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IMI Workshop II: 結晶転位の先進数理解析

(Advanced Mathematical Investigation for Dislocations)

at IMI オーディトリアム（W1-D413） 九州大学伊都キャンパス

1 Program (2018 年 9 月 10 日（月）-11 日（火）)

9 月 10 日（月）

13:00-13:05	オープニング	
13:05-13:55	中川淳一（新日鐵住金）	数学と物質・材料との連携への展開 -転位と回位の数学的記述を事例に-
14:10-15:00	東田賢二（佐世保高専）	結晶中の転位観察と塑性変形現象：現状と課題
15:00-15:30	休憩	
15:30-16:20	時弘哲治（東京大学)	液晶における転位と準周期性
16:30-17:15	松谷茂樹（佐世保高専）	先進数理解析と結晶の転位問題
19:00-	懇親会 *	

9 月 11 日（火）

10:00-10:30	社会数理実践研究 (東大数理)	- 結晶構造の数学的記述 Growth -
10:45-12:15	甘利俊一（理化学研究所）	転位の連続体の動的理論：微分幾何によるアプローチ
12:15-14:00	昼休憩	
14:00-15:30	砂田利一（明治大学）	Certain Arithmetic Quasicrystals
15:30-16:00	ティータイム	
16:00-16:50	上坂正晃 (北海道大学)	結晶のらせん転位に関する変分問題的アプローチ
16:50-16:55	クロージング,	

*: 懇親会:
日時：9 月 10 日 (月) 19:00〜
場所：海峯魯 (かいほうろ) 天神西通り
`https://kaihouro-tg.owst.jp/`
`https://tabelog.com/fukuoka/A4001/A400103/40035725`
会費：6000 円 (飲み放題付)
ご出席ご希望の方は松谷（smatsu @ sasebo.ac.jp) に 8 月末頃までにご連絡ください.
席に限りがありますので，参加ご希望の場合はお早めにお知らせ頂ければ幸いです。

2 概要

9 月 10 日（月）

1. **13:05-13:55 中川淳一（新日鐵住金） 数学と物質・材料との連携への展開-転位と回位の数学的記述を事例に-**

   (Propulsion of Collaboration between Mathematics and Materials -Topics regarding Mathematical Description for Dislocation and Disclination-)

   Disordered structures in a crystal, such as lattice defects, are a primary factor in determining the mechanical properties of materials. For example, the plasticity observed in the macro-scale world is caused by the lattice defect called as dislocations in the micro-scale world. We have been studying mathematical properties of the lattice defects in the Study Group Workshop and the FMSP mathematical research on real world problems of the University of Tokyo. In these activities, the behavior of the screw dislocation observed by material scientists was described by a simple formula. It was found that the mathematical essence of the formula was monodromy. Then, the monodromy was described using a bundle whose fibers

constitute a discrete group, such as $\mathbb{Z}$. Furthermore it was found that both the screw and edge dislocations, what is more, disclination were described by encoding the symmetry arising from the original lattice using Thurston's monodromy, which was composed of local charts of the graph corresponding to the lattice defects, and a coordinate change of these charts. The topics mentioned above are problems in mathematics originating from problems in materials and industry. Progress on the problem is advancing mathematically year by year through interdisciplinary discussions among the field of mathematics, materials and industry, what is more, among different fields of mathematics. In this workshop, I hope to go through the next stage where their theories make consistent mathematically and pragmatic progress with the social cooperation of mathematics.

2. **14:10-15:00 東田賢二（佐世保高専）結晶中の転位観察と塑性変形現象：現状と課題**

   (On observation of dislocations and phenomena of plastic deformation in crystals)

   In this talk, several observation results of dislocations and phenomena of plastic deformation in crystals are reported. The experimental results exhibit that dislocations essentially control the mechanical behaviours of crystals such as plastic deformation and fracture. A plastic deformation phenomenon called "kink deformation" is introduced, since it attracts interests not only from materials engineering but also from mathematical field. The properties of dislocations and related phenomena play important roles for the next generations.

3. **15:30-16:20 時弘哲治（東京大学) 液晶における転位と準周期性**

   (Quasi-periodicity and dislocation in liquid crystals)

   液晶と超伝導体の統計力学的な類似性から，液晶におけるらせん転位は超伝導体における磁束の進入とみなすことができる．この類似によって，第２種超伝導体のアブリコソフ相に対応する液晶の相として TGB 相が存在することが知られている．この TGB 相における準周期性と準結晶の分類に表れる整数論における類数との関連などについてお話したい．

   By the analogy between liquid crystals and super conductors in statistical physics, a screw dislocation in a liquid crystal corresponds to a magnetic vortex in a super conductor. According to this analogy, there exists the twisted grain boundary (TGB) phase in liquid crystals that is an analogue of the Abrikosov phase in super conductors. In this talk, we wish to explain relations of the quasi-periodicity of TGB phase to the classification of quasi-crystals in terms of class numbers in number theory.

4. **16:30-17:15 松谷茂樹（佐世保高専）先進数理解析と結晶の転位問題**

   (Advanced mathematical investigation and dislocations in crystal lattice)

   産業における重要な問題は，一般的には一つの数学分野や，一つの科学分野の枠内で解かれることはない．それらは多岐に亘る数学分野，更には多岐に亘る科学分野と関係している．その原型と呼べるものが，ベルヌーイ・オイラーの弾性曲線の研究にある．それをプロトタイプとして私はそのような研究を先進数理解析と名付けている．講演では，弾性曲線のベルヌーイ・オイラーらの研究を紹介した後に，先進数理解析の重要性を述べる．また，先進数理解析の例として，らせん転位の離散的幾何に関する結果と，鉄鋼のキンク現象とエラスティカの関係についての最近の結果を報告する．

   Crucial problems in industry, basically, cannot be solved in the framework of a single mathematical field or a single field in science. They are related to a variety of mathematical fields and wider scientific knowledge. The study of Bernoulli-Euler's elastic curve (elastica) is a nice prototype. I call such a study *advanced*

mathematical investigation. In this talk, after I give a short review of their study of elastica, I explain what is the advanced mathematical investigation. As examples of the investigation, I report the discrete geometry of screw dislocation and recent study of kink phenomenon using the elastica.

9 月 11 日（火）

1. **10:00-10:30 社会数理実践研究 (東大数理) - 結晶構造の数学的記述 Growth -**

   (FMSP mathematical research on real world problems of the University of Tokyo - Mathematical Description of Crystal Lattice Structure, Growth -)

   The mathematical research on real world problems is an educational program for doctor course students in FMSP (Leading Graduate Course Frontiers of Mathematical Science and Physics) of the University of Tokyo. Nippon Steel & Sumitomo Metal Corporation is a proposer of the theme for the program, and has provided several themes for students who major in geometry or algebra. In this talk, the growth is highlighted as a theme that is interesting in mathematics and important in materials. The growth is defined as a sequential representation of the graphical structure of a crystal lattice. The first growth corresponds to the coordination number of crystals, which is used as a numerical index to describe the crystalline structure in material science. The number of the nth growth was counted step by step and the numerical sequences at $n \to \infty$ is a quasi-polynomial, i.e. the coefficients are periodic functions with integral period. The generating functions can be derived from the quasi-polynomial and showed symmetrical properties. We have been studying the mathematical conditions such that the growth becomes a quasi-polynomial and the relationship between the growth of a crystal lattice and the growth of the crystal group.

2. **10:45-12:15 甘利俊一（理化学研究所） 転位の連続体の動的理論：微分幾何によるアプローチ**

   (Space-Time Theory of Continuously Distributed Dislocations: Differential-Geometrical Approach)

   金属材料はミクロには結晶構造を有するため，結晶のひずみ（欠陥）がその強度に重要な役割を果たす．欠陥はミクロに見れば転位や転傾であるが，マクロにはこれらが連続に分布していると考えてよい．この様相を記述するのに，捩率を含むリーマン空間の理論が 1950 1960 年代に日本及びヨーロッパにおいて展開された．

   その理論はいまではほとんど忘れ去られた感があるが，ここでもう一度掘り起こして考えてみたい．特に転位などの欠陥が運動する動的転位の連続体を，4 次元物質時空間の捩率－曲率として扱う理論について紹介したい．

   Metals have crystal structures and defects of such structures are responsible for their strength. Defects are typically dislocations and disclinations from the microscopic point of view, but they are continuously distributed from the macroscopic point of view. Riemannian and non-Riemannian theories had been developed in Japan and Europe in 1950-1970 for elucidating these aspects.

   However, it looks mostly forgotten in the present days. We review these theories again. We recapitulate the four-dimensional continuum theory of moving dislocations in which motion, creation and annihilation of dislocations are described as torsions and curvatures of a four-dimensional material space-time.

3. **14:00-15:30 砂田利一（明治大学）Certain Arithmetic Quasicrystals**

   In this talk, motivated by the 31st entry dated 1796 September 6 in Gauss's Mathematisches Tagebuch (Mathematical Diary), I will deal with a class of discrete sets defined arithmetically in the Euclidean space. Asymptotic behaviors of primitive Pythagorean and Eisenstein triples are discussed in connection with the notion of quasicrystals.

4. **16:00-16:50 上坂正晃 (北海道大学) 結晶のらせん転位に関する変分問題的アプローチ**

(Approach using variational problem toward a dislocation of a crystal)

結晶の転位はミクロな現象であるが，その生成や動きがマクロな金属の性質に大きな影響を与えるという意味でマルチスケールの問題であると考えることができる．そうした問題にアプローチするためには，均質化法などのような，離散的なミクロモデルと連続的なマクロモデルを結びつける極限操作が必要である．特に，エネルギーの変分問題として転位の問題を取り扱おうとすると，Γ収束などの変分問題において都合の良い収束の概念を取り扱う必要がある．

本講演ではΓ収束を用いた転位のモデルについて，これまでにできている 1 次元のモデルを紹介するとともに，2 次元ではどういう結果が得られるのかについて紹介したい．特に 2 次元でのらせん転位モデルを考えようとすると，トポロジカルな性質がエネルギーに大きく関わってくることを示す．

また，もう一つ別の話題として，elastica の問題から発生する異なるタイプのエネルギーにおいて，Γ収束によってキンク構造が生じ得ることを紹介する．これはすぐに転位の理論に結びつくものではなく，むしろ医学に由来する全く違う問題から考察されたものであるが，転位の理論への応用が可能かどうかについて議論したいと思っている．

Dislocation of a crystal itself is a microscopic phenomenon and it is also considered as a multiscale problem since the generation and movement of it gives a big influence on macroscopic property of metal. To approach to this problem, The limit procedure, like homogenization for example, to connect a discrete microscopic model with a continuous macroscopic model is necessary. Especially, we need to treat the suitable concept of the convergence like Γ-convergence when treating this problem as energy minimization problem.

In this talk, We introduce one- and two-dimensional model of dislocation and their Γ-convergence results. Especially, we show that on two-dimensional problem, topological property affects the limit energy.

In addition, we show the generation of kink structure from the energy arising from elastica problem. This problem is not directly related to the theory of dislocation and it is arised from another phenomena origined from medical phenomena. I'd like to discuss whether this result can be connected with dislocation theory.