INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 19, Number 1, Pages 85–100

A SCALAR AUXILIARY VARIABLE (SAV) AND OPERATOR SPLITTING COMPACT FINITE DIFFERENCE METHOD FOR PERITECTIC PHASE FIELD MODEL

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Abstract. Peritectic crystallization is a process in which the solid phase precipitated in the form of solid solution reacts with the liquid phase to form another solid phase. The process can be described by a phase field model where two continuous phase variables, ϕ and ψ, are introduced to distinguish the three different phases. We discretize the time variable with a scalar auxiliary variable (SAV) method that can ensure the unconditional energy stability. Moreover, the SAV method only requires solving a linear system at each time step and therefore reduces the computational complexity. The space variables in a two-dimensional region are discretized by an operator splitting method equipped with a high order compact finite difference formulation. This approach is effective and convenient since only a series one-dimensional problems need to be solved at each step. We prove the unconditional energy stability theoretically and test the order of convergence and energy stability through numerical experiments. Simulations of peritectic solidification demonstrate the patterns formed during the process.

Key words. Peritectic crystallization, phase field model, scalar auxiliary variable (SAV) method, operator splitting, compact finite difference method.

1. Introduction

Peritectic crystallization occurs when the solution of alloy is cooled down to critical temperature and one solid phase, denoted by α, precipitated in the form of solid solution reacts with the liquid phase to form another solid phase, denoted by β. This process is similar to eutectic crystallization where the two different solid phases precipitated simultaneously from the solution. The mathematical modeling of both processes has gradually matured with the application of phase field model. In a typical phase field model, a variable, usually denoted by ϕ, takes two different values in solid and liquid, e.g. $+1$ and -1, changes smoothly between the two values in the region around the interface and diffuses with a limited width. Another variable, ψ, is used to distinguish the α-solid and β-solid in the same way. The discrete position of the interface can be defined as the set of all points where the phase field takes a specific value, e.g. 0. In other words, the phase field model does not track the location of the interface explicitly, unlike the sharp-interface approach such as level-set method, hence is effective in simulations of complicated patterns formed in alloy solidification.

Concerning the peritectic process, Trivedi [26] proposed a one-dimensional model to explain the formation of peritectic banded structure in pure diffusion controlled growth. This model is improved by P. Mazumder, R. Trivedi and A. Karma [20] under the assumption of a planar solidification front and incorporation with a fully two-dimensional convection flow field. A. Wheeler et al [29] proposed a phase field model for eutectic solidification which is then developed for both eutectic and peritectic phase transitions [21]. Based on [29], T. S. Lo, A. Karma and M. Plapp

Received by the editors January 28, 2021 and, in revised form, May 7, 2021.
2000 *Mathematics Subject Classification.* 65M06, 65M12, 65P99, 35Q99.
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[19] developed a phase field model of the formation of microstructure mode during directional solidification of amorphous unstable peritectic alloys. This model will be discussed and solved numerically in the following sections.

As the evolution of phase field model is driven by energy dissipation, it is crucial to imitate this physical law in numerical approximation. Numerical schemes that satisfy discrete energy dissipation law are energy stable. X. Yang and D. Han [32] developed a series of linear, unconditionally energy stable numerical schemes for solving the phase field crystal model. The temporal discretizations are based on the first order Euler method, the second order backward differentiation formulas (BDF2) and the second order Crank-Nicolson method, respectively. K. Cheng, W. Feng and C. Wang [4] proposed an energy stable numerical scheme for the Cahn-Hilliard equation by the long stencil fourth order finite difference approximation. In the temporal approximation, a second order BDF stencil is applied with a second order extrapolation formula applied to the concave diffusion term, as well as a second order artificial Douglas-Dupont regularization term, for the sake of energy stability. K. Cheng, C. Wang and S. M. Wise [5] proposed an energy stable numerical scheme for the strongly anisotropic Cahn-Hilliard model that is discretized in space by the Fourier pseudospectral method. C. Elliott and A. Stuart [11] construct an energy stable scheme with the convex splitting method that was applied to solve Cahn-Hilliard equation by D. Eyre [12]. W. Chen et al [3] combined the convex splitting method with a variable step BDF-2 approach and mixed finite element method to approximate the Cahn-Hilliard equation and obtained second order rate of convergence. Although the convex splitting method is unconditionally energy stable, a nonlinear system has to be solved at every time level. J. Zhu et al [37] proposed an efficient numerical method for the phase field model that maintains the energy stability by adding an artificial stabilization term. However, this approach is difficult to extend to high-order schemes.

F. Guilln-Gonzlez and G. Tierra [15, 2] proposed the invariant energy quadratization (IEQ) method to solve the interface diffusion problem. The IEQ method can be effectively extended to the higher-order schemes and only require solving linear systems with variable coefficients at each time step [31]. The IEQ method is then developed by J. Shen [23, 24] to scalar auxiliary variable (SAV) method and is widely used in numerical approximations for phase field and related problems [1, 6, 13, 34, 35, 28, 36]. In addition to maintaining unconditional energy stability, only linear systems with *constant* coefficients need to be solved at each step. And, unlike IEQ method, the SAV approach reduces the system to *de-coupled* Poisson type equations for multi-component models. In this paper, we apply the SAV method for time discretization in the numerical approximations of the peritectic phase transition.

To account for the two-dimensional space variable, we implement an operator splitting approach equipped with a high order compact finite difference scheme [14, 30]. The 2D Poisson problem is separated into two 1D equations that are solved by fourth-order compact finite difference schemes. The operator splitting method has been widely used to approximate high dimensional problems. C. Zhang et al [33] proved the nonlinear stability and convergence of a second-order operator splitting scheme applied to the "good" Boussinesq equation. Y. Cheng et al [7] proposed a fast explicit operator splitting method for the epitaxial growth model with slope selection. This approach is modified by X. Li, Z. Qiao and H. Zhang [16] with a compact center-difference scheme. C. Liu, C. Wang and Y. Wang [17] suggested a