pi X_2) + 2,\ x_2 = X_2 + 0.1X_1,\ x_3 = X_3$

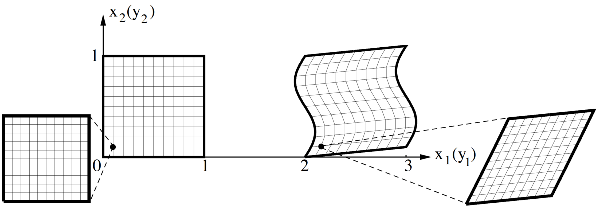


Figure 2.3: Example of an inhomogeneous deformation. The reference configuration on the left deforms to the deformed configuration on the right under the deformation described in Eq. (2.16). Notice that under sufficient magnification, an inhomogeneous deformation can be approximated locally by a homogeneous deformation.

Continuum kinematics

- Deformation gradient $\mathbf{F} = (\nabla \mathbf{x})_{\mathbf{ij}} = \frac{\partial x_i}{\partial X_j} = \boldsymbol{I} + \frac{\partial u_i}{\partial X_j}$
- $\mathbf{F}(\mathbf{x}) = \nabla \mathbf{x}(\mathbf{X})$
- e.g.: $F_{m,n} = \begin{pmatrix} 1/\sqrt{2} & -\sqrt{2} & 0 \\ 1/\sqrt{2} & \sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$
- All homogenous deformation can be written as $\mathbf{x} = \mathbf{F}\mathbf{X} + \mathbf{c}$
- $\mathbf{F}$ is a constant matrix
- $\mathbf{c}$ is a translation vector

Deformation of a continuous body

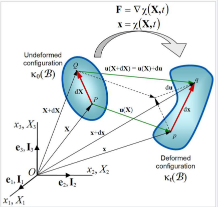


Figure 2. Deformation of a continuum body.

- infinitesimal element of a continuous body $d\mathbf{X} = (dX_1, dX_2, dX_3)$
- It is possible to show that (using Taylor expansion around a point of deformation) $d\mathbf{x} = \mathbf{F}(\mathbf{X}) \cdot d\mathbf{X} = \mathbf{F}_{ik} d\mathbf{X}_k$
- $dx_i = X_i + dX_i + u(X_k + dX_k) - (X_i + u_i)$
- $u(X_k + dX_k) \approx u_i(X_k) + \frac{\partial u_i}{\partial X_k} dX_k$
- Therefore $dX_i = dx_i + \frac{\partial u_i}{\partial X_k} dX_k = (\delta_{ik} + \frac{\partial u_i}{\partial X_k} dX_k)$
- $\mathbf{F}(\mathbf{X}) = \nabla \mathbf{x}(\mathbf{X})$

Non-linear strain tensor: Cauchy-Green

- Consider two line elements in the reference configuration $d\boldsymbol{X}^{(1)}$, $d\boldsymbol{X}^{(2)} \Longrightarrow d\boldsymbol{x}^{(1)}$, $d\boldsymbol{x}^{(2)}$
- $d\boldsymbol{x}^{(1)} \cdot d\boldsymbol{x}^{(2)} = (\boldsymbol{F} d\boldsymbol{X}^{(1)}) \cdot (\boldsymbol{F} d\boldsymbol{X}^{(2)}) = d\boldsymbol{X}^{(1)}(\boldsymbol{F}^T \boldsymbol{F}) d\boldsymbol{X}^{(2)} = d\boldsymbol{X}^{(1)} \boldsymbol{C} d\boldsymbol{X}^{(2)}$
- The right Cauchy-Green strain: $\boldsymbol{C} = \boldsymbol{F}^T \boldsymbol{F}$
- Cauchy-Green strain: $C_{ij} = F_{kl} F_{kj}$
- $\boldsymbol{I}$ is the identity matrix
- Properties: symmetric, positive and non-linear with respect to $\boldsymbol{F}$
- $\boldsymbol{C}^T (\boldsymbol{F}^T \boldsymbol{F})^T = \boldsymbol{F}^T (\boldsymbol{F}^T)^T = \boldsymbol{F}^T \boldsymbol{F} = \boldsymbol{C}$

Non-linear strain tensor: Green-Lagrange

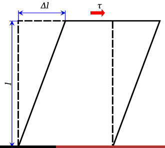
- Variation of lengths: $d\boldsymbol{X}^{(1)} = d\boldsymbol{X}^{(2)} = d\boldsymbol{X} = dl_0\boldsymbol{n}_0 \rightarrow d\boldsymbol{x}^{(1)} = d\boldsymbol{x}^{(2)} = d\boldsymbol{x} = dl\boldsymbol{n}$
- $|\boldsymbol{n}_0| = |\boldsymbol{n}| = 1$
- $dl^2 - dl_0^2 = |d\boldsymbol{x}|^2 - |d\boldsymbol{X}|^2 = d\boldsymbol{X}2\boldsymbol{E}d\boldsymbol{X} - d\boldsymbol{X}\cdot d\boldsymbol{X} = 2(d\boldsymbol{n}_0\boldsymbol{E}d\boldsymbol{n}_0)dl_0^2$
- Green-Lagrange: $\boldsymbol{E} = \frac{\boldsymbol{F}^T\boldsymbol{F}-\boldsymbol{I}}{2}$
- $\frac{dl^2-dl_0^2}{dl_0^2} = 2d\boldsymbol{n}_0\boldsymbol{E}d\boldsymbol{n}_0$
- Relative length variation in direction of $\boldsymbol{n}_0$
- The diagonal components of the Lagrangian finite strain tensor are related length change of elements
- What is the physical meaning ?
- Take a line element in the 1-direction $d\boldsymbol{X}_1 = [d\mathbf{X_1}, 0, 0]$‘
- Define the stretch: $\lambda = \frac{|d\boldsymbol{x}_1|}{|d\boldsymbol{X}_1|} \Longrightarrow \lambda^2 = (\frac{|d\boldsymbol{x}_1|}{|d\boldsymbol{X}_1|})^2 = d\boldsymbol{X}_1\boldsymbol{C}d\boldsymbol{X}_1 = C_{11}$
- compression: $\lambda < 1$, extension: $\lambda > 1$ and unstretched : $\lambda = 1$
- $\Longrightarrow \boldsymbol{E}_{11} = \frac{1}{2}(C_{11} - 1) = \frac{1}{2}\lambda^2 - 1$
- The square of the stretch of this element is λ_1^2 then $E_{11} = \frac{\lambda_1^2-1}{2}$

Physical interpretation of the finite strain tensor

- Variation of angles: $d\boldsymbol{X}^{(1)} = dl_0^{(1)}\boldsymbol{n}_0; d\boldsymbol{X}^{(2)} = dl_0^{(2)}\boldsymbol{m}_0 \rightarrow$ $d\boldsymbol{x}^{(1)} = dl^{(1)}\boldsymbol{n}; d\boldsymbol{x}^{(2)} = dl^{(2)}\boldsymbol{m}$
- Let θ denote the angle between the deformed elements which were initially parallel to X_1 and X_2
- $\boldsymbol{n}_0 \cdot \boldsymbol{m}_0 = \cos(\theta_0)$ and $\boldsymbol{n} \cdot \boldsymbol{m} = \cos(\theta)$
- $d\boldsymbol{x}^{(1)} \cdot d\boldsymbol{x}^{(2)} - d\boldsymbol{X}^{(1)} \cdot d\boldsymbol{X}^{(2)} = d\boldsymbol{X}^{(1)} 2\boldsymbol{E} d\boldsymbol{X}^{(2)} - d\boldsymbol{X}^{(1)} \cdot d\boldsymbol{X}^{(2)} =$ $2(d\boldsymbol{n}_0 \boldsymbol{E} d\boldsymbol{m}_0) dl_0^{(1)} dl_0^{(2)}$
- The angle between two vectors is given by: $\cos(\theta) = \frac{d\mathbf{x_1}}{|d\mathbf{x_1}|} \cdot \frac{d\mathbf{x_2}}{|d\mathbf{x_2}|}$
- e.g., $\cos(\theta) = \frac{\cos(\theta_0) + 2(\boldsymbol{E}\boldsymbol{m}_0) \cdot \boldsymbol{n}_0}{\sqrt{(\boldsymbol{E}+1)\boldsymbol{n}_0 \cdot \boldsymbol{n}_0}\sqrt{(\boldsymbol{E}+1)\boldsymbol{m}_0 \cdot bm_0}}$

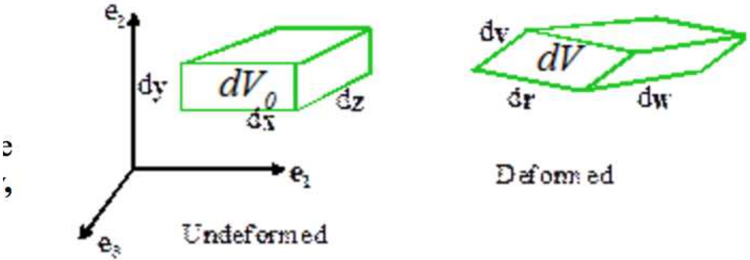
Example: shear

- Shear: $\boldsymbol{F} = \boldsymbol{I} + \alpha(\boldsymbol{e}_1 + \boldsymbol{e}_2)$ such that $\boldsymbol{e}_1 \perp \boldsymbol{e}_2$
- Let's choose $\boldsymbol{e}1 = (1,0)$ and $\boldsymbol{e}2 = (0,1)$ and α is the shear strength
- $x_1 = X_1 + \alpha X_2, x2 = X2, x3 = X3$
- $F_{m,n} = \begin{pmatrix} 1 & \alpha & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ $C_{m,n} = \begin{pmatrix} 1 & \alpha & 0 \\ \alpha & 1+\alpha^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
  $E_{m,n} = \begin{pmatrix} 0 & \alpha & 0 \\ \alpha & \alpha^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
- $\cos(\theta) = \frac{2E_{12}}{\sqrt{2E_{11}+1}\sqrt{2E_{22}+1}}$
- The off-diagonal components of the Lagrangian finite strain tensor are related to shear strain



Volume change

- Consider a differential material volume dV at some material point that goes to dv after deformation
- How to measure the volume change ?
- Reference volume: $dV_0 = d\mathbf{Z}.(d\mathbf{X} \times d\mathbf{Y})$
- Deformed volume: $dv = d\mathbf{W}.(d\mathbf{R} \times d\mathbf{V})$
- It is easy to show that the volume change: $J = dv = (det\mathbf{F}(\mathbf{X}))dV_0$



Polar decomposition theorem

- A rotation matrix: $\boldsymbol{R}$ such that $\boldsymbol{R}\boldsymbol{R}^T = \boldsymbol{R}^T\boldsymbol{R}$=**I** ($det\boldsymbol{R} = I$).
- Polar decomposition theorem: For any matrix **F** with $det\mathbf{F} > \mathbf{0}$, there exists an unique rotation $\boldsymbol{R}$ and an unique positive-definite symmetric matrix $\boldsymbol{U}$ such that

$$\boldsymbol{F} = \boldsymbol{R}\boldsymbol{U}$$

- how to calculate it ? Calculate the Cauhy-Green strain tensor $\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}$ and then $\boldsymbol{U} = \sqrt{\boldsymbol{C}}$, i.e. Find the eigenvalues $\{\gamma_1, \gamma_2, \gamma_3\}$ and eigenvectors $\{\boldsymbol{u}_1, \boldsymbol{u}_2, \boldsymbol{u}_3\}$ of $\boldsymbol{C}$ calculate $\mu_i = \sqrt{\gamma_i}$ and then $\boldsymbol{U}$ is the matrix with eigenvalues $\{\mu_1, \mu_2, \mu_3\}$ and the corresponding eigenvectors such that

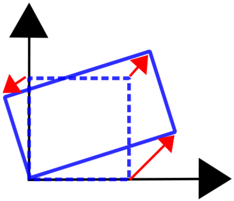
$$\boldsymbol{U} = \mu_1\boldsymbol{u}_1 \otimes \boldsymbol{u}_1 + \mu_2\boldsymbol{u}_2 \otimes \boldsymbol{u}_2 + \mu_3\boldsymbol{u}_3 \otimes \boldsymbol{u}_3$$

$$\boldsymbol{R} = \boldsymbol{F}\boldsymbol{U}^{-1}$$

- Ajoute un example

Polar decomposition example

- Example of deformation: $x_1 = 1.3X_1 - 0.375X_2$ and $x_2 = 0.75X_1 + 0.65X_2$
- $F_{m,n} = \begin{pmatrix} 1.3 & -0.375 & 0 \\ 0.75 & 0.65 & 0 \\ 0 & 0 & 1 \end{pmatrix}$



Polar decomposition example

- Example of deformation: $x_1 = 1.3X_1 - 0.375X_2$ and $x_2 = 0.75X_1 + 0.65X_2$
- $F_{m,n} = \begin{pmatrix} 1.3 & -0.375 & 0 \\ 0.75 & 0.65 & 0 \\ 0 & 0 & 1 \end{pmatrix}$, $\boldsymbol{F}^T\boldsymbol{F} = \begin{pmatrix} 2.25 & 0 & 0 \\ 0 & 0.563 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \boldsymbol{U}^T\boldsymbol{U}$
- $U_{m,n} = \begin{pmatrix} \sqrt{2.25} & 0 & 0 \\ 0 & \sqrt{0.563} & 0 \\ 0 & 0 & 1 \end{pmatrix}$
- $\boldsymbol{F}\boldsymbol{U}^{-1} = \boldsymbol{R}\boldsymbol{U}\boldsymbol{U}^{-1} = \boldsymbol{R} = \begin{pmatrix} 0.86 & -0.5 & 0 \\ 0.5 & 0.86 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cos(\theta) & -\sin(\theta) & 0 \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Linear strain

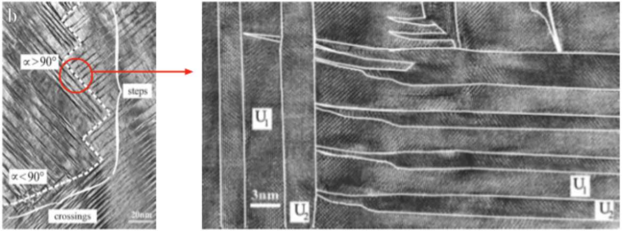
- The Green-Lagrange strain: $\boldsymbol{E} = \boldsymbol{F}^T\boldsymbol{F} - \boldsymbol{I}$
- How it looks in terms of displacement ?
- $\boldsymbol{E} = \frac{1}{2}(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i} + \frac{\partial u_i}{\partial X_j}\frac{\partial u_j}{\partial X_i})$
- For small deformation $\frac{\partial u_i}{\partial X_j} \ll 1$, we obtain
- $\epsilon = \frac{1}{2}(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i})$
- It works well up to $1 - 2\%$ of deformation

Linear strain (2)

- Infinitesimal volume change: $\mathbf{tr}(\epsilon) = \epsilon_{ii}$
- rotation: $\omega = \frac{1}{2}(\frac{\partial u_i}{\partial X_j} - \frac{\partial u_j}{\partial X_i})$
- additive decomposition of deformation gradient:
- $\frac{\partial u_i}{\partial X_j} = \epsilon_{ij} + \omega_{ij}$

Comparaison small-strain and large deformation (2)

- Apply a pure rigid body rotation $\boldsymbol{F} \to \boldsymbol{RF}$
- Calculate non-linear strain:
  $\boldsymbol{E} = \boldsymbol{F}^T\boldsymbol{F} = (\boldsymbol{RF})^T\boldsymbol{RF} = \boldsymbol{F}^T\boldsymbol{R}^T\boldsymbol{RF} = \boldsymbol{F}^T\boldsymbol{F}$
- Calculate linear strain:
  $\epsilon = (\boldsymbol{F}^\mathbf{T} + \boldsymbol{F} - 2\mathbf{I})/2 = (\boldsymbol{RF})^\mathbf{T} + \boldsymbol{RF} \neq (\boldsymbol{F}^\mathbf{T} + \boldsymbol{F} - 2\mathbf{I})/2$



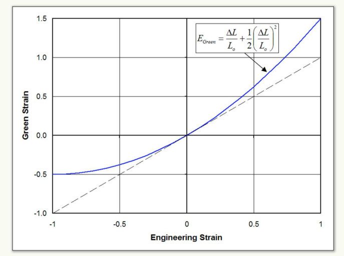
collision between laminates

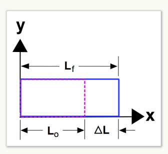
needle bending, tapering and splitting in $Ni_{65}Al_{35}$

Boullay et al., Phys. Rev. (2001), Acta.Mater., (2002)

Comparaison small-strain and large deformation

- Uniaxial loading: elongate a bar of length L_0 by ΔL
- Lagrangian displacement: $u(\boldsymbol{X}) = \frac{\boldsymbol{X}}{L_0}(L_f - L_0)$
- $\alpha = \frac{\Delta L}{L_0}$
- Uniaxial tension $F_{11} = 1 + \frac{\partial u}{\partial X} = 1 + \alpha$
- $C_{11} = \alpha + \frac{\alpha^2}{2}$
- $\epsilon_{11} = \alpha$



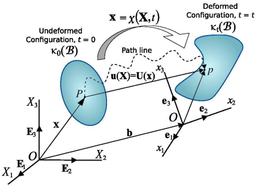


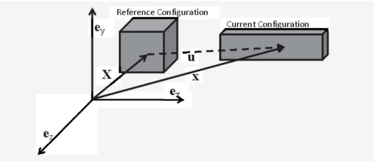
A brief recall: Eulerian coordinates

- We consider a ball thrown vertically under a gravity field g
- Newton equation: $F = m\ddot{\mathbf{x}} = mg$
- Lagrangian coordinates: $x(X_0, t) = X_0 + V_0 t - \frac{gt^2}{2}$
- Velocity at Lagrangian coordinates: $V(X_0, t) = \frac{dx(X_0,t)}{dt} = V_0 - gt$
- Now find the time t using the equation of coordinates $x(X_0, t) \rightarrow$ $t = \frac{V_0 - \sqrt{-2gx + 2gX_0 + V_0^2}}{g}$
- Insert the solution into velocity at Lagrangian coordinates $V(X_0, t)$
- Eulerian description (fixed frame): $V(x) = -(V_0 - [2g(X - X_0)]^{1/2})$
- It implies $V^E(x, t) = V^L(X_0, t)$
- $\frac{df^L}{dt} = \frac{\partial f^E}{\partial t} + \frac{\partial f^E}{\partial x}\frac{\partial x}{\partial t} \rightarrow \frac{DF}{dt} = \frac{\partial f^E}{\partial t} + \mathbf{v} \cdot \nabla f^E$

Continuum kinematics

- Eulerian description of deformation $\boldsymbol{X}(\boldsymbol{x}) = \boldsymbol{x} - \boldsymbol{U}(\boldsymbol{x})$
- Spatial coordinates: $\boldsymbol{x} = (x_1, x_2, x_3)$
- $\boldsymbol{U}(\boldsymbol{x})$ is the displacement vector
- Deformation: $\boldsymbol{X}(\boldsymbol{x}) = (X_1(\boldsymbol{x}), X_2(\boldsymbol{x}), X_3(\boldsymbol{x}))$
- One can show that $\boldsymbol{U}(\boldsymbol{x}) = \boldsymbol{u}(\boldsymbol{X})$





Continuum kinematics

- What happens to deformation gradient $\boldsymbol{F}$?
- $\boldsymbol{F}(\boldsymbol{x}) = \nabla \mathbf{X}(\mathbf{x}) = \boldsymbol{F}^{-\mathbf{1}}(\boldsymbol{X})$
- Deformation gradient $\boldsymbol{F}^{-1} = (\nabla \boldsymbol{x})_{ij} = \frac{\partial X_i}{\partial x_j} = \boldsymbol{I} - \frac{\partial U_i(\boldsymbol{x})}{\partial \boldsymbol{x}_j}$
- All homogenous deformation can be written as $\boldsymbol{X} = \boldsymbol{F}^{-1}\boldsymbol{x} + \boldsymbol{c}$
- $\boldsymbol{F}^{-1}$ is a constant matrix which is the inverse of $\boldsymbol{F}$
- **c** is a translation vector

The Left Cauchy-Green Strain

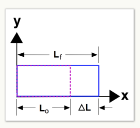
- define strain as $\frac{l^2-l_0^2}{l^2}$
- Consider two line elements in the reference configuration $d\boldsymbol{x}^{(1)}$, $d\boldsymbol{x}^{(2)} \Longrightarrow d\boldsymbol{X}^{(1)}$, $d\boldsymbol{X}^{(2)}$
- $d\boldsymbol{X}^{(1)} \cdot d\boldsymbol{X}^{(2)} = (\boldsymbol{F}^{-1} d\boldsymbol{x}^{(1)}) \cdot (\boldsymbol{F}^{-1} d\boldsymbol{x}^{(2)}) = d\boldsymbol{X}^{(1)} (\boldsymbol{F}^{-T} \boldsymbol{F}^{-1}) d\boldsymbol{X}^{(2)} = d\boldsymbol{X}^{(1)} \boldsymbol{b}^{-1} d\boldsymbol{X}^{(2)}$
- The left Cauchy-Green strain: $\boldsymbol{b} = \boldsymbol{F}\boldsymbol{F}^T$
- The left Cauchy-Green strain: $b_{ij} = F_{ik} F_{jk}$
- How it is related to the the right Cauchy-Green strain ?
- $\boldsymbol{C} = \boldsymbol{F}^{-1} \boldsymbol{b} \boldsymbol{F}$, and $\boldsymbol{b} = \boldsymbol{F} \boldsymbol{C} \boldsymbol{F}^{-1}$

Non-linear strain tensor: Euler-Almansi

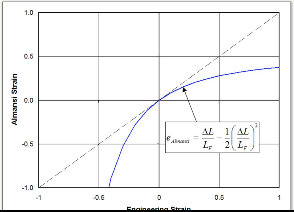
- $\frac{|d\boldsymbol{x}|^2 - |d\boldsymbol{X}|^2}{2}$
- This time use $d\boldsymbol{X} = \boldsymbol{F}^{-1} d\boldsymbol{x}$
- $d\boldsymbol{x} \cdot d\boldsymbol{x} - d\boldsymbol{X} \cdot d\boldsymbol{X} = d\boldsymbol{x} \cdot d\boldsymbol{x} - (\boldsymbol{F}^{-1} d\boldsymbol{x})(\boldsymbol{F}^{-1} d\boldsymbol{x}) =$
  $d\boldsymbol{x} \cdot (\boldsymbol{I} - \boldsymbol{F}^{-T}\boldsymbol{F}^{-1}) \cdot d\boldsymbol{x} = d\boldsymbol{x} \cdot \boldsymbol{e} \cdot d\boldsymbol{x}$
- Almansi-Euler: $\boldsymbol{e} = (\boldsymbol{I} - \boldsymbol{F}^{-T}\boldsymbol{F}^{-1})$
- The diagonal components of the Euler finite strain tensor are related length change of elements (again!!)

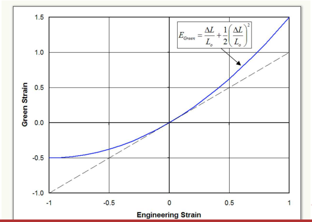
Uniaxial tension with the Almansi strain tensor

- Lagrangian displacement: $\boldsymbol{U}(\boldsymbol{X}) = \frac{\boldsymbol{X}}{L_0}(L_f - L_0)$



- Eulerian displacement: $\boldsymbol{U}(\boldsymbol{x}) = \frac{\boldsymbol{x}}{L_F}(L_f - L_0)$
- $\frac{d\boldsymbol{U}(\boldsymbol{x})}{d\boldsymbol{x}} = \frac{\Delta L}{L_f}$
- $e_{11} = \frac{d\boldsymbol{u}(\boldsymbol{x})}{d\boldsymbol{x}} - \frac{1}{2}(\frac{d\boldsymbol{u}(\boldsymbol{x})}{d\boldsymbol{x}})^2 = \frac{\Delta L}{L_f} - \frac{1}{2}(\frac{\Delta L}{L_f})^2$



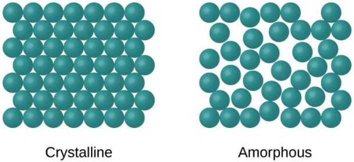


Linear strain for Eulerian-Almansi

- Almansi-Euler: $\boldsymbol{e} = (\boldsymbol{I} - \boldsymbol{F}^{-T}\boldsymbol{F}^{-1})$
- How it looks in terms of displacement ?
- $\boldsymbol{e} = \frac{1}{2}(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{\partial U_i}{\partial x_j}\frac{\partial U_j}{\partial x_i})$
- For small deformation $\frac{\partial U_i}{\partial X_j} \ll 1$, we obtain
- $\epsilon^{\textbf{Eulerian}} = \frac{1}{2}(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i})$
- $\epsilon^{\textbf{Lagrangian}} = \frac{1}{2}(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i})$
- Important conclusion: for small deformations, both Eulerian and Lagrangian strains are equivalent
- $\boldsymbol{U}(\boldsymbol{x}) = \boldsymbol{u}(\boldsymbol{X}) \Longrightarrow \epsilon^{\textbf{Eulerian}} = \epsilon^{\textbf{Lagrangian}}$

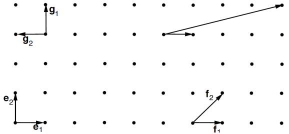
Crystalline solids

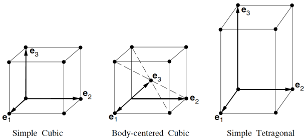
- A solid is said to be crystal if atoms are arranged in a way that their positions are exactly periodic
- Crystalline solids are solids in which the atoms, ions, or molecules are arranged in a definite repeating pattern
- It is also possible for a liquid to freeze before its molecules become arranged in an orderly pattern. The resulting materials are called amorphous solids or noncrystalline solids (or, sometimes, glasses)
- There is also quasi-crystals with no translation symmetry but with order

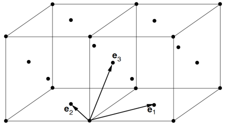


Bravais Lattices

- A Bravais lattice $L(\boldsymbol{e}, \boldsymbol{o})$ is an infinite set of points in three-dimensional space generated by the translation of a single point $\boldsymbol{o}$ through three linearly independent lattice vectors $\{\boldsymbol{e}_1, \boldsymbol{e}_3, \boldsymbol{e}_3\}$: $\Longrightarrow L(\boldsymbol{e}, \boldsymbol{o}) = \{\boldsymbol{x} : \boldsymbol{x} = m^i \boldsymbol{e}_i\}$, where m^1, m^2, m^3 are integers.
- The lattice vectors $\{\boldsymbol{e}_1, \boldsymbol{e}_3, \boldsymbol{e}_3\}$ define an a unit cell.

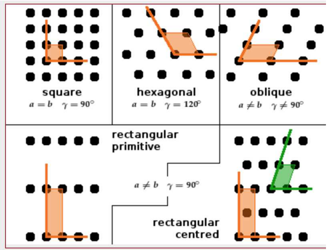


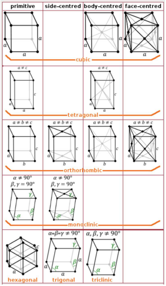




Bravais Lattices

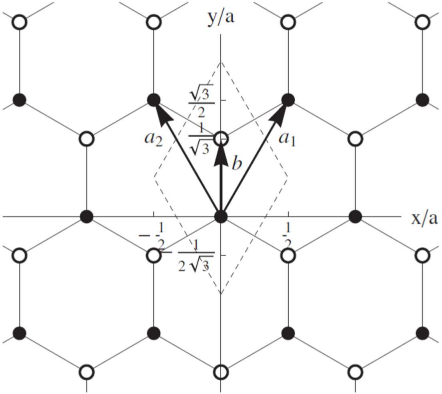
- All of the points in the lattice can be accessed by properly chosen primitive translation vectors
- The parallelepiped formed by the primitive translation vectors can be used to tile all of space
- A primitive unit cell (containing only one lattice point) can be chosen





Non-Bravais Lattices

- More than 1 primitive translation vectors
- We observe it graphene or in alloys with more than 1 atom



Same notions

- It is conventional to denote a direction in a lattice by $\boldsymbol{d} = u\boldsymbol{e}_1 + v\boldsymbol{e}_3 + w\boldsymbol{e}_3$
- A class of crystallographically equivalent directions is denoted by $<uvw>$
- The lattice vectors $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ define an a unit cell.
- For example, in a simple cubic lattice with lattice vectors chosen parallel to the edges $<100>\{[100], [\bar{1}00], [0\bar{1}0], [0\bar{1}0], ...\}$.
- A crystallographic plane with its normal (hkl); h, k and l are numbers are defined as normal plane to a direction
- Reciprocal vectors$\{\boldsymbol{e}^1, \boldsymbol{e}^2, \boldsymbol{e}^3\} \longrightarrow \boldsymbol{e}_i \cdot \boldsymbol{e}^j = 1$ if $i = j$
- Normal to the plane is given by $\boldsymbol{n} = h\boldsymbol{e}^1 + k\boldsymbol{e}^2 + l\boldsymbol{e}^3$
- $\{hkl\}$ denotes a class of equivalent planes

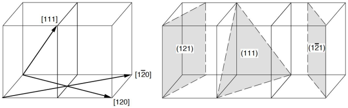


Figure 3.2: Some directions (left) and planes (right) in a lattice.

Deformation of Lattices and Symmetry

- Consider two Bravais lattices $L(\boldsymbol{e}, \boldsymbol{o})$ and $L(\boldsymbol{f}, \boldsymbol{o})$ generated by lattice vectors $\{\boldsymbol{e}_i\}$ and $\{\boldsymbol{f}_i\}$
- There is a matrix $\boldsymbol{F}$ with $\det\boldsymbol{F} \neq 0$ such that $\boldsymbol{f}_i = \boldsymbol{F}\boldsymbol{e}_i$
- There are some deformations which map a Bravais lattice back to itself. This is a consequence of the symmetry in a lattice $\longrightarrow \boldsymbol{e}_i = m_i^j \boldsymbol{f}_j$ such that $\boldsymbol{m}$ has integer entries with $\det\boldsymbol{m} = \pm 1$
- $\boldsymbol{f}_1 = \boldsymbol{e}_1,\ \boldsymbol{f}_2 = \boldsymbol{e}_1 + \boldsymbol{e}_2,\ \boldsymbol{f}_3 = \boldsymbol{e}_3\ m_{m,n} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
- $\boldsymbol{H}\boldsymbol{e}_i = m_i^j \boldsymbol{e}_j$
- Therefore, the set of deformations that map a lattice back into itself is given by $\longrightarrow G(\boldsymbol{e}_i) = \{\boldsymbol{H} : \boldsymbol{H}\boldsymbol{e}_i = m_i^j \boldsymbol{e}_i\}$
- $G(\boldsymbol{e}_i)$ is a symmetry group $GL(2, Z)$ or $GL(3, Z)$

The Cauchy-Born hypothesis

- Our goal is to obtain a continuum theory
- The Cauchy-Born hypothesis says that the lattice vectors deform according the deformation gradient: $\boldsymbol{e}_i = \boldsymbol{F}(\boldsymbol{x})\boldsymbol{e}_i^o$
- The lattice vectors behave like material filaments

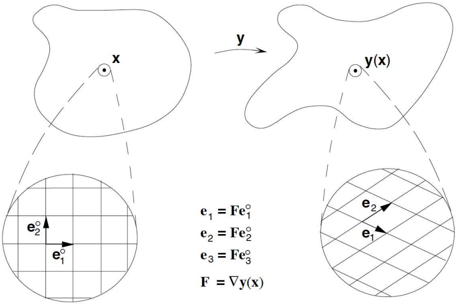


Figure 3.4: Lattice-continuum link using the Cauchy-Born Hypothesis. The lattice vectors deform according to the deformation gradient.

The Cauchy-Born hypothesis (2)