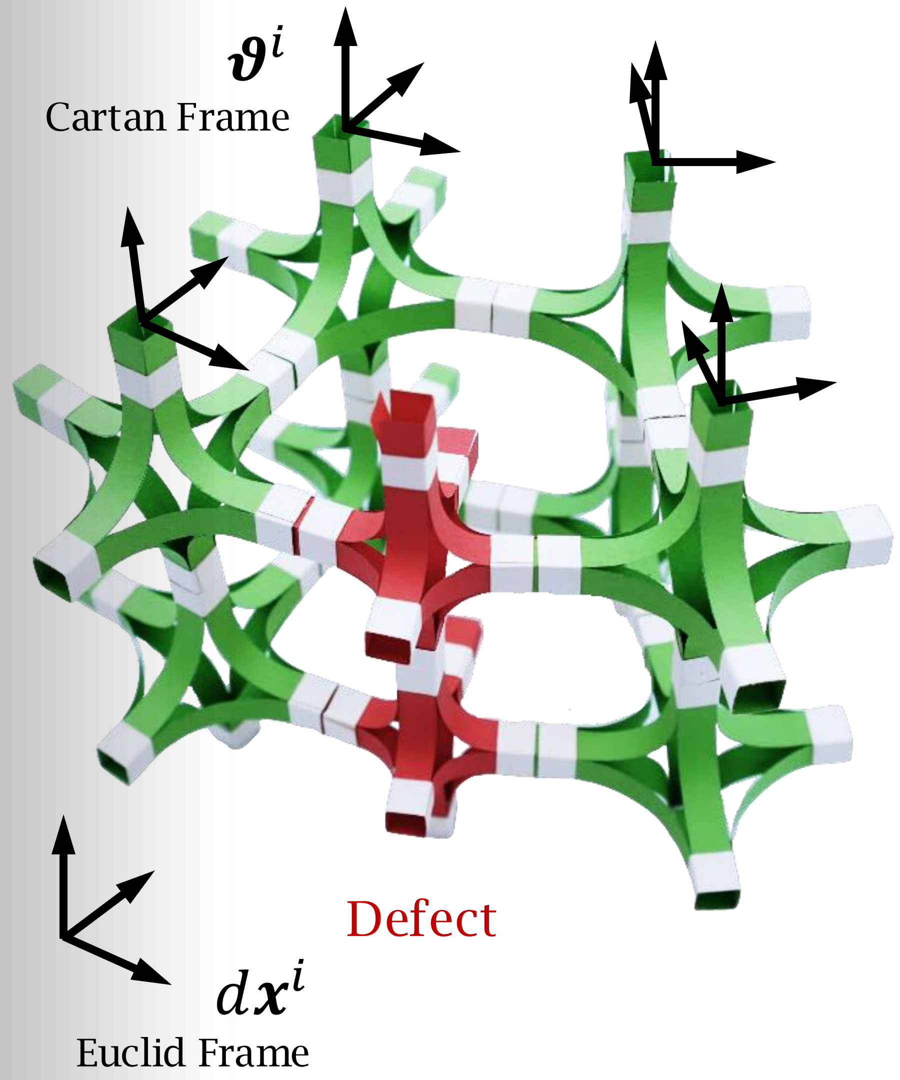
Materials Science on Riemann-Cartan manifold

- Reformulation of Volterra Defects -

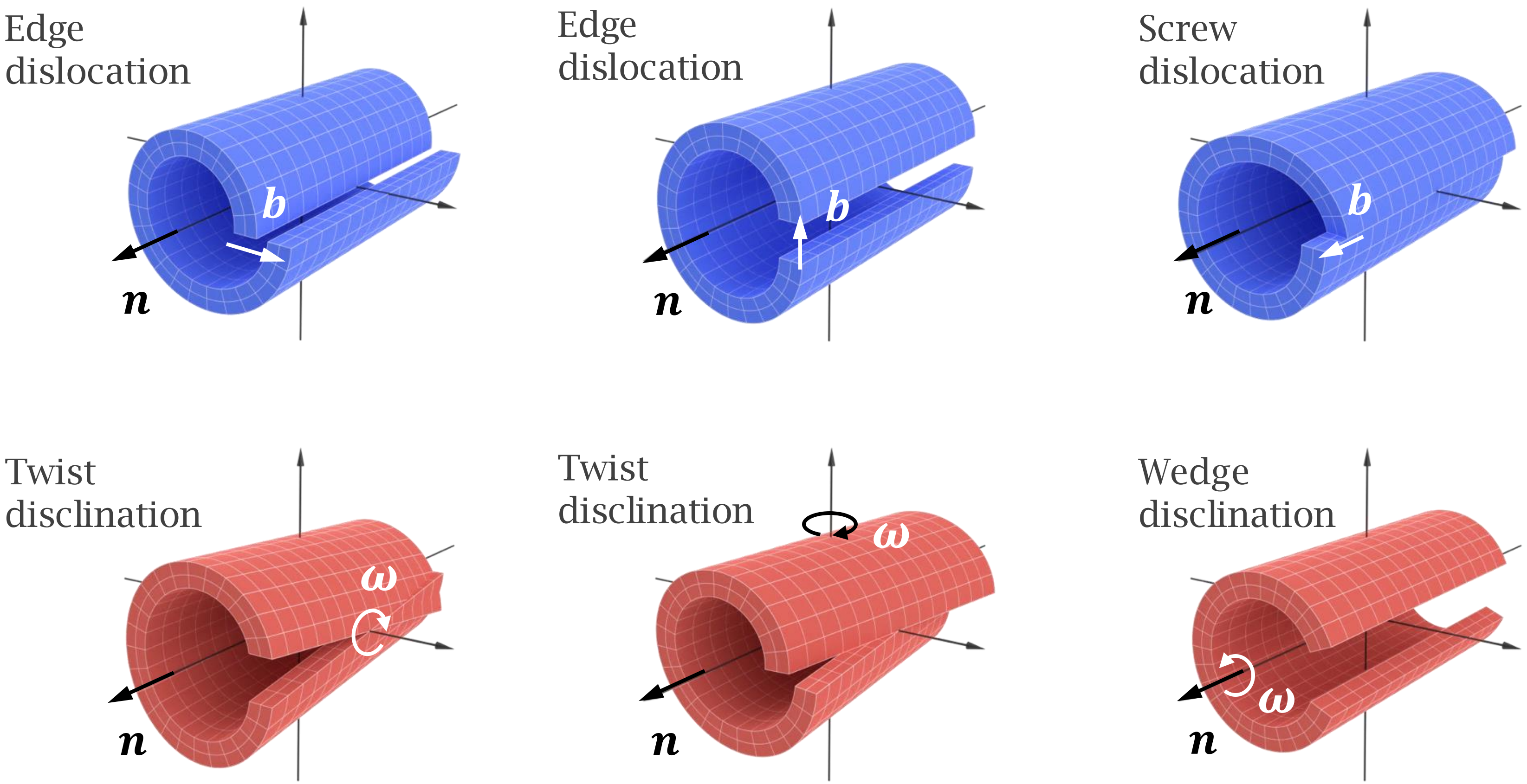
Nonlinear Mechanics Division, Osaka University
Ryuichi Tarumi and Shunsuke Kobayashi



Introduction

Volterra defects: classification of dislocations and disclinations

Vito Volterra
(1860 - 1940)



Introduction

A brief history of the theory of dislocation

Vito Volterra
(1860 - 1940)

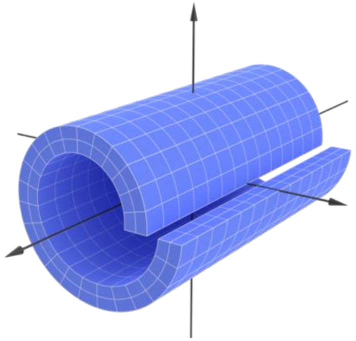
Euclidean Space

- V. Volterra (1907)
- G.I. Taylor (1934)
- E. Orowan (1934)
- R. Peierls (1940)
- F.R.N. Nabarro (1947)
- T. Mura (1964)
- W. Noll (1967)
- A.C. Eringen (1983)
- D.G.B. Edelen (1988)
- M.O.Katanaev (1992)
- L.M. Zubov (1997)
- M. Lazar (2000-)
- Acharya (2010-)

10 20 30 40 50 60 70 80 90 2000 10 20

Year

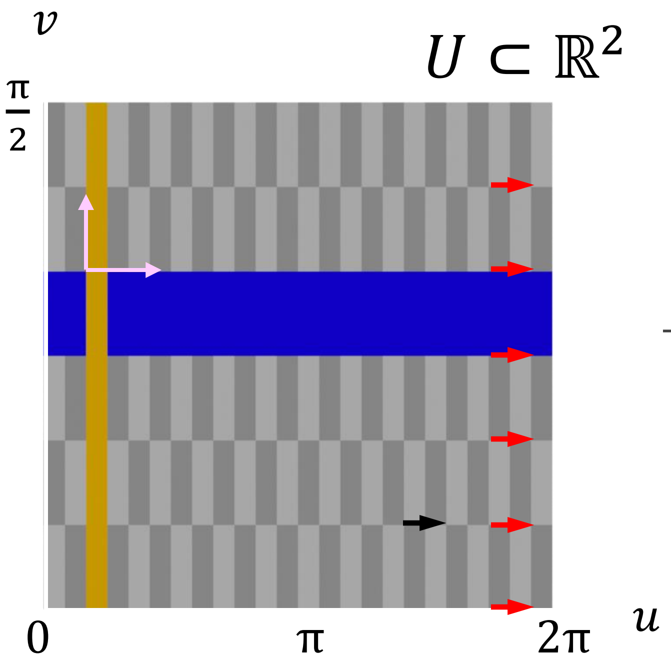
Differential Geometry



- K. Kondo (1955)
- B.A. Bilby (1955)
- E. Kroner (1959)
- S. Amari (1962)
- R. de Wit (1981)
- J. Wenzelburger (1998)
- Yavari & Goriely (2012)
- Kobayashi & Tarumi (2024)

Introduction

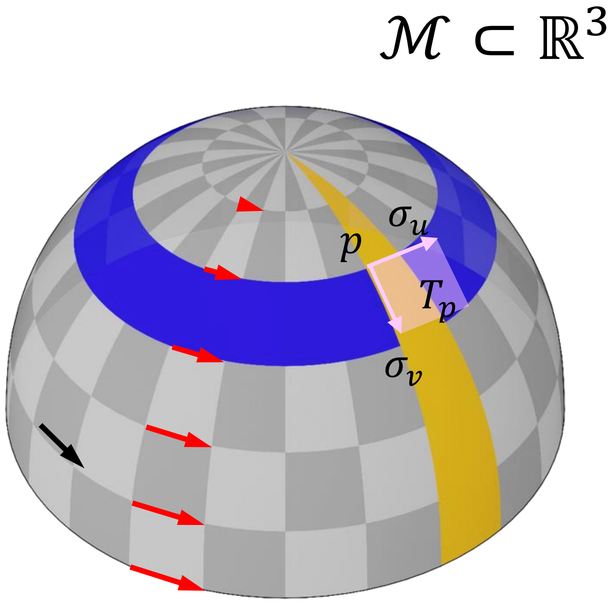
A map ϕ from 2D Euclidean space to a semi-spherical surface



$$\phi : U \to \mathcal{M}$$

$$\phi(u, v) = \begin{cases} x = r \sin u \cos v \\ y = r \sin u \sin v \\ z = r \cos u \end{cases}$$

$$N = (\sin u \cos v \,, \sin u \sin v \,, \cos u)$$



Plane (coordinate)

Riemannian manifold

Introduction

The first and second fundamental forms of a curved surface

$$\mathcal{F}_1 = Edu^2 + 2Fdudv + Gdv^2$$

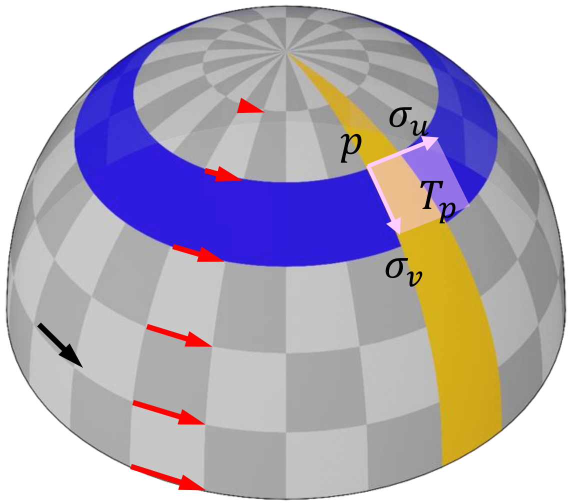
$$\begin{cases} E = \langle \phi_u, \phi_u \rangle = r^2 \sin^2 v \\ F = \langle \phi_u, \phi_v \rangle = 0 \\ G = \langle \phi_v, \phi_v \rangle = r^2 \end{cases} \quad g_{ij} = \begin{pmatrix} E & F \\ F & G \end{pmatrix} = \begin{pmatrix} r^2 \sin^2 v & 0 \\ 0 & r^2 \end{pmatrix}$$

Riemannian metric

$$\mathcal{F}_2 = edu^2 + 2fdudv + gdv^2$$

$$\begin{cases} e = \langle \phi_{uu}, N \rangle = -r \sin^2 v \\ f = \langle \phi_{uv}, N \rangle = 0 \\ g = \langle \phi_{vv}, N \rangle = -r \end{cases} \quad W = \frac{1}{EG - F^2} \begin{pmatrix} eG - fF & fG - gF \\ fE - eF & gE - fF \end{pmatrix}$$

Weingarten matrix



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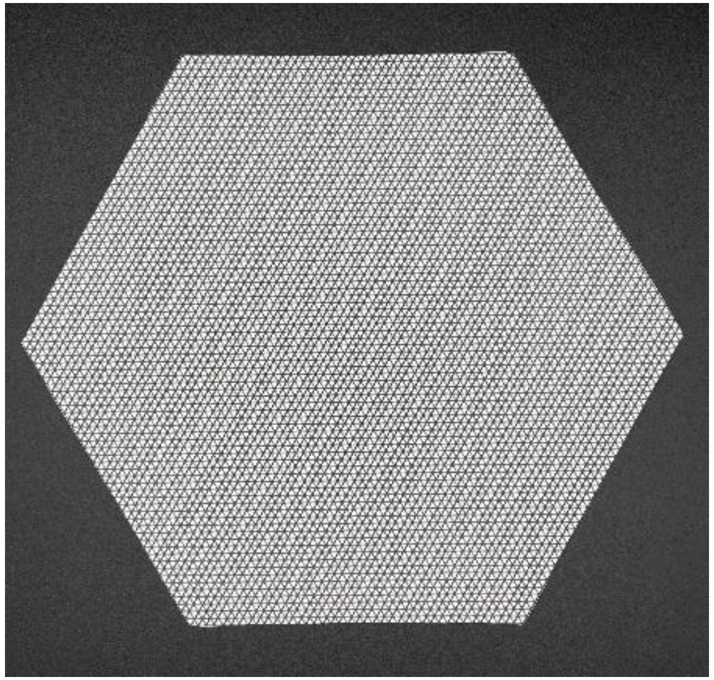
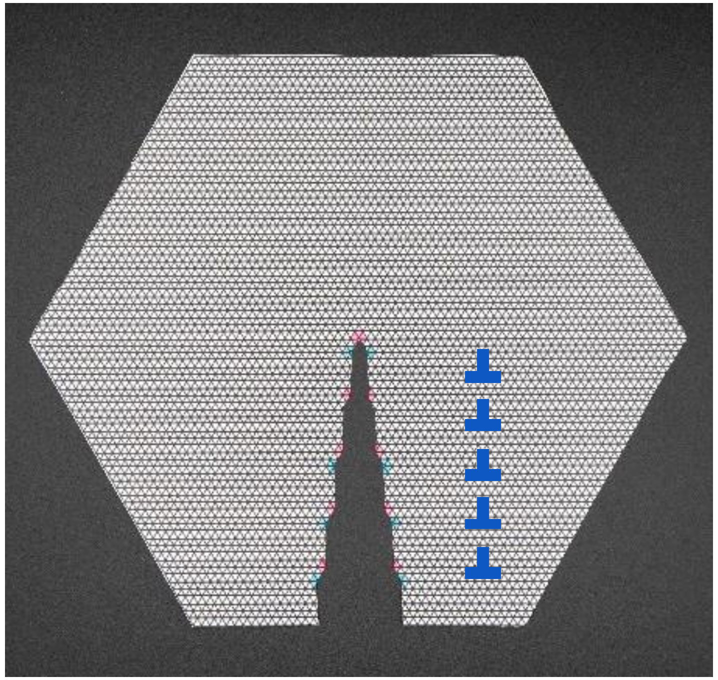
Weingarten matrix

Introduction

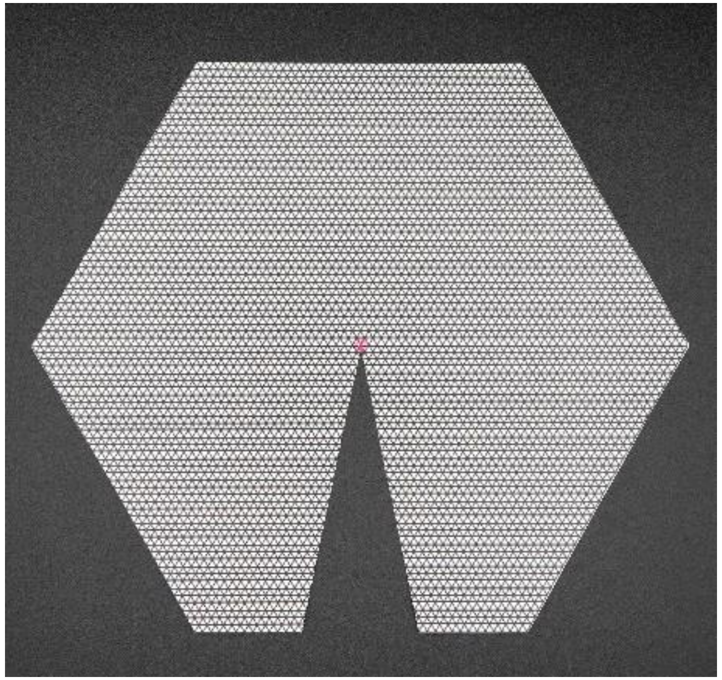
Volterra defects made by 'Kirigami' lattice



Perfect crystal

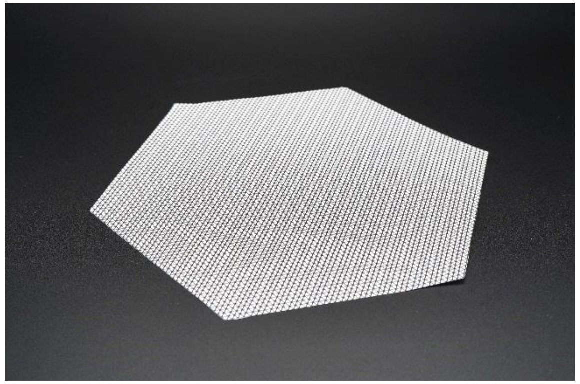


Edge dislocation array



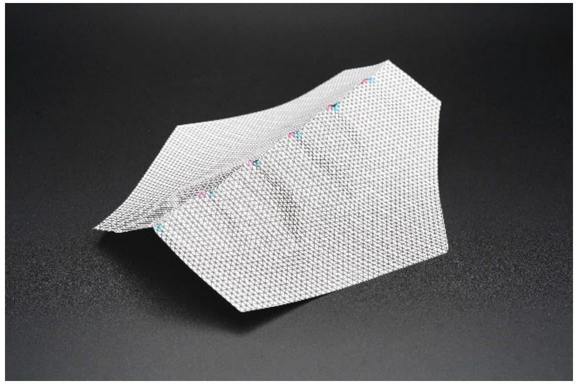
Wedge disclination

Introduction



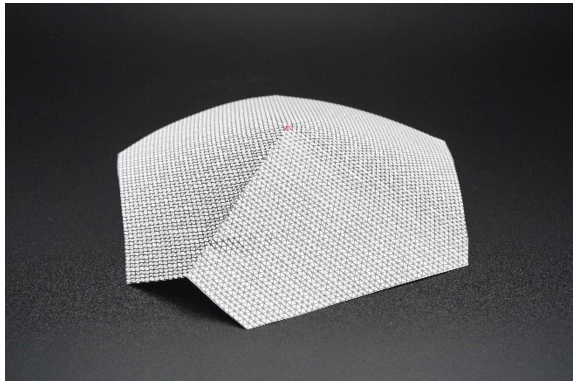
Perfect crystal

- Only a perfect crystal can exist in 2D plane
- Plastic deformation: a curved surface in 3D space (Riemannian manifold)
- Elastic deformation: embedding of a curved surface into 2D plane

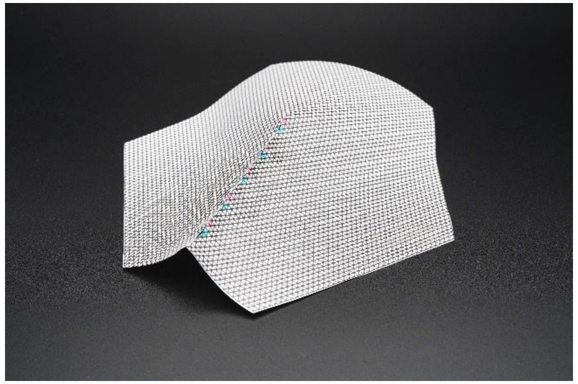


Grain boundary

Dislocation pair



Disclination



Dislocation array

Curvature represents the plastic deformation due to Volterra defects

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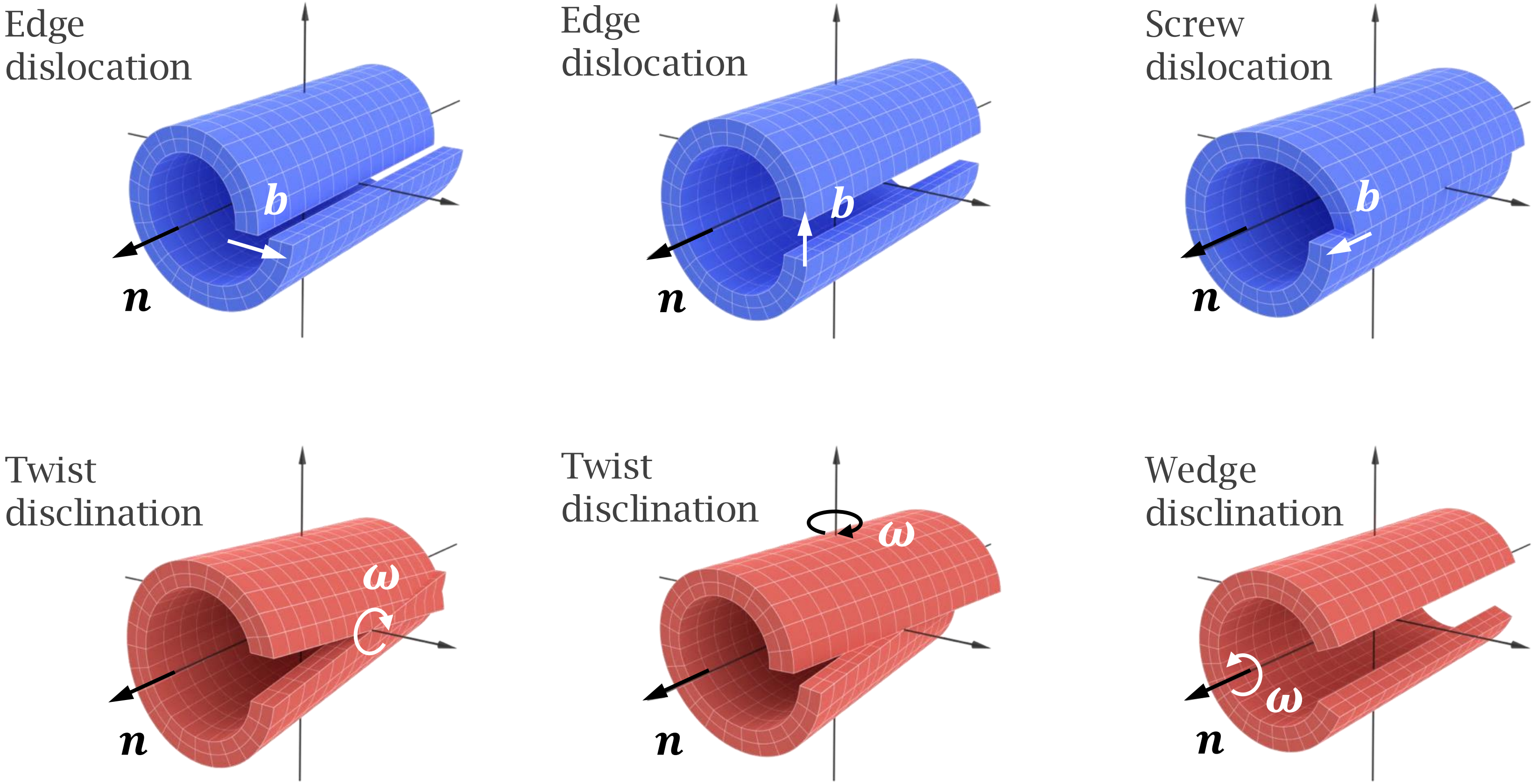

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1. Geometrical frustration

- What is the origin of stress in crystalline solids?
- Remove stress singularity at the core of dislocation

S. Kobayashi & R. Tarumi, Royal Society Open Science (In Press)

2. Biot-Savart law for dislocations

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- Analytical solution of plastic deformation fields

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4. Materials Geometry & Information Geometry

- Statistical analysis for materials science

1. Geometrical frustration

Riemann-Cartan Manifold

- Cartan structure equations for Riemann-Cartan manifold

$$\tau^i = d\vartheta^i + \omega^i_j \wedge \vartheta^j$$

$$\Omega^i_j = d\omega^i_j + \omega^i_k \wedge \omega^k_j$$

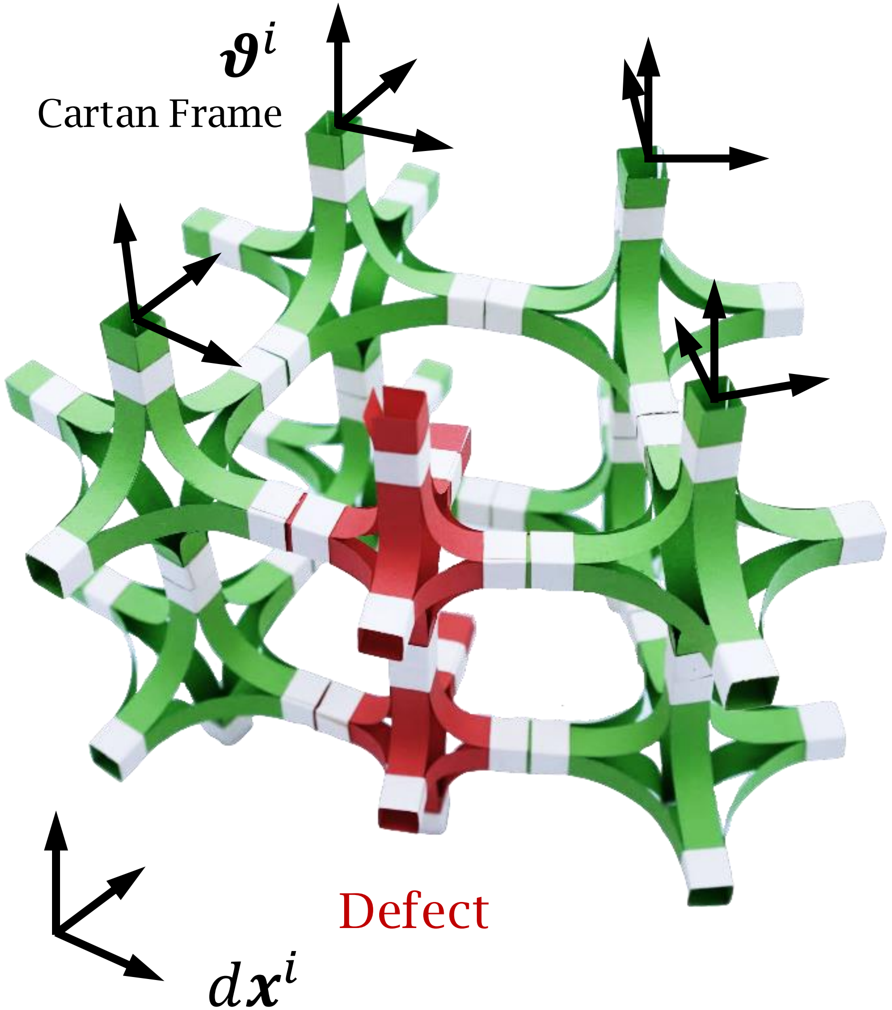
- $\vartheta^i : \mathrm{TM} \to M \times \mathbb{R}^3$: Cartan moving frame $\boldsymbol{\vartheta}^i$ for dislocations

$$\vartheta^i = \left(d\psi^i + \Theta^i\right) dx^j \otimes E_i$$

Helmholtz decomposition

- Dislocation density and torsions 2-form

$$\tau^i = * \alpha^i = f b^i n_l \epsilon_{ljk} dx^j \wedge dx^k \otimes E_i$$



1. Geometrical frustration

Kinematics on Riemannian manifold

- Three different configurations: reference, intermediate and current configurations.

$$(\mathcal{M}, g, \nabla) \xrightarrow{F_p} (\mathcal{M}, g_B, \nabla_B) \xrightarrow{F_e} (\mathcal{M}, g_C, \nabla_C)$$

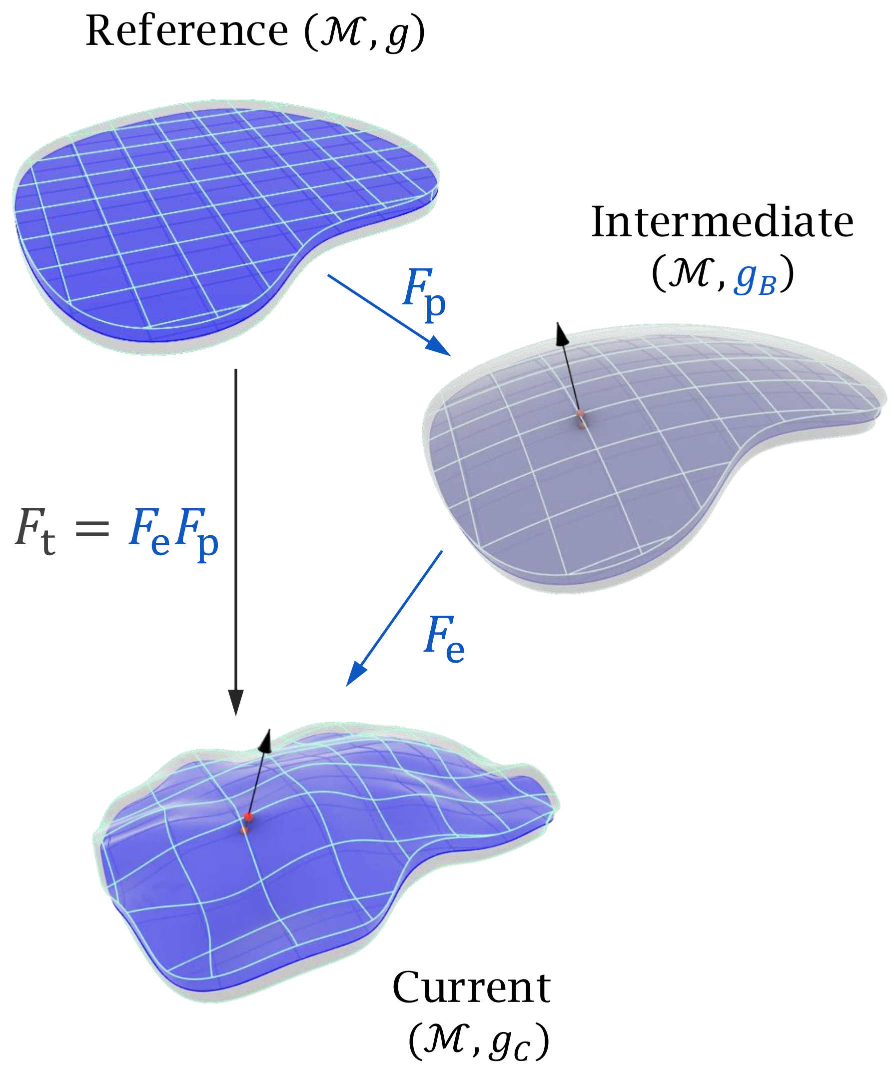
Reference ($\mathbb{R}^3$) Intermediate Current ($\mathbb{R}^3$)

- Kinematics is described by the two deformation gradients: F_p and F_e.

$$F_t = F_e F_p$$ Multiplicative decomposition

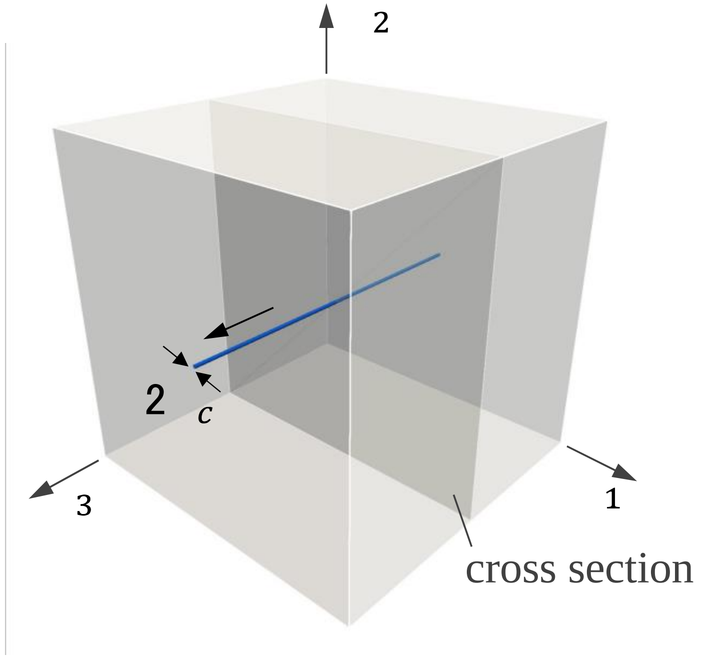
- Elastic embedding from the intermediate to the current configuration

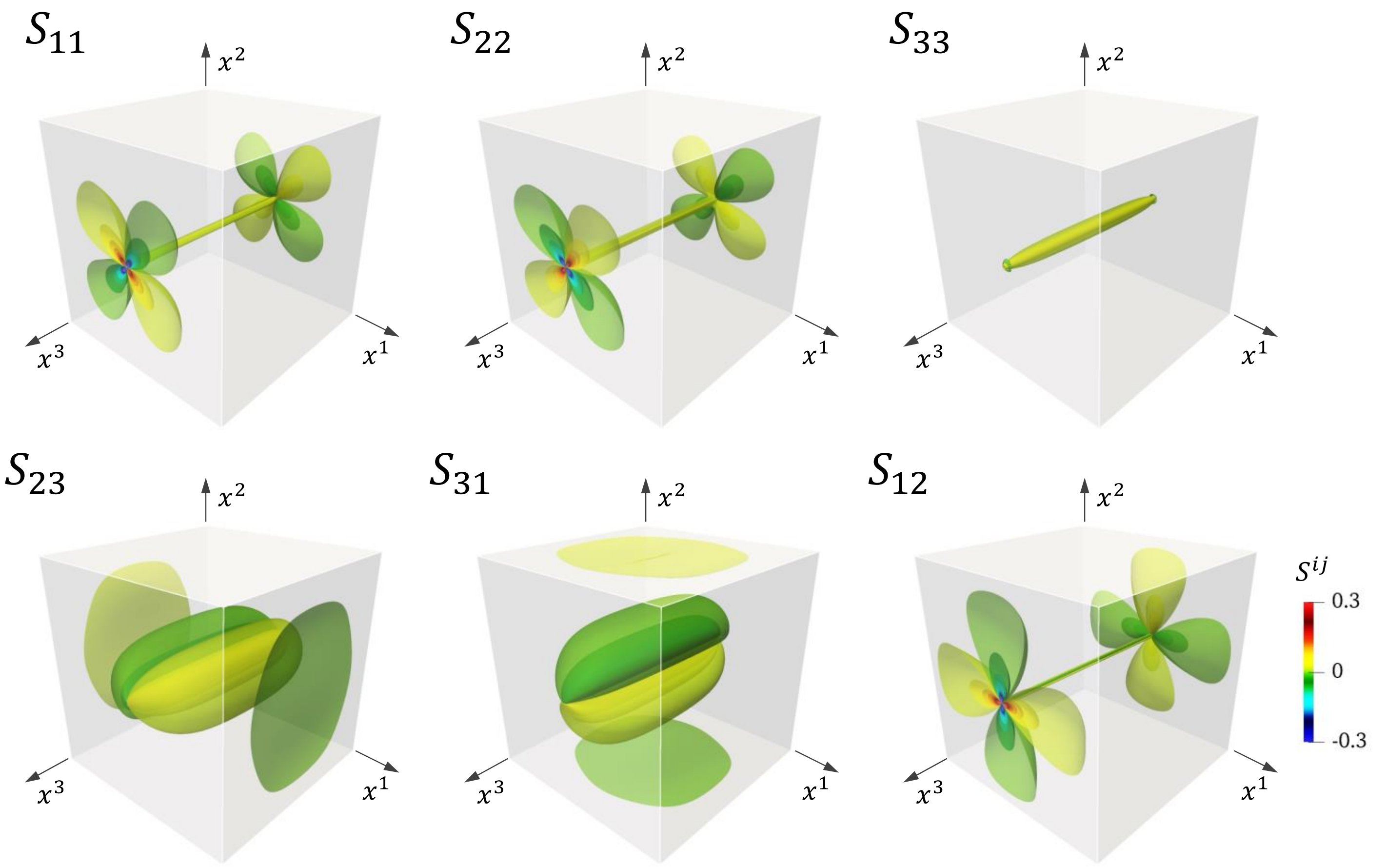
$$W[y] = \int_{\mathcal{M}} C^{ijkl} \frac{(g_C - g_B)_{ij}}{2} \frac{(g_C - g_B)_{kl}}{2} dV$$



1. Geometrical frustration

Internal stress fields of screw dislocation (2nd-Piola-Kirchhoff stress)





S. Kobayashi & R. Tarumi, Royal Society Open Science (in press)

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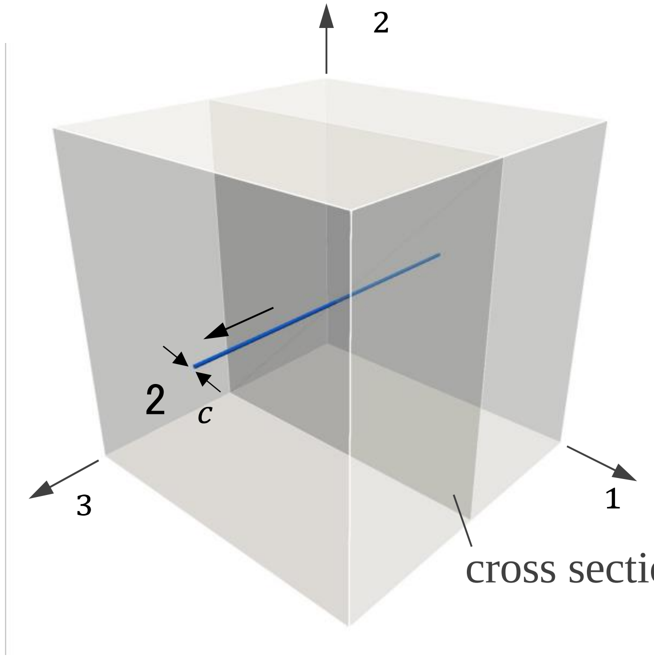

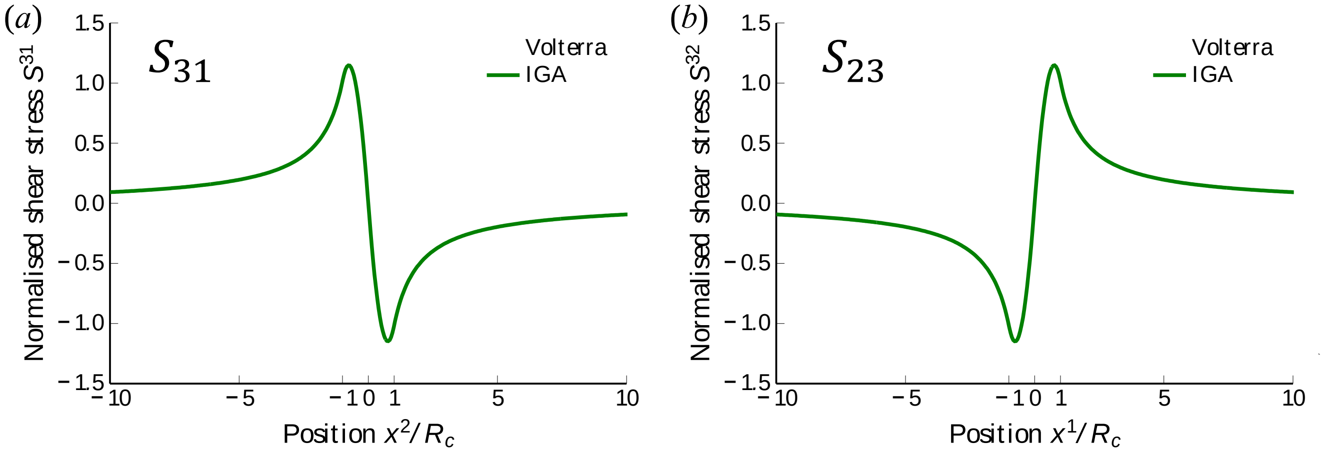

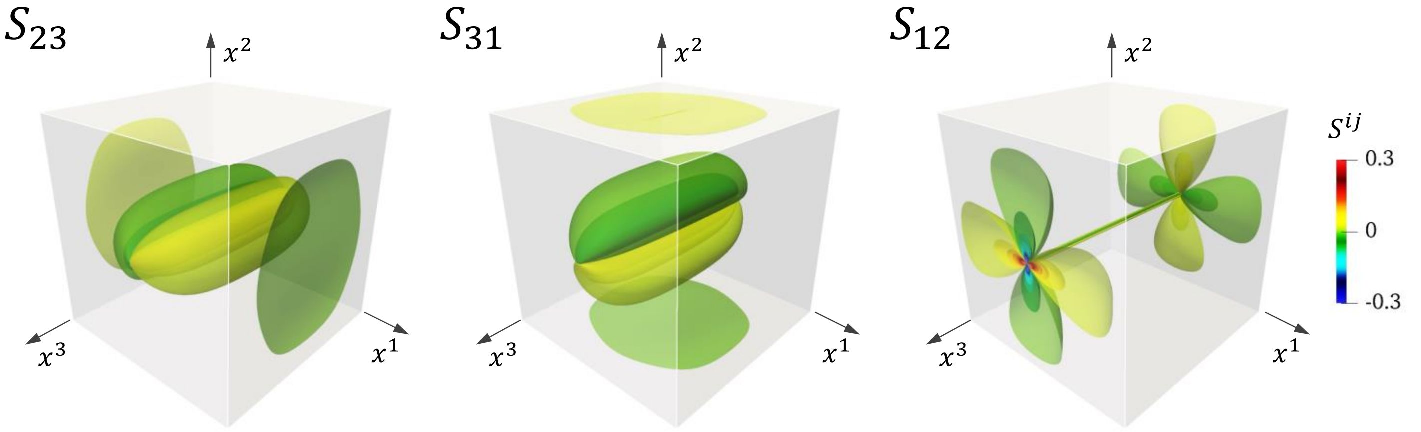

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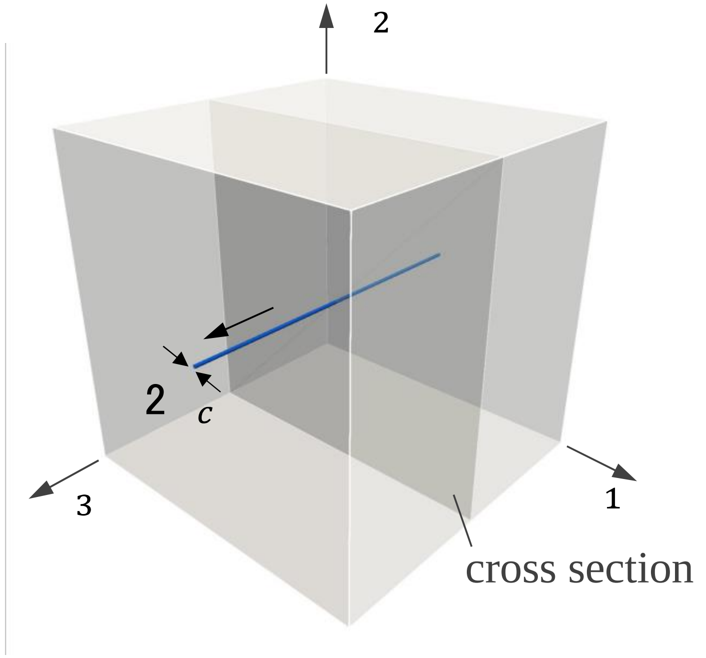
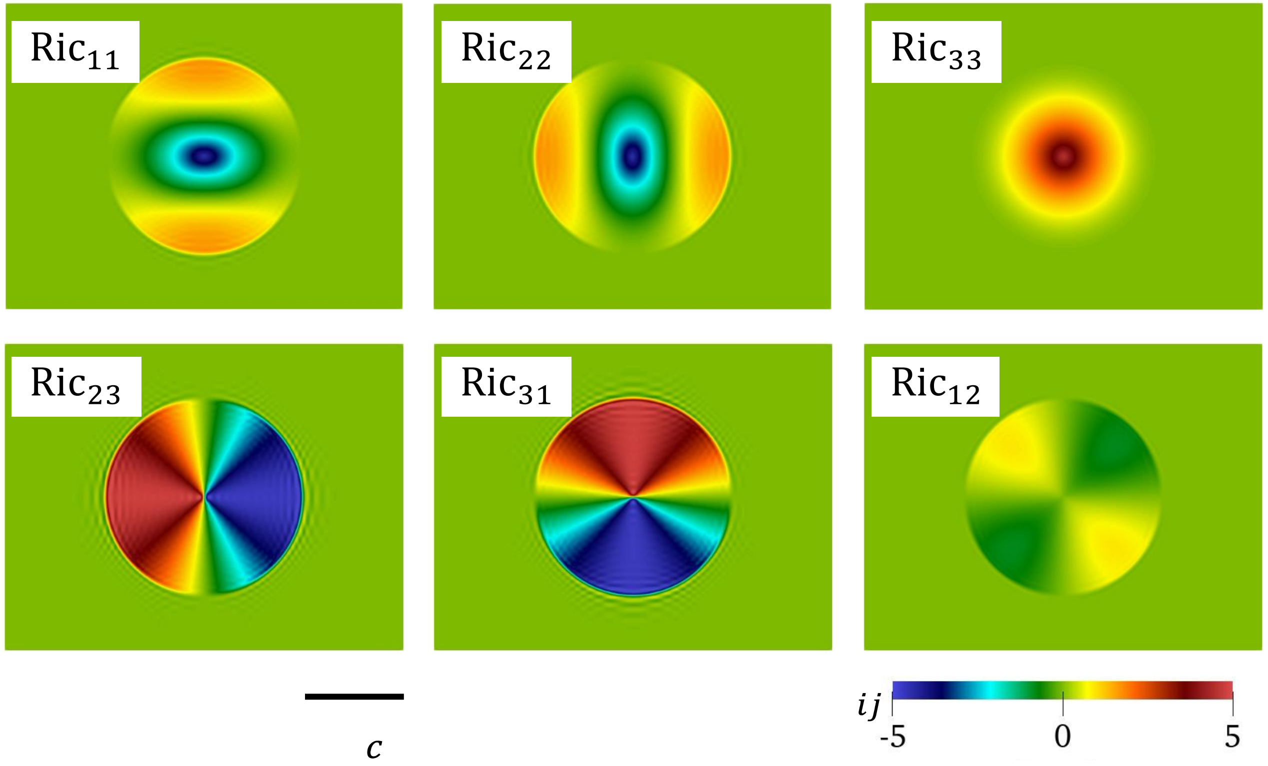
1. Geometrical frustration

Geometrical frustration of screw dislocation inside the dislocation core

$$\mathrm{Ric}[\vartheta] = R^{k}_{ikj}[dx^i \otimes dx^j]$$





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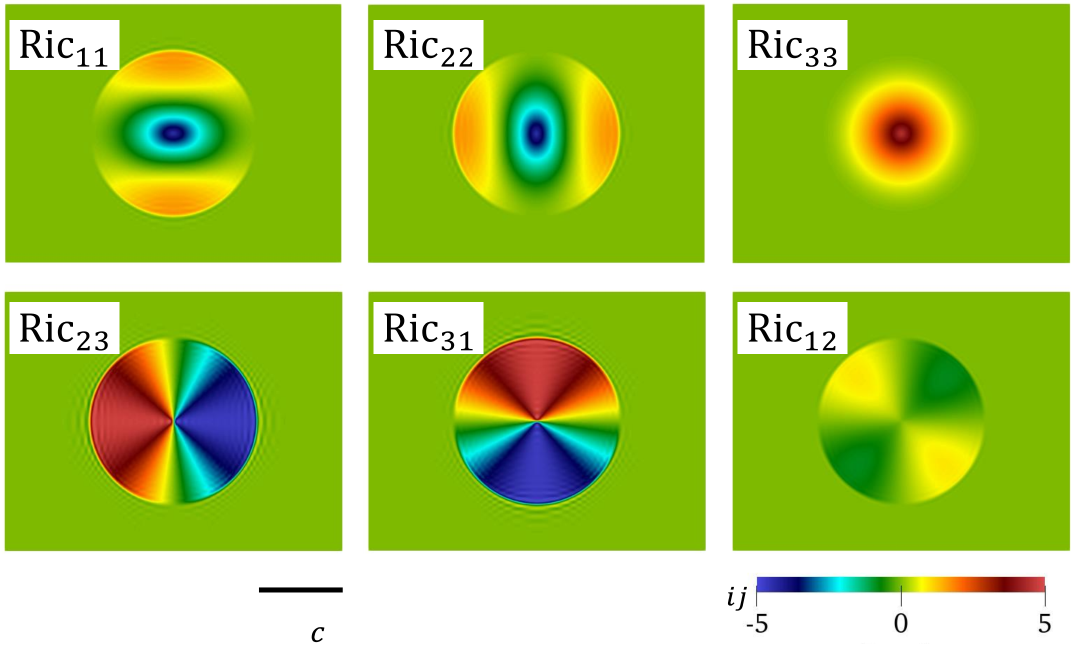
1. Geometrical frustration

Duality between the stress and Ricci curvature



$$\mathrm{Ric}[\vartheta] = R^{k}_{ikj}[dx^i \otimes dx^j]$$

Euclidean Space

Reference (Perfect Crystal) $\xrightarrow{\boldsymbol{F}}$ Current (Plastic+Elastic)

Reference (Perfect Crystal) $\xrightarrow{\boldsymbol{F}_p}$ Intermediate (Plastic) $\xrightarrow{\boldsymbol{F}_e}$ Current (Plastic+Elastic)

Differential Geometry

Remove geometrical frustration

$$\boldsymbol{F}_e = \boldsymbol{F}\,\boldsymbol{F}_p^{-1}$$

Stress equilibrium equation
(Minimize strain energy)

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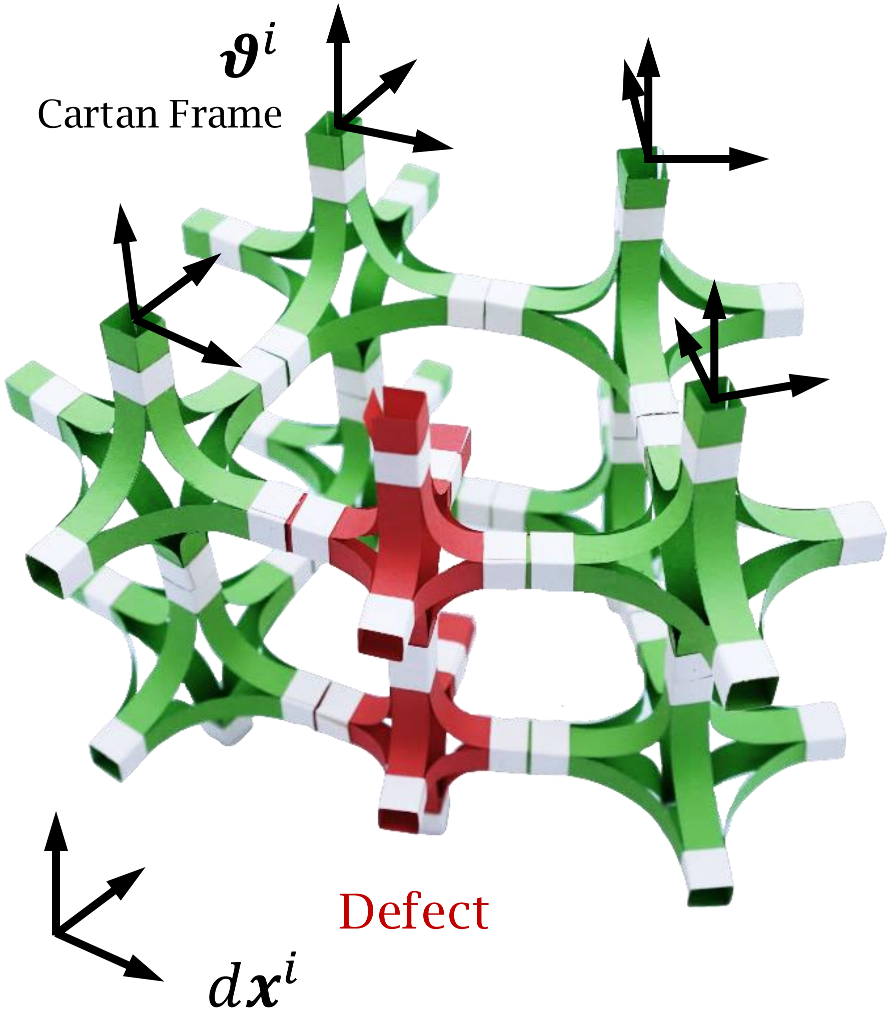

2. Biot-Savart law for dislocations

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Dislocation Plasticity
(Plastic deformation of dislocation)

$$\nabla \times \Theta^i = \tau^i$$

$$\nabla \cdot \Theta^i = 0$$

電磁気学
(Ampere & Gauss Law)

$$\partial_y \Theta^i_1 - \partial_x \Theta^i_2 = 0$$

$$\partial_x \Theta^i_1 + \partial_y \Theta^i_2 = 0$$

複素関数論
(Cauchy-Riemann Equations)

Theorem : Biot-Savart Law for Dislocation

Let α^i be a dislocation density given in an infinite medium. Then, analytical integration of the dual exact form, *i.e.*, plastic displacement gradient of the dislocation, is given by the following form:

$$\boldsymbol{\Theta}^i(\boldsymbol{x}) = \frac{1}{4\pi} \int \frac{* \boldsymbol{\tau}^i(\boldsymbol{\xi}) \times (\boldsymbol{x} - \boldsymbol{\xi})}{\|\boldsymbol{x} - \boldsymbol{\xi}\|^3} dV$$

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Electromagnetics
(Ampere & Gauss Law)

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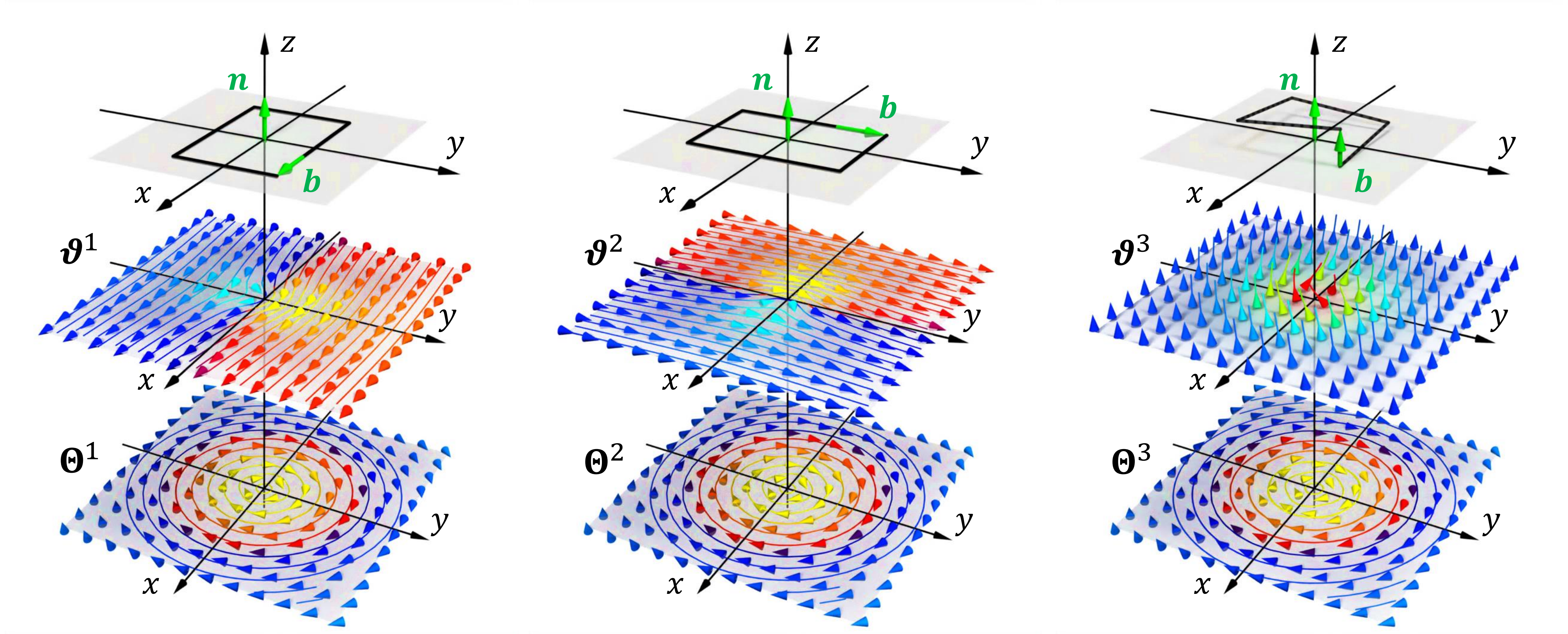
2. Biot-Savart law for dislocations



Edge dislocation

Edge dislocation

Screw dislocation

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Dislocation Plasticity
(Plastic deformation of dislocation)

Electromagnetics
(Ampere & Gauss Law)

Complex Function
(Cauchy-Riemann Equations)

Theorem : Complex Potential for Dislocations

Plastic displacement gradients $\boldsymbol{\Theta}^i$ of a dislocation can be obtained from the complex potential of plastic deformation in such a way that

$$\Psi(x,y) = -\mathbb{i}\frac{b}{2\pi}\log z\,, \qquad \Theta^i_1 = \mathrm{Re}\left(\frac{d\Psi}{dz}\right), \qquad \Theta^i_2 = \mathrm{Im}\left(\frac{d\Psi}{dz}\right)$$

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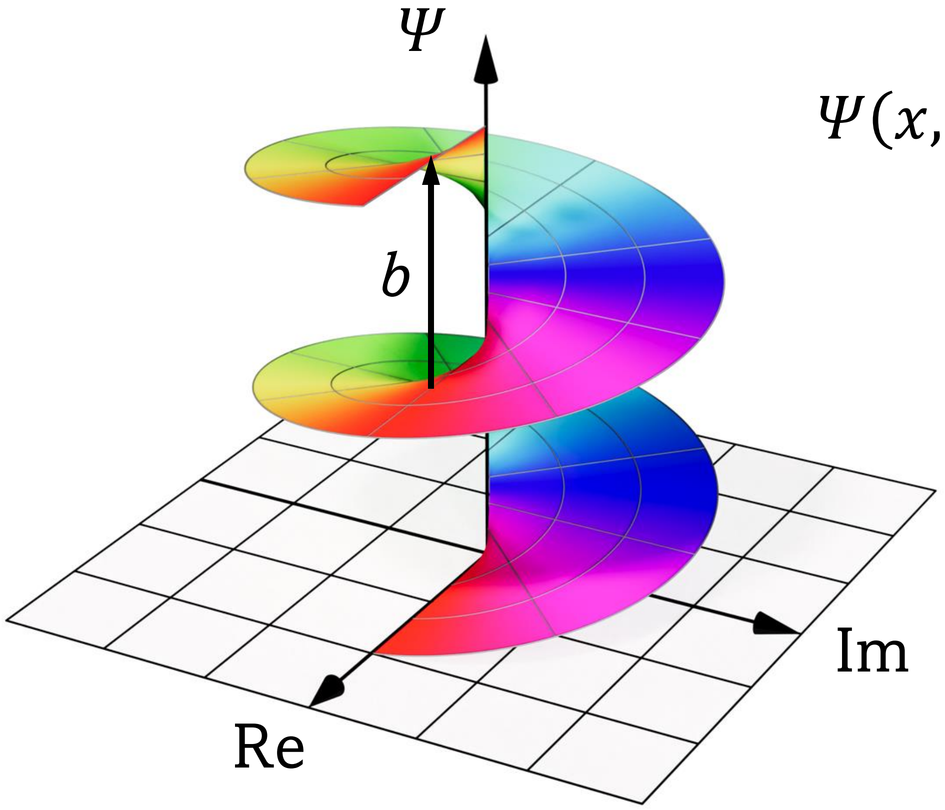
2. Biot-Savart law for dislocations

Polar representations of plastic deformation potential Ψ



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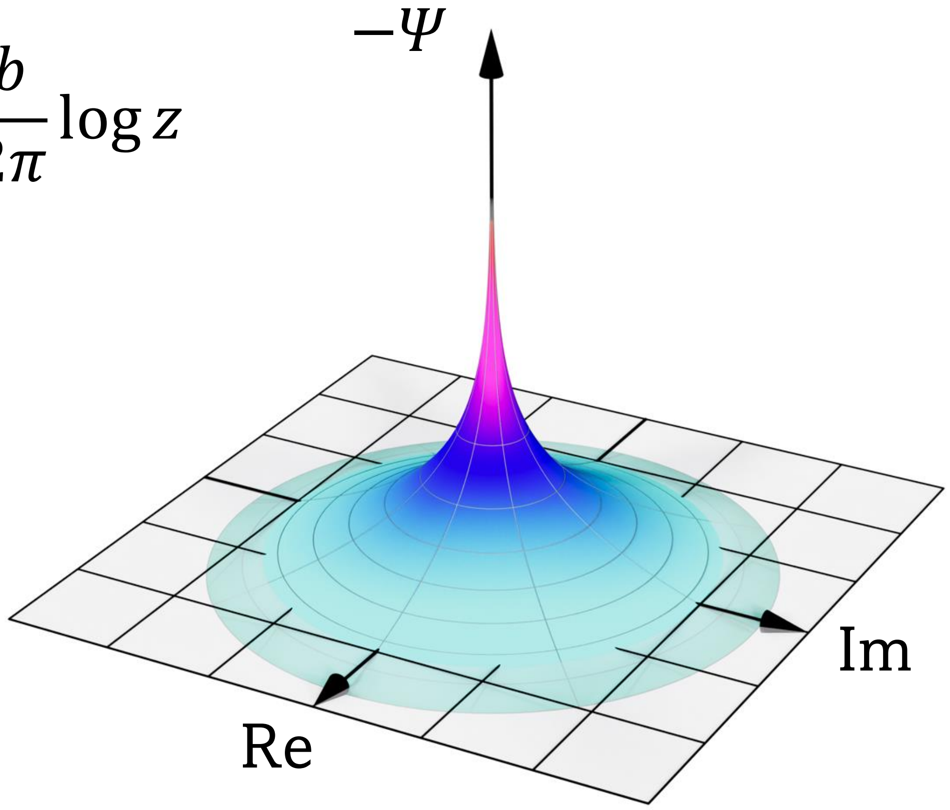

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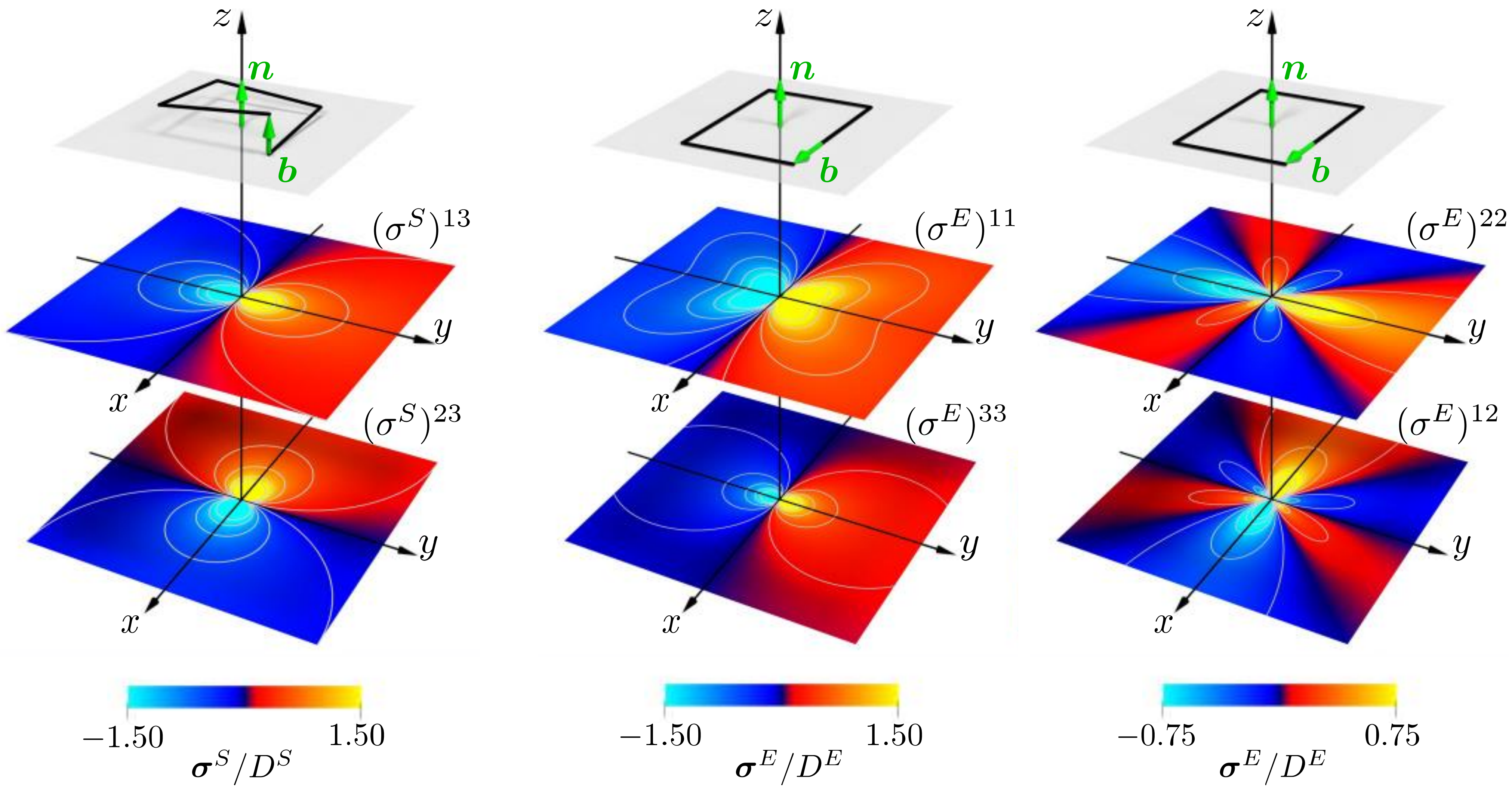

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   - Geometrical definition of Volterra defects
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4. **Riemann-Cartan Geometry & Information Geometry**
   - Unification of materials science using differential geometry

3. Reconsideration of Volterra defects

Classification of 1-D topological defects by Volterra

Volterra Process for defect

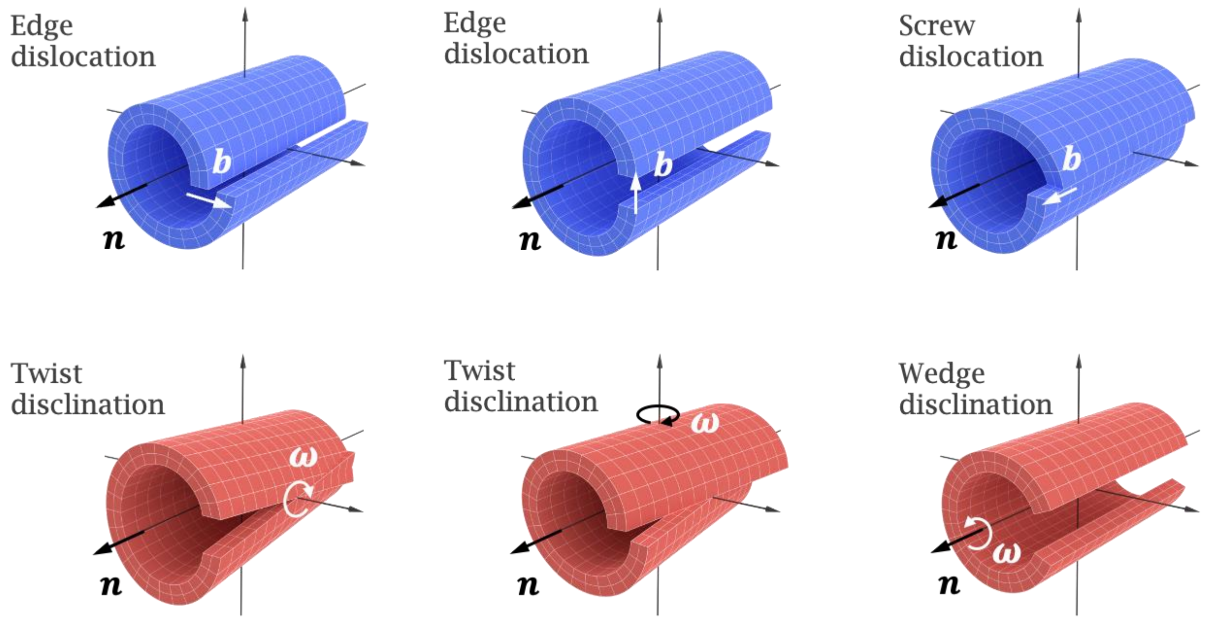
$$\boldsymbol{\psi}(\boldsymbol{x}) = \mathcal{R}(\boldsymbol{x})\boldsymbol{x} + \mathcal{T}(\boldsymbol{x})$$

Deformation Rotation Translation

Mathematical issues

- Geometrical definition of disclinations
- Dislocations and disclinations relation

Objective



Clarify the relation between Volterra defects based on the differential geometry

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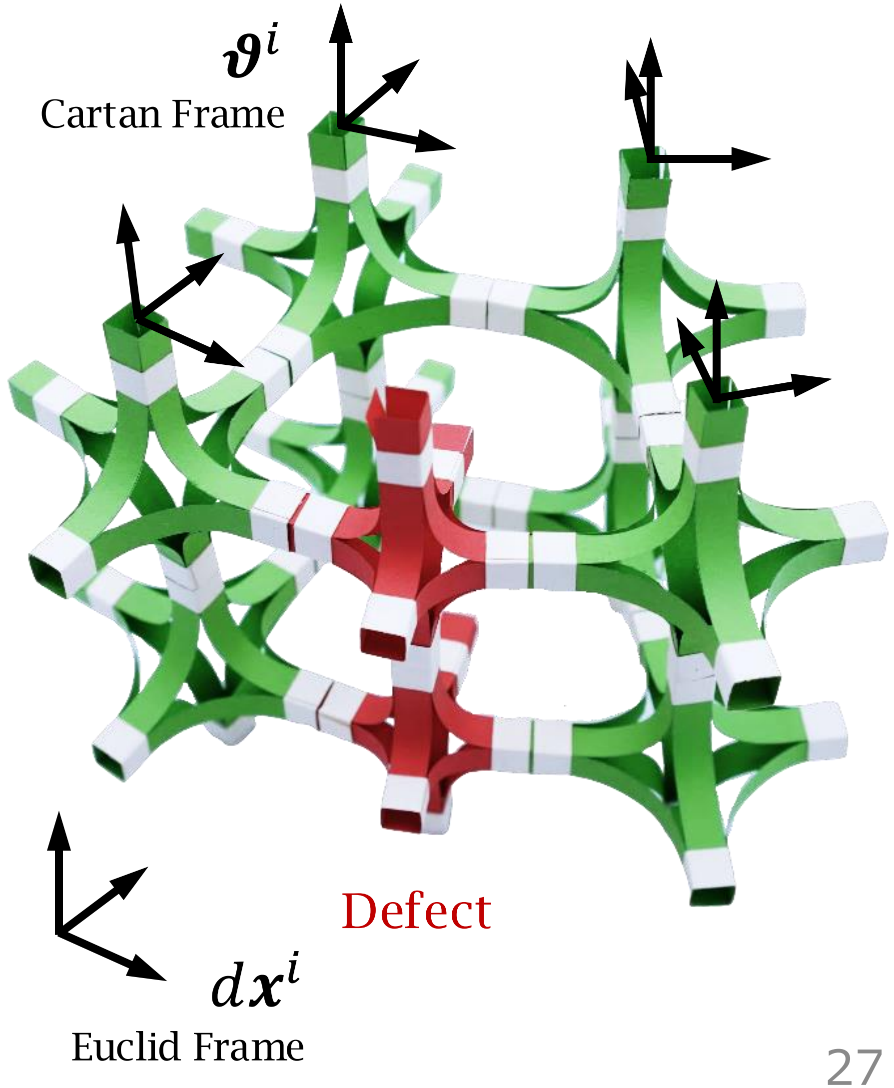
Deformation Rotation Translation

Cartan moving frame and Helmoltz decompositioin

$$\boldsymbol{\vartheta}^i(\boldsymbol{x}) = d\boldsymbol{x}^i + \boldsymbol{\Theta}^i(\boldsymbol{x})$$

Cartan Frame Euclid Frame Plastic Deformation



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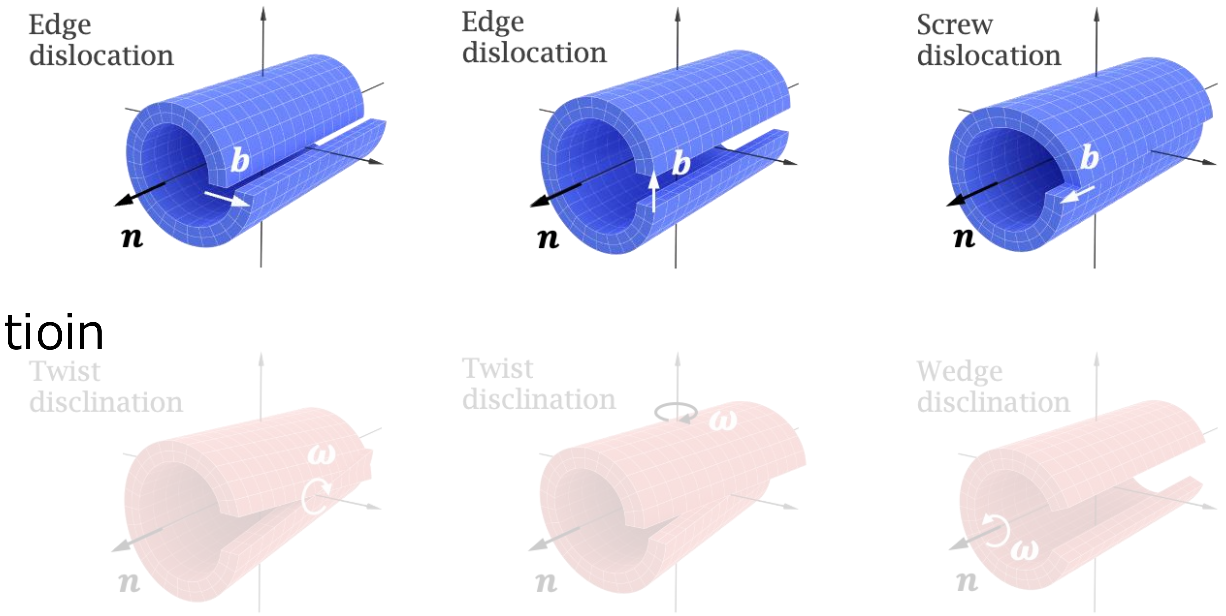

Cartan moving frame and Helmoltz decompositioin

$$\boldsymbol{\vartheta}^i(\boldsymbol{x}) = d\boldsymbol{x}^i + \boldsymbol{\Theta}^i(\boldsymbol{x})$$

Cartan Frame Euclid Frame Plastic Deformation

Local moving frame

$$\boldsymbol{\vartheta}^i(\boldsymbol{x}) = d\boldsymbol{x}^i + d\mathcal{T}(\boldsymbol{x}) \longrightarrow$$

Definition of dislocations by torsions

$$\tau^i = b\delta(x,y)dx \wedge dy$$

$$\boldsymbol{\Omega} = (0,0,0)$$

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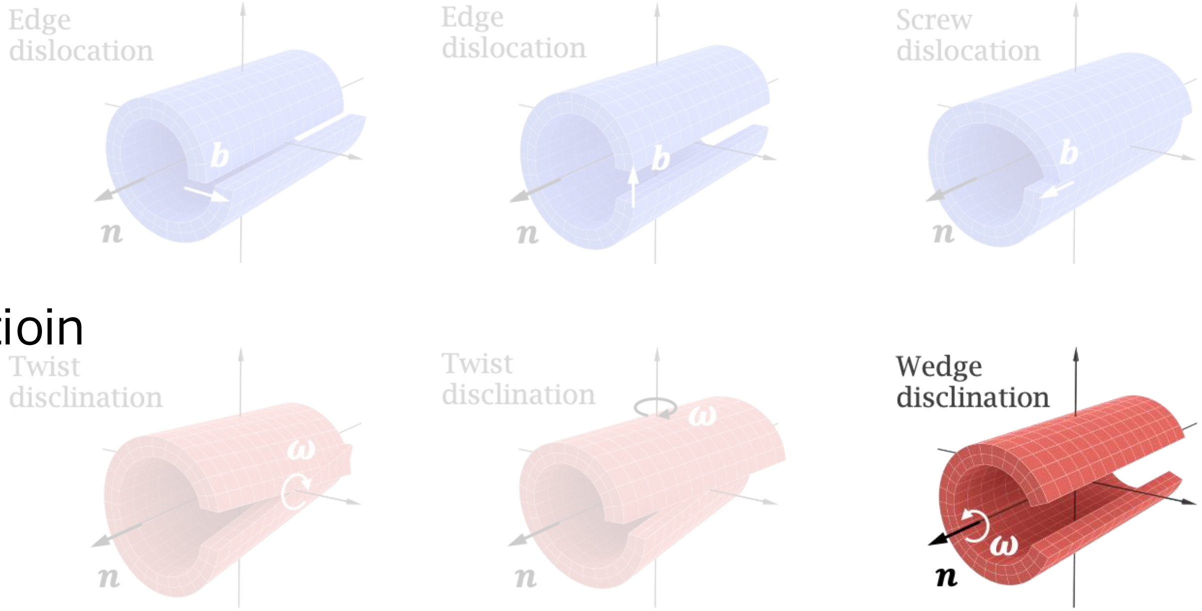
Deformation Rotation Translation



Cartan moving frame and Helmoltz decompositioin

$$\boldsymbol{\vartheta}^i(\boldsymbol{x}) = d\boldsymbol{x}^i + \boldsymbol{\Theta}^i(\boldsymbol{x})$$

Cartan Frame Euclid Frame Plastic Deformation

Local moving frame

$$\boldsymbol{\vartheta}^i(\boldsymbol{x}) = d\boldsymbol{x}^i + \mathcal{R}^{-1}d\mathcal{R}(\boldsymbol{x})\boldsymbol{x} \longrightarrow \Omega^1_2 = \phi\delta(x,y)dx \wedge dy$$

Definition of disclinations by curvature

$$\boldsymbol{\tau} = (0,0,0)$$

S. Kobayashi K. Takemasa & R. Tarumi (to be submitted)

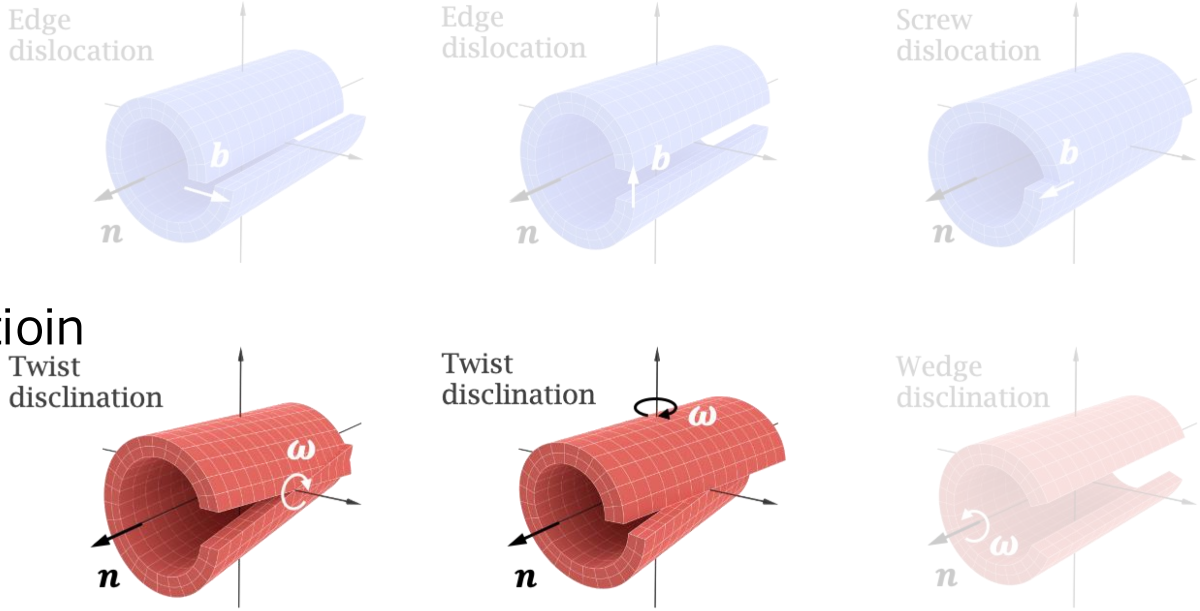
3. Reconsideration of Volterra defects

Classification of 1-D topological defects by Volterra

Volterra Process for defect

$$\boldsymbol{\psi}(\boldsymbol{x}) = \mathcal{R}(\boldsymbol{x})\boldsymbol{x} + \mathcal{T}(\boldsymbol{x})$$

Deformation Rotation Translation



Cartan moving frame and Helmoltz decompositioin

$$\boldsymbol{\vartheta}^i(\boldsymbol{x}) = dx^i + \boldsymbol{\Theta}^i(\boldsymbol{x})$$

Cartan Frame Euclid Frame Plastic Deformation

Local moving frame

$$\boldsymbol{\vartheta}^i(\boldsymbol{x}) = dx^i + \mathcal{R}^{-1}d\mathcal{R}(\boldsymbol{x})\boldsymbol{x} \longrightarrow$$

Twist disclination cannot be defined ⋯

$$\Omega^2_3 = \omega\delta(x,y)dx\wedge dy$$

$$\tau^1 = \frac{\omega z}{2\pi}\delta(x,y)dx\wedge dy$$

S. Kobayashi K. Takemasa & R. Tarumi (to be submitted)

3. Reconsideration of Volterra defects

Revision of Volterra Process

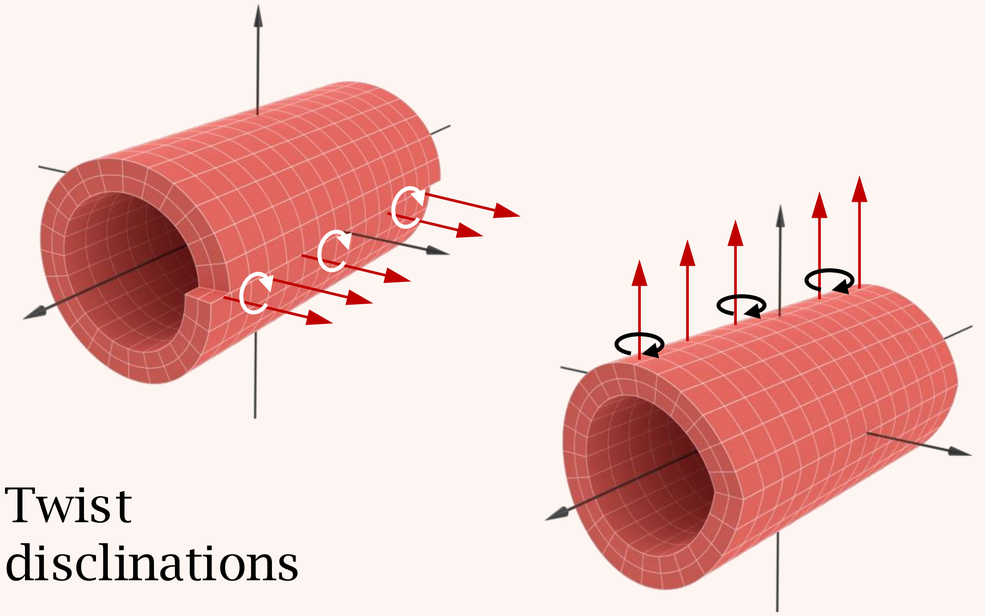
$$\boldsymbol{\psi}(\boldsymbol{x}) = \mathcal{R}(\boldsymbol{x})(x, y, z)$$

$$\boldsymbol{\psi}(\boldsymbol{x}) = \begin{pmatrix} \cos\frac{\phi}{2\pi}\theta & 0 & \sin\frac{\phi}{2\pi}\theta \\ 0 & 1 & 0 \\ -\sin\frac{\phi}{2\pi}\theta & 0 & \cos\frac{\phi}{2\pi}\theta \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Copy of rotation along z-axis

$$\boldsymbol{\psi}(\boldsymbol{x}) = \mathcal{R}(\boldsymbol{x})(x, y, 0) + (0,0,z)$$

$$\boldsymbol{\psi}(\boldsymbol{x}) = \begin{pmatrix} \cos\frac{\phi}{2\pi}\theta & 0 & \sin\frac{\phi}{2\pi}\theta \\ 0 & 1 & 0 \\ -\sin\frac{\phi}{2\pi}\theta & 0 & \cos\frac{\phi}{2\pi}\theta \end{pmatrix}\begin{pmatrix} x \\ y \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ z \end{pmatrix}$$



Twist disclinations

True definition of twist disclinations by curvature

$$\Omega_3^2 = \phi\delta(x, y)dx \wedge dy$$

$$\boldsymbol{\tau} = (0,0,0)$$

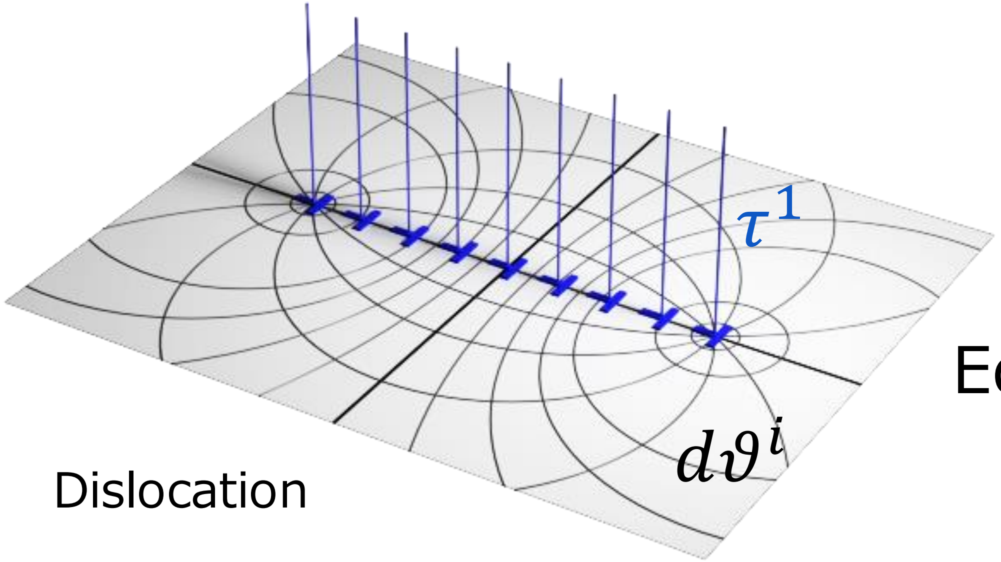
3. Reconsideration of Volterra defects

Theorem-1 : Wedge disclination dipole at the ends of dislocation array

Weitzenbock cnct.	Cartan Equations	Levi-Civita cnct.
$\tau^i = d\vartheta^i + \omega^i_j \wedge \vartheta^j$ $\Omega^i_j = d\omega^i_j + \omega^i_k \wedge \omega^k_j$	$\tau^i = d\vartheta^i + \omega^i_j \wedge \vartheta^j$ $\Omega^i_j = d\omega^i_j + \omega^i_k \wedge \omega^k_j$	$0 = d\vartheta^i + \omega^i_j \wedge \vartheta^j$ $\Omega^i_j = d\omega^i_j + \omega^i_k \wedge \omega^k_j$

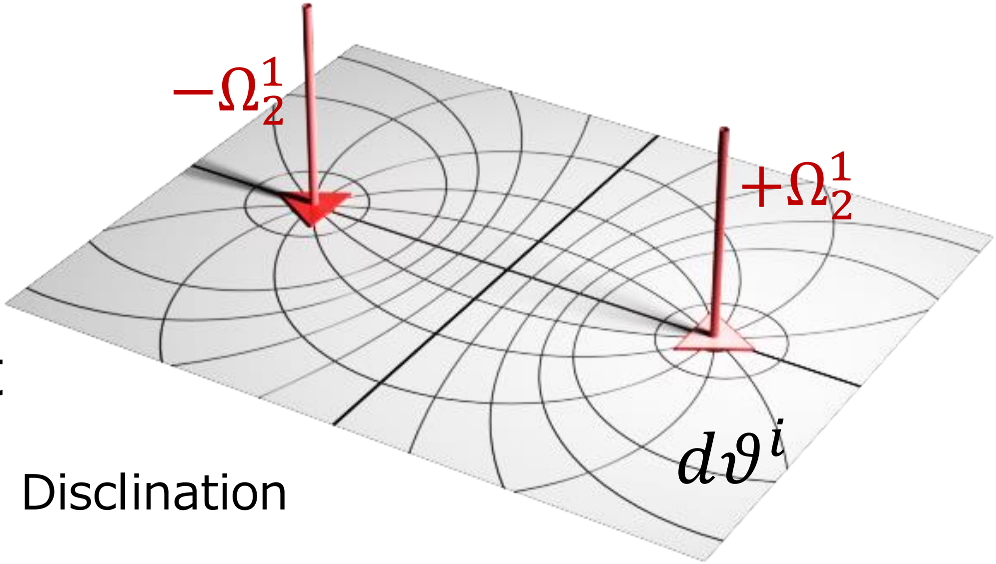
$$\tau^1 = b\rho\delta(y)(H(x+L) - H(x-L))dx \wedge dy$$

$$\Omega^1_2 = b\rho(\delta(x-L,y) - \delta(x+L,y))dx \wedge dy$$



Dislocation

Equivalent



Disclination

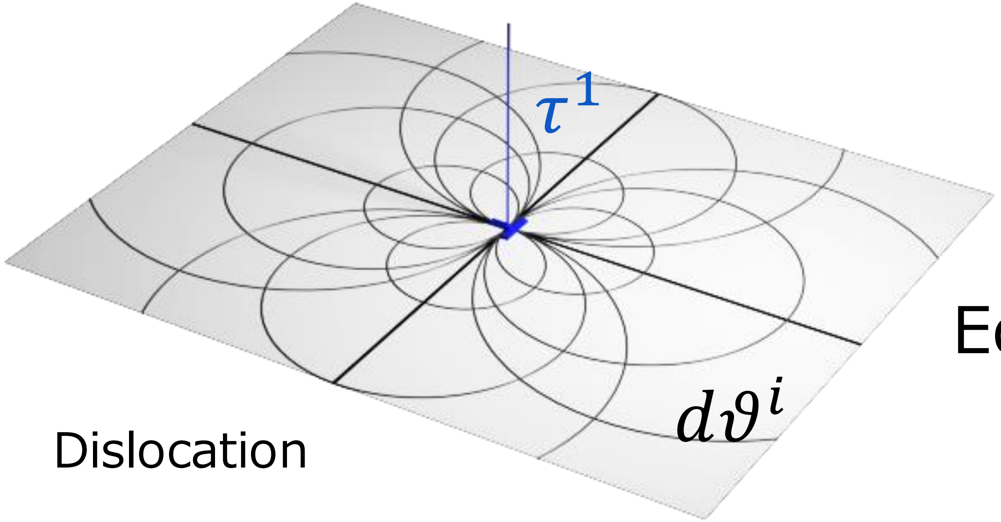
3. Reconsideration of Volterra defects

Theorem-2 : Edge dislocation is equivalent to wedge disclination dipole

Weitzenbock cnct.	Cartan Equations	Levi-Civita cnct.
$\tau^i = d\vartheta^i + \omega^i_j \wedge \vartheta^j$	$\tau^i = d\vartheta^i + \omega^i_j \wedge \vartheta^j$	$0 = d\vartheta^i + \omega^i_j \wedge \vartheta^j$
$\Omega^i_j = d\omega^i_j + \omega^i_k \wedge \omega^k_j$	$\Omega^i_j = d\omega^i_j + \omega^i_k \wedge \omega^k_j$	$\Omega^i_j = d\omega^i_j + \omega^i_k \wedge \omega^k_j$

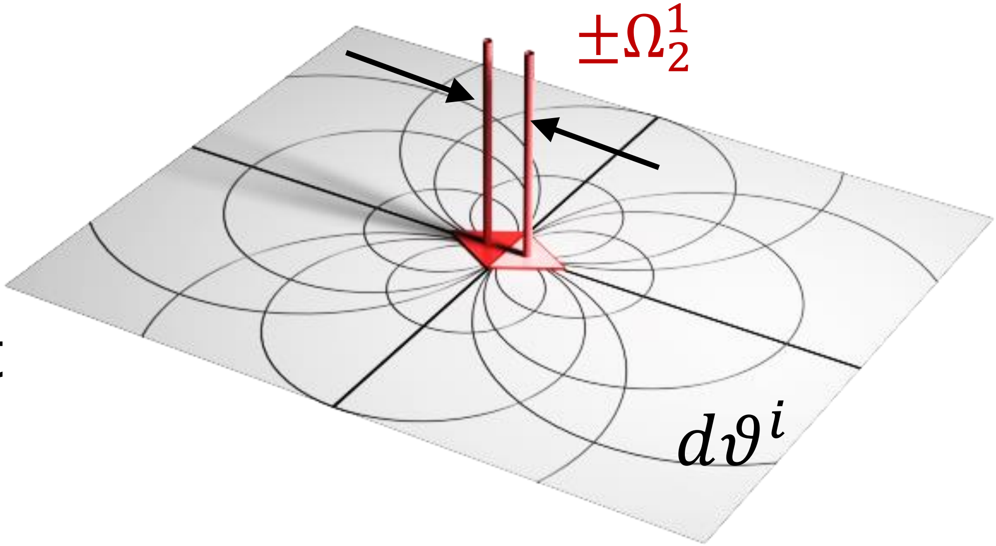
$\tau^1 = b\delta(x,y)\, dx \wedge dy$

$\lim_{L\to 0} \Omega^1_2 = \pm\infty$



Dislocation

Equivalent



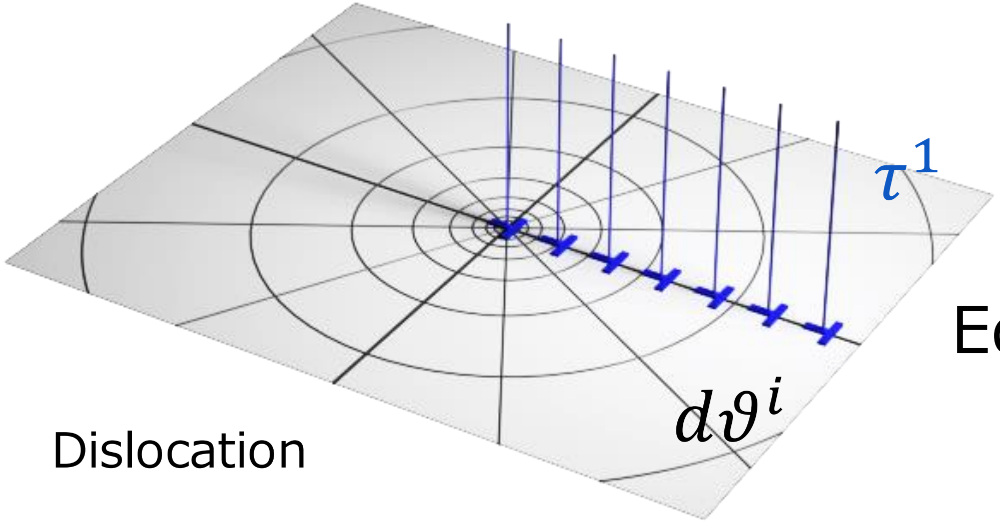
3. Reconsideration of Volterra defects

Theorem-3 : Existence of disclination monopole at semi-infinite array of dislocations

Weitzenbock cnct.	Cartan Equations	Levi-Civita cnct.
$\tau^i = d\vartheta^i + \omega^i_j \wedge \vartheta^j$ $\Omega^i_j = d\omega^i_j + \omega^i_k \wedge \omega^k_j$	$\tau^i = d\vartheta^i + \omega^i_j \wedge \vartheta^j$ $\Omega^i_j = d\omega^i_j + \omega^i_k \wedge \omega^k_j$	$0 = d\vartheta^i + \omega^i_j \wedge \vartheta^j$ $\Omega^i_j = d\omega^i_j + \omega^i_k \wedge \omega^k_j$

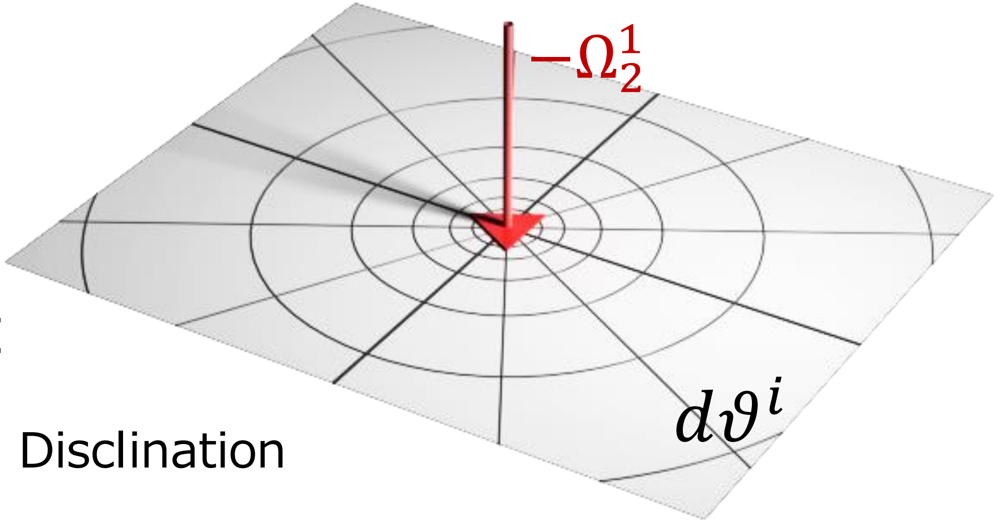
$$\tau^1 = b\rho\delta(y)H(x)dx \wedge dy$$

$$\Omega^1_2 = -b\rho\delta(x,y)dx \wedge dy$$



Dislocation

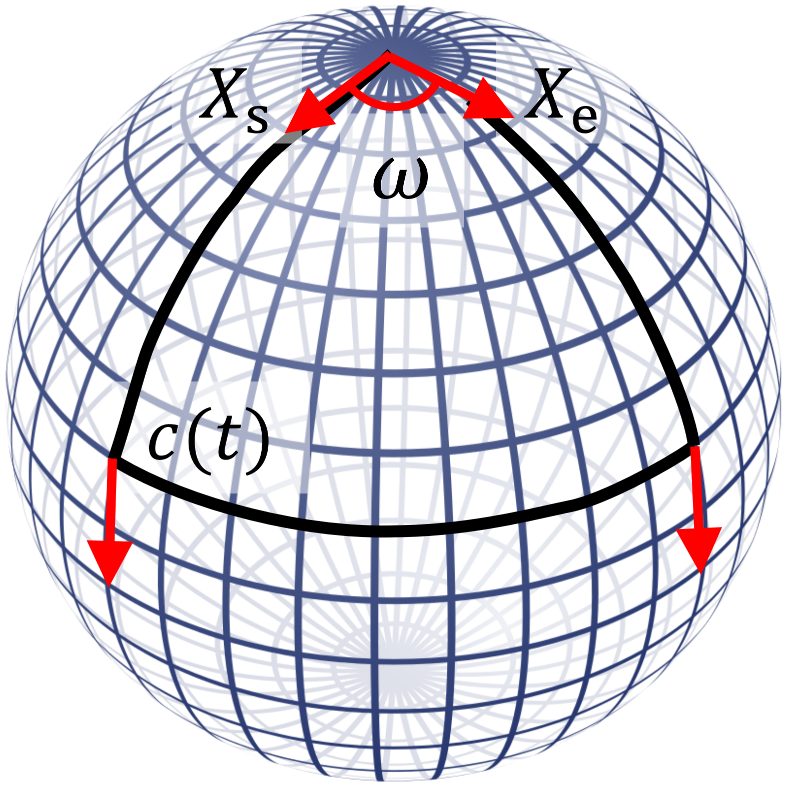
Equivalent



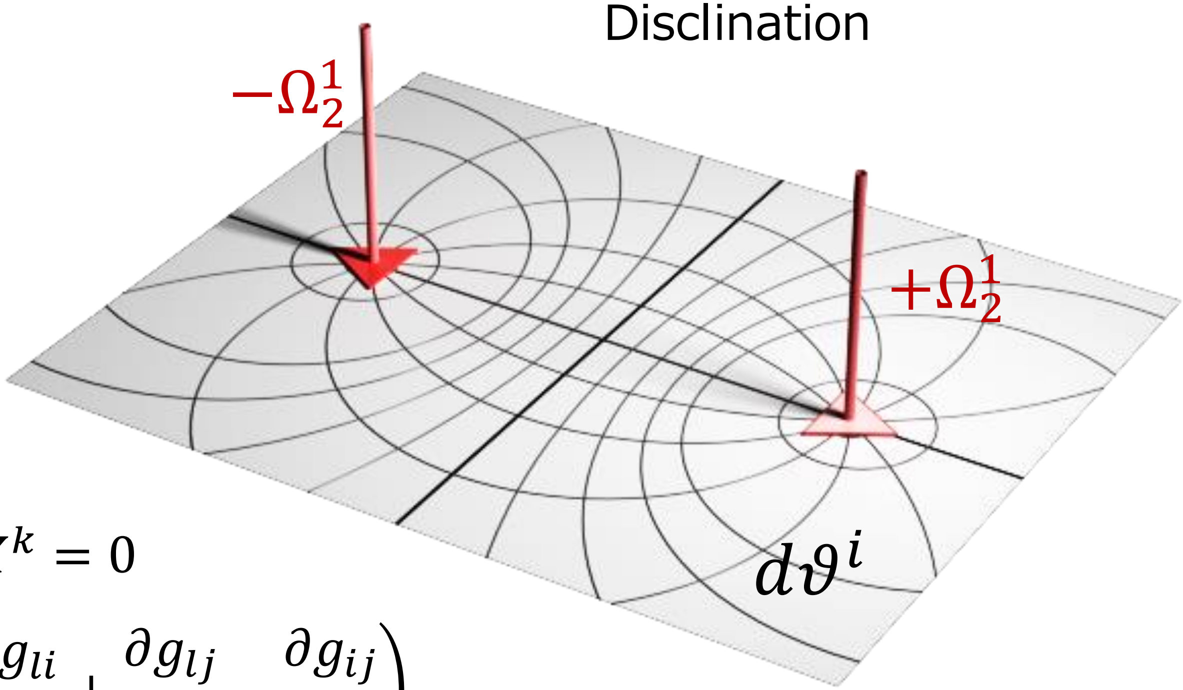
Disclination

3. Reconsideration of Volterra defects

Frank vector of disclination can be measured using holonomy on Riemannian mfd



Parallel transportation of vector



$$\frac{\partial X^i}{\partial t} + \Gamma^i_{jk}\dot{c}^j X^k = 0$$

$$\Gamma^k_{ij} = \frac{g^{-1}_{kl}}{2}\left(\frac{\partial g_{li}}{\partial x_j} + \frac{\partial g_{lj}}{\partial x^i} - \frac{\partial g_{ij}}{\partial x^l}\right)$$

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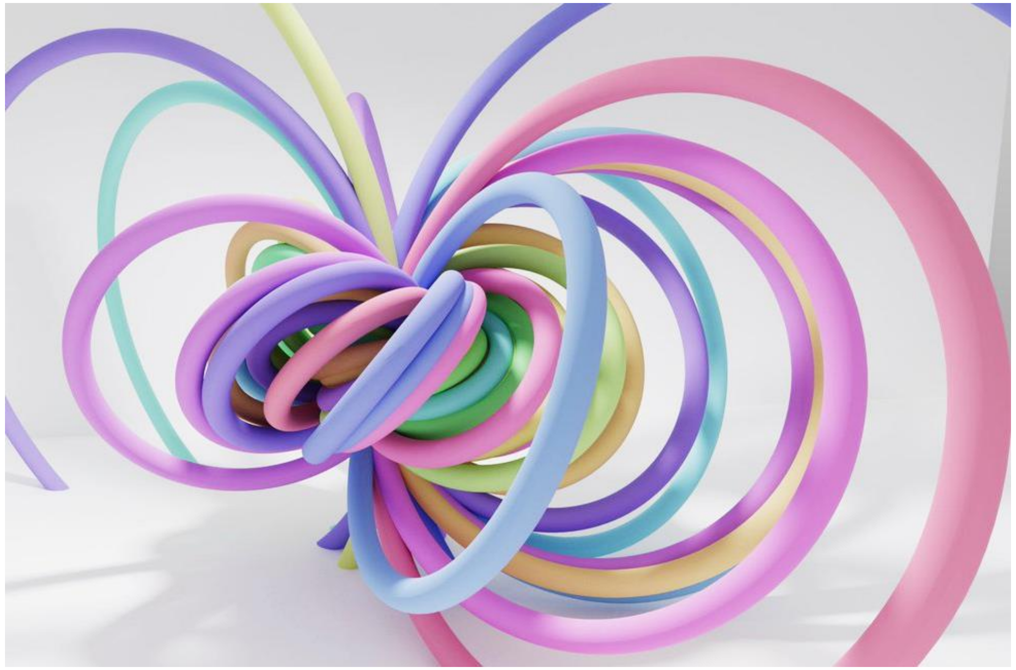
4. Riemann-Cartan & Information Geometry

JSPS KAKENHI, Promotion of Innovative Area A (5 years, 1.5 Billion YEN, Deadline: May 2025)

Materials Science

×

Differential Geometry



In this research field, we will create a new academic discipline called "**Material Geometry**" by integrating "Materials Science" and "Differential Geometry." By establishing a common academic foundation for a wide range of materials, we aim to lead the next generation of materials mechanics research, which will deepen traditional materials science in a more integrated manner.

4. Riemann-Cartan & Information Geometry

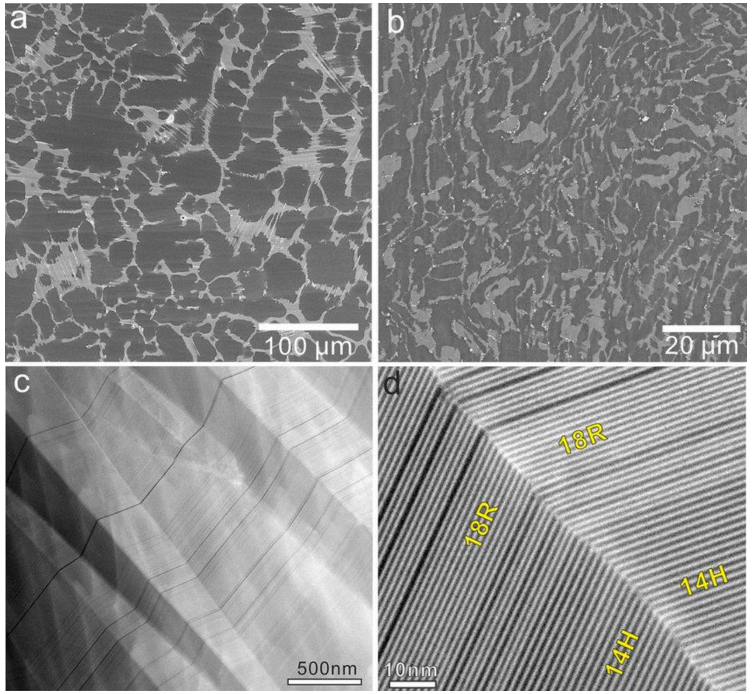
- 材料科学は高強度化によるCO2削減、医療材料、環境保護など産業基盤に直結（材料の国際戦略）
- 国際的に高い競争力を持つ構造材料や、高機能性材料の研究開発は進むが、基本原理が未解明のものが多く、効率的な応用展開に繋がらない（基本原理の解明・学術の普遍化）
- 人類が使用する実用材料の剛性比は1,000万倍を超えるため、材料種ごとに専門分野が分かれている。微分幾何学による共通の学術基盤を構築し、イノベーションを促進（学術基盤の共通化）
- JST「ナノ力学」は、材料の多様性から相乗効果を生み出す革新的な試みで、専門分野を超えた研究者の横の繋がりが生まれ始めている。相乗効果は萌芽的な段階にあるが、この方向性を維持することが重要（多様性の創出）

Young's modulus of industrial materials

4. Riemann-Cartan & Information Geometry

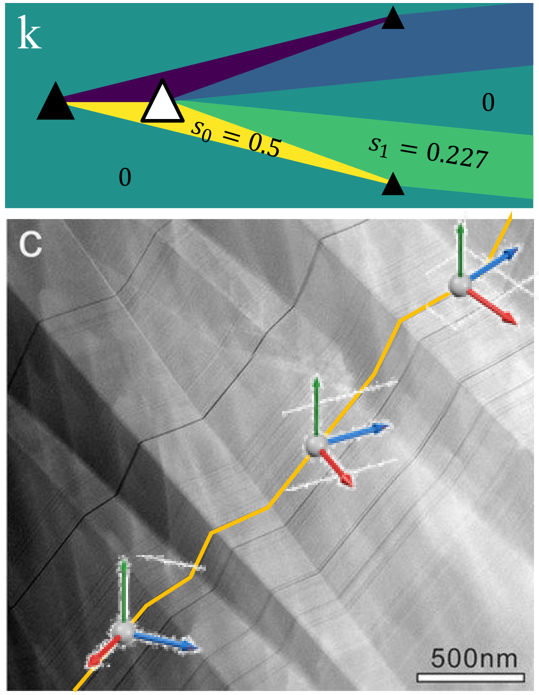
Application of **Riemann-Cartan geometry** for analysis of kink deformation

Kink Analysis



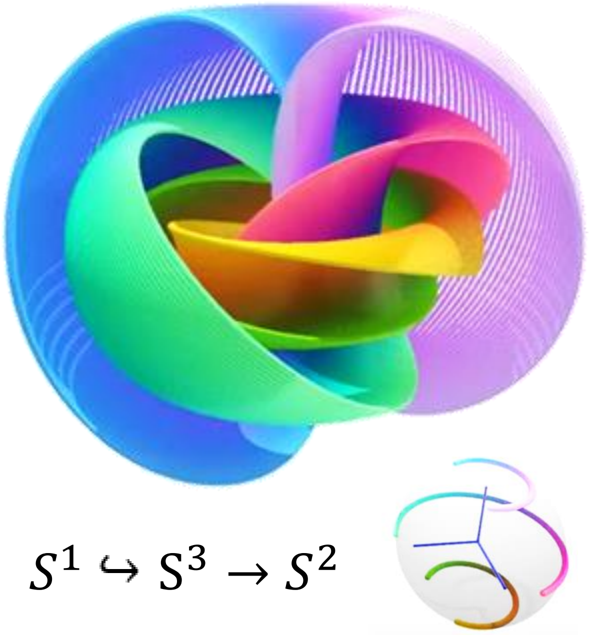
電子顕微鏡によるキンク界面構造の精密解析
+ 力学特性と構造・組織の関係

Topological Defects



Rank-1接続解析による回位の検出
+ 塑性フラストレーションのエネルギー評価

Hopf Fibration



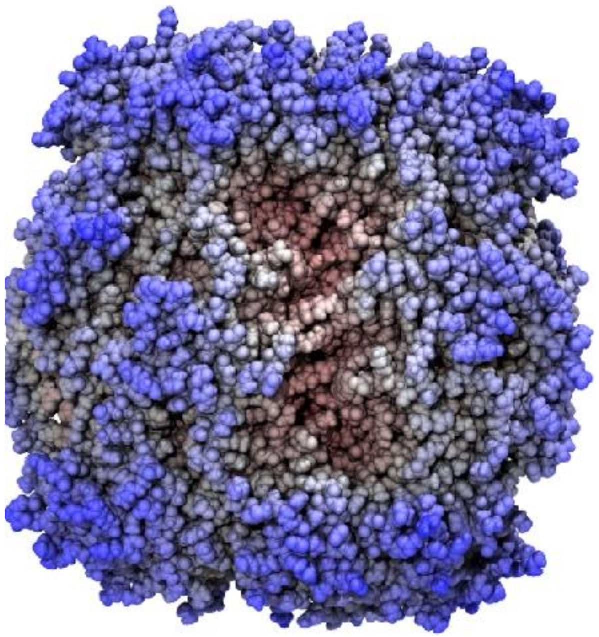
$$S^1 \hookrightarrow S^3 \rightarrow S^2$$

強化原理の普遍化
（位相微分幾何学によるキンク構造解析）

4. Riemann-Cartan & Information Geometry

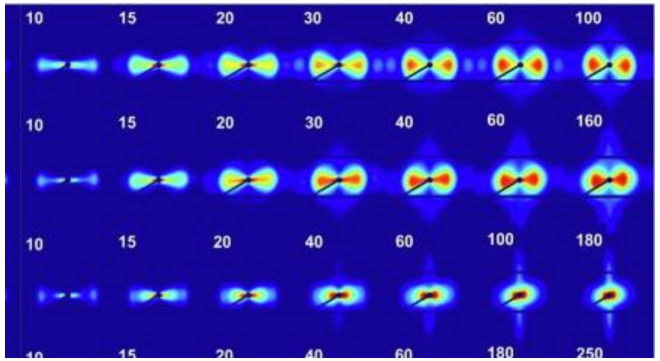
Application of **information geometry** for statistical mechanics of polymers and soft matters

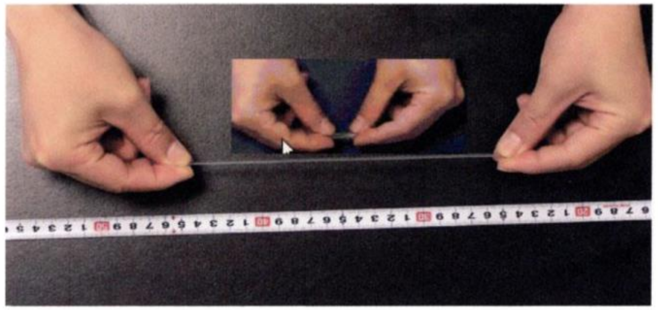
Nonlinear Mechanics



ソフトマテリアルの分子設計と力学特性
+ 熱延伸による高分子の高強度化

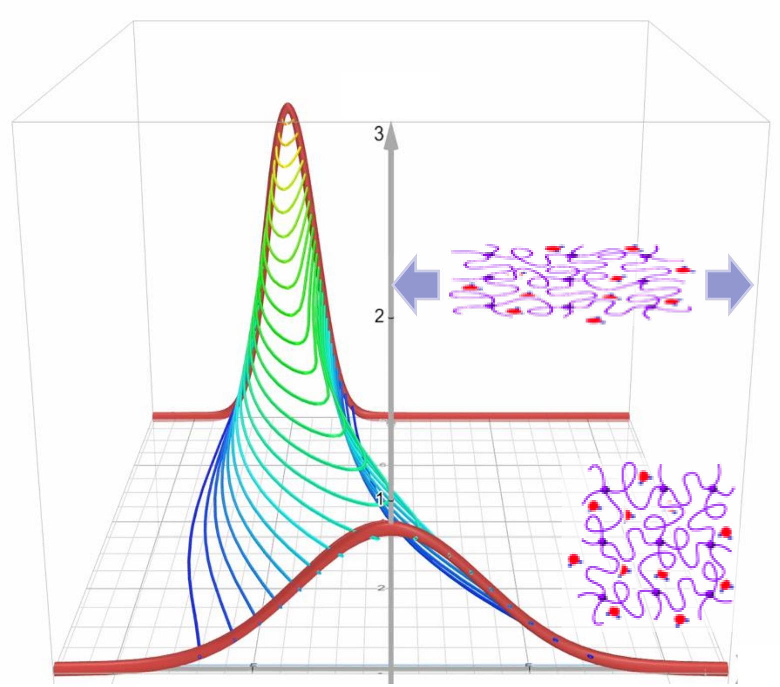
X-Ray Scattering and Diffraction





分子鎖ネットワークの配向度・結晶化計測
+ 分子動力学計算力との比較・検証

Information Geometry



グラフ理論による分子鎖の位相幾何学解析
+ 確率密度分布の時間発展評価（情報幾何学）