IMI Workshop I:
Mathematics in Interface, Dislocation and Structure of Crystals
at Nishijin Plaza, Kyushu University

Abstracts
In this workshop, experts of various mathematical fields gather together to discuss
problems related to mathematics in interface, dislocation and structure of crystals
from broad range of viewpoints, expecting to have progress in constructing mathe-
matical models of these objects.

1 Program

Aug. 28
13:00-13:05 Opening
13:05-13:50 Junichi Nakagawa (Nippon Steel & Sumitomo Metal Co.)
Algebraic analysis of orientation relationship created by phase transition in crystals
14:10-14:55 Tomohiro Takaki (Kyoto Inst. of Tech.)
Phase-field simulations of dendrite solidification and grain growth
15:15-16:00 Karel Svadlenka (Kyoto Univ.)
Numerical analysis of moving interfaces: the level-set and phase-field approaches
16:00-16:30 Tea Time
16:30-17:15 Philip Broadbridge (La Trobe Univ./IMI, Kyushu Univ.)
Exact solution of nonlinear boundary value problems for surface diffusion
17:30-19:30 One-coin party (1F)*
(Discussion, with two beer cans and snacks of one-coin = 500 yen/person)

Aug. 29
9:45-10:30 Kenji Higashida (Nat. Inst. of Tech., Sasebo College)
On observation of dislocations in crystals
10:50-11:35 Akihiro Nakatani (Osaka Univ.) / Xiao-Wen Lei (Fuku Univ.)
Analysis of stress field of kink boundary based on lattice defect theory
11:55-12:40 Kazutoshi Inoue (AIMR, Tohoku Univ.)
Structure of tilt grain boundaries from mathematical perspective
12:40-14:10 Lunch
14:10-14:40 FMSP Mathematical Research on Real World Problems, Group G,
The University of Tokyo
Hokuto Konno (The Univ. of Tokyo), Tsukasa Ishibashi (The Univ. of Tokyo),
Sho Ejiri (The Univ. of Tokyo), Junichi Nakagawa (Nippon Steel & Sumitomo Metal Co.),
Yasuhiro Wakabayashi (The Univ. of Tokyo)
Lattice defects from monodromy
15:00-15:45 Shizuo Kaji (Yamaguchi Univ.)
Geometry of closed kinematic chain
15:45-16:10 Tea Time
16:10-17:30 Discussion slot
19:00-21:00 Banquet 5,000yen *)
Souen**) *) Please let us know if you’d like to attend it by Aug. 15, Shigeki Matsutani smatsu@sasebo.ac.jp
Aug. 30

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Presentation Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:45-10:30</td>
<td>Patrick van Meurs (Kanazawa Univ)</td>
<td>Discrete-to-continuum limits of moving straight edge dislocations in 2D</td>
</tr>
<tr>
<td>10:50-11:35</td>
<td>Masaaki Uesaka (Hokkaido Univ.)</td>
<td>Anti-plane deformation model of screw dislocation and its related variational problem</td>
</tr>
<tr>
<td>11:55-12:40</td>
<td>Pierluigi Cesana (IMI, Kyushu Univ)</td>
<td>Variational models of lattice defects</td>
</tr>
<tr>
<td>12:40-14:10</td>
<td>Lunch</td>
<td></td>
</tr>
<tr>
<td>14:10-14:30</td>
<td>Junichi Nakagawa (Nippon Steel &amp; Sumitomo Metal Co.)</td>
<td>Sequence representation of graph structure of crystal (Growth)</td>
</tr>
<tr>
<td>14:30-14:50</td>
<td>Tea Time</td>
<td></td>
</tr>
<tr>
<td>14:50-16:55</td>
<td>Discussion slot</td>
<td></td>
</tr>
<tr>
<td>16:55-17:00</td>
<td>Closing</td>
<td></td>
</tr>
</tbody>
</table>

**On discussion slots:**

**Purpose of discussion slots:** 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. As mentioned above, this conference is arranged so that experts in various fields gather together and discuss problems related to crystals whose origin is in industry. Its prototype is in the style of mathematical studies in industry.

It is expected that participants discuss mathematical problems with those from various fields. It is also expected that the discussions stimulate their own works and generate a new intermediate field of study.

Consequently, there is no rule for discussing problems. Every one will be able to participate in any group to discuss problems with her/his own interest. The one-coin party is also set for similar discussions accompanied with some drinks and snacks.

**Utilities:** We have three rooms including the main room for the discussions. In each room, there are a projector and a white board. You can also use the lobby.

**Report:** There is no duty to report the results of the discussions: however, if you think that your discussions should be shared with others, then we can arrange such occasions in the discussion slots.

Furthermore, we will need to report the discussion slots in the proceedings of this conference later. Therefore, the organizers would appreciate it if you could record briefly the contents of the discussions made during the discussion slots. Thank you.
2 Aug. 28

1. 13:05-13:50, Junichi Nakagawa (Nippon Steel & Sumitomo Metal Co.) Algebraic analysis of orientation relationship created by phase transition in crystals

Polycrystalline materials such as iron acquire their properties from various thermo-mechanical treatments. In many cases, the low temperature behaviors of these materials are sought from high temperature processes, such as re-heating, rolling and cooling, that are followed by phase transitions. The microstructure of polycrystalline materials at low temperatures is an important parameter, and it is greatly involved in plastic deformation. Therefore, the improvement of products designed for a given application requires the formation of an adapted low temperature microstructure, obtained from the high temperature state, which can also be characterized by its microstructure. A grain (for example $\beta$), which is defined by a set of crystals with the same orientation, is transformed into many grains of the same phase (for example $\alpha$) with an orientation relationship. We refer to them as daughter crystals. These daughter crystals ($\alpha$), which have an orientation relationship with the parent crystal ($\beta$), are called variants, and they are algebraically identified with left co-sets. C. Cayron who is a physicist in crystallography dealt with variants using algebraic analysis and proposed a method for reconstructing parent crystals from the observed daughter crystals. Our intention is to redefine the way of describing the method using mathematics and obtain a comprehensible representation mathematically in order to understand Cayron’s way of thinking.

2. 14:10-14:55, Tomohiro Takaki (Kyoto Inst. of Tech.) Phase-field simulations of dendrite solidification and grain growth

Phase-field studies of dendrite growth and grain growth are introduced. In the dendrite growth, the competitive growth among multiple dendrites is investigated. In the grain growth, the true behaviors of ideal grain growth are investigated by the very-large simulation.

3. 15:15-16:00, Karel Svadlenka (Kyoto Univ.) Numerical analysis of moving interfaces: the level-set and phase-field approaches

There are several well-established efficient numerical methods for simple interfaces evolving according to various rules, such as the curve-shortening flow or surface diffusion. Recently, the focus of researchers in this field has shifted towards numerical solution of interfacial networks with junctions, especially in the anisotropic or non-symmetric setting (for example, different surfaces tensions for each interface in the mean curvature flow).

In this talk, I will briefly review the two basic approaches to evolving interfaces that can be extended to the multiphase anisotropic/non-symmetric case including topological changes: the phase-field method and the level-set method (in particular, its simplified version proposed by Merriman, Bence and Osher). I will present an overview of the state of the art methodologies and their range of applicability, mentioning also some results of my own.

4. 16:30-17:15 Philip Broadbridge (La Trobe Univ./IMI, Kyushu Univ.) Exact solution of nonlinear boundary value problems for surface diffusion

Curvature-driven surface diffusion on crystalline surfaces is modelled by a fourth order nonlinear diffusion equation. There is a class of nonlinear weakly anisotropic models that is fully integrable. Exact solutions are constructed for development of a grain boundary groove and for smoothing of an initial ramp dislocation.

Even for linear fourth order “diffusion”, there are strange overshoot phenomena that are no longer prescribed by maximum principles of second order diffusion.

There are additional phenomena due entirely to the nonlinearity. For example, in a solvable quasilinear model, the depth of a grain boundary groove remains bounded as the dihedral angle approaches vertical.
At a dislocation point of infinite curvature, the quasilinear Mullins model should be extended to a fully nonlinear degenerate model to account for Gibbs-Thompson evaporation-condensation. An exactly solvable fully nonlinear degenerate diffusion model shows that unlike in the quasilinear model, deposition rate at the dislocation point is bounded, and the slope remains discontinuous for a finite delay time.

My group is currently working on classical and non-classical symmetry reductions of the fourth-order evolution of crystal surfaces near cores with cylindrical phase boundaries.

3 Aug. 29

1. 9:45-10:30 Kenji Higashida (Nat. Inst. of Tech., Sasebo College) On observation of dislocations in crystals

In this talk, several observation results of dislocations in crystals are reported. Some experimental results exhibit that the properties of dislocations should play more important roles in materials for the next generations. (Since terminology in experimental material science is quite different from mathematics, this talk is given in Japanese though slides are written in English.)

2. 10:50-11:35 Akihiro Nakatani (Osaka Univ.) / Xiao-Wen Lei (Fukui Univ.) Analysis of stress field of kink boundary based on lattice defect theory

An expression of the displacement field of the continuum limit of uniformly distributed dislocations on a finite straight segment in an infinite elastic body is formulated as a closed-form. The exact solution based on the linear elasticity is applied to describe the elastic field near a kink boundary in magnesium alloy with long-period stacking ordered structure. Stress singularity of line of intersection between two kink boundaries will be discussed in detail by an asymptotic analysis as well as computational analysis.

3. 11:55-12:40 Kazutoshi Inoue (AIMR, Tohoku Univ.) Structure of tilt grain boundaries from mathematical perspective

Functional materials are often used in a polycrystalline form, and their electrical and physical properties are strongly affected by crystalline defects such as dislocations and grain boundaries (GBs). Structures and properties of GBs have been intensively studied both experimentally and numerically for decades. Simplified system of bicrystals has been often investigated in order to determine individual contributions from various components to the macroscopic properties. Many studies have been mainly focused on special commensurate GBs with a short periodicity. However, any GB deviated from a typical commensurate orientations can have a rather long periodicity which are well described by the structural-unit model. It has been shown that the structures of symmetrical tilt GBs can be described by a part of quasi-periodical arrangements structural units as a realization of the lowest energy structure under an assumption that the structure may change as continuously as possible as a function of misorientations. Consequently, two types of structural units are arranged in a way that GB dislocations are maximally separated. Because of this property, the periodicity and the arrangement of structural units in symmetrical tilt GBs can be closely related to the distribution of rational numbers that is well represented by the Farey sequence. We have systematically predicted the arrangement of structural units in various types of GBs in ceramic materials by utilizing the Farey sequence. The atomic configurations in GBs were characterized by the aberration-corrected scanning transmission electron microscopy, showing a nice agreement with the prediction.
4. 14:10-14:40 FMSP Mathematical Research on Real World Problems, Group G, The University of Tokyo, Lattice defects from monodromy, by Hokuto Konno (The Univ. of Tokyo), Tsukasa Ishibashi (The Univ. of Tokyo), Sho Ejiri (The Univ. of Tokyo), Junichi Nakagawa (Nippon Steel & Sumitomo Metal Co.), Yasuhiro Wakabayashi (The Univ. of Tokyo)

We study some lattice defects in terms of monodromy in the sense of William Thurston. This description of lattice defects enables us to encode some special structure of it which arises from original lattice structure.

5. 15:00-15:45 Shizuo Kaji (Yamaguchi Univ.) Geometry of closed kinematic chain

Consider a system consisting of rigid bodies connected to each other. Such a system can be modelled by a graph with edges labelled by elements of the Euclidean group SE(3), where each cycle satisfies a certain closedness condition. We are particularly interested in a system consisting of hinges. To each vertex is assigned one degree-of-freedom, namely the rotation angle, and the configuration space of the system is described by the real solution to a system of polynomial equations. We found an interesting family of systems on cycle graphs, whose configuration spaces form positive dimensional real algebraic varieties. They are a type of so called Kaleidocycle, but exhibit intriguing properties such as anti-symmetry and constant bending energy. This is joint work with Eliot Fried, Michael Grunwald, and Johannes Schoenke at OIST.

4  Aug. 30

1. 9:45-10:30 Patrick van Meurs (Kanazawa Univ) Discrete-to-continuum limits of moving straight edge dislocations in 2D

The starting point is a 2D interacting particle system which models n Volterra dislocations of edge type. We assume a linear drag law for the motion of the dislocations. Our main result is the rigorous passage to the limit \( n \to \infty \) of the corresponding evolution equations for the dislocations. The proof relies on the theory of Wasserstein gradient flows and advanced functional analysis on the weak form of the model equations. Interestingly, the limiting dynamics for the dislocation density differs from the prediction in the celebrated engineering paper by Groma and Balogh from 1999.

2. 10:50-11:35 Masaaki Uesaka (Hokkaido Univ.) Anti-plane deformation model of screw dislocation and its related variational problem

As a microscopic model of screw dislocation, Hudson and Ortner [1] propose the lattice model based on anti-plane dislocation. They prove that in this model, the state corresponding to the screw dislocation is a globally stable equilibrium under appropriate conditions for the interaction energy. In this talk, we attempt to obtain the upscale model of the anti-plane deformation model in terms of \( \Gamma \) -convergence. The main point is that the discrete system which takes value in \( S^1 \) is naturally derived from the model. We also point out the mathematical difficulty of this discrete model.

3. 11:55-12:40 Pierluigi Cesana (IMI, Kyushu Univ.) Variational models of lattice defects

A martensitic phase-transformation is a first-order diffusionless transition occurring in elastic crystals and characterized by an abrupt change of shape of the underlying crystal lattice. It is the basic activation mechanism for the so-called Shape-Memory effect. The re-organization of the crystalline structure is not only accompanied by the formation of sharp interfaces delimiting the various martensitic variants but also by presence of defects and mismatches. In this talk I will present a modeling approach for topological defects based on variational (energy-minimization) methods. Considering disclinations (angular defects
caused by the mismatch measured around a loop in a planar lattice) I will present a linearized theory based on a continuum model describing the formation of a “nested” hierarchical martensitic microstructure containing a disclination at the center. The microstructure is described by the solution to a differential inclusion problem. I will then introduce the Gamma-Convergence approach to the description of dislocations (linear defects often observed in metal subject to shear stress). Comparisons are reported for numerical and analytical solutions and experimental observations.

4. 14:10-14:30 Junichi Nakagawa (Nippon Steel & Sumitomo Metal Co.) Sequence representation of graph structure of crystal (Growth)

We define the growth as a sequence representation of graph structure of crystal. The first growth corresponds to the coordination number of crystals. We will show the generation functions of some growths and their symmetrical properties.