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A Splitting Scheme for the Numerical Solution of the KWC System

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Abstract. We consider a splitting method for the numerical solution of the regularized Kobayashi-Warren-Carter (KWC) system which describes the growth of single crystal particles of different orientations in two spatial dimensions. The KWC model is a system of two nonlinear parabolic PDEs representing gradient flows associated with a free energy in two variables. Based on an implicit time discretization by the backward Euler method, we suggest a splitting method and prove the existence as well as the energy stability of a solution. The discretization in space is taken care of by Lagrangian finite elements with respect to a geometrically conforming, shape regular, simplicial triangulation of the computational domain and requires the successive solution of two individual discrete elliptic problems. Viewing the time as a parameter, the fully discrete equations represent a parameter dependent nonlinear system which is solved by a predictor corrector continuation strategy with an adaptive choice of the time step size. Numerical results illustrate the performance of the splitting method.

AMS subject classifications: 65M12,35K59,74N05

Key words: Crystallization, Kobayashi-Warren-Carter system, splitting method.

1. Introduction

The Kobayashi-Warren-Carter (KWC) system is an orientation field based multi-phase field model describing the growth of single crystal particles of different orientations in two spatial dimensions. It has been originally suggested in [19, 31] (cf. also [25, 32]) and further studied in [14–16]. We refer to the monograph [25] for further references. The KWC model is a system of two nonlinear parabolic PDEs representing gradient flows associated with a free energy in two variables, namely the orientation angle and the orientation order (local degree of crystallinity). In particular, the equation with regard to the orientation angle is a second order total variation flow. A mathematical analysis of the KWC system has been provided in [11, 18, 21, 22] mainly focusing on results concerning the existence of a solution. Splitting methods for the numerical solution of PDEs go back to the seminal

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work [24] and have been further studied in [28] (cf. also the monographs [13,30] and the review article [20] as well as the references therein).

In this paper, we consider a standard regularization of the total variation flow and focus on an approximation of the thus regularized KWC system by a splitting scheme based on an implicit discretization in time by the backward Euler method. The splitting allows to treat the problems in the orientation angle and the orientation order independently at each time step. We prove the existence and energy stability of a solution. For discretization in space we use Lagrangian finite elements with respect to a geometrically conforming, shape regular, simplicial triangulation of the computational domain. Considering the time as a parameter, the fully discrete nonlinear equations represent a parameter dependent nonlinear system which is solved by a predictor-corrector continuation strategy (cf. [6,17]). This strategy consists of constant continuation as a predictor and Newton's method as a corrector and features an adaptive choice of the time step. Numerical results are provided that illustrate the performance of the splitting scheme.

In this paper, we use standard notation from Lebesgue and Sobolev space theory (cf., e.g., [29]) and the theory of functions of bounded variation (cf., e.g., [1,7,12]) and functions of weighted bounded variation (cf. [2]). In particular, for a bounded domain $\Omega \subset \mathbb{R}^d, d \in \mathbb{N}$, we refer to $L^p(\Omega), 1 \leq p < \infty$, as the Banach space of p-th power Lebesgue integrable functions on Ω with norm $\|\cdot\|_{0,p,\Omega}$ and to $L^\infty(\Omega)$ as the Banach space of essentially bounded functions on Ω with norm $\|\cdot\|_{0,\infty,\Omega}$. Given a Muckenhoupt weight function ω of class $\mathscr{A}_p, 1 \leq p < \infty$, [23, 27], the space $L^p(\Omega;\omega)$ is the Banach space of weighted p-th power Lebesgue integrable functions u on Ω with norm $\|u\|_{0,p,\omega,\Omega} := (\int_\Omega \omega |u|^p \ dx)^{1/p}$.

Further, we denote by $W^{s,p}(\Omega), s \in \mathbb{R}_+, 1 \leq p \leq \infty$, the Sobolev spaces with norms $\|\cdot\|_{s,p,\Omega}$. We note that for $p = 2$ the spaces $L^2(\Omega)$ and $W^{s,2}(\Omega) = H^s(\Omega)$ are Hilbert spaces with inner products $(\cdot,\cdot)_{0,2,\Omega}$ and $(\cdot,\cdot)_{s,2,\Omega}$. In the sequel, we will suppress the subindex 2 and write $(\cdot,\cdot)_{0,\Omega}, (\cdot,\cdot)_{s,\Omega}$ and $\|\cdot\|_{0,\Omega}, \|\cdot\|_{s,\Omega}$ instead of $(\cdot,\cdot)_{0,2,\Omega}, (\cdot,\cdot)_{s,2,\Omega}$ and $\|\cdot\|_{0,2,\Omega}, \|\cdot\|_{s,2,\Omega}$.

Moreover, for a Muckenhoupt weight function ω of class $\mathscr{A}_1$ we denote by $BV(\Omega;\omega)$ the Banach space of functions $u \in L^1(\Omega;\omega)$ such that

$$\mathrm{var}_\omega u(\Omega) := \sup \Big\{ -\int_\Omega u \nabla \cdot \mathbf{q} \ dx, \mathbf{q} \in C_0^1(\Omega;\mathbb{R}^2), |\mathbf{q}| \leq \omega \text{ in } \Omega \Big\} < \infty,$$

equipped with the norm

$$\|u\|_{BV(\Omega;\omega)} := \|u\|_{0,1,\omega,\Omega} + \mathrm{var}_\omega u(\Omega).$$

2. The Kobayashi-Warren-Carter system

The Kobayashi-Warren-Carter system is an orientation field based multi-phase field approach where the associated free energy functional is given in terms of an orientation field Θ, which locally describes the crystallographic orientation, and a structural order parameter ϕ, which is called the orientation order and describes the local degree of crystallinity.