Symposium on Mathematics for Various Disciplines 19
Mathematical Aspects of Surface and Interface Dynamics 14
表面・界面ダイナミクスの数理 14
October 25 (Wed.) – October 27 (Fri.), 2017
Lecture Hall / Room 056, Graduate School of Mathematical Sciences, University of Tokyo

Abstracts

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

Lecture 1: Crystal growth and atomic steps

In the first lecture, we discuss the "modeling of non-equilibrium interface dynamics in crystal growth". We present models at different scales, from atomistic descriptions to the continuum, and show how relations between these models can be based on asymptotic analysis. If time allows, we shall also present some basic properties of kinetic roughening.

1 introduction
- Models and scales to model surfaces and interfaces
- Atomic steps and surface dynamics

2 Kinetic Monte Carlo
- Master Equation
- KMC algorithm
- KMC Simulations

3 Phase field models
- Diffuse interfaces models
- Asympotics
- Phase field simualtions

4 BCF Step model
- Burton-Cabrera-Frank step model
- Multi-scale analysis

5 Nonlinear interface dynamics
- Preamble in 0D
- Nonlinear dynamics in 1D 6 Kinetic Roughening
- Fractal interfaces
- Continuum models

7 Conclusion

Marcel J. Rost (Universiteit Leiden)

When vapor deforms metal:
Thermodynamics of deposition flux dependent intrinsic film stress

The growth of polycrystalline films at temperatures above ˜0.2 of the melting temperature is accompanied by compressive stress development after film closure.
Mysteriously, a significant part of this stress has a reversible nature: it disappears when the deposition is stopped and re-emerges upon resumption. Chason [1] even showed the corresponding inverse behavior during electrochemical etching.

All these observations clearly point towards a steady-state, flux (deposition or etching rate) dependent equilibrium phenomenon, which should, therefore, be treated properly by thermodynamics.

It has been suggested that the variation of the surface chemical potential upon starting/stopping of the deposition may cause adatoms to diffuse in/out of the grain boundaries leading to the development/relaxation of the intrinsic compressive film stress.
However, film growth involves a myriad of atomic processes such that the mystery is not yet solved and new mechanisms and ideas are still published frequently.

Based on atomic scale live observations during the growth observed with a Scanning Tunneling Microscope [2], I present here an analytical derivation, in which we address, for the first time, the reason ***why*** additional atoms want to get incorporated in the grain boundaries. This background delivers the required driving force independently of the precise way the atoms get incorporated. In this sense we are not proposing a new model, but delivering the basis for all different models proposed.

To derive the driving force, we calculate the variation of the chemical potential of the surface, the grain boundaries, and the film. Surprisingly, using pure thermodynamic arguments, our results fully agree with the magnitude of the reversible compressive stress:
the tremendous stress levels observed in the experiments can indeed be explained by the flux induced density variations in the extremely dilute adatom gas on the surface! [3]

[1] Shin and Chason; Phys. Rev. Lett. **103**, 056102 (2009)
[2] M. J. Rost; Phys. Rev. Lett. **99**, 266101 (2007)
[3] A. Saedi and M. J. Rost; Nature Communications, **7:10733** (2016)

Tatsu-Hiko Miura (University of Tokyo)

Mathematical and numerical analysis of the Hamilton-Jacobi equation on an evolving surface

In this talk we consider the first-order Hamilton-Jacobi equation on a two-dimensional evolving hypersurface. Our aim is to establish the existence and uniqueness of a viscosity solution as well as to give a numerical scheme and an error estimate. The numerical scheme we construct on a triangulated surface is based on a viscous approximation and a finite volume scheme. By analyzing our scheme we show the convergence of a numerical solution to a viscosity solution, which establishes the existence result. Also, a comparison principle and an error estimate are proved by a standard technique of doubling of variables.

This talk is based on a joint work with Prof. Charles M. Elliott (University of Warwick) and Prof. Klaus Deckelnick (Otto von Guericke University Magdeburg).

Dionisios Margetis (University of Maryland)

The trouble with crystal facets

Below the roughening transition temperature, crystal surfaces have distinct line defects, steps, at the nanoscale. At larger scales, macroscopic plateaus, facets, on these surfaces are evident. This talk will touch upon aspects of the following question: Can facet evolution be described by a continuum theory that is consistent with the physics of steps? I will discuss recent progress and open challenges in this direction. Emphasis will be placed on simplified situations in which the discrete dynamics of steps can be described by a large system of ordinary differential equations. This system plausibly gives rise to a fourth-order partial differential equation (PDE) for surface diffusion at the macroscopic scale. In this context, the facet amounts to a free boundary problem for this PDE.

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

Lecture 2: Wetting and dewetting of thin films

The subject of the second lecture is the "wetting and dewetting of thin films". After a presentation of the static properties of wetting of solids and liquids, we will focus on the dynamics of dewetting. Three main questions will be addressed. The first one is the role of anisotropy, and especially singular crystalline anisotropy. The second topic is the influence of the wetting potential on ultra-thin films. The third topic is the case of solids immersed in liquid solutions.

1 Static Wetting of liquids and Solids
2 Dynamics of wetting
3 Consequences of singular anisotropy
  Experimental evidences
  2D SOS KMC
  Dewetting of thin films: KMC vs model
4 Wetting potential
  Mesoscopic Continuum thin film model
  Derivation of the TL Boundary Condition
  Accelerated mass shedding
  KMC study of magic heights
5 Immersed solids
  Introduction
  Model equations
  Pressure solution
6 Conclusions

Yuki Kimura (Hokkaido University)

Direct TEM observation of nucleation processes in a solution

In recent years, several innovated works have reported nanoscale nucleation pathways from a solution. Most of them cannot be explained based on classical view of nucleation, such as nucleation via metastable phases, nucleation beginning from a inside of a pre-nucleated amorphous or dense-liquid, and aggregation of precursor particles. Development of an innovative tool for transmission electron microscope (TEM), liquid cell, allows us to observe a nanoscale phenomenon in an aqueous solution, and gives us a chance to find a direct evidence of a nucleation pathway. Here, we will report some results of nucleation processes of lysozyme protein and calcium carbonate.

Ken Shirakawa (Chiba University)

Mathematical approaches to Kobayashi–Warren–Carter type models of grain boundary motions

In this talk, a class of mathematical models of grain boundary motions, called *Kobayashi–Warren–Carter type models,* is considered. Each mathematical model is based on the original phase-field system by [Kobayashi–Warren–Carter, Physica D **140** (2000), 141–150], which consists of two order parameters to reproduce the *orientation order* and *orientation angle* of grains in a polycrystal. Under appropriate notations and assumptions, the mathematical theories for Kobayashi–Warren–Carter type models will be expounded, via the representative topics in mathematical analysis, such as the *solvability, large-time behavior,* and so on.

Takeshi Ohtsuka (Gunma University)

Growth rate of a crystal surface by several screw dislocations and grouping of dislocation centers by the effective growth rate

In this talk we consider the growth rate of a crystal surface with several screw dislocations under the setting by the classical paper by Burton et al. in 1951. We refine or correct their predictions on the growth rate with multiple spiral steps. In particular, we present some new observations on the relation between the distribution of screw dislocations with co-rotating orientations and the effective growth rate of the surface. We also improve the Burton et al.'s theory which is based on the grouping centers into effective centers.

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

Lecture 3: Adhesion and dynamics of membranes

The third lecture will be devoted to "Adhesion and dynamics of membranes". We will first discuss static properties of adhesion dynamics on rough or patterned substrates. Then, the dynamics of adhesion will be addressed. We first focus on the combined roles of bending rigidity and confinement. This gives rise to a sublte interplay between frozen states and coarsening dynamics. Finally, we discuss the consequences of shear on the nonlinear dynamics of membranes.

1 Statics: Adhesion on rough and patterned substrates
- 1D model
- Membranes in 2D – the case of Graphene
- Filaments at Finite Temperature

2 Dynamics of adhesion/ Modeling confined membranes
- Dynamics: frozen patches and order-disorder transition
- Numerical solutions of membrane dynamics
- Linear stability analysis
- Stability of kinks and steady-state solutions
- Robustness of frozen states
- Finite tensions
- Potential asymmetry
- Thermal fluctuations

3 Conclusion

Koichi Sudoh (Osaka University)

Phase-field simulation of void formation by annealing of hole patterns on Si(001)

High temperature annealing of hole patterns with high-aspect-ratios on silicon surfaces results in formation of various void structures in the substrate, through surface-diffusion-driven evolution involving topological changes. We have studied phase-field simulation using Cahn-Hilliard equation with a concentration dependent mobility to understand and predict the void structure formation process. We show that the numerical simulation with suitable parameters which approximately achieve the deep quench limit qualitatively reproduces the experimentally observed evolution involving topological changes.

Robert Nürnberg (Imperial College London)

Numerical approximation of (crystalline) anisotropic surface diffusion

Surface diffusion is a classic example for a geometric evolution equation, with many applications in Material Sciences. Computational methods to approximate such flows are usually based on one of three approaches: (i) parametric methods, (ii) phase field methods or (iii) level set methods.

In this talk we begin by reviewing a variational formulation for the parametric approach for isotropic surface diffusion, which leads to an unconditionally stable, fully discrete finite element approximation. In addition, the scheme has excellent mesh and volume conservation properties.

On introducing a special class of anisotropies, these properties of the scheme can be generalized to the case of anisotropic surface diffusion. In particular, the considered class of anisotropies allows to approximate crystalline surface energies, which lead to faceted equilibrium shapes with corners and edges.

Finally, we mention how the same class of anisotropies can also be applied in the phase field context, where it once again leads to unconditionally stable, fully discrete finite element approximations.

References:
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J. W. Barrett, H. Garcke, and R. Nürnberg, On the stable discretization of strongly anisotropic phase field models with applications to crystal growth, ZAMM Z. Angew. Math. Mech., 93(10–11):719–732, 2013.
J. W. Barrett, H. Garcke, and R. Nürnberg, Stable phase field approximations of anisotropic solidification, IMA J. Numer. Anal., 34(4):1289–1327, 2014.