Zusammenfassung des Projektes:
"Optimization problems governed by Cahn-Hilliard variational inequalities"

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Summary

The aim of this project is to develop efficient numerical methods to *control interface evolution* governed by Cahn-Hilliard variational inequalities. The applications range from quantum dot formation in *crystal growth* of heteroepitaxial *thin films* and *grain growth* to void evolution in microelectronic devices. In all these applications a certain location of phases or special properties of the interface distribution are of importance.

The Cahn-Hilliard model is a conserved phase field model based on a diffuse (not sharp) interface. The underlying free energy is related to the interfacial thickness and includes an obstacle potential, where we focus on a double obstacle version. The model is usually formulated as a non-standard *variational inequality of fourth order*. Despite it is not obvious whether a particular designed simultaneous approach for the control problem, also called 'first discretize then optimize', would be more efficient, fast simulation methods are required. The current state of the art provides numerical simulation mainly to study the evolution and various appearing phenomena. While the convergence of these methods are established, they are in general not efficient and not fast enough to be used for control purposes. There exists only one approach for an efficient solver so far, namely the preconditioned *Uzawa type method* for the variational inequality developed by Gräser and Kornhuber. However there are certain limitations of their ansatz (concerning the dependence of the efficiency on the interfacial thickness) which we would like to avoid. Hence, either their method has to be revised or a new method has to be developed for the Cahn-Hilliard model, in order to have an efficient simulation solver for the overall control problem.

The semi-implicit time discretization of the Cahn-Hilliard model can be viewed itself as a control problem with possibly *nonlinear constraints, control box constraints* and a highly *complex cost function*, which includes semi-norms and non local behaviour of the control function. Hence the evolution of interfaces can be simulated by a sequence of optimization problems, where the inputs change with time. The control of interface evolution can be seen as a process of *nested optimization*. This will be the starting point for our numerical approach. In order to solve the control problem corresponding to the Cahn-Hilliard model we wish to study the application of the *primal-dual active set strategy* and/or a *semi-smooth Newton method*. While on the first glance the optimization formulation falls into the class, where convergence is guaranteed, it is not obvious whether all convergence conditions are fulfilled. This is one of the first issues which has to be clarified. Here, due to the time stepping local convergence is sufficient. The next question to clarify is how to apply the primal-active set strategy efficiently due to the semi-norms in the

cost function. Issues as *preconditioning, adaptivity and efficient time stepping* must be approached. As a first ansatz for preconditioning we think of a transfer or an extension of the preconditioner developed by Gräser and Kornhuber which is based on linear *Schur complements* associated with successive approximations of active constraints combined with *monotone multigrid methods*. Moreover, the dependency of the conditioning on the interfacial thickness has to be studied in detail. One may have to develop a problem adapted preconditioner which can be based on *deflation methods*. A rigorous ansatz for adaptivity for our problems could be based e.g. on the work of Morin, Nochetto and Siebert. The goal is to derive a mesh independent, *superlinear convergent* method where the dependence on the interfacial thickness is moderate.

In practical applications the Cahn-Hilliard variational inequality has to be coupled either to an elliptic system containing an elasticity system and the Laplace equation for the electrical potential or to a nonlinear heat equation. However, so far no algorithms with a convergence speed independent of the mesh size are known. Since the optimization formulation of the extended Cahn-Hilliard equations is an extended version of the optimization formulation of the Cahn-Hilliard equations, we see that an efficient solver for the Cahn-Hilliard equation formulated as optimization problem is a major step to construct an efficient solver for the more general case. In the first application period one of our goals is to develop a fast solver for the extended system. Either we extend the ideas of Gräser and Kornhuber. Or, when efficient methods based on the ideas of the semi-smooth Newton method are developed for Cahn-Hilliard variational inequalities, these have to be generalised to the extended versions. Exploiting the structure will be important in order to develop an efficient algorithm.

The final goal is to solve *optimal control problems* in which the extended versions of the Cahn-Hilliard variational inequality act as constraints. In addition to the *highly nonlinear constraints* the cost functional is often *non-convex* and gradient based. For the first application period we plan to study this optimal control problem analytically. We wish to derive first and second order optimality conditions as well as the *existence of Lagrange multipliers*, which is also necessary to apply and analyze methods such as *SQP methods*. We would like to point out that the structure of the control problem includes state box constraints. However, these box constraints can be hidden in the solution operator concerning the variational inequality, such that we suspect that these 'concealable' state constraints will not lead to major difficulties as they are typically known for control problems with non-variational PDE constraints. Since it does not seem promising to obtain smoothness of the solution operator concerning the variational inequality and of the remaining constraints, we target the application of a semi-smooth Newton method also for this overall control problem. However, first more theoretical insight into the problem is necessary, to derive possible *'semi-smooth' derivatives* (e.g. a slanting function). In a second application period it is planned to design and implement a fast solver for the optimal control problem with superlinear convergence. *Optimal design problems* involving Cahn-Hilliard variational inequalities shall also be an issue.