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Mini-Workshop: Multiscale Modelling in Epitaxial Growth

Organised by
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Introduction by the Organisers

Thin film epitaxy is a modern technology of growing single crystals that inherit atomic structures from substrates. Various mathematical models and numerical algorithms are proposed to be used for describing epitaxial growth processes. Due to the underlying multiscale phenomena, which range from the interaction of single atoms at steps up to an engineering scale, on which the transport of material to the surface in a MBE (molecular beam epitaxy) furnace needs to be described, the models can be distinguished by the relevant length scales they are living on

(a) discrete atomic models: Individual atoms are the basic degrees of freedom and single hoppings to neighbouring lattice sites are simulated by kinetic Monte Carlo methods. A n example are the so-called Solid-on-Solid models.
(b) discrete-continuous models: The atomic distance in the growth direction is discrete, but the atomic distance in the lateral direction is coarse grained. The steps are assumed to be smooth curves and serve as free boundaries for an adatom diffusion equation on terraces. These models are known as Burton-Cabrera-Frank models.
(c) continuous models: The atomic processes at steps are neglected , the overall surface is assumed to be smooth and phenomenological equations describe directly the height of the growing film. An example is the Villain equation.

The main goal in modelling epitaxial growth is to bridge the gap between these different models and to describe growth process on a continuous scale by incorporating atomic effects. The focus of this workshop was to bring together materials scientists, theoretical physicists and applied mathematicians to exchange ideas on the three different regimes (a),(b) and (c). The mini-workshop consisted of three introducing lectures, one for each approach and several lectures which focus on connections both in an analytical and numerical fashion. The contributions ranged from quantum-chemistry, molecular dynamics and kinetic Monte Carlo to step flow and continuum models. Several multiscale approaches have been considered to combine at least two of these models.

Besides the mathematical aspects of modelling epitaxial growth also the connection to experimental results was dealt with in order to drive the recent theoretical developments into a direction which is relevant for a large variety of industrial applications. The mini-workshop was also used to give young researchers the opportunity to be introduced into such an actual interdisciplinary field.

Multiscale Modelling in Epitaxial Growth

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Abstracts

Fronttracking for Epitaxial Growth by a Cellular Automaton Algorithm

Rainer Backofen

(joint work with Frank Haußer, Axel Voigt)

The description of steps is a crucial part in the numerical modelling of step flow or island growth. There are a lot of different methods, e.g. level sets, parametric finite elements or phasefield methods. Each of them have their advantages and disadvantages. But for all this methods faceting of the steps or strong anisotropic properties are numerically hard to treat[1].
In cases of strong anisotropic growth laws Gandin and Rappaz [1] introduced a cellular automata (CA) algorithm for the description of grain growth in metallurgical solidification.We present first steps to adapt this algorithm to epitaxial island growth.

In the presence of strong anisotropies the growth of an island is limited by its slowest growing directions. In these directions the island form facets. A complete representation of such an island is given by the normal directions of the facets and their distances from a central point. A set of facet normals together with a distance to a point defines an evolution element. In order to take into account local effects such as island impingement or spatially varying growth velocities, a local description of the island is needed. Thus the step or island boundary is approximated by a set of local evolution elements defined at points near the step. In figure 1 the evolution algorithm is shown.

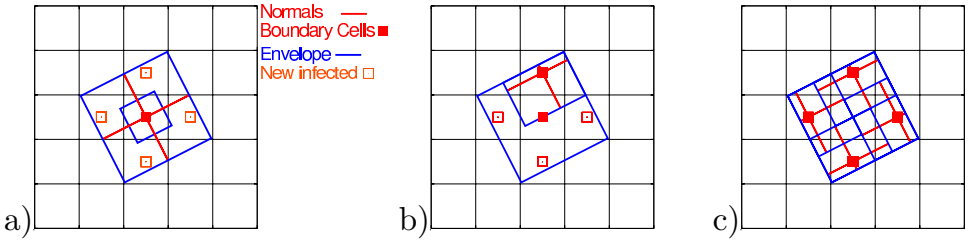

FIGURE 1. a) An island is nucleated in a cell and successively grows until adjacent cells are inside the envelope. b) Adjacent cells are infected, that is, the island is represented by a evolution element defined at the new infected cell. c) The whole island is now locally defined by evolution elements defined in cells nearby

The CA uses a regular structured grid. Every grid cell has a state, ξ_i : terrace, no terrace or boundary. In the boundary cells are additionally evolution elements defined to track the step.

[1] at least compared to a isotropic case

The driving force for the step evolution is derived by a standard Burton-Cabrera-Frank (BCF) type model [1]. The adatom density ρ_i at the terrace Ω_i of atomic height is described by the diffusion equation

$$\rho_i - D\Delta\rho_i = F - \tau^{-1}\rho_i \quad \text{in} \quad \Omega_i(t) \tag{1}$$

where F and $\tau^{-1}\rho_i$ model the flux onto the surface and evaporation. The steps (terrace boundaries) Γ_i are free boundaries with normal velocity v_i governed by the adatom fluxes toward the steps and edge diffusion.

$$v_i = -D\nabla\rho_i \cdot \vec{n_i} - \rho v_i + D\nabla\rho_{i-1} \cdot \vec{n_i} + \nu\partial_{ss}\kappa_i \tag{2}$$

Until now we use thermodynamic boundary conditions at the steps

$$\rho_i = \rho_i = \rho_{eq}(1 + \mu\kappa_i) \quad \text{on } \Omega_i \tag{3}$$

To solve this set of equations, we use a operator splitting approach, as in Bänsch et al. [2]. The step evolution is modelled with the CA, which is coupled to the FEM algorithm for adatom diffusion, see figure 2.

As a first test case a circular island is treated. To approximate an isotropic situation evolution elements with 90 facets are used, see figure 3 a),b).

The instabilities of the island growth is triggered by the approximation of the step by a polygon. For a slightly tilted evolution element with five facets the instabilities are clearly caused by the prescribed anisotropy of the growth algorithm,see figure 3 c).

The next major step will be to connect the anisotropy of the growth algorithm to physical situations.

Another important issue is the effective derivation of a smooth and nearly equidistant polygon from the CA description of the island. Since the implementation of topological changes and incorporation of faceting is very natural, the algorithm seems to be worth further considerations.

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Lattice Gas Models and Kinetic Monte Carlo Simulation of Epitaxial Crystal Growth

Michael Biehl

A brief introduction is given to the Kinetic Monte Carlo (KMC) simulation of epitaxial crystal growth. Molecular Beam Epitaxy (MBE) serves as a particularly clear-cut prototype situation, but many of the aspects discussed here would carry

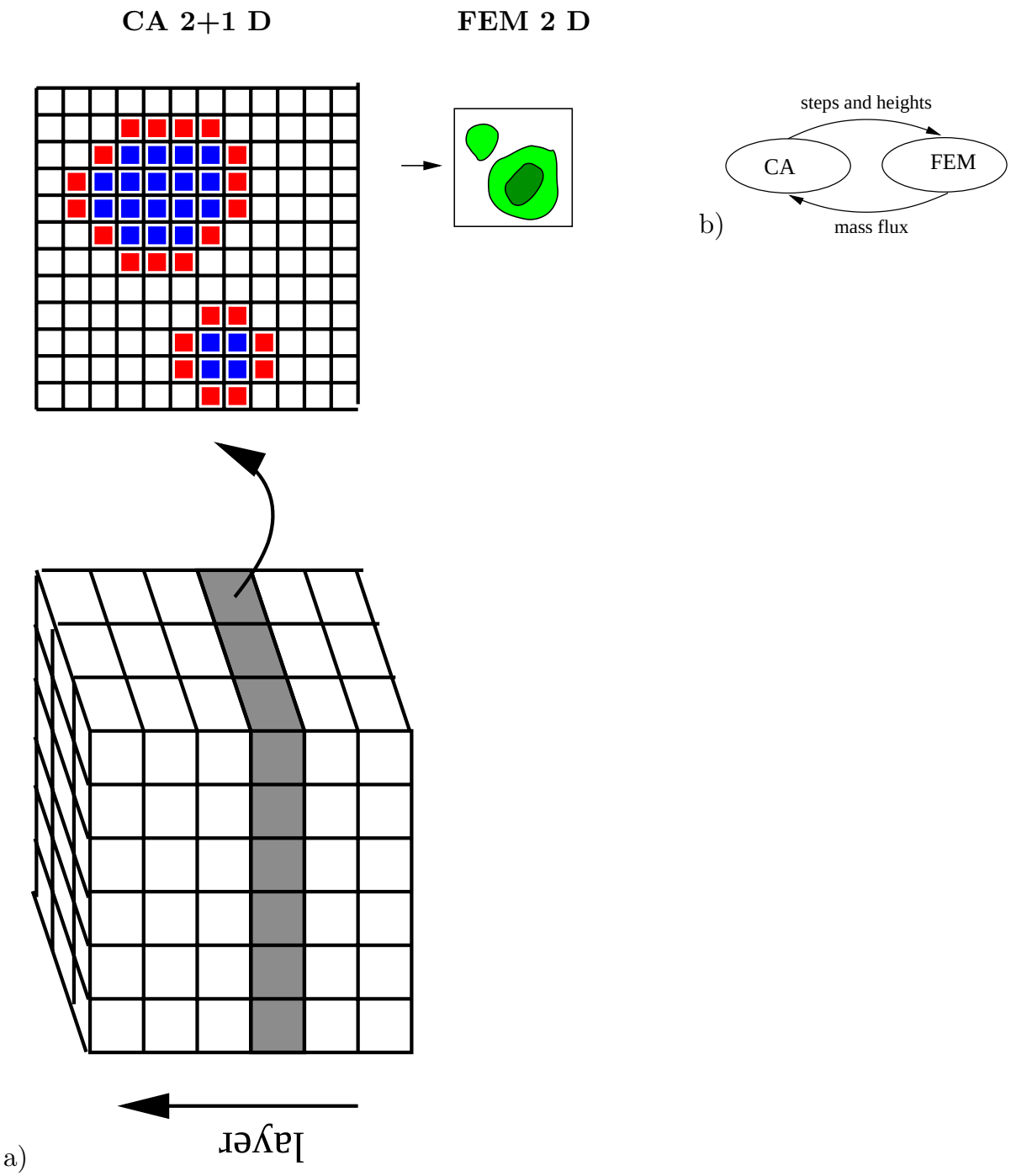

FIGURE 2. a) For each atomic layer a CA grid is defined. In each layer the islands of the corresponding height are defined. The steps are then transferred as polygons to the FEM calculation of adatom diffusion, the FEM algorithm then calculates the growth velocity of the steps, b).

over to other techniques. MBE has become a standard experimental setup for the production of high quality crystals, such as thin magnetic films or nano-scale

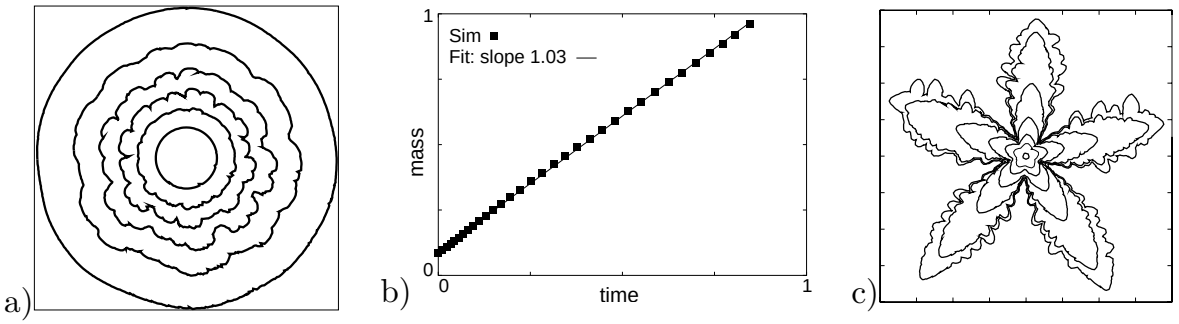

FIGURE 3. a) Envelope of the island. Curvature effects are not taken into account, so the growth is instable for small islands. The instability is driven by fluctuations in the definition of the steps. b) Overall mass conservation is 3%. c) Five sided evolution element. The instability is triggered by the anisotropy of the evolution element. (mass conservation $\approx 10\%$) .

semiconductor structures. At the same time it provides a framework in which to develop theoretical and computational concepts for the description of growth and more general non-equilibrium processes.

Different approaches to the modelling and simulation of MBE and similar growth techniques have been applied. They range from the full microscopic quantum mechanics treatment of the dynamics to the coarse grained description in terms of, for instance, stochastic differential equations. Here, the focus will be on discrete models such as lattice gas and Solid-On-Solid (SOS) models and the corresponding Kinetic Monte Carlo techniques. Various levels of simplification or sophistication have been employed in this context, depending on the precise goal of the investigation.

This contribution is far from giving an exhaustive review of the field. It is intended to provide a brief discussion of the basic concepts of KMC simulations and their strengths and limitations in the modelling of crystal growth processes. The following example books and review articles give a detailed and more complete overview of, both, the physics of epitaxial growth and the KMC method. They also provide plenty of further references.

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M. Kotrla, N.I. Pananicolaou, D.D. Vvedensky, and L.T. Wille (eds.), Proc. of the NATO Advanced Research Worshop on *Atomistic Aspects of Epitaxial Growth* Kluwer, Dordrecht 2001.

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Off-lattice Kinetic Monte Carlo Simulation of strained hetero-epitaxial growth

Michael Biehl

An off-lattice, continuous space Kinetic Monte Carlo algorithm is introduced and discussed [1, 2, 3, 4], which allows to study various phenomena known from strained, hetero-epitaxial crystal growth [5, 6].

As a starting point, we study a simplifying, 1+1 dimensional model with Lennard-Jones interactions. It exhibits, for instance, the appearance of misfit dislocations at a characteristic layer thickness [6, 3].

The focus of this talk is on the appearance of strain induced multilayer islands or *dots* upon a persisting wetting layer, i.e. the so-called Stranski-Krastanow growth mode [5, 7, 8, 9]. The transition from monolayer to multilayer islands occurs at a critical film thickness. Its dependence on the model parameters (lattice misfit, growth rate, and temperature) is investigated quantitatively. We find that for sufficiently large deposition rates the properties of the mounds is governed by the lattice mismatch only [8, 9].

The method is also applied in the context of surface alloy formation of immiscible metals on appropriate substrates. Two competing mechanisms for the emergence of nano-scale stripe structures are investigated [10].

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A Multiscale Approach to the Modelling of Chemical Vapor Deposition

Carlo Cavallotti

Computational material science of thin solid films has undergone great advancements in the last years. Significant progress has been made not only in the prediction and description of the surface and bulk properties of the materials, but also, from an engineering point of view, in the comprehension of the influence that the operating conditions of the growth process have on the desired material properties. An approach that has recently proved successful in the description of the thin film deposition processes is the multiscale modeling approach. It is based on the fact that growth of materials with well controlled morphological and compositional properties is a processes complicated by chemical and physical phenomena that occurs on time and length scales that can differ even by several orders of magnitude. I present a multiscale approach that has been developed to investigate the Chemical Vapor Deposition of epitaxial thin films at different time and length scales. The multiscale approach here outlined is designed to investigate the influence that gas phase and surface reactions have on the morphological and compositional evolution of thin solid films deposited by chemical vapor deposition. Atomic scale energetic and kinetic parameters, when not available from the literature, are estimated by means of quantum chemistry computations. The local gas phase composition, fluid dynamic and thermal fields are evaluated by integration of mass, energy and momentum equations at the reactor scale using kinetic and thermodynamic data calculated with quantum chemistry. The morphology of the film is finally investigated using 3 dimensional Kinetic Monte Carlo, which inputs are the gas phase fluxes calculated at the reactor scale and the kinetic parameters determined at the atomic scale. The calculation of kinetic parameters for CVD processes by means of quantum chemistry is usually performed by means of density functional theory (DFT). DFT calculations can be essentially of two different types, depending on the choice of the basis set between plane waves and Gaussian basis functions. While the first type of calculations has the advantage of treating more correctly systems with delocalized electrons, such as metals, the second offers the possibility to systematically increase the dimension of the basis set used for the calculations, and thus describe in higher detail the electronic density distribution. Since our analysis is focused mainly on semiconductors, in which electrons are usually localized within covalent bonds and atomic orbitals, we choose to perform our atomic scale calculations using gaussian basis functions with gradient corrected

functionals, such as B3LYP [1]. Surface processes are studied using clusters of different dimension to represent the surface structure. We choose to investigate the morphology evolution of the thin solid films with 3 Dimensional Kinetic Monte Carlo, that has the advantage over other mesoscale models to require as inputs kinetic constants or diffusion parameters that can be directly calculated by means of quantum chemistry. Our implementation of KMC follows the theory outlined by Weinberg [2], with direct tracking of real time and a rejection free choice of the random transition. The starting conditions of the KMC simulation are the surface structure at time 0, the surface temperature and the fluxes of gas phase species towards the surface. The output of a KMC simulation consists in the detailed surface morphology of the film after the deposition of a certain amount of layers. It is thus possible to determine the growth regime of the film, be it 3 dimensional, terrace step flow or 2 dimensional. The reactor scale modeling of CVD processes can nowadays be considered as a mature field. Several commercial CFD codes dedicated to CVD are in fact available and have been tested in many different occasions against experimental data. However, being the focus of our research the integrated multiscale modeling of the CVD process, we still rely on the use of our codes when the intent is that of linking together consistently KMC and reactor scale models [3]. The multiscale approach here proposed was used to investigate the epitaxial CVD of Si and ZnSe and the selective Metal Organic CVD of AlGaAs and InP [4, 5]. The results of the calculations were compared with experimental data with the aim of improving our understanding of the growth process.

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Configurational continuum modelling of crystal surface evolution

Navot Israeli
(joint work with Daniel Kandel)

We propose a novel approach to continuum modelling of dynamics of crystal surfaces. Our model follows the evolution of an ensemble of step configurations, which are consistent with the macroscopic surface profile. Contrary to the usual approach where the continuum limit is achieved when typical surface features consist of many steps, our continuum limit is approached when the number of step configurations of the ensemble is very large. The model is capable of handling singular surface structures such as corners and facets and has a clear computational advantage over discrete models.

Thermal decay and Ostwald ripening in homoepitaxy

Frank Haußer
(joint work with Axel Voigt)

The thermal relaxation of isolated (single layer) homoepitaxial islands and craters and of isolated nanomounds is simulated using a 2+1 dimensional step flow model. Numerical simulations based on adaptive finite elements are used to study decay rates of these structures in the diffusion limited and attachment-detachment limited regime under the influence of anisotropic effects.

Configurational continuum modelling of crystal surface evolution

Navot Israeli
(joint work with Daniel Kandel)

The behavior of classical physical systems is typically described in terms of equations of motion for discrete microscopic objects (e.g. atoms). The dynamics of the microscopic objects is usually very erratic and complex. Nevertheless, in many cases a smooth behavior emerges when the system is observed on macroscopic length and time scales (e.g. in fluid flow through a pipe). A fundamental problem in physics is to understand the emergence of the smooth macroscopic behavior of a system starting from its microscopic description. A useful way to address this problem is to construct a continuum, coarse-grained model, which treats the dynamics of the macroscopic, smoothly varying, degrees of freedom rather than the microscopic ones. The derivation of continuum models from the microscopic dynamics is far from trivial. In most cases it is done in a phenomenological manner by introducing various uncontrolled approximations.

In this work we address the above problem in the context of the dynamics of crystal surfaces. The evolution of crystal surfaces below the roughening transition proceeds by the motion of discrete atomic steps which are separated by high symmetry orientation terraces. One can model step motion by solving the diffusion problem of adatoms on the terraces with appropriate boundary conditions at step edges. This approach was introduced long ago by Burton, Cabrera and Frank [1], and was further developed by other authors [2]. The resulting models are capable of describing surface evolution on the mesoscopic scale with significant success [3, 4]. However, such models pose a serious challenge for numerical computations, and can be solved only for small systems.

Several attempts were made to construct continuum models for stepped surfaces [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17], in order to understand their large scale properties. The general idea behind these attempts is that step flow can be treated continuously in regions where every morphological surface feature is composed of many steps. If we label surface steps by the index n, the continuum limit in these models is obtained by taking n to be continuous. The outcome of these attempts are partial differential equations for surface evolution. Such continuum models are

fairly successful in describing the evolution of smooth surfaces with very simple morphologies. However, they suffer from fundamental drawbacks, which do not allow generalizations to more complex and realistic situations.

The most severe drawback is that below the roughening temperature, crystal surfaces have singularities in the form of corners and macroscopic facets. The latter are a manifestation of the cusp singularity of the surface free energy at high symmetry crystal orientations. The assumption that every surface feature is composed of many steps clearly breaks down on macroscopic facets where there are no steps at all. Thus, existing continuum models fail conceptually near singular regions. Several authors have tried to overcome this problem by solving a continuum model only in the non-singular parts of the surface and then carefully match the boundary conditions at the singular points or lines[11, 12, 13, 14]. In most cases however it is not at all clear how these matching conditions can be derived. Another approach is to round the surface free energy cusp [15, 16, 17], replacing true facets by relatively flat but analytic regions. This method implicitly assumes that the surface free energy derived for non singular orientations determines the dynamics on facets as well. This assumption is often found to be false because steps near facet edges obey different dynamics than steps in the sloping parts of the surface[12, 13].

In this work we propose a conceptually new definition of the continuum limit, which we term Configurational-Continuum[18]. Configurational-Continuum allows construction of continuum models, which are free of all the limitations of standard continuum models discussed above. It provides a rigorous way of deriving the continuum model directly from the discrete step equations of motion. Like other continuum models, Configurational-Continuum has a clear computational advantage over the discrete step model due to the small number of discretization points it requires for the description of smooth surface regions in a numerical scheme.

Our key observation in deriving Configurational-Continuum is that a continuous surface height profile defines an *ensemble* of microscopic step configurations which are all consistent with the continuous profile. The continuous profile in this picture evolves as the upper envelope of the ensemble with each configuration obeying the microscopic step dynamics. We derive the envelope equation of motion in the continuum limit when the number of configurations in the ensemble is very large. In contrast to the situation in standard continuum models, this Configurational-Continuum limit is exact.

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Universality classes for step bunching?

Joachim Krug
(joint work with V. Tonchev, S. Stoyanov)

In a remarkable recent paper [1], Pimpinelli and coworkers proposed a classification of step bunching instabilities in terms of scaling exponents characterizing the shape of the bunches and the time evolution of their size. The scaling exponents α, β and γ are defined through the relations

$$N \sim W^{\alpha}, \quad l_{\min} \sim N^{-\gamma}, \quad N \sim L \sim t^{\beta} \tag{4}$$

between the number of steps N in a bunch, the width W of the bunch, the minimal terrace size $l_{\min}$ in the bunch and the spacing L between bunches. The second and third of theses scaling relations have been observed experimentally in electromigration-induced step bunching on surfaces vicinal to Si(111) [2, 3].

Pimpinelli et al. derive the scaling exponents by dimensional analysis of a continuum height equation of the generic form

$$\frac{\partial h}{\partial t} = -\frac{\partial}{\partial x}\left[Bm^{\rho} + K\frac{\partial^2}{\partial x^2}m^{n}\right], \tag{5}$$

where $m = \partial h/\partial x > 0$ is the slope of the surface, assumed to be positive, the exponent ρ characterizes the instability mechanism and n is the exponent of the step-step interactions (usually $n = 2$). In this talk I address two questions: First, how can equations of the form (5) be derived from the underlying step dynamics? Second, are the scaling exponents correctly given by the dimensional analysis employed in [1]?

With regard to the first question, we show that an equation of the form (5) with $\rho = -1$ follows whenever the destabilizing part of the step dynamics can be assumed to be *linear* in the step spacings [4]. Examples for such kind of linear step dynamics include growth with strong inverse Ehrlich-Schwoebel barriers [5], as well as sublimation with conventional Ehrlich-Schwoebel barriers [6], and surface electromigration [7], provided attachment to the steps is slow. The latter implies

an additional mobility factor $1/m$ in front of the coefficient K of the stabilizing term in (5) [8, 9]. In a well-defined sense, these three problems therefore belong to the same universality class. The corresponding prediction of the theory of [1] for the scaling exponents is

$$\alpha = 1 + \frac{2}{n}, \quad \gamma = \frac{2}{2+n}, \quad \beta = \frac{1}{2}. \tag{6}$$

To address the second question, we have analyzed the stationary solutions of (5), which are characterized by the condition of constant current. For the universality class of interest it reads

$$J = \frac{B}{m} + \frac{K}{m}\frac{d^2}{dx^2}m^n \equiv J_0. \tag{7}$$

Interpreting m^n as a particle coordinate, this is Newton's equation for motion in a one-dimensional potential. The bunch shape corresponds to a trajectory starting at and returning to $m = 0$.

In analyzing this problem, it is important to realize that the mean current J_0 is not an adjustable integration constant; instead, it is forced by the microscopic boundary conditions to remain at the value $J_0 = B/m_0$ that it would have on the initial undisturbed vicinal surface of slope m_0 [6, 7]. For large bunches (large slopes) this implies that the mean current J_0 much exceeds the destabilizing part B/m inside the bunch, which is therefore irrelevant for the shape of the bunch. The latter is instead determined by the balance between the stabilizing step-step interaction term and the mean current. This problem was first analyzed by Nozières [8]. It gives rise to a bunch profile with the characteristic Pokrovsky-Talapov singularity

$$h(x) - h(x_0) \sim (x - x_0)^{3/2} \tag{8}$$

near the edges x_0 of the bunch. The scaling exponent for the minimal terrace size (i.e., the maximum value of the slope) turns out to be $\gamma = 2/(n+1)$, in contradiction to (6). This is because the relevant part of the current is in fact independent of the slope, so that the dimensional analysis should be carried out with $\rho = 0$ rather than with $\rho = -1$.

Numerical integration of the step dynamical equations shows good agreement with the expression for the minimal terrace size $l_{\min}$ derived through the above analysis, with regard to the scaling exponent γ as well as with regard to the prefactor in the scaling law [6, 10]. Similar agreement is found for the size l_1 of the *first* terrace in the bunch. On the other hand, the numerics indicates that the exponents α and β, which describe, in a sense, the *global* properties of bunches, are correctly given by the expressions (6) derived by dimensional analysis assuming $\rho = -1$. In particular, the scaling relation $\gamma = 1 - 1/\alpha$ suggested by trivial geometric considerations seems to be violated. We conjecture that this is related to the distinctly asymmetric bunch shape, which is not captured by the (manifestly symmetric) solutions of (7). In particular, the scaling of the size of the last terrace in the bunch (which is in fact hard to unambiguously identify) is completely different from that of the first terrace. Qualitatively, the asymmetry in

the bunch shape is related to the drift of bunches and the exchange of steps between bunches. Further work is needed to clarify to what extent these phenomena, and thus, the overall scaling of the bunch morphology, can be captured by continuum height equations.

The talk is based on joint work with Vesselin Tonchev and Stoyan Stoyanov.

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Surface Electromigration of single Islands

Philipp Kuhn
(joint work with Joachim Krug)

Surface electromigration is the biased diffusion of adatoms in the presence of an electric field. In order to understand the influence of this effect on the morphology of the surface we investigate the motion of a single island on a flat surface. We utilise a continuum approach where the island edge is treated as a continuous curve which evolves due to the competition between capillary forces and the electromigration force. We present an exact solution for the case without capillarity, and show numerical evidence for an oscillatory instability induced by crystal anisotropy in the step edge mobility.

Upper bounds on coarsening rates

Felix Otto
(joint work with Robert Kohn)

We consider two standard models of surface-energy-driven coarsening: a constant-mobility Cahn-Hilliard equation, whose large-time behaviour corresponds to Mullins-Sekerka dynamics; and a degenerate-mobility Cahn-Hilliard equation, whose large-time behaviour corresponds to motion by surface diffusion. Arguments based on scaling suggest that the typical length scale should behave as $l(t) \approx t^{1/3}$ in the first case and $l(t) \approx t^{1/4}$ in the second. We prove a weak, one-sided version of this assertion – showing, roughly speaking, that no solution can coarsen faster than the expected rates. Our results constrains the behaviour in a time-averaged sense

rather than pointwise in time, and it constrains not the physical length scale but rather the perimeter per unit volume.

Discretization and numerical tests of a diffuse-interface model with Ehrlich-Schwoebel barrier

Patrick Penzler, Tobias Rump
(joint work with Felix Otto)

We consider a step–flow model for epitaxial growth, as proposed by Burton, Cabrera and Frank. This type of model is discrete in the growth direction but continuous in the lateral directions. The effect of the Ehrlich–Schwoebel barrier, which limits the attachment rate of adatoms to a step from an upper terrace, is included. Mathematically, this model is a 2+1–dimensional dynamic free boundary problem for the steps. In [Nonlinearity 17, 477(2004)] a diffuse–interface approximation which reproduces an arbitrary Ehrlich–Schwoebel barrier has been proposed. It is a version of the Cahn–Hilliard equation with variable mobility. In this talk, we propose a discretization for this diffuse–interface approximation. Our approach is guided by the fact that the diffuse–interface approximation has a conserved quantity and a Liapunov functional. We obtain an implicit finite volume discretization of symmetric structure. We test the discretization by comparison with the matched asymptotic analysis. We also test the diffuse–interface approximation itself by comparison with theoretically known features of the original free boundary problem. More precisely, we investigate quantitatively the phenomena of step–bunching and the Bales–Zangwill instability.

Phase field models for step flow growth

Olivier Pierre-Louis

The relation between phase field and discontinuous models for crystal steps is analyzed. - Different formulations of the kinetic boundary conditions of the discontinuous model are first presented. We show that: (i) step transparency, usually interpreted as the possibility for adatoms to jump through steps, may be seen as a modification of the equilibrium concentration engendered by step motion. (ii) The interface definition (i.e. the position of the dividing line) intervenes in the expression of the kinetic coefficients only in the case of fast attachment kinetics. (iii) We also identify the thermodynamically consist ent reference state in the kinetic boundary conditions. - Asymptotic expansions of the phase field models in the limit where the interface width is small, lead to various discontinuous models: (1) A phase field model with one global concentration field and variable mobility is shown to lead to a discontinuous model with fast step kinetics. (2) A phase field model with one concentration field per terrace allows one to recover arbitrary step kinetics (i.e. arbitrary strong Ehrlich-Schwoebel effect and step transparency). - Quantitative agreement is found in the linear and nonlinear regimes, between the

numerical solution of the phase field models and the analytical solution of the discontinuous model.

Phase-field models for epitaxial growth

Andreas Rätz
(joint work with Axel Voigt)

Different phase field models are proposed as an approximation of classical sharp interface models of Burton-Cabrera-Frank type. The motion of island boundaries of discrete atomic layers is determined by the time evolution of an introduced phase-field variable. In order to describe attachment-detachment kinetics in epitaxial growth a reduced mobility is applied for the modelling of the asymmetry in the kinetic boundary conditions, while an increased mobility is used for the approximation of edge diffusion along the free boundary. We apply matched asymptotic expansion to determine the asymptotic limit of vanishing interfacial thickness and show the reduction to classical sharp interface models. Furthermore an adaptive finite element discretization and numerical results are shown.

Continuum ("height") models for surface growth, an overview

Martin Rost

In crystal growth models the surface is often represented by a height field h(x,t). Its dynamics can be derived on heuristic grounds yielding equations of the form ht(x,t) =3D =85, where the growth velocity above the substrate point x and at time t depends on the present surface configuration h. This talk attempts to give an introductory overview on the use of continuum height field dynamics for crystal growth focussing on three key issues: (i) thermodynamic and kinetic basis for its derivation, (ii) symmetries and conserved quantities, also in connection to analogous approaches in other fields, and (iii) typical applications and results, also linking it to more detailed crystal growth models.

Quasicontiuum Monte Carlo: A computational method for surface growth calculations

Peter Smereka
(joint work with Jason Devita, Giovanni Russo, Len Sander)

Epitaxial growth on surfaces is of central importance both for applications and as a very interesting example of statistical processes out of equilibrium. This growth process is commonly modeled by Kinetic Monte Carlo (KMC) and continuum models. In KMC each adatom is represented individually; therefore, it automatically includes internal noise processes. However, when there are many adatoms, (e.g. close to equilibrium) these simulations slow down considerably. A deterministic continuum model which represents the adatoms as a continuous

fluid does not have this problem, and should be much faster. There has been considerable work in the development of such models for epitaxial growth (see [1] references therein). In some cases they have been quite successful, but in other cases they have failed to reproduce the structures seen in experiment. One reason for such problems is that deterministic continuum models neglect important fluctuations. In this talk we present a method of dealing with some fluctuations without giving up the advantages of a continuum treatment. We call this approach Quasi-Continuum Monte Carlo (QCMC). The most important use of this method will be in cases where fluctuations are important, but which would be difficult to treat with KMC because of the presence of a large number of adatoms.

The first version of our QCMC algorithm goes as follows: we treat the islands on the surface as crystals containing discrete atoms which occupy the sites of a lattice. To illustrate the method we use a square lattice. On the other hand, the adatoms are treated as a continuum whose density, ρ, is governed by:

$$\partial_t \rho = D\nabla^2 \rho + F. \tag{9}$$

In practice, we solve this equation numerically on a discrete grid which is commensurate with the crystal lattice. On the surface of the island, we include boundary conditions that model both attachment and detachment processes. We then compute the velocity of the interface as one would have for a continuum model. However, in QCMC we interpret this in a way that includes fluctuations. For example, when attachment is the only process we compute the total flux onto the island boundary and when the total flux exceeds one atom, then one or more adatoms are attached to the boundary at random with the probability proportional to the normal speed. For more details see [4]. We have shown that this method agrees quite well with KMC and retains the advantages of a continuum method. This approach is similar to the dielectric breakdown model[3] which can be considered a generalization of diffusion limited aggregation[2]. Our method has been extended to multi-layer growth including nucleation in [5].

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Semi-implicit level set methods for curvature and surface diffusion motion

Peter Smereka

We introduce semi-implicit methods for evolving interfaces by mean curvature flow and surface diffusion using level set methods.

Regularized anisotropic curve shortening flow

Axel Voigt
(joint work with Frank Haußer)

Realistic interfacial energy densities are often non convex, which results in backward parabolic behaviour of the corresponding anisotropic curve shortening flow, thereby inducing phenomena such as the formation of corners and facets. Adding a term being quadratic in the curvature to the interfacial energy yields a regularized evolution equation for the interface, which is fourth order parabolic. Using a semi-implicit time discretization, we present a variational formulation of this equation, which allows the use of linear finite elements. The resulting linear system is shown to be uniquely solvable. We also present numerical examples. The described algorithm can also be used to solve Willmore flow.

A general finite element framework for Burton-Cabrera-Frank equations

Axel Voigt
(joint work with Eberhard Bänsch, Frank Haußer)

An adaptive finite element method is presented for step flow models in homoepitaxial growth. Such problems consist of an adatom (adsorbed atom) diffusion equation on each terrace; boundary condition on steps between the terraces including thermodynamic or kinetic conditions; and a normal velocity law for the motion of the steps, which is determined by a two-sided flux, together with edge-diffusion. Mathematically speaking it is a 2+1 model and it is solved using independent meshes, a two-dimensional mesh for the adatom diffusion and a one-dimensional mesh for the boundary evolution. The diffusion equation is discretized using linear composite finite elements in space and an implicit scheme in time in the case of attachment limited growth (kinetic boundary conditions). For diffusion limited growth (thermodynamic boundary conditions) a penalty method is applied. The evolution of the steps included surface diffusion, curvature flow and forcing terms. Its governing equation is solved by a semi-implicit front-tracking method using linear parametric finite elements. Simple adaptive techniques are employed in solving the adatom diffusion equation as well as the boundary motion problem.

Levelset formulation for fourth order geometric evolution problems

Ulrich Weikard
(joint work with Ulrich Clarenz, Frank Haußer, Axel Voigt)

A level set formulation of anisotropic surface diffusion is derived using the gradient flow perspective. Starting from single embedded surfaces and the corresponding gradient flow, the metric is generalized to sets of level set surfaces using the identification of normal velocities and variations of the level set function in time via the level set equation. The approach in particular allows to identify the natural dependent quantities of the derived variational formulation. Furthermore, spatial and temporal discretization are discussed and some numerical simulations in two and three dimensions are presented.

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