Symposium on Mathematics for Various Disciplines 21

Mathematical Aspects of Surface and Interface Dynamics 16
表面・界面ダイナミクスの数理 16

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Lecture Hall / Room 056, Graduate School of Mathematical Sciences, The University of Tokyo

Abstracts

Dionisios Margetis (University of Maryland)

Lecture 1: On the fundamentals of crystal surface morphological evolution

The goal with this lecture is to introduce basic physical and mathematical concepts permeating epitaxial relaxation and growth. In materials science, the design of novel devices requires understanding how structures on crystal surfaces evolve and fluctuate across several scales, from the atomistic to the full continuum. In this talk, I will review a few related models and their underlying principles. First, I will introduce the main mechanisms of crystal surface motion from a physics perspective, exemplifying the role of surface diffusion. Second, I will review past theories that aim to describe crystal surface morphological evolution above and below the roughening transition temperature.

Hiroyoshi Mitake (The University of Tokyo)

On large-time behavior for birth-spread type nonlinear PDEs

In this talk, we introduce birth-spread type nonlinear partial differential equations which is motivated by a crystal growth phenomenon.

Mathematically, an interesting nonlinear phenomenon in terms of asymptotic speed of solutions appears which is sensitive to the shapes of source terms.

We discuss properties of large-time asymptotic speed, and also present recent results on large-time asymptotic profile of solutions.

Salvador Moll (Universitat de València)

The constrained total variation flow

Let $(\mathcal{N}, g)$ be a complete, n-dimensional Riemannian manifold (embedded as a surface in the Euclidean space $(\mathbb{R}^N, |\cdot|)$ with some $N \geq n$). Given an open, bounded domain $\Omega \subset \mathbb{R}^m$ with smooth boundary $\partial\Omega$ and $1 \leq p < \infty$, we consider the formal steepest descent flow with respect to L^2 distance of the energy functional

$$\boldsymbol{u} \in C^1(\overline{\Omega}, \mathcal{N}) \mapsto E_p(\boldsymbol{u}) = \frac{1}{p}\int_\Omega |\nabla \boldsymbol{u}|^p.$$

The flow is formally given by the system

$$\begin{cases} \boldsymbol{u}_t = \pi_{\boldsymbol{u}} \mathrm{div}\,(|\nabla \boldsymbol{u}|^{p-2}\nabla \boldsymbol{u}) & \text{in }]0,T[\times\Omega, \\ \boldsymbol{\nu}^\Omega \cdot |\nabla \boldsymbol{u}|^{p-2}\nabla \boldsymbol{u} = 0 & \text{in }]0,T[\times\partial\Omega. \\ u(0,x) = u_0(x) & \text{in } \Omega \end{cases} \tag{1}$$

where, $\pi_{\boldsymbol{p}}\colon T_{\boldsymbol{p}}\mathbb{R}^N \equiv \mathbb{R}^N \to T_{\boldsymbol{p}}\mathcal{N}$ denotes the orthogonal projection onto $T_{\boldsymbol{p}}\mathcal{N}$ at a point $\boldsymbol{p} \in \mathcal{N}$ and ν^{Ω} the outer unit normal to $\partial\Omega$.

In this talk I will present some recent results in collaboration with L. Giacomelli, M. Łasica and J. Mazón about solvability of the system (1) in the limit case $p = 1$. The talk will be divided into two main parts.

In the first part of the talk I will introduce the 1-harmonic flow in the context of image denoising; starting with the celebrated paper [4] in which the target $\mathcal{N} = \mathbb{R}$ (with the standard metric); i.e.: the standard total variation flow. I will also make an overview of known results about $p-$ harmonic maps and $p-$harmonic flows; i .e. minimizers of the energy functional E_p or solutions to the system (1).

The second part of the talk will be devoted to solving the system (1) in the case $p = 1$ in different scenarios:

(a) In the case that the initial data $u_0 \in W^{1,\infty}(\Omega;\mathcal{N})$ and with the hypothesis that the sectional curvature of $\mathcal{N}$ is bounded by above, existence (in a maximal time interval) and uniqueness of regular solutions is obtained. In the case of non–positive sectional curvature, we obtain that the solutions exist for all time and that they converge to a constant in finite time. These results are contained in [3].

(b) The case that $\mathcal{N}$ is a hyperoctant of the $n-$dimensional sphere. Here, I will introduce a proper notion of solution for general $BV-$ initial data and I will show existence of solutions to the system. This is contained in [2]. In the case that $n = 2$, uniqueness of solutions can be proved (see [1])

(c) The case of Ω being 1-dimensional; i.e. $\Omega =]a, b[$ with $a < b \in \mathbb{R}$. Here I will present existence of solutions for generic BV initial data. In the case that the sectional curvature of $\mathcal{N}$ is non–positive, uniqueness will be also shown.

References

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Dionisios Margetis (University of Maryland)

Lecture 2: From discrete schemes to macroscopic laws: Reconciling step motion with crystal facet evolution

In this lecture, I will focus on derivations and implications of deterministic macroscopic laws for the relaxation of crystal surface morphologies at temperatures below the roughening transition. At the nanoscale, the surface motion is described by discrete equations for the positions of line defects, steps, according to the Burton-Cabrera-Frank model. At the macroscale, it is plausible to use Partial Differential Equations (PDEs) for the surface height or slope. Such PDEs are usually of fourth order (under surface diffusion) and nonlinear. The focus of this talk will be the connection between descriptions at the nanoscale and the macroscale when macroscopic plateaus, facets, are present. Notably, in this regime large-scale surface phenomena may exhibit an effective behavior dominated by microscale events of step annihilations. This talk will address these issues via selected examples.

Olivier Pierre-Louis (Université Claude Bernard Lyon 1/CNRS)

Growth and dissolution in confinement: dynamics within contacts

This is joint work with Luca Gagliardi. Confinement constrains growth in many natural environments, such as in geology or in biomineralization. One key issue for the growth and dissolution of confined crystals is the understanding of the dynamics in the contact regions between the crystal and the surrounding environment. We have therefore developed a thin film model [1] describing the dynamics of growth or dissolution at the interface between the crystal and the substrate, including diffusion, hydrodynamics, interface kinetics, disjoining pressure effects, and a loading force.

We first apply the model to the study of pressure solution, i.e., dissolution under load [1]. We find that when the disjoining pressure diverges like a power law with the distance, contacts are flat and the dissolution rate increases as a power-law of the loading force. In contrast, disjoining forces decaying exponentially with the distance lead to pointy contact with a dissolution rate independent of the load.

Two different conditions are studied in growth.

First, during growth with no (or small) applied force, we find that a cavity forms within the contact region. The subsequent growth of this cavity gives rise to growth rims. This study is performed in collaboration with experimentalist at the University of Oslo [2]. The model predicts that the formation of the cavity becomes subcritical (first order) when attractive interactions such as van der Waals forces come into play at the nano-scale [3]. Hydrodynamics and attachment-detachment kinetics can also hinder or prevent the formation of the cavity.

Second, we analyze the crystallization force produced by a crystal growing between two parallel plates [4]. The crystallization force in slow growth is consistent with thermodynamic predictions in equilibrium. However, non-equilibrium effect can lead to strong deviations from the thermodynamic prediction.

References

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Yoshihiro Kangawa (Kyushu University / Nagoya University)

Influence of surface reconstruction on the impurity incorporation in GaN MOVPE

GaN is attracting attention as a next generation power device material. To develop a power device beyond 1kV breakdown voltage, it is necessary to reduce carrier concentration less than 1×10^{16} cm^{-3}. In the present talk, I would like to discuss incorporation mechanisms of unintentionally doped carbon during GaN MOVPE based on ab initio based-approach to understand how to reduce the impurity concentration in the films. First, p-T surface phase diagrams for GaN(0001) and GaN(000-1) MOVPE were obtained to understand the surface reconstructions under the typical growth conditions. Next, relative energy changes in the system with substitutional carbon in subsurface layers were analyzed. The calculation results suggest that in addition to the change of chemical potential of the gas phase, the next crucial factors for impurity incorporation are Fermi level pinning and accompanying surface band bending. This implies that these effects are responsible for facilitating or hindering the incorporation of impurities and dopants.

Toru Ujihara (Nagoya University)

High-quality SiC crystal grown with solution method by controlling macro-step structure

We have developed the growth technology for high-quality SiC crystal based on a solution method. In this method, the SiC seed crystal dipped to the Si-X-Y solvent can grow in a carbon crucible at high temperature (1800-2000 deg.C). There are two key technologies for high-quality crystal growth as follows: (1) Macro-steps on the growth surface causes the structural conversion from threading dislocations which are perpendicular to the growth direction to the different dislocations which are parallel to the growth direction and (2) the solution flows against macro-step flow direction avoid the formation of over-developed macro-step which becomes the origin of void formation. In addition, we recently developed the fast prediction model of CFD simulation by machine learning.

Hiroki Hibino (Kwansei Gakuin University)

Crystal growth of two-dimensional materials and heterostructures

Two-dimensional (2D) materials and their heterostructures are attracting huge attention due to their wide potential applications. Because large-scale, high-quality 2D crystals are prerequisites for many of the applications, crystal growth of 2D materials has been intensively studied. In this presentation, we review our research to understand the growth mechanism of 2D materials and to better control the growth processes.

Dionisios Margetis (University of Maryland)

Lecture 3: From atoms to step flow:
The atomistic origin of the Burton-Cabrera-Frank model

In this talk, I will discuss recent progress, and open challenges, in linking the Burton-Cabrera-Frank (BCF) model of step flow to descriptions for the hopping of atoms on crystal surfaces. Starting from a many-atom master equation of a kinetic restricted solid-on-solid model in 1+1 dimensions, I will show how one can extract a coarse-grained, nonlinear mesoscale description that defines the motion of a line defect on the surface. This approach reveals that the BCF theory is valid in a regime of low density of adsorbed atoms. For high enough supersaturations, I will explain how ingredients of the BCF model acquire nonlinear corrections.

Jian-Guo Liu (Duke University)

Dynamics of a degenerate PDE model of epitaxial crystal growth

Epitaxial growth is an important physical process for forming solid films or other nanostructures. It occurs as atoms, deposited from above, adsorb and diffuse on a crystal surface. Modeling the rates that atoms hop and break bonds leads in the continuum limit to degenerate 4th-order PDE that involve exponential nonlinearity and the p-Laplacian with p=1, for example. We discuss a number of results in physical derivation, computation and analysis for such models.