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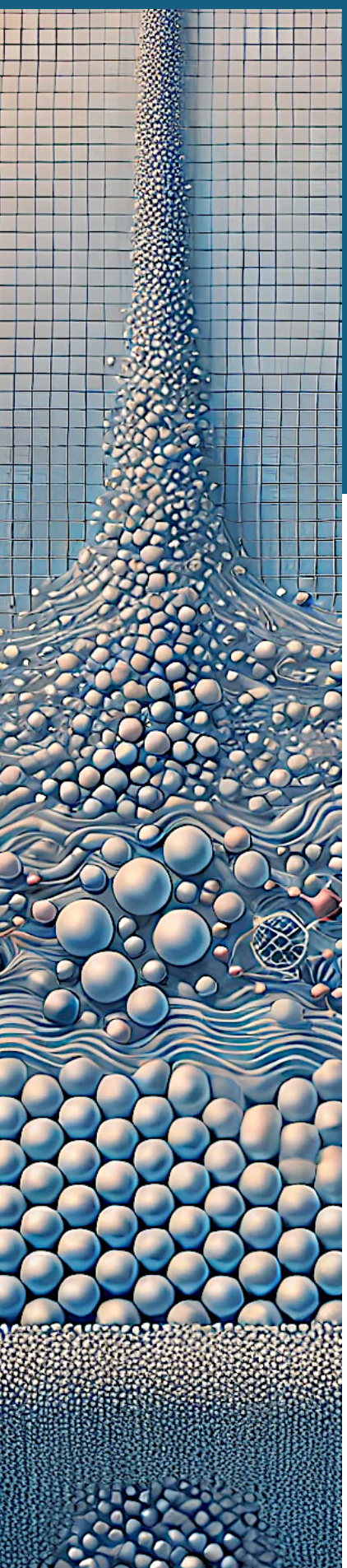

International Workshop

Advancements in Mesoscale Materials Modeling

Cutting-edge formulations, simulations, and applications

2nd-4th December 2024

Institute of Scientific Computing

TU Dresden

Key Topics

- Pattern formation and physical phenomena at the mesoscale
- Elasticity and plasticity of diverse materials
- Modeling of defects like dislocations and grain boundaries
- Advancements in modeling techniques (PFC, MD, MC)
- Analogies across different scales and systems
- Novel applications

Organizers: Marco Salvalaglio, Axel Voigt | TU Dresden

DFG Deutsche Forschungsgemeinschaft

Förderverein für Mathematik zu Dresden e.V.

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Venue

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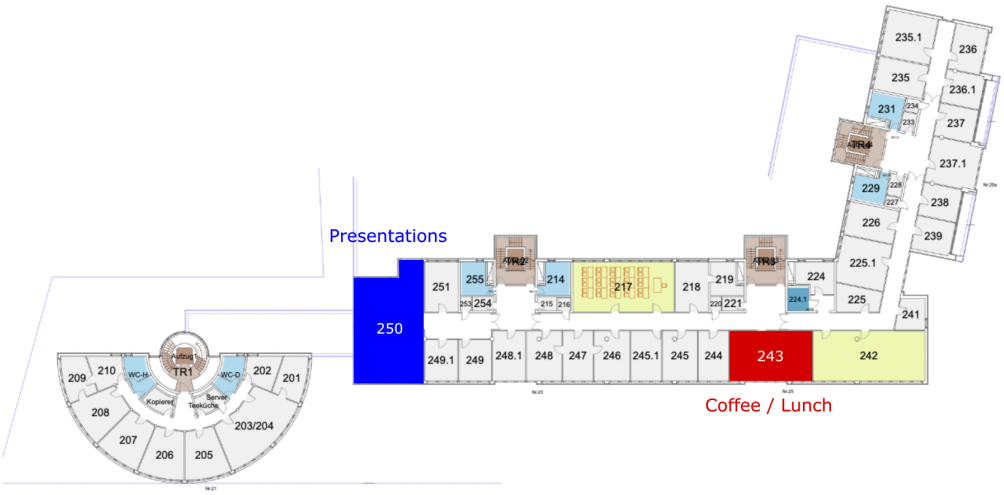
Institute of Scientific Computing – TU Dresden
Zellescher Weg 21-25, 01217 Dresden.



Presentations: Second Floor, Room 250

Coffee Break, Light Lunch: Second Floor, Room 243

Program & Index of Abstract

Monday – 2nd Dec. 2024

10.00 Registration & Welcome Coffee

10.45 Opening

11.00 Ken Elder – Defect nucleation in phase field crystal models

11.45 Håkan Hallberg – Assessing grain boundary structures and properties from phase field crystal simulations

12.30 Marcello De Donno – Mesoscale field theory for quasicrystals

13.00 Lunch

14.00 Marco Salvalaglio – Grain boundaries are Brownian ratchets

14.45 Simiso K. Mkhonta – Phase field crystal modeling of graphene-like materials growing on liquid substrates

15.30 Maik Punke – Hybrid-PFC: coupling the phase-field crystal model and its amplitude-equation formulation

16.00 Coffee Break

16.30 Steven M. Wise – (Online) A non-isothermal phase field crystal model with lattice expansion

17.15 Peter Galenko – Kinetic phase field *versus* atomistic data of simulation in fast crystal growth

Evening Suggestion: Christmas Markets Walk-around

Tuesday – 3rd December 2024

9.00 Hartmut Löwen – Mesoscale modelling of active matter

9.45 Lea Happel – Moving towards morphogenesis - Understanding cellular systems with multiphase field models

10.30 Coffee Break

11.00 Zhi-Feng Huang – Field-theory modeling of nonreciprocity: Two-dimensional active odd crystals and chiral patterns

11.45 Andreas M. Menzel – Induced deformations of soft magnetoelastic composite materials by magnetization effects on mesoscopic scales

12.30 Rainer Backofen – Flow patterns and interface dynamics in two-dimensional active systems

13.00 Lunch – Group Photo

14.00 Luiza Angheluta – (online) From crystals to biological tissues: How topological defects control deformations and flows

14.45 Igor Zlotnikov – Physical phenomena governing biomineral morphogenesis in molluscs

15.30 Nadia Bihari Padhan – Phase separation dynamics: Hyperuniformity and non-hyperuniformity in passive and active hydrodynamic systems

16.00 Coffee Break

16.30 Michael te Vrugt – Microscopic derivations of phase field crystal models

19.00 Social Dinner
Kleinert's Spezialitäten Dresden, Friedrich-Wieck-Straße 45B, 01326 Dresden.

Wednesday – 4th December 2024

9.00 Olivier Pierre-Louis – Controlling the shape of fluctuating nanoscale clusters

9.45 Roberto Bergamaschini – Simulating morphological evolutions by convolutional neural networks

10.30 Coffee Break

11.00 Hamza Oudich – Phase-field modeling of elastic microphase separation

11.30 Max Rosenkranz – Inverse design of spinodoid metamaterials

12.00 Abel H. G. Milor – Describing the local geometry of architected structures with persistent homology

12.30 Lunch

13.30 Brandon Runnels – Multiscale modeling of grain boundary plasticity

14.15 Anne-Sophie Sur – A variational damage-plasticity model considering stress triaxiality effects

15.00 Emma Radice – Phase field modelling of anisotropic solid-state dewetting on patterned substrates

15.30 Conclusions & Coffee / Get-Together

Defect Nucleation in Phase Field Crystal Models

Ken Elder[1], Vidar Skogvoll[2] and Luiza Angheluta[3]

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Defects like dislocations and vortices have a strong influence on material properties and their response to external forces. However, determining the nucleation criteria for such defects under various conditions is challenging. In this work, we study the spontaneous nucleation of dislocations using the phase field crystal approach in its amplitude formulation. By performing the stability analysis of a strained crystal lattice, we identify the critical strain for a given quenching depth for a linear instability. Numerical simulations validate that, for dissipative systems, this instability leads to the nucleation of bound vortical defects in the amplitudes corresponding to dislocations in the crystal lattice as illustrated in Fig. 1

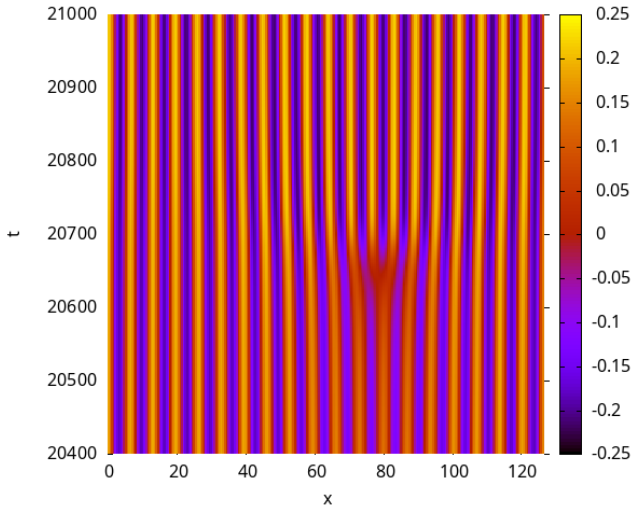

Figure 1: Nucleation of an extra wavelength due to a linear instability of a strained state in the 1D Swift-Hohenberg equation.

Assessing Grain Boundary Structures and Properties from Phase Field Crystal Simulations

Håkan Hallberg, Kevin H. Blixt

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Materials having a crystalline microstructure, such as metals and ceramics, derive their properties from a microstructure consisting of crystalline grains, demarcated by grain boundaries (GBs). The grains and the locally varying properties of the internal GB interface network impact key material properties and overall material performance. A complete description of GB structures and properties is not easily gained, however, due to a significant variation with local crystallography. In fact, while the thermodynamic and kinetic properties of bulk phases often can be mapped in detail, GBs defy any simple description due to their variability and highly individualistic nature. The lack of a means to provide a general and accurate description of GBs poses a severe challenge when trying to establish numerical models of crystalline materials and their microstructure evolution. This challenge lies at the background of the present work, driven by an interest to address important phenomena such as recrystallization, grain growth and solid-state phase transformations.

In this work, it is demonstrated how phase field crystal (PFC) simulations can be used to evaluate central aspects of GB structures and properties. Particular attention is given to the full anisotropy of GB energy, which remains a challenge in numerical models of GB evolution. GB energy is also intimately linked to GB stiffness, which is shown to be accessible from PFC simulations [2]. While ideal minimum-energy GB structures are rarely encountered in actual polycrystals, they are usually the only structures considered when characterizing GBs. It is shown how PFC, when combined with γ-surface sampling, provides a tool to evaluate the structural multiplicity of GBs when accounting for both macroscopic and microscopic GB degrees of freedom [4]. Additional aspects of PFC modeling of crystal interfaces, including the interaction between particles and migrating GBs [1], handling of interfaces in crystal structures beyond FCC/BCC [4], as well as methods for evaluation of nanoscale deformation fields from PFC are also discussed. The aim is to highlight both possibilities and challenges in using PFC as a tool to assess GB structures and properties.

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Mesoscale Field Theory for Quasicrystals

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[4] *Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany*

We present a comprehensive mesoscale field theory that unifies the modeling of growth, elasticity, and dislocations in quasicrystals by building on the density-wave representation of their atomic structure [1]. We rely on the amplitude expansion of the phase-field crystal model, describing slowly-varying complex amplitudes corresponding to the characteristic Fourier modes of the microscopic density field of the quasicrystal. To study the evolution of these amplitudes, we introduce a free energy functional and assume non-conserved dissipative dynamics. This approach enables the self-consistent emergence of elasticity, including both phononic and phasonic deformations, as well as defect nucleation and motion.

Our theory provides critical insights into the formation of semi-coherent interfaces between misoriented quasicrystals, and offers detailed predictions on dislocation kinematics. By deriving the equations of motion for the amplitudes, we demonstrate that the elasticity and the dislocation behavior align with the predictions of classical continuum mechanics, thereby bridging the gap between the micro- and macroscopic scales.

Furthermore, our theory can be regarded as a mesoscale Landau theory for phase transitions in quasicrystals, encompassing both mechanical aspects. Through this framework, we establish a self-consistent connection between the microscopic quasicrystalline order and the resulting macroscopic properties, paving the way for broader mesoscale investigations into quasicrytalline systems. This work not only advances the understanding of the mechanics of quasicrystals, but also sets the stage for future explorations of complex material behaviors at the mesoscale.

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Grain boundaries are Brownian ratchets

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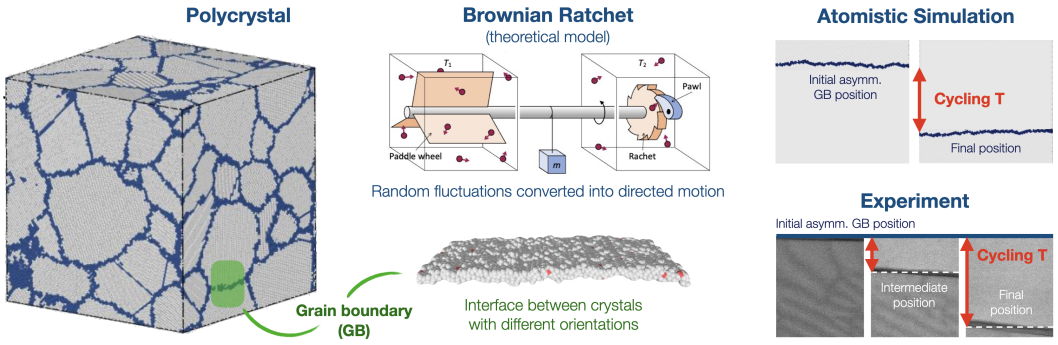
The migration of grain boundaries (GBs), interfaces between crystalline domains with different orientations, is the fundamental mechanism behind microstructure evolution in polycrystals. It thus affects key material properties, including mechanical strength and thermal stability. The velocity of a migrating GB is traditionally described as proportional to a driving force depending on the local GB curvature, stress field, and chemical potential jumps across the GB [1], while the proportionality constant is identified as GB mobility. This presentation illustrates that the actual dynamic of GBs deviates from this picture: GB mobility generally depends on the direction of migration or, equivalently, on the sign of the driving force, with important implications for both bicrystals and entire microstructures [2]. By means of molecular dynamics and phase-field crystal simulations for a wide range of GB types and driving forces, it is shown that nearly all nonsymmetric GBs exhibit direction-dependent mobilities and, therefore, unidirectional motion under oscillatory driving forces. We analyze these results with a Markov chain model, which allows for interpreting this behavior in terms of nucleation barriers for disconnections –steps with dislocation character– mediating GB motion. Importantly, such analysis indicates that directional motion can also be realized simply by cyclic thermal annealing, i.e., GB behaves as a "Brownian ratchets" [3] like, for instance, molecular motors. Simulations are corroborated by in situ experimental observations of directional migration upon cycling thermal annealing. Oscillating driving forces and cycling thermal annealing are finally shown to accelerate grain growth/shrinkage in polycrystals with a potentially great impact on materials processing and microstructure tailoring [2].



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Phase field crystal modeling of graphene-like materials growing on liquid substrates

Simiso K. Mkhonta[1]

[1] *Physics Department, University of Eswatini*

Recent experiments have shown that large high-quality crystal monolayers can be grown thousand times faster on a molten substrate than on a solid. In this talk, I will present phase field crystal (PFC) model simulations demonstrating that liquid substrate fluctuations can play a significant role in enhancing the domain coarsening dynamics, surpassing that of a free-standing system. The results also reveal that disordered hyperuniform structures can emerge from the interplay of the adlayer particle diffusion and the substrate noise. Hence liquid substrates can also provide a strategy for synthesizing disordered hyperuniform thin films with promising applications in photonics.

Hybrid-PFC: coupling the phase-field crystal model and its amplitude-equation formulation

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The so-called phase-field crystal (PFC) model emerged as a prominent framework to model crystalline systems [1, 2]. Indeed, it describes crystalline materials through a continuous order parameter related to the atomic number density and its dynamic at relatively large (diffusive) time scales. It describes solidification and crystal growth, including capillarity, elasticity, nucleation, and motion of defects.

The amplitude expansion of the PFC model (APFC) was developed to overcome the length scale limitations in the PFC framework [3]. This coarse-grained version of the PFC has been used to examine many phenomena, including liquid/solid fronts, dislocation nucleation and motion, as well as strained films. However, the APFC is limited to small rotation angles with respect to a reference lattice, which prevents an accurate description of large angle GBs [4]. Although requiring sophisticated numerical implementation and so far being demonstrated for very simple systems, some approaches were developed to overcome this issue [5]. It remains, however, that the APFC model proves too coarse to inspect accurately microscopic effects while reaching large scales.

This talk builds on the recent investigations in [6], where we propose a hybrid multiscale PFC-APFC framework with PFC accuracy in regions of interest (e.g., at defects and interfaces) while exploiting the coarse resolution of the APFC model elsewhere. In the proposed method, these two models are coupled, leveraging an advanced pseudo-spectral method for spatial discretization. We showcase the capabilities of this newly proposed method via selected numerical investigations that focus on GB structures and the anisotropic solidification of two-dimensional crystals. Benchmarks against standard PFC and APFC models are reported. We also show a proof of concept for its application to describe large-angle GBs, providing a practical solution to a crucial limitation of the APFC model.

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A Non-Isothermal Phase Field Crystal Model with Lattice Expansion

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[2] *Institute of Scientific Computing, TU Dresden, Dresden 01067, Germany*

The phase field crystal modeling framework describes materials at atomic space scales on diffusive time scales. It has been used to study grain growth, fracture, crystallization, and other phenomena. In this talk I will describe some recent work with collaborators developing a thermodynamically consistent phase field crystal model that includes heat transport and lattice expansion and contraction. We use the theory of non-equilibrium thermodynamics, a formalism developed by Alt and Pawlow, and Onsager's principle to give consistent laws of entropy production, and mass and energy conservation [1]. I will show some phase diagram calculations and some preliminary numerical simulation results involving heat transport during solidification. Time permitting, I will discuss some ideas on developing entropy and energy stable numerical methods.

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Kinetic phase field *versus* atomistic data of simulation in fast crystal growth

Peter Galenko

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The results of atomistic simulations of the crystallization process reveal a complex temperature dependence in the velocity of the crystal–liquid interface featuring an increase up to a maximum at 10-30% undercooling below the equilibrium melting temperature followed by a gradual decrease of the velocity at deeper levels of undercooling. At the qualitative level, such nonmonotonous behavior of the crystallization front velocity is consistent with kinetic theories [1, 2, 3, 4, 5], where the almost linear increase in the interface velocity in the vicinity of the melting temperature is defined by the growth of the thermodynamic driving force for the phase transformation, while the decrease in atomic mobility with a further increase in the undercooling drives the velocity although the maximum and into a gradual decrease at lower temperatures. At the quantitative level, however, the kinetic theories fail to describe the results of atomistic simulations in the whole range of temperatures with a single set of parameters for some of the model materials.

To describe crystal-liquid interface propagation in the widest range of temperatures the predictions of the kinetic phase field theory [6] formulated for small and large driving forces on solidification and melting are used. These predictions were made as atomistically informed using travelling wave solutions of the phase field equation describing nonlinear behavior in velocity and dynamic width of the interface. Within the kinetic crossover from slow to fast mode of the crystal-liquid interface propagation, the predictions are compared with molecular dynamics simulation as well as with experimental data on the rapid dendritic solidification of binary alloys. Particularly, it is shown that the transition from crystal to glass formation is accompanied by an abrupt drop in the interface velocity at the highest experimentally accessible undercooling. Finally, the description of quantum crystallization of liquid helium is considered within the kinetic phase field theory [6].

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Mesoscale modelling of active matter

Hartmut Löwen[1]

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While ordinary materials are typically composed of inert "passive" particles, active matter comprises objects or agents which possess an intrinsic propulsion [1]. Examples are living systems like schools of fish, swarms of birds, pedestrians and swimming microbes but also artificial particles equipped with an internal motor such as robots and colloidal Janus particles. In this talk I shall discuss various aspects of mesoscopic field theories for active matter. First of all, a systematic derivation for non-reciprocal interactions is proposed establishing a novel Active Model N which is used to describe vision-cone like interactions [2]. Numerical solution of the equations reveals hitherto unknown structures such as "active yarn". Second, numerical evidence for a universality of hyper-uniformity in active field theories is presented [4]. Finally a model for a quantum active particle is proposed by unifying quantum mechanics with mesoscopic stochastic trajectories [1].

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Moving towards morphogenesis - Understanding cellular systems with multiphase field models

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The multiphase field model is a powerful and versatile tool for modelling epithelial systems and has been shown to capture important biological properties such as solid-liquid transitions, neighbour relationships, and rosette formation [1]. The high local resolution and cell-based modelling approach make it a well-suited model to study the interplay between local and global behaviour in dense cellular systems, for example a $p-$atic order introduced by the cell shape [2] or the emergence of global rotational motion due to single cell properties [1].

To get closer to real-world examples of morphogenesis and tissue deformation, the multiphase field model has been generalised to surfaces [4]. After a closer look at exemplary stationary surfaces such as the sphere or the cylinder to understand the interplay between substrate curvature and cell behaviour [4, 1], we investigate cellular systems on evolving surfaces. A Helfrich energy, which depends on the properties of individual cells is used to link the behaviour at the cell and tissue level.

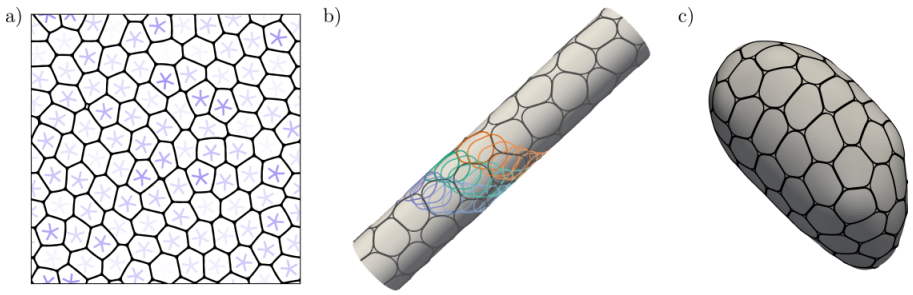

Figure 1: Multiphase field models are powerful tool to model a) $p-$atic order n) global rotational motion and c) surface deformation due to properties of individual cells.

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Field-Theory Modeling of Nonreciprocity: Two-Dimensional Active Odd Crystals and Chiral Patterns

Zhi-Feng Huang

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Continuum density-field type approaches play an important role on achieving the bridging between microscopic and mesoscopic scales of structures or patterns in complex systems. In this talk such type of modeling on nonequilibrium active matter systems governed by nonreciprocal interactions that violate Newton's third law will be discussed. This includes some findings from two newly developed continuum field models based on a generic field-theory framework. They demonstrate the novel behavior of matter becoming active by nonreciprocity, through the results of two-dimensional (2D) active pattern formation induced by single-species nonreciprocity and active crystals with odd elasticity. The first model, termed Active Model N, incorporates effects of vision-cone type nonreciprocal force interactions. It leads to the emergence of new types of active chiral patterns breaking 2D parity-time symmetry, in particular dynamical patterns of flowing active branches and interwoven self-knitting "active yarn", as a result of nonreciprocal phase transitions and the simultaneous development of micro- and bulk phase separations. The second model is built upon a new density-field description for transverse interaction and the resulting nonreciprocal internal torque, and its incorporation with the phase field crystal (PFC) model, termed T-PFC. The model generates a variety of interesting phenomena for odd crystals, such as odd elasticity, self-rotation of crystallites, dislocation self-propulsion, unbinding of a dislocation dipole instead of annihilation, dislocation proliferation, and a dynamical state of self-kneading whorls in polycrystals. The results well agree with those observed in recent experiments and particle-based or molecular dynamics simulations of active and living chiral crystalline systems formed by magnetic colloids, swimming bacteria, and starfish embryos.

Induced deformations of soft magnetoelastic composite materials by magnetization effects on mesoscopic scales

Andreas M. Menzel[1]

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One of our major directions is to establish links between mesoscopic features and overall, macroscopic behavior of soft composite materials. Our principal example system is given by magnetic elastomers [1]. They consist of rather rigid, magnetizable particles on the scale of ten to hundred micrometers, embedded in soft elastic polymeric solids.

Generally, these materials feature several interesting properties. They are addressable from outside by magnetic fields. Particularly, their elastic moduli can therefore be tuned by external magnetic stimuli [2]. For instance, through magnetization, magnetic elastomers can become an order of magnitude stiffer.

Besides such magnetorheological effects, we mainly focus on magnetostrictive phenomena. These can be exploited in the field of soft actuators. Specifically, we have developed an analytical theory that quantitatively describes the coupled displacements and rotations of particles under external forcing or mutual interactions in an elastic background material [3, 4]. For a spherical example system, we have derived explicit analytical expressions to quantify the overall deformation in response to such locally applied internal forces [5].

Using these scale-bridging links, we are now able to analytically calculate global deformations as a function of the spatial arrangement of the contained magnetizable particles. The consequences of several different types of particle positioning have been considered [6, 7].

As a perspective, such scale-bridging connections open the opportunity of optimizing the material behavior as a function of the mesoscopic structure [8]. We will devote major efforts to this direction in the future.

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Flow Patterns and Interface Dynamics in Two-Dimensional Active Systems

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We employ a generalized Navier-Stokes (GNS) model to simulate two-dimensional active flow systems. The investigation includes both single-phase flows and two-phase systems where active and passive phases coexist. Structures of the flow fields, dynamic interactions between phases, and interface behaviors are explored using a range of quantitative measures. A key focus is placed on understanding large-scale ordering phenomena. Special emphasis is given to identifying and characterizing hyperuniform states [1], which may arise under certain conditions.

Active flow is driven by active particles that induce energy input throughout the fluid. In the generalized Navier-Stokes (GNS) model, this is represented by a negative viscosity for fluid fluctuations within a certain bandwidth [2]. For low levels of activity, the flow exhibits a hyperuniform structure characterized by the formation of microscopic vortices, with a mean distance defined by the unstable bandwidth of the viscosity. These vortices are transient, appearing and vanishing over time. As activity increases, unsteady flow structures of larger length scales emerge. At very high levels of activity, the flow condenses into two dominant macroscopic vortices, which ultimately destroy the hyperuniform structure of the flow [3].

An interface between active and passive flows is deformed by fluctuations in the active flow. At low activity levels, this deformation results in a slightly fluctuating planar interface. As activity increases, the amplitude of the separating interface grows. At high activity levels, the interface may break up, leading to the formation of smaller active and passive domains. Typically, the number of passive domains exceeds that of the active domains. Within these domains, the energy of the fluid rises with increasing activity; however, the flow does not condense into macroscopic vortices. The phase distribution and, thus, the combined flow field lack hyperuniformity.

Here we will discuss these phenomena by analyzing the flow field with different local and global measures in order to get deeper insight into active flow and the interaction of active and passive phases.

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From crystals to biological tissues: How topological defects control deformations and flows

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Topological defects, as localised regions where order breaks down, determine the properties of systems with collective order, represented by an order parameter. In physical systems, such defects have finite cores within which the singular behavior of the order parameter is regularised. This finite core size of topological defects provides a natural length scale for material properties induced by topological defects. We propose a non-singular field theory for topological defects in systems with broken rotational symmetry, such as liquid crystals, crystals or superfluids. In Landau-type theories, the order parameter is a smooth field that changes both in magnitude and orientation, with a topological defect corresponding to a singularity in the orientation field and a vanishing magnitude. The phase singularity defined the topological charge, while the vanishing magnitude shapes the defect core. Using both of these properties, we can define a smooth defect density field that is topological conserved and accurately tracks the evolution of defects. We apply this formalism to characterise flow and deformation patterns induced by topological defects in the context of crystal plasticity [1] and tissue morphogenesis [2].

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Physical Phenomena Governing BioMineral Morphogenesis in Molluscs

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Mollusks, as well as many other living organisms, have the ability to shape mineral crystals into unconventional morphologies and to assemble them into complex functional mineral-organic structures, an observation that inspired tremendous research efforts in scientific and technological domains. Despite these, a biochemical toolkit that accounts for the formation of the vast variety of the observed mineral morphologies cannot be identified yet. Herein, phase-field modeling of molluscan shell formation, an intensively studied biomineralization process, is used to identify key physical parameters that govern mineral morphogenesis (Figure 1). Manipulating such parameters, various properties ranging from the morphology of a single mineral building block to that of the entire shell assembly are reproduced [1, 2, 3]. The results support the hypothesis that the control over mineral morphogenesis in mineralized tissues happens via regulating the physico-chemical environment, in which biomineralization occurs: the organic content manipulates the geometric and thermodynamic boundary conditions, which in turn, determine the process of growth and the form of the biomineral phase. We demonstrate that phase-field modeling is a powerful approach for the identification of thermodynamic and kinetic parameters that govern the formation of biogenic mineralized assemblies and has the potential of providing explicit guidelines for the morphogenetic control of synthetically formed bioinspired materials systems.

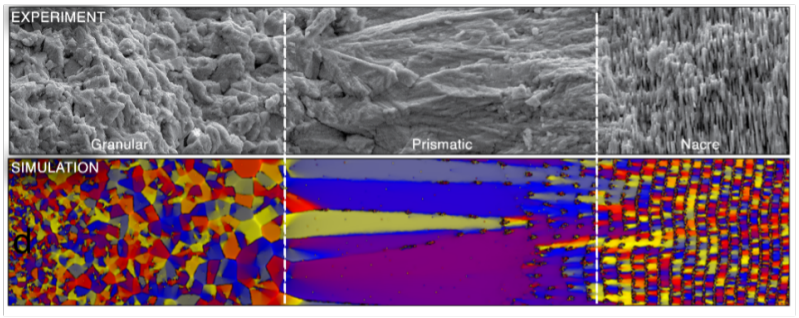

Figure 1: Phase-field simulation of an entire thickness of the shell of the cephalopod N. pompilius having three ultrastructural layers made entirely of aragonite (Bottom, from left to right: granular, prismatic and nacre). For comparison, the actual microstructure of the shell is also presented (Top).

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Phase Separation Dynamics: Hyperuniformity and Non-Hyperuniformity in Passive and Active Hydrodynamic Systems

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Active matter systems display a wide range of fascinating behaviours, driven by internal mechanisms that sustain their dynamics and self-organization without external input. One such example is motility induced phase separation (MIPS), which shows the spontaneous emergence of dense and dilute phases from an initially uniform state of microswimmers. Such phase separation in dry active systems, without hydrodynamic interactions, has been shown to exhibit hyperuniform behaviour, similar to passive phase separation in binary fluid mixtures[1, 2]. We demonstrate the role of hydrodynamic interactions in influencing hyperuniformity in a wet active system described by active Model H [3]. Our direct numerical simulations reveal that, while passive Model H shows hyperuniformity, the interplay of activity and hydrodynamic interactions suppresses hyperuniformity in active Model H, especially when the activity generates contractile stress in the fluid. In Fig. 1, we illustrate $\phi(\mathbf{r})$ and its spectral density $S(k)$ for both passive and active Model H. The dynamics of passive Model H exhibit complete phase separation with hyperuniform structures, as evidenced by the ring structure in the spectral density, where large-scale fluctuations of $\phi(\mathbf{r})$ are suppressed. In contrast, the active Model H dynamics result in arrested phase separation due to contractile stress, leading to a uniform spectral density across a wide range of length scales, which indicates a non-hyperuniform structure.

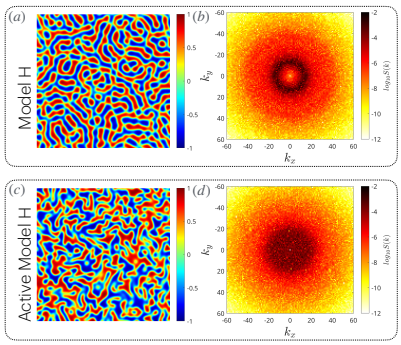

Figure 1: Pseudocolor plot of the order parameter $\phi(\mathbf{r}, t)$ at a representative time: (a) during domain coarsening in Model H and (c) in the statistically steady state of active Model H with contractile active stress. (b) and (d) show the corresponding spectral densities $S(k)$ in the (k_x, k_y) plane.

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Microscopic derivations of phase field crystal models

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Phase field crystal (PFC) models are a widely used tool in modeling phase transitions and nonequilibrium dynamics in materials science. Via dynamical density functional theory, they can be systematically derived from the microscopic equations of motion governing the individual particles the system consists of [1]. This can be done also for systems with orientational degrees of freedom, such as liquid crystals or active matter.

In this talk, I will present some recent results on deriving PFC (and similar) models for particles with orientational degrees of freedom and on the collective dynamics that they predict. First, I will discuss a PFC model for mixtures of active and passive particles [1]. Second, I will present a recently developed theory (*Active Model N*) for particles with nonreciprocal interactions [2], which exhibits a variety of notable pattern formation effects such as the formation of self-knitting 'active yarn' structures (see Fig. 1). Finally, I discuss some recent progress on developing PFC models for biaxial liquid crystals [4].

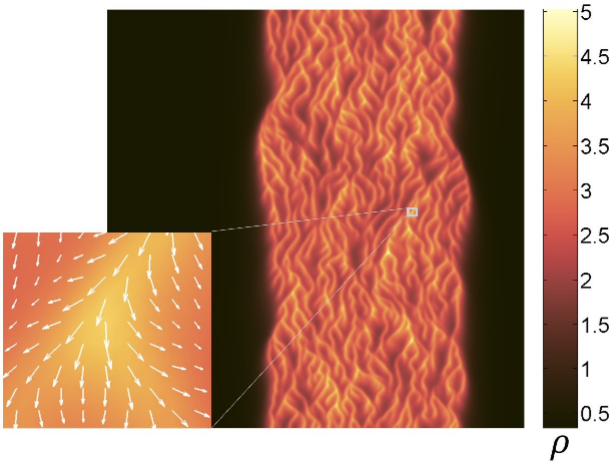

Figure 1: Active yarn pattern. (Reproduced from Ref. [2])

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Controlling the shape of fluctuating nanoscale clusters

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We have investigated how one can manipulate the shape of a small cluster of colloids (or nano-particles) using an external field in the presence of thermal fluctuations. This problem can be formulated as a minimization of first passage times in configuration space. We obtain the optimal solution using Dynamic Programming. We then show how the efficiency in Reinforcement-Learning approaches vanishes at the nanoscale due to thermal fluctuations

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Simulating morphological evolutions by Convolutional Neural Networks

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In the last decade, Neural Networks (NN) have attracted a lot of interest given their potential exploitation as general approximators to surrogate computationally-intensive calculations without accuracy losses. Convolutional NNs (CNN) can be conveniently used for the mapping of morphological evolution problems in the continuum, thanks to their inherent encoding of spatial correlations, opening the way toward large-scale and long-time simulations. As a first approach [1], we employ a CNN to obtain fast, yet-accurate predictions of just one term in the evolution equation, i.e. the most time-consuming one, and perform the time integration using its prediction. In particular, we consider the case of heteroepitaxial growth which would require to numerically solve, e.g. by Finite Element Methods, the mechanical equilibrium problem at each time step, and replace it by a trained CNN model (see Fig. 1a). A second approach [2] instead relies on a CNN to directly predict the entire time-evolution sequence from a few, or just a single, initial frame, using a recurrent architecture to encode time correlations. The method is successfully applied to reproduce Cahn-Hilliard-like dynamics from spinodal decomposition simulations, including anisotropic elasticity (an example in Fig.1b), to the shape evolution of crystalline particles by surface diffusion. The advantages and limitations of both strategies are critically discussed.

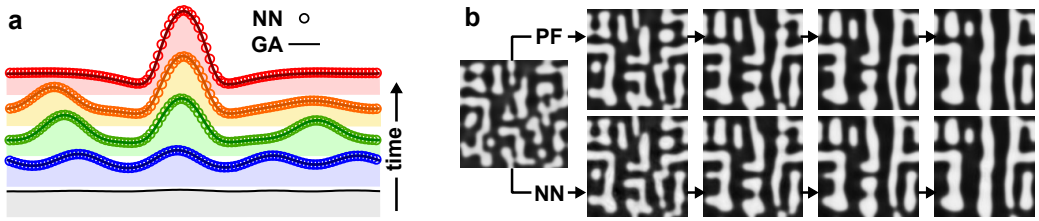

Figure 1: (a) Time evolution of the profile of a heteroepitaxial film as obtained by computing strain by a Green's function approximation and predicting it by NN. (b) Simulation of spinodal decomposition for a strained alloy with cubic elastic anisotropy obtained by phase-field (PF) vs. its NN prediction.

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Phase-field modeling of elastic microphase separation

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Spinodal decomposition is a process where an initial homogeneous but unstable mixture spontaneously separates into two or more stable phases with a distinctive arrangement termed *spinodal structure*. This process can be modeled with the *Cahn-Hilliard equation* [1] which is based on the definition of a chemical energy density depending on an order variable, i.e. the phase field, representing the smooth transition between the unstable initial mixture and the stable phases. Spinodal structures are characterized by a length scale that, if no competing processes are accounted for, coarsens over time until complete segregation of the stable phases. Recent studies suggest that for certain mixtures involving a solid matrix, the elastic parameters of the matrix govern the coarsening stage and can even arrest it, a phenomenon that is denoted as elastic microphase separation [2].

In this work, we propose a phase-field model that captures the main features of elastic microphase separation observed in [2]. We extend the Cahn-Hilliard free-energy functional [1] to include the elastic strain energy density as well as an additional coupling term. The model is first investigated in 1D and the results show that the mechanical deformation controls both the composition of the stable phases and the initial characteristic length of the spinodal structure. Moreover, we numerically show that the proposed coupling is able to predict the arrest of the coarsening phase at a length scale controlled by the model parameters. The formulation is then extended to the multi-dimensional setting and compared to experimental results. The numerical results show excellent agreement with the experimental evidence, especially in terms of initial and arrested pattern morphology.

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Inverse design of spinodoid metamaterials

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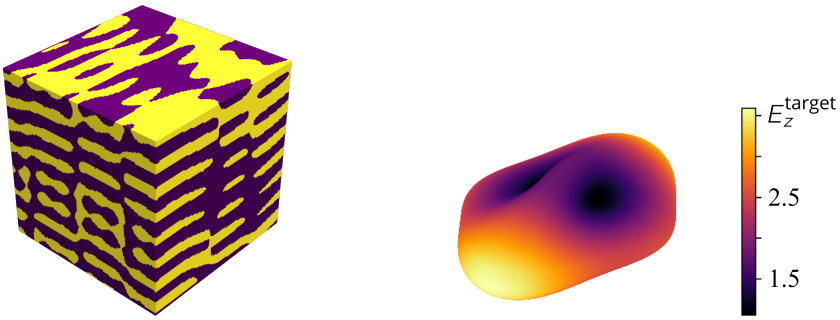
Mechanical *metamaterials* or architected materials are becoming increasingly popular due to rapid developments in additive manufacturing. These metamaterials exhibit mechanical properties that differ greatly from those of their base material and are highly customizable. This freedom in design naturally raises the question: How can we systematically find a structure that matches some given requirements? Thus, within a single class of metamaterials, the goal of *inverse design* is to map some desired *properties* $\mathcal{P}^*$ onto a tuple of *structure parameters* $\mathcal{S}^*$, such that the structure generated with these parameters has exactly these properties.

This presentation firstly introduces some general approaches [1, 2] to solving the inverse design problem before considering the special case of *spinodoid metamaterials* [1] with linear elastic properties. Initially, a *surrogate model* for the forward mapping $\mathcal{S} \mapsto \mathcal{P}$ is generated where the focus is on data efficient sampling and modeling. *Permutation equivariant neural networks* are used to take into account the symmetries inherent to the spinodoid structure parameters. Using this learned function, optimal structure parameters $\mathcal{S}^*$ can be determined given some desired properties $\mathcal{P}^*$. The effectiveness of both the surrogate model as well as the inverse design algorithm is demonstrated. Exemplarily, some obtained structures are shown for requirements with increasing complexity, as for example in Fig. 1. Finally, a possible extension to more complex elastic or even inelastic properties is outlined.

Goal: Find $\mathcal{S}^*$, such that (i) $E_z \geq E_z^{\text{target}}$, (ii) $E_x/E_y = 2$ and (iii) $\rho \to \min$.



(a) Structure obtained with $\mathcal{S}^*$.

(b) Elastic surface of the structure.

Figure 1: Example of an inverse design problem and the respective solution for spinodoid metamaterials.

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Describing the local geometry of architected structures with persistent homology

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Metamaterials are artificial architected materials, achieving superior properties in comparison with bulk ones thanks to their structural arrangement. If they are highly promising for a wide range of applications, from optics to mechanics, apprehending their geometry is challenging due to their complex and disordered configuration. In this regard, the persistent homology [1] emerged as a great method to grasp their geometrical organization and to apply it to the design and inverse design of metamaterials. Indeed, this mathematical tool originating from the topology allows us to capture the local geometry of the structure and to convert it into numerical information suitable for statistical analysis, for example via machine learning models [2]. We discuss the application of this local geometry description to point patterns [3] and we show that the local geometrical features as described by the persistent homology, although picturing the structure on short scales, are able to capture with great accuracy properties only appearing on large scales, for instance, the hyperuniformity of the arrangement. Furthermore, we present several examples of the applications of persistent homology to inverse design problems, including parameter estimation and pattern generation. Finally, we discuss the highly promising extensions offered by these results to the case of hyperuniform fields, with a large range of applications to the engineering of metamaterials.

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Multiscale modeling of grain boundary plasticity

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Grain boundary (GB) migration is one of key underlying processes behind mechanisms ranging from recrystallization and solidification to work hardening. GBs have been repeatedly identified as the least understood of all material defects, a well-earned designation resulting from their wide range of behaviors over a very large configurational space. GB migration, in particular, exhibits a strong sensitivity to loading type, with a single boundary able to exhibit a wide range of behaviors under varied boundary conditions. Understanding these behaviors is essential to the analysis and design of many structural materials, and the talk consists of four talks. First, we present work at the atomic scale, using atomistic simulations and optimal transportation theory to provide a systematic way for predicting shuffling mechanisms. Second, we look at boundary migration as a dissipative process within a thermodynamic framework inspired by crystal plasticity. This approach unifies motion by driving force, shear coupling, mode switching, and stagnation as special cases of a general continuum evolution law for boundary motion. The model employs the principle of minimum dissipation potential, and introduces "dissipation energy" as an intrinsic GB property, measured using molecular dynamics. Agreement of dissipation energies across driving forces provides verification for the framework. Third, the mechanistic framework is applied directly to a phase field model for boundary migration. It is shown that, by combining nonconvex boundary energy, elasticity, and the principle of minimum dissipation potential, preferential boundary migration occurs spontaneously through the emergence of horizontally moving steps, which we identify as so-called phase field disconnections. A variety of boundaries are considered, including symmetric and asymmetric tilt boundaries. Fourth, we present "network plasticity," an extreme multiscale model designed to convey realistic microstructural information to viable continuum length scales.

Phase Field modeling, crack propagation, variational models

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Ductile fracture is associated with plastic deformation and the development of voids in the material, which leads to a gradual fracture evolution. This work aims to capture the complex micromechanical processes such as void nucleation, growth and coalescence that govern the material behaviour on the material scale in a phenomenological sense and to regularise the fracture model across a damage zone. A model is proposed that includes triaxiality effects, i.e. captures the hydrostatic stresses arising under necking during plastic deformation. The hydrostatic stress is related to void nucleation and growth in the material, and is relevant for the prediction of ductile fracture initiation. Local models such as the well-known Gurson-Tvergaard-Needleman model [1], [2], which directly considers the porosity evolution in the material and thus accounts for triaxiality effects, suffer from the disadvantage of not being well-defined when it comes to the localisation of porosity.

In this context, the aim is to provide a variational phase-field model that can account for triaxiality effects and does not consider the porosity as an additional damage variable. The proposed formulation considers the modified Cam-Clay plasticity model that goes back to [3] and is originally developed for geomechanics. The variationally consistent phase-field plasticity model imitates the plastic yielding of the Gurson-Tvergaard-Needleman model and is thus able to qualitatively capture ductile fracture.

The behaviour of the proposed model is studied with numerical simulations for high strength steel. These show for various benchmark tests that the model is suitable for predicting ductile fracture initiation and propagation for a linear geometry.

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Phase field modelling of anisotropic solid-state dewetting on patterned substrates

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We present a phase-field model for simulating the solid-state dewetting of anisotropic crystalline films on non-planar substrates. This model exploits two order parameters to trace implicitly the crystal free surface and the substrate profile in both two and three dimensions. First, we validate the model by comparing numerical simulation results for planar substrates with those obtained by a conventional phase-field approach and by assessing the convergence toward the equilibrium shape predicted by the Winterbottom construction. We then explore non-planar geometries, examining the combined effects of surface-energy anisotropies and parameters controlling the contact angle. Our findings reveal that crystalline particles on curved supports lose self-similarity and exhibit a volume-dependent apparent contact angle, with opposite trends for convex versus concave profiles. Additionally, we investigate the migration of faceted particles on substrates with variable curvature. Applying this model to experimentally relevant cases like spheroidal and pit-patterned substrates demonstrates various behaviors that could be leveraged to direct self-assembly of nanostructures, from ordered nanoparticles to interconnected networks with complex topology

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