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BOOK OF ABSTRACTS

**Modeling of Crystalline Interfaces
and Thin Film Structures:
A Joint Mathematics-Physics Symposium**

Workshop Organized by

Ulrike DIEBOLD, Irene FONSECA, and Paolo PIOVANO

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Derivation of linear elasticity from atomistic energies with multiple wells

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A rigorous derivation of linear elastic theories from non linear elasticity has been provided in terms of Γ -convergence for both continuum and atomistic models mainly in the case of single well potentials (see for example [2, 3, 4]). On the other hand, energies with multiple wells naturally arise in many models, as for example in the gradient theory of solid-solid phase transitions. In the recent paper [1], it has been shown that linear elasticity can be rigorously derived from multi-well energies by adding a singular higher order term which penalizes the transitions between the wells and turns out to be necessary in order to recover good compactness properties of minimizing sequences of displacement fields. In this talk I will present a recent result in collaboration with G. Lazzaroni and M. Palombaro for the derivation of linear elasticity from a general class of atomistic energies with multiple wells for crystalline materials, showing that the role of the singular term in the continuum model in penalizing jumps from one well to another is played in this setting by interactions beyond nearest neighbours.

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Wrinkling of a thin elastic sheet on a compliant sphere

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Wrinkling of thin elastic structures can be viewed as a way how they avoid compressive stresses. While the question of where the wrinkles appear is (mostly) well-understood, understanding properties of wrinkling is not trivial. Considering a variational viewpoint, the problem amounts to minimization of an elastic energy, which can be written as a non-convex membrane energy singularly perturbed by a higher-order bending term. To understand the global minimizer (ground state), the first step is to identify its energy, in particular how it depends on the small physical parameter (thickness). To explain this approach I will focus on one specific example: a disk-shaped thin elastic sheet bonded to a compliant sphere. There the leading-order behavior of the energy determines the macroscopic deformation of the sheet and provides insight about the length scale of the wrinkling. The next-order correction then provides insight about how the wrinkling pattern should vary across the film, and is in particular related to the form of transition between different wrinkling patterns.

Some results on the relaxation of the area functional for graphs in dimension two and codimension two

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Let us consider the functional

$$A(u, \Omega) = \int_{\Omega} \sqrt{1 + |\nabla u_1|^2 + |\nabla u_2|^2 + \left(\frac{\partial u_1}{\partial x} \frac{\partial u_2}{\partial y} - \frac{\partial u_1}{\partial y} \frac{\partial u_2}{\partial x} \right)^2} dx dy,$$

defined on smooth maps $u = (u_1, u_2) : \Omega \subset \mathbf{R}^2 \rightarrow \mathbf{R}^2$; $A(u, \Omega)$ gives the value of the two-dimensional area in \mathbf{R}^4 , of the graph of u . We shall discuss some aspects of the relaxation of $A(\cdot, \Omega)$, in particular its values on nonsmooth maps, for instance on piecewise constant maps [1], [2]. We shall show that the evaluation of the relaxation is related to the solution of certain Plateau-type problems, with various sort of boundary conditions.

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Homogenization of oscillating networks

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We consider the asymptotic behaviour of integral energies with convex integrands defined on one-dimensional networks contained in a region of the three-dimensional space with a fast-oscillating boundary as the period of the oscillation tends to zero, keeping the oscillation themselves of fixed size. The limit energy, obtained as a Γ -limit with respect to an appropriate convergence, is defined in a ‘stratified’ Sobolev space and is written as an integral functional depending on all, two or just one derivative, depending on the connectedness properties of the sublevels of the function describing the profile of the oscillations. In the three cases, the energy function is characterized through an usual homogenization formula for p -connected networks, a homogenization formula for thin-film networks and a homogenization formula for thin-rod networks, respectively. This is work in collaboration with Valeria Chiadò Piat [3], and is related to previous work on fast oscillating boundaries [1] and on the homogenization of singular structures (e.g. in [2, 4, 5]).

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Crystalline evolution of mean-convex sets

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In a recent paper [4], T. Laux and G. De Philippis have studied the mean curvature flow of (strictly) mean convex sets and characterized its major properties. In this talk we essentially address the same questions however in the nonsmooth case. We show that given an appropriate definition of strict “mean convexity” relative to an arbitrary surface tension (including crystalline), we can recover the same results, using mostly variational proofs based on [1, 5] and the recent theory for crystalline flows [3, 2] In particular, this flow is (as expected) unique and decreasing. This is a joint work with Matteo Novaga (U. Pisa).

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Does the N -clock model approximate the XY -model?

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The N -clock model is a two-dimensional ferromagnetic spin model on the square lattice in which the spin field is constrained to take values in a set of N equi-spaced points of the unit circle. It is usually considered as an approximation of the XY model, for which instead the spin field is allowed to attain all the values of the unit circle. In the theory of superconductivity the latter models phase transitions mediated by the formation and the interaction of co-dimension 2 topological defects as in the well-known Ginzburg-Landau functional. A breakthrough result by Fröhlich and Spencer (CMP 1981) shows that the same kind of phase transitions appear in the N -clock model for N large enough. By a variational analysis we find the explicit rate of divergence of N (with respect to the number of interacting lattice points) for which the N -clock model asymptotically behaves like the XY model at zero temperature. We moreover exhaustively discuss all the other regimes of N and we show how Cartesian Currents can detect the energy concentration on sets of co-dimension smaller or equal than 2. The results presented are contained in a recent paper in collaboration with G. Orlando (TUM) and M. Ruf (EPFL).

On the jerky crack growth in elastoplastic materials

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The purpose of the talk is to show that in elastoplastic materials cracks can grow only in an intermittent way. This result is rigorously proved in the framework of a simplified model.

Pinning of interfaces by localized dry friction

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We consider a differential inclusion to model the propagation of an interface, e.g., a phase boundary, in an environment with obstacles. The interaction of the interface with the obstacles is governed by a localized dry friction. The model implies that energy has to be expended to pass across an obstacle. Hence, the interface becomes arrested until enough curvature is accumulated such that it is energetically more favorable to pass across the obstacle. The treatment of our model in the context of pinning and depinning requires a comparison principle. We prove this property and hence the existence of viscosity solutions. Moreover, under reasonable assumptions, they are equivalent to weak solutions. Our main results asserts that for obstacles distributed according to a Poisson point process, interfaces become pinned, leading to the emergence of a rate-independent hysteresis. This is joint work with Luca Courte and Ulisse Stefanelli.

Assembly and stability of nanoclusters during thin film deposition

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We consider epitaxial nanoclusters (NCs) formed by deposition on crystalline surfaces where NCs can be either two- or three-dimensional (depending on the relative strength of adhesion to surface energy). NC assembly is described by appropriate theories for nucleation and growth during deposition. Extensive theoretical efforts attempted to develop a beyond-mean-field for homogeneous nucleation of homoepitaxial 2D NCs to predict NC size distributions, and the stochastic geometry of the spatial NC distribution [1]. Recent efforts have also provided a precise description with ab-initio kinetics of far-from-equilibrium growth shapes [2]. For heteroepitaxial 3D NCs, nucleation is often heterogeneous, and modeling of growth shapes is more challenging as it must account for interlayer transport. In this presentation, we focus on post-deposition evolution which can involve either Ostwald Ripening - OR (dissolution of smaller NCs and growth of larger NCs), or Smoluchowski Ripening - SR (NC diffusion and coalescence) [3]. OR for 2D NCs can provide perfect 2D realizations of classic LSW theory in some systems. However, “anomalous” behavior has been observed in others [4], and the presence of even trace additives can accelerate OR due to mass transport by complex formation (where analysis involves appropriate reaction-diffusion equations) [5]. For SR of 2D NCs, the size-dependence of NC diffusion, and the dynamics of coalescence or sintering are of central interest. For 3D NCs, a long-standing debate about whether OR or SR dominates is being answered by in-situ experimental imaging. For both 2D and 3D epitaxial NCs, we present recent modeling related to SR revealing a complex oscillatory size dependence of NC diffusivity, and also analyzing evolution during NC coalescence.

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How a minimal surface leaves a thin obstacle

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In this talk I will present recent results on the optimal regularity of the solution to the thin obstacle problem for nonparametric minimal surfaces with zero obstacle.

A detailed analysis of the global structure of the related free boundary, in particular its local finiteness in measure and its rectifiability, will be also considered.

This is joint work with Emanuele Spadaro (U. Roma La Sapienza).

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Variational approach to the dynamics of multiphase models with density constraints

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We study the dynamics of a multiphase model given as a gradient flow of non local energies subject to a global density constraint when the interaction energy is given by a potential of coulomb type possibly singular at the origin. Due to the presence of the density constraint and the singularity of the interaction potential, we provide an approximation by particle systems whose motion is ruled by a suitable regularisation of the potential accounting for the non-congestion constraint.

Connectedness of drops in convex potentials

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An old conjecture of Almgren states that for every convex and coercive potential $g : \mathbb{R}^d \rightarrow \mathbb{R}$, every convex and one-homogeneous anisotropy $\Phi : \mathbb{R}^d \rightarrow \mathbb{R}^+$ and every volume $V > 0$, the minimizers of

$$\min_{|E|=V} \int_{\partial E} \Phi(\nu) d\mathcal{H}^{d-1} + \int_E g dx$$

are convex. I will review the known results on this problem and present recent progress obtained with G. De Philippis on the connectedness of the minimizers for smooth potentials and anisotropies. Our proof is based on the introduction of a new “two-point function” which measures the lack of convexity and which gives rise to a negative second variation of the energy.

Discrete energies with surface scaling: interactions beyond nearest neighbours versus non-interpenetration

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We present some discrete models for crystals with surface scaling of the interaction energy. We assume that at least nearest and next-to-nearest neighbour interactions are taken into account. Our purpose is to show that interactions beyond nearest neighbours have the role of penalising changes of orientation and, to some extent, they may replace the positive-determinant constraint that is usually required when only nearest neighbours are accounted for.

From joint works in collaboration with R. Alicandro and M. Palombaro [1, 2].

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A Sharp Interface Model for Solid-State Dewetting Problems

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In this talk we will present a sharp interface model for solid-state dewetting of thin films with anisotropic surface energies. The morphology evolution of thin films is governed by surface diffusion and contact line migration. This is joint work with Irene Fonseca and Gianni Dal Maso.

Dynamics of a degenerate PDE model of epitaxial crystal growth

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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 analytical results for such models, some of which involve subgradient dynamics for Radon measure solutions and a new notion of weak solutions.

Ultra-thin Co films: structure and magnetism

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Ultra-thin magnetic films have been of interest as their low-dimensionality and the presence of interfaces sensitively modify the structural and magnetic properties [1]. From a technological view, such films present possibilities for applications in terms of recording density, fast domain wall motion and the presence of exotic magnetic domains. In this respect, among elemental metals cobalt is arguably the most studied one in ultra-thin film and multilayer configurations due to the magnetic anisotropy perpendicular to the film plane and the observation of chiral domain structures such as *skyrmions* [2]. In the first part of the talk, the structural aspects of cobalt films grown on heavy metal substrates such as W(110) and Re(0001) will be treated. Along with the substrate interface and the hcp-fcc Co phase transition, we will also consider the subsequent growth of a graphene overlayer on the cobalt film [3]. In the second part, we will focus on the magnetic properties of cobalt films with perpendicular magnetization. In particular, we will show how x-ray speckles can be applied to studies of periodic magnetic domain patterns observed in such films. X-ray speckles, which had been developed for imaging aperiodic objects based on ideas from x-ray crystallography [4], provide interesting opportunities when combined with other x-ray imaging methods.

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Analysis of a perturbed Cahn-Hilliard model for Langmuir-Blodgett films

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A one-dimensional evolution equation including a transport term is considered; it models a process of thin films deposition. Existence and uniqueness of solutions, together with continuous dependence on the initial data and an energy equality are proved by combining a minimizing movement scheme with a fixed-point argument. Finally, it is shown that, when the contribution of the transport term is small, the equation possesses a global attractor and converges to a purely diffusive Cahn-Hilliard equation.

This is joint work with Marco Bonacini and Elisa Davoli.

The surface diffusion flow with elasticity in two and three dimensions

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We prove short-time existence and uniqueness for the surface diffusion flow with a non-local forcing of elastic type. We also establish long-time existence and asymptotic behavior for a suitable class of strictly stable initial data. To the best of our knowledge these are the first rigorous results for a surface diffusion evolution equation with elastic stress and without curvature regularization.

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Chiral domain walls and domain wall tilt in ferromagnetic nanostrips

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Recent advances in nanofabrication make it possible to produce multilayer nanostructures composed of ultrathin film materials with thickness down to a few monolayers of atoms and lateral extent of several tens of nanometers. At these scales, ferromagnetic materials begin to exhibit unusual properties, such as perpendicular magnetocrystalline anisotropy and antisymmetric exchange, also referred to as Dzyaloshinskii-Moriya interaction (DMI), due of the increased importance of interfacial effects. The presence of surface DMI has been demonstrated to fundamentally alter the structure of domain walls. Here we use the micromagnetic modeling framework to analyse the existence and structure of chiral domain walls, viewed as minimizers of a suitable micromagnetic energy functional. We explicitly construct the minimizers in the one-dimensional setting, both for the interior and edge walls, for a broad range of parameters. Using variational methods we analyze the asymptotics of the two-dimensional magnetization patterns in samples of large spatial extent in the presence of weak applied magnetic fields and present an analytical theory of domain wall tilt. We show that under an applied field the domain wall remains straight, but tilts at an angle to the direction of the magnetic field that is proportional to the field strength for moderate fields and sufficiently strong DMI.

This is joint work with V. V. Slastikov, A. G. Kolesnikov, and O. A. Tretiakov. Support by NSF via grants DMS-1313687 and DMS-1614948 is gratefully acknowledged.

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The 0-fractional perimeter

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I will present a unified point of view on fractional perimeters and Riesz potentials. Denoting by H^s - for $s \in (0, 1)$ - the s -fractional perimeter and by J^s - for $s \in (-d, 0)$ - the s -Riesz energies acting on characteristic functions, I will show that the functionals H^s and J^s , up to a suitable additive renormalization diverging when $s \rightarrow 0$, belong to a continuous one-parameter family of functionals, which for $s = 0$ gives back a new object we refer to as 0-fractional perimeter. All the convergence results with respect to the parameter s and to the renormalization procedures are obtained in the framework of Γ -convergence. As a byproduct of our analysis, we obtain the isoperimetric inequality for the 0-fractional perimeter. These results are in collaboration with L. De Luca and M. Ponsiglione.

Derivation of linearised polycrystals from a 2D system of edge dislocations

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Many solids in nature exhibit a polycrystalline structure. A *single phase polycrystal* is formed by many individual crystal grains, having the same underlying periodic atomic structure, but rotated with respect to each other. The region separating two grains with different orientation is called *grain boundary*. Since the grains are mutually rotated, the periodic crystalline structure is disrupted at grain boundaries. As a consequence, grain boundaries are regions where dislocations occur, inducing high energy concentration.

We will discuss a variational model that describes the emergence of polycrystalline structures as a result of elastic energy minimisation. The setting is that of linearised planar elasticity. Starting from the variational semi-discrete model for edge dislocations introduced in [2] within the so-called core radius approach, we derive by Γ -convergence as the lattice spacing tends to zero, a limit energy given by the sum of a plastic term, acting on the dislocation density, and an elastic term, which depends on the symmetric strains. Minimisers under suitable boundary conditions are piece-wise constant antisymmetric strain fields, representing in our model a polycrystal whose grains are mutually rotated by infinitesimal angles. In this respect our result can be regarded as a linearised version of the Read-Shockley formula [3]. This is joint work with S. Fanzon and M. Ponsiglione [1].

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On the optimization of Riesz-like potentials

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In this talk, we will discuss the extrema of functionals of the type

$$P(E) + \iint_{E \times E} g(|y - x|) dx dy,$$

where $E \subseteq \mathbb{R}^N$ is a set of finite perimeter with an assigned volume, $P(E)$ is its perimeter, and $g : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ is a given concave function. This problem is currently deeply studied by several people, with a particular emphasis on the case when $g(t) = t^{\alpha-N}$ for some $0 < \alpha < N$. We will describe the general question and some of the main known facts, and we will discuss in particular the case of the small volume, and the stability of the extrema (this last, central issue is studied in several papers, see for instance [1, 2, 3]).

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Novel Functionalities in Atomically Controlled Oxide Heterostructures by Pulsed Laser Deposition

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In recent years, it has been shown that novel functionalities can be achieved in oxide heterostructures in which the interfaces are atomically controlled, in terms of atomic stacking as well as in terms of the local symmetry. I will highlight the recent developments in atomic controlled growth of epitaxial oxides by pulsed laser deposition, with a focus on heterostructures showing manipulated magnetic and electronic properties. Emergent phenomena in oxide heterostructures such as interface charge transfer [1], two dimensional electron gas and ferromagnetism between two non-magnetic materials, are induced by the dedicated coupling between spin, orbital, charge and lattice degrees of freedom. Developing strategies to engineer these intimate couplings in oxide heterostructures is crucial to achieve new phenomena and to pave the path towards novel functionalities with atomic scale dimensions. Strong oxygen octahedral coupling has recently been demonstrated, which transfers the octahedral rotation from one oxide into the other at the interface region. As a result, we possess control of the lateral magnetic and electronic anisotropies by atomic scale design of the oxygen octahedral rotation [2].

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Electronic transport properties of graphene doped by gallium – application of density functional theory

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In this work we present the effect of low dose gallium (Ga) deposition ($< 4\text{ML}$) performed in UHV (10^{-7}Pa) on electronic doping and charge carrier scattering in graphene grown by chemical vapor deposition. In situ graphene transport measurements performed with a graphene field-effect transistor structure show that at low Ga coverages a graphene layer tends to be strongly n-doped with an efficiency of 0.64 electrons per one Ga atom, while the further deposition and Ga cluster formation results in removing electrons from graphene (less n-doping) [1]. These experimental results are supported by density functional theory (DFT) calculations and explained as a consequence of distinct interaction between graphene and Ga atoms in case of individual atoms, layers, or clusters. We will present application of DFT for calculations of Ga atom clustering on graphene. According to DFT simulations, gallium starts to form stable clusters from three atoms. However, when the van der Waals correction is involved, a parallel geometry up to size of four atoms is preferred. This leads to an increase of absolute values of doping of graphene by electrons from Ga atoms. In addition, we will show that gallium atoms can diffuse along the graphene sheet across a small diffusion barrier of 0.11 eV. This barrier can be additionally reduced by application of external electric field, which was simulated by ionization of the simulated structure. The work is a joint collaboration with David Nezval, Miroslav Bartošík, Jindřich Mach, Jakub Piastek, Pavel Procházka, Vojtěch Švarc, and Miroslav Konečný.

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Effective theories and energy minimizing configurations for heterogeneous multilayers

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We will report on recent advances in deriving effective theories for thin sheets consisting of multiple layers with (slightly) mismatching equilibria, see [1, 2]. While the regime of finite bending energy is well understood by now, the talk will focus on energy scaling regimes beyond Kirchhoff's theory leading to linearized Kirchhoff, von Kármán and linearized von Kármán functionals with a spontaneous curvature term. We will also investigate optimal energy configurations and find that the von Kármán scaling is critical for their generic shape.

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Grain boundary dynamics: a disconnection perspective

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The motion of grain boundaries (GBs) and the relative motion of crystals that meet at a GB are describable in terms of the motion of line defects that are constrained to the GB. These line defects (disconnections) are characterized by both a Burgers vector (dislocation character) and steps (step character). The set of possible disconnections b, h are determined by the relative orientations of the two grains that meet at the GB. At low temperature, GB dynamics is controlled by the disconnections with the lowest formation energies for any driving force. This gives rise to classical “shear coupling” behavior. At high temperature, it is possible to form disconnections of multiple nodes (this is responsible for GB sliding). While single mode disconnection dynamics may be important in bicrystals, GB migration in polycrystals require the activation of multiple modes. A Kosterlitz-Thouless transition may occur at high temperature which changes the fundamental nature of how disconnections move. We present a combination of theory and molecular dynamics and kinetic Monte Carlo simulations to demonstrate these effects. While discrete disconnections dynamics can describe many of the fundamental behaviors, the goal is a continuum equation of motion for GBs and the junctions at which they meet. We present some recent results on the development of such continuum approaches. Some key references are listed below [1, 2, 3, 4, 5, 6, 7].

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Interfaces between crystalline organic semiconductor nanostructures and 2D materials

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Crystalline films of small conjugated molecules offer attractive potential for fabricating organic solar cells, organic light emitting diodes (LEDs), and organic field effect transistors (OFETs) on flexible substrates. Here, the novel two-dimensional (2D) van der Waals materials like conducting graphene (Gr), insulating ultra-thin hexagonal boron nitride (hBN) or semiconducting transition metal dichalcogenides come into play. Gr for instance offers potential application as a transparent conductive electrode in organic solar cells and LEDs replacing indium tin oxide, whereas hBN can be used as ultra-thin flexible dielectric in OFETs. Since small conjugated molecules like the rod-like molecules para-hexaphenyl (6P) or pentacene fit well to the honeycomb structure of 2D materials, their growth can be expected in a lying configuration. This has indeed been observed for growth of 6P on Pt(111) supported Gr by low-energy electron microscopy (LEEM) and by micro-beam low-energy electron diffraction (μ -LEED) revealing the epitaxial relation between substrate and the molecular overlayer [1]. A similar interface can be assumed for the self-assembly of crystalline 6P needles on exfoliated, wrinkle-free Gr, where atomic-force microscopy (AFM) reveals several 10 nm wide, a few nm high, and tens of μ m long needles along discrete substrate directions [2]. For 6P on ultrathin hBN, such needles grow almost along the armchair direction of the substrates which could be supported by density functional theory (DFT) calculations of the energetically favorable molecular adsorption site [3]. AFM based manipulation in conjunction with molecular dynamics simulations revealed friction anisotropy and preferential sliding directions between the 6P nanocrystals and both 2D substrates [4]. For needle-like nanocrystals of the polar molecule dihydrotetraazaheptacene (DH7) on hBN, electrostatic force microscopy (EFM) revealed light-induced charge spreading depending on the polarization direction of light [5]. Here, DFT was not only employed to reveal the molecular adsorption site but also the most probable crystal structure as well as the optical properties of the molecules.

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Microscopical justification of the winterbottom shape

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In this talk we will discuss the microscopical derivation of a continuum model for the Winterbottom problem, i.e., the problem of determining the equilibrium shapes for droplets attached to a wall. Our strategy consists in showing that properly defined atomistic energies of crystalline configurations Γ -converge, as the number of atoms grows, converge to a surface energy which is minimized by the Winterbottom shape. The work generalizes the result [?] which deals with the equilibrium shape of particles in a free crystalline configuration (without a substrate) where it was that the limit minimizing configuration is the Wulff shape. This problem finds applications in the framework of growth of thin films over substrates. This is a joint work with Paolo Piovano (University of Vienna).

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Low-volume fraction martensitic microstructures close to interfaces

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In this talk, I shall discuss recent analytical results on variational models for martensitic microstructures. We consider (singularly perturbed) multiwell elastic energy functionals and the associated nonconvex vectorial minimization problems. We shall discuss in particular needle-like microstructures and geometrically linearized models in the limit of low volume fraction. This talk is based on joint works with S. Conti, J. Diermeier, M. Lenz, N. Lüthen, D. Melching, and M. Rumpf.

