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A FINITE ELEMENT METHOD FOR ANISOTROPIC CRYSTAL GROWTH ON SURFACES

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Abstract. Phase transition problems on curved surfaces can lead to a panopticon of fascinating patterns. In this paper we consider finite element approximations of phase field models with a spatially inhomogeneous and anisotropic surface energy density. The problems are either posed in $\mathbb{R}^3$ or on a two-dimensional hypersurface in $\mathbb{R}^3$. In the latter case, a fundamental choice regarding the anisotropic energy density has to be made. One possibility is to use a density defined in the ambient space $\mathbb{R}^3$. However, we propose and advocate for an alternative, where a density is defined on a fixed chosen tangent space, and is then moved along geodesics to the other tangent spaces. Our numerical method can be employed in all of the above situations, where for the problems on hypersurfaces the algorithm uses parametric finite elements. We prove an unconditional stability result for our schemes and present several numerical experiments, including for the modelling of ice crystal growth on a sphere.

Key words. Crystal growth, hypersurface, phase field, anisotropy, finite elements, stability.

1. Introduction

Crystal growth on curved surfaces can lead to a multitude of interesting patterns. This phenomenon is one example of a phase change problem on a surface. Other applications involve phase separation on surfaces, the formation of two phases in vesicles or in lipid raft formation, see [1, 14, 35, 37, 42, 45, 49, 50, 52, 54, 63]. In this paper we numerically approximate interface evolutions on manifolds governed by an inhomogeneous, anisotropic interfacial energy by using a phase field approach. A particular application we have in mind is dendritic ice crystal growth on surfaces like soap bubbles, see, e.g., the fascinating pictures in [1], partly reproduced in Figure 1. Other possible applications are dendritic growths on aircraft bodies or metal shaped bodies, see [60], and phase separation on surfaces, see [54, 53, 30, 52, 42]. In the latter case one solves a Cahn–Hilliard equation on a surface with either an isotropic or an anisotropic surface energy.

Although phase field models in the Euclidean space have received a lot of attention, see [44, 40, 26, 61, 58, 59, 29, 3], not much is known for (anisotropic) phase field approaches for interface evolution problems on surfaces. Similarly, while for anisotropic phase field models in the Euclidean space a lot is known for the analysis and numerical analysis, see [33, 61, 43, 10, 11, 38, 39] and the references therein, not much is known for anisotropic models on surfaces.

There have been some numerical computations for phase field models describing crystal growth on surfaces, see [50, 63, 45]. However, no numerical analysis has been performed so far. In what follows, we will first introduce the governing equations leading to an anisotropic phase field model on a surface. This system reduces to an anisotropic Cahn–Hilliard equation in situations in which some terms involving time derivatives are neglected. On a surface the interfacial energy is defined on the tangent spaces of the surface. Here, a reasonable choice on how to choose the

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anisotropy when the tangent space changes has to be taken, in order to model physically realistic situations. We basically consider two cases. In the first case we fix an anisotropy in $\mathbb{R}^3$ and then restrict the anisotropy to the respective tangent spaces. The advantage is that the anisotropic density need not depend on space, and existing physical models and numerical methods can be easily extended from flat domains to surfaces. However, it will turn out that this choice has certain undesirable properties. A second choice is obtained by moving an anisotropy given on one fixed tangent space along geodesics to the other tangent spaces. This allows, for example, to choose a six-fold anisotropy on all tangent spaces, see Section 3.2.

For the numerical analysis, we generalize anisotropies introduced by Barrett, Garcke and Nürnberg in [4, 10, 12] to the surface case. This enables us to show stability bounds as well as to prove existence and uniqueness results for fully discrete approximations. These results are shown both for the case of a smooth potential, as well as for the case of an obstacle potential. We remark that the anisotropies can also depend on space, i.e., they can be inhomogeneous. We will then demonstrate the effect of an inhomogeneous energy with the help of numerical simulations. In addition, we will show the effect of different choices of the anisotropy. In particular, in the case where a 3d-anisotropy is restricted to the tangent spaces, the form of the anisotropy can change heavily from tangent space to tangent space. We observe a change from a six-fold anisotropy to a four-fold anisotropy. Moreover, a convergence experiment is presented using an explicit solution constructed by Rätz in [52]. Finally, computations for spinodal decomposition and crystal growth are also presented, where the latter leads to snow crystal growth on manifolds.

Let us now discuss literature related to this work. Basic information on parametric methods for curvature flow and its anisotropic variants can be found in [26, 51, 31, 6, 15, 16, 27, 28, 3]. Related are also the works [47, 48] for curvature flows on graphs. In the computer graphics literature also anisotropies on manifolds have been used and we refer to [56, 57, 64] for details. Phase separation on manifolds using the Cahn–Hilliard model on surfaces has been studied numerically in [54, 30, 52, 42, 22, 49]. Analytic results for inhomogeneous anisotropies can be found in [19, 2, 27].

The outline of this paper is as follows. In Section 2 we present the governing phase field equations on a surface in its strong and weak formulation. In Section 3 we present the different choices of the anisotropy and state and prove certain qualitative properties. Section 4 is devoted to a fully discrete finite element approximation of the anisotropic phase field equations on surfaces. We also state existence, uniqueness and stability results. Their proofs are mostly straightforward extensions of the results in [12] to surfaces and to spatially dependent anisotropies. Finally in Section 5 we present several numerical computations which demonstrate convergence as well as several qualitative properties of solutions.

2. The mathematical model and its weak formulation

2.1. The underlying anisotropic interfacial energy. Let $\mathcal{M} \subset \mathbb{R}^3$ be a given stationary smooth manifold, with or without boundary. We let n denote a continuous unit normal field on $\mathcal{M}$, and m the outer conormal on $\partial\mathcal{M}$. Let $(\Gamma(t))_{t\in[0,T]}$ be a family of evolving curves on $\mathcal{M}$. Then we consider a general anisotropic energy of the form

$$\mathcal{E}(\Gamma) = \int_\Gamma \gamma(z, \nu_{\mathcal{M}}(z))\, \mathrm{d}\mathcal{H}^1(z) = \int_\Gamma \gamma(\cdot, \nu_{\mathcal{M}})\, \mathrm{d}\mathcal{H}^1,$$