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Fast High Order and Energy Dissipative Schemes with Variable Time Steps for Time-Fractional Molecular Beam Epitaxial Growth Model

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Dedicated to the memory of Professor Zhongci Shi

Abstract. In this paper, we propose and analyze high order energy dissipative time-stepping schemes for time-fractional molecular beam epitaxial (MBE) growth model on the nonuniform mesh. More precisely, $(2-\alpha)$-order, second-order and $(3-\alpha)$-order time-stepping schemes are developed for the time-fractional MBE model based on the well known L1, L2-1_σ, and L2 formulations in discretization of the time-fractional derivative, which are all proved to be unconditional energy dissipation in the sense of a modified discrete nonlocal-energy on the nonuniform mesh. In order to reduce the computational storage, we apply the sum of exponential technique to approximate the history part of the time-fractional derivative. Moreover, the scalar auxiliary variable (SAV) approach is introduced to deal with the nonlinear potential function and the history part of the fractional derivative. Furthermore, only first order method is used to discretize the introduced SAV equation, which will not affect high

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order accuracy of the unknown thin film height function by using some proper auxiliary variable functions $V(\xi)$. To our knowledge, it is the first time to unconditionally establish the discrete nonlocal-energy dissipation law for the modified L1-, L2-1_σ-, and L2-based high-order schemes on the nonuniform mesh, which is essentially important for such time-fractional MBE models with low regular solutions at initial time. Finally, a series of numerical experiments are carried out to verify the accuracy and efficiency of the proposed schemes.

AMS: 65M06, 65M15, 41A05, 41A25

Key words: Time-fractional molecular beam epitaxial growth, variable time-stepping scheme, SAV approach, energy stability.

1 Introduction

The technique of molecular beam epitaxy (MBE) is among the most refined methods for the growth of thin solid films and is of great importance for applied studies. It allows to grow high-quality crystalline films, and form structures with high precision in the vertical direction, such as monolayer-thin interfaces or atomically flat surfaces. The macroscopic evolution of the growing film is directly related to movement of adatoms on surfaces and their various bonding configurations, thus it is attractive to use atomic-scale simulations for a theoretical description of epitaxial growth. However, in order to reach the length and time scales of interest for various applications, the continuous models have to be used. Several different types of MBE models including atomistic models [9, 24], continuum models [26, 48], and hybrid models [6, 14], have been derived and investigated to better understand the thin film growth mechanisms behind its technological applications. Among these models, the continuum model has been attracting particular interest in the community by modeling the epitaxial growth via partial differential equations with structure of gradient flow:

$$\frac{\partial \phi}{\partial t} = -M \frac{\delta E(\phi)}{\delta \phi}, \tag{1.1}$$

where ϕ is a scaled height function of the thin film, M represents a positive mobility parameter, and $\frac{\delta E(\phi)}{\delta \phi}$ is functional derivative in term of a total free energy $E(\phi)$ in L^2 sobolev space. It is worth to mention that the above MBE model (1.1) satisfies the following energy dissipation law

$$\frac{d}{dt} E(\phi) = \Big(\frac{\delta E(\phi)}{\delta \phi}, \frac{\partial \phi}{\partial t} \Big) = -\frac{1}{M} \Big\| \frac{\partial \phi}{\partial t} \Big\|^2 \leq 0, \tag{1.2}$$