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IMI Workshop II: 材料科学における幾何と代数 I

(Geometry and Algebra in Material Science I)

九州大学マス・フォア・インダストリ研究所　On-line 研究会 (Zoom)
(2020 年 9 月 7 日 (月)-8 日 (火))

1 Program

9 月 7 日 (月)

11:00-11:05	オープニング	
11:05-11:45	川原一晃 (東京大学)	界面接合の実験と数理
11:45-13:30	昼休憩	
13:30-14:10	熊野知二 (日本製鉄 (株))	材料技術者のための四元数と行列を用いた対応格子関係の導出
14:30-15:10	小林舜典 (大阪大学)	Geometrical modeling and numerical analysis on dislocations in solid
15:30-16:10	下川智嗣 (金沢大学)	Relationship between the development of lattice defects and mechanical properties in solid materials through atomic simulations
16:30-17:10	田中良巳 (横浜国立大学)	ゲルの破壊と浸透圧の力学

9 月 8 日 (火)

11:00-11:30	山岸弘幸 (都立高専)	正多面体における離散ソボレフ不等式の最良定数
11:35-12:05	關戸啓人 (京都大学)	C_{60} における離散ソボレフ不等式の最良定数
12:05-14:00	昼休憩	
14:00-14:40	田中　守 (都城高専)	結晶構造に近いアモルファス構造のモデル化とパーコレーション
15:00-15:40	松江要 (IMI)	有限時間特異性: 力学系的アプローチ
16:00-16:30	中川淳一 (東大数理)	東京大学大学院数理科学研究科ＦＭＳＰ社会数理実践研究：結晶と準結晶に動機付けられた数学の問題 II
16:30-16:35	クロージング	

オンラインのため，参加にあたっては，下記の参加申込をお願いします.

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IMI Workshop II: Geometry and Algebra in Material Science I

On-line conference in Kyushu University (Zoom)
September 7 (Mon) - 8 (Tue), 2020

September 7 (Mon)

11:00-11:05	Opening	
11:05-11:45	Kazuaki Kawahara (The Univ. of Tokyo)	Experiments and mathematics of interface structure
11:45-13:30	Lunch	
13:30-14:10	Tomoji Kumano (Nippon Steel Corp.)	A derivation of coincidence site lattice relations utilizing quaternion and matrix for material engineers
14:30-15:10	Shunsuke Kobayashi (Osaka Univ.)	Geometrical modeling and numerical analysis on dislocations in solid
15:30-16:10	Tomotsugu Shimokawa (Kanazawa Univ.)	Relationship between the development of lattice defects and mechanical properties in solid materials through atomic simulations
16:30-17:10	Yoshimi Tanaka (Yokohama Nat. Univ.)	Fracture of gels and mechanics of osmosis

September 8 (Tue)

11:00-11:30	Hiroyuki Yamagishi (TMCIT)	The best constant of discrete Sobolev inequality on regular polyhedra
11:35-12:05	Hiroto Sekido (Kyoto Univ.)	The best constant of discrete Sobolev inequality on C_{60} fullerenes
12:05-14:00	Lunch	
14:00-14:40	Mamoru Tanaka (NIT, Miyakonjo)	A model of amorphous structure similar to crystal structure and percolation
15:00-15:40	Kaname Matsue (IMI)	Finite-time singularity: a dynamical system approach
16:00-16:30	Junichi Nakagawa (The Univ. of Tokyo)	Mathematical research on real-world problems is an educational program for doctorate course students in FMSP (Leading Graduate Course Frontiers of Mathematical Science and Physics) of the University of Tokyo : Problems in Mathematics Motivated by Crystals and Quasi-Crystals II
16:30-16:35	Closing	

To participate this conference, please apply below

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2 概要

9 月 7 日 (月)

1. **11:05-11:45 川原一晃 (東京大学)　界面接合の実験と数理**

(Experiments and mathematics of interface structure)

川原一晃 [1]，井上和俊 [2,3]，斎藤光浩 [1]，荒船竜一 [4]，林俊良 [5] 高木紀明 [6]，川合眞紀 [7]，幾原雄一 [1,3]

1. 東京大学総合研究機構，2. JST さきがけ，3. 東北大学材料科学高等研究所，4. 物質・材料研究機構，5. National Chiao Tung University ，6. 京都大学人間・環境学研究科，7. 分子科学研究所

グラフェンやシリセンなどの 2 次元物質と基板の界面や機能性材料の多結晶体の粒界は材料の機能や電子状態に大きな影響を及ぼす [1,2]．機能特性や電子状態の解明には原子構造を明らかにする必要がある．界面は 2 次元の面で接しているため，構造解析には 2 次元格子整合の概念が利用される．本研究では，2 次元格子整合を代数的整数論を用いて議論し，2 つの格子を重ねてできる超構造の周期および対称性は代数体の不変量であるイデアル類群により決まることを明らかにした [3]．さらに，実験的にある超構造が観測されたとき，その構造モデルを構築するアルゴリズムを導出した．本講演では 2 次元格子整合理論を応用した金属基板上の 2 次元ハニカムシートの構造および立方晶系材料の粒界構造の解析への応用についても述べる．

Kazuaki Kawahara[1], Kazutoshi Inoue[2,3], Mitsuhiro Saito[1], Ryuichi Arafune[4], Chun-Liang Lin[5]
Noriaki Takagi[6], Maki Kawai[7], Yuichi Ikuhara[1,3]

1. Institute of Engineering Innovation, The University of Tokyo, 2. JST-PRESTO, 3. WPI Research Center, Advanced Institute for Materials Research, Tohoku University, 4. National institute for material science, 5. National Chiao Tung University, 6. Garduate school of human and environmental studies, Kyoto University, 7. Institute for molecular science

Interface between a two-dimensional (2-D) material such as graphene and silicene with the substrate, as well as grain boundaries in polycrystalline functional materials have a great influence on the function and electronic state of the material [1,2]. To elucidate the properties and electronic states, it is necessary to determine the interface atomic structure. Since 2-D lattices are in contact with each other at a 2-D plane, the concept of 2-D lattice matching is used for structural analysis. In this study, 2-D lattice matching is classified by the ideal class group that is an invariant of algebraic number field [3]. The period and symmetry of superstructure formed by two 2-D lattices is determined by the ideal class group. As an application of this theory, an algorithm to construct a structural model for a superstructure is derived. We will discuss the application of the 2-D lattice matching theory to the structural analysis of 2-D honeycomb sheet grown on metal substrate and grain boundary of cubic polycrystalline materials.

[1] C.-L. Lin, et al., Phys. Rev. Lett. 110, 076801 (2013).

[2] K. Inoue, et al., J. Mater. Sci. 52, 4278 (2017).

[3] K. Kawahara, et al., e-J. Surf. Sci. Nanotech. 13, 365 (2015).

2. **13:30-14:10 熊野知二 (日本製鉄 (株))　材料技術者のための四元数と行列を用いた対応格子関係の導出**

(A derivation of coincidence site lattice relations utilizing quaternion and matrix for material engineers)

Grain-oriented silicon steel is mainly used as the core material of transformers, and it is manufactured by applying secondary recrystallization phenomena. The driving force of this phenomena is the grain boundary energy, which would be characterized by coincidence site lattice (CSL) relations. CSL relations are determined by the arrangement of lattice points in three-dimensional space and have already been shown mathematically by using advanced mathematics. However, their derivation processes are difficult for material engineers to understand due to their abstractness. Therefore, in this study, a derivation of CSL relations is attempted in order to enable them to easily understand the derivation. This study contributes to industrial mathematics by helping them understand the essence of the mathematical method in order to apply the relations appropriately.

A derivation method for CSL relations is proposed using the hexagonal lattice in the case of an axial ratio of $\sqrt{(8/3)}$ as an example. This method involves applying the scale rotation of a quaternion, and it is thus named the quaternion-matrix method.

The matrix specifying the ΣN-CSL relation of a certain lattice system is expressed by a similarity transformation using the matrix comprising its primitive translation vectors and is given as the following transformation matrix: $\mathbf{H}_i = \mathbf{E}_i^{-1}\mathbf{E}_R\mathbf{E}_i$. Based on the rational number properties for elements of the transformation matrix, the following formula is derived:

$N = N_0^2 + 2N_1^2 + 6N_2^2 + 3N_3^2$, $N_i \in \mathbb{N}+$, $N : \Sigma$ value.

Here, $(N_0N_1N_2N_3)$ is specified by the integrality (lattice point) and irreducibility (unit cell) among the elements of $\mathbf{H}_i$.

Finally, a quaternion for the CSL relation formation is thus derived, and based on the polar form of the quaternion, the CSL relation could be derived.

3. **14:30-15:10 小林舜典 (大阪大学) Geometrical modeling and numerical analysis on dislocations in solid**

The aim of this study is to construct a framework to calculate the internal stress field of a crystalline solids for an arbitrary distribution of dislocations. Based on the standard assumptions in kinematics, the original problem is divided into the two parts; plastic and elastic defromations. We introduce three diffeomorphic manifolds called the reference, intermediate and equilibrium states. The reference and equilibrium states are in the Euclidean space while the intermediate state is a Riemannian manifold which accompanies an affine connection with non-zero torsion and vanishing curvature. The first part of the problem, *i.e.*, plastic deformation, is to find the Reimannian metric for a given distribution of dislocations. By using the equivalence of torsion and dislocation density tensors, we employ the Cartan first structure equation as a geometrical constraint between the torsion and metric. To simplify the analysis, we take a pullback of the structure equation and consider the constraint condition on the reference state. The solution must satisfy additional constraint conditions required from the Helmholtz decomposition of a vector-valued 1-form. Finally, the conditions are cast into an optimization problem to minimize the residual norm of the structure equation. We obtained the metric as well as affine connection of the intermediate state by solving the variational problem numerically. The second-half of the problem is relatd to the elastic deformation. By definition, the Riemannian metric of the equilibrium state is obtained from the displacement from the reference state. It indicates that Riemannian metric of the intermediate state behaves as a geometric constraint of the elastic part. In the present geometrical framework, elastic deformation is understood as an embedding map of the Riemannian manifold to Euclidean space. We obtained the deformation so that it minimizes the strain energy functional as in usual elasticity. We employed isogeometric analysis to solve the variational problems, *i.e.*, Galerkin method which uses NURBS as the basis function. Numerical analysis is conducted for several configuration of dislocations including dislocation loops, forest dislocations and polygonization structure for kink deformations.

4. **15:30-16:10 下川智嗣 (金沢大学) Relationship between the development of lattice defects and mechanical properties in solid materials through atomic simulations**

Plastic deformation of solid materials occurs through lattice defects. There are various various morphologies of lattice defects, including vacancy as 0-dimensional, dislocations and disclinations as 1-dimensional, grain boundaries as 2-dimensional defect, and precipitates as 3-dimensional. The mechanism of the release of elastic strain energy stored in the materials due to the motion, development and interaction of these lattice defects governs the mechanical properties of solid materials. Although the indirect interactions of lattice defects through their mechanical fields can be expressed theoretically, the direct interactions between the lattice defects must be expressed explicitly in terms of the structure of the atoms. In this presentation, the relationship between the development of the lattice defects and mechanical properties in solid materials through atomic simulations. First, the fundamental issues of dislocations, grain boundaries, and disclinations are explained, then the mechanism of dislocation generation from grain boundaries as an interaction of lattice defects is described in detail, and the relationship between this phenomenon and the fracture properties of materials is explained. In addition, the method of combining atomic and continuum regions, the problems of lattice defects in new materials (high-entropy alloy), and the relationship between the statistic properties of intermittent plasticity and mechanical properties of materials are discussed.

5. **16:30-17:10　田中良巳 (横浜国立大学)　ゲルの破壊と浸透圧の力学**

(Fracture of gels and mechanics of osmosis)

前半では，ゲルの破壊現象の幾つかの興味ある側面を議論する．例えば，1) き裂先端線に形成される巨視的な欠陥構造の形成や，2) 多量の溶媒を含むゲルを高強度化するメカニズム，また 3) き裂先端での溶媒の混合にゲル網目の応力発生の共役現象について述べる．講演の後半では，上述の 3) に関連していわゆる浸透圧というものの力学をソフトマター物理学に知見に基づき考察する．

In the former half of this talk, I will describe some interesting aspects of fracture of gels; concretely, 1) formation of a sort of giant defects on the crack front lines, 2) a mechanism for remarkable reinforcement

of watery gels, and 3) stress diffusion coupling by mixing of two solvents occurring around the crack the front. In the latter half, I will discuss the mechanics of the so-called osmotic pressure based on soft matter physics.

9 月 8 日 (火)

1. **11:00-11:30 山岸弘幸 (都立高専) 正多面体における離散ソボレフ不等式の最良定数**

   (The best constant of discrete Sobolev inequality on regular polyhedra)

   正多面体上の頂点に同一の原子を置き，頂点同士を線形バネで繋いだ古典力学モデルを考える．このモデルに外力をかけた時の変位 (たわみ) を，バネのポテンシャルエネルギーの定数倍で評価する不等式が離散ソボレフ不等式である．定数倍の内，最も小さい定数が最良定数であり，正多面体における離散たわみ問題を記述する離散ラプラシアンのムーア・ペンローズ一般化逆行列 (擬グリーン行列) の対角成分の最大値で与えられる．不等式の等号を達成するベクトルも擬グリーン行列の列ベクトルで構成される．離散ソボレフ不等式の最良定数は古典力学モデルのかたさの指標であり，定数が小さいとモデルが固いことを意味している．最良定数を比べることで，見た目ではわかりにくい多面体のかたさを比較する事ができる．

   The best constants of discrete Sobolev inequalities corresponding to regular polyhedra are found. We treat a classical mechanical model of regular polyhedra. Its neighboring two atoms are connected by a linear spring with uniform spring constant. The best constants stand for rigidities of these polyhedra. Thus we can expect the best constant of Sobolev inequalities have connections with physical properties of materials with crystal structure. The discrete Sobolev inequality shows that the maximum of deviation of a polyhedron is estimated from above by a constant multiples of the potential energy. That is, if the best constant is smaller, the model is more rigid. In the background, there is a discrete version of a bending problem. The solution is expressed by using Moore-Penrose generalized inverse matrix (pseudo Green matrix) of discrete Laplacian. Using a pseudo Green matrix, we have the best constant and the vector, which attain the equality.

2. **11:35-12:05　關戸啓人 (京都大学)C_{60} における離散ソボレフ不等式の最良定**

   (The best constant of discrete Sobolev inequality on C_{60} fullerenes)

   C_{60} フラーレンとは，炭素原子 n 個からなる球状の分子である．最初に発見された C_{60}，フラーレンは，バッキーボールと呼ばれる切頂二十面体の形をしている C_{60} フラーレンで，クロトー，カール，スモーリーらによって発見された．全ての炭素原子は他の 3 つの炭素原子と結合しており，5 員環と 6 員環のみからなるもののみを考えると，C_{60} フラーレンは 1812 個の異性体が存在することが知られている．ここで，各炭素原子が線形バネでつながっている古典力学モデルを考えて，かたさの指標として離散ソボレフ不等式の最良定数用いる．C_{60} フラーレンの全 1812 個の異性体について，最良定数を求めることで，C_{60} フラーレンの中で最もかたいフラーレンはバッキーボールであることがわかった．

   C_{60} fullerene is a molecule composed of 60 carbon atoms in the form of a hollow sphere. Kroto, Curl, and Smalley found the first C_{60} fullerenes called "buckyball" with the shape of a truncated icosahedron. We assume that each carbon atom bonds to 3 other atoms, and fullerenes contain only pentagonal and hexagonal faces. In this assumption, it is known that there are 1812 non-isomorphic C_{60} fullerenes. We consider the classical mechanical model, that is, we consider that carbon atoms are connected by uniform linear springs. Then we introduce the best constant of the discrete Sobolev inequality for the criteria of rigidity. We calculate the best constants of the discrete Sobolev inequality for all the C_{60} isomers, and we show the most rigid C_{60} fullerene is backyball.

3. **14:00-14:40　田中　守 (都城高専)　結晶構造に近いアモルファス構造のモデル化とパーコレーション**

   (A model of amorphous structure similar to crystal structure and percolation)

   相変化記録材料は，書き換え可能な CD, DVD, BD のような記録メディアに使われている．これらの材料の反射性は結晶構造とアモルファス構造で非常に異なり，急速な「結晶-アモルファス」構造変化により記録・消去が行われる．これまでのいくつかの研究により，結晶相とアモルファス相の局所原子配置が大まかに似ていることが示唆されている．ここでは，結晶構造とアモルファス構造をとる相変化材料のグラフによるモデル化について紹介する．これは平田秋彦先生との共同研究である．　また，このモデル化に関連する平面グラフのパーコレーションにおいて，無限クラスターの数，半径，大きさについて考察する．

   Phase-change recording materials are used for recording media such as rewritable compact discs (CD), digital versatile discs (DVD), and blu-ray discs (BD). The recording/erasing mechanism is driven by fast "amorphous-crystal" structural change, because the reflectivity of crystal is quite different from that of amorphous in these materials. Previously some studies suggested that local atomic configurations in amorphous phase is largely similar to that in crystalline phase. In this talk, we introduce a model of phase change materials which has amorphous structure and crystal structure. This is a collaborative research with Professor A. Hirata. We also consider the expected number of infinite clusters, and the exponential tail decay of the radius and the size of a cluster in a percolation of planer graphs related to this model.

4. **15:00-15:40　松江要 (IMI) 有限時間特異性: 力学系的アプローチ**

   (Finite-time singularity: a dynamical system approach)

   本講演では常微分方程式の解で，有限時刻で特異な振る舞いをする物の特徴付けを論じます．非線型性に付随する適切な時間・空間の (コンパクト化を含む) 特異性解消と力学系の基礎理論を用いて，数学的・数値的に記述が容易でない「爆発・絶滅」解やその派生物である「コンパクトン・急冷」解の包括的な記述が可能になることを示します．この特徴付けは (精度保証付き) 数値計算による解の定性・定量的記述も可能となっており，様々な時間依存する「特異性」の記述や計算の基礎的な考え方を与えると期待されます．

   This talk aims at describing finite-time singularities for solutions of ordinary differential equations. We mainly prove that appropriate desingularizations of time and space variables (including compactifications) with standard theory of dynamical systems provide comprehensive description of blow-up solutions, finite-time extinction as well as their secondary objects such as compacton and quenching solutions which are difficult to describe the behavior both mathematically and numerically. Our characterization also enables qualitative and quantitative descriptions of these phenomena through (rigorous) numerics, which will provide a fundamental idea to study time-dependent “singularities” of various kinds.

5. **16:00-16:30 中川淳一 (東大数理) 東京大学大学院数理科学研究科ＦＭＳＰ社会数理実践研究：結晶と準結晶に動機付けられた数学の問題 II**

   (Mathematical research on real-world problems is an educational program for doctorate course students in FMSP (Leading Graduate Course Frontiers of Mathematical Science and Physics) of the University of Tokyo： Problems in Mathematics Motivated by Crystals and Quasi-Crystals II)

   Mathematical research on real-world problems is an educational program for doctorate course students in FMSP (Leading Graduate Course Frontiers of Mathematical Science and Physics) of the University of Tokyo. The academic-Industry collaboration Program ‘Mathematical Innovation in Data Science’ has started up in April 2018 provided Nippon Steel Corporation with funds, affiliated with the Graduate School of Mathematical Science, the University of Tokyo has proposed themes for the program, and provided several themes for doctoral students who mainly major in algebra or geometry.

   We have discussed problems in mathematics motivated by crystals and quasi-crystals are highlighted as themes of interest in mathematics and important in materials for several years. I am going to speak at this workshop on the outcomes regarding quasi-crystal. A quasi-crystal, is a structure that is ordered but not periodic. A quasi-crystalline pattern can continuously fill all available space, but it lacks translational symmetry. We try to grasp the problem as a difference in quasi-polynomial type compared with crystal and as the mathematical way of tiling in space by atoms.