Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. **16**, No. 1, pp. 1-23

DOI: 10.4208/aamm.OA-2021-0193
February 2024

# A Hessian Recovery Based Linear Finite Element Method for Molecular Beam Epitaxy Growth Model with Slope Selection

Minqiang Xu[1,2] and Qingsong Zou[3,*]

[1] *College of Science, Zhejiang University of Technology, Hangzhou, Zhejiang 310023, China*
[2] *School of Computer Science and Engineering, Sun Yat-Sen University, Guangzhou, Guangdong 510275, China*
[3] *School of Computer Science and Engineering, and Guangdong Province Key Laboratory of Computational Science, Sun Yat-Sen University, Guangzhou, Guangdong 510275, China*

Received 3 June 2021; Accepted (in revised version) 19 May 2022

**Abstract.** In this paper, we present a Hessian recovery based linear finite element method to simulate the molecular beam epitaxy growth model with slope selection. For the time discretization, we apply a first-order convex splitting method and second-order Crank-Nicolson scheme. For the space discretization, we utilize the Hessian recovery operator to approximate second-order derivatives of a $C^0$ linear finite element function and hence the weak formulation of the fourth-order differential operator can be discretized in the linear finite element space. The energy-decay property of our proposed fully discrete schemes is rigorously proved. The robustness and the optimal-order convergence of the proposed algorithm are numerically verified. In a large spatial domain for a long period, we simulate coarsening dynamics, where 1/3-power-law is observed.

**AMS subject classifications**: 65N30, 45N08

**Key words**: Molecular beam epitaxy, Hessian recovery, linear finite element method, superconvergence.

## 1 Introduction

In recent years, the molecular beam epitaxy (MBE) growth approach has become a powerful tool for thin-film deposition of single crystal [15,43]. So MBE growth technique has been widely applied in material science, especially in semi-conductor manufacture and

*Corresponding author.
*Emails:* mqxu@zjut.edu.cn (M. Xu), mcszqs@mail.sysu.edu.cn (Q. Zou)

 

nano-technology industry. In previous works, there are mainly three types of mathematical modelings to study dynamics of the MBE growth process: atomistic models [2, 19], continuum models [23, 31, 42] and hybrid models [6, 14].

We are interested in the continuum model with slope selection introduced by Moldovan and Golubovic [29]. It describes the evolution of the MBE growth with isotropic symmetry current, of which the governing equation takes the form [22]:

$$\begin{cases} \partial_t u = -\varepsilon\Delta^2 u + \nabla\cdot(|\nabla u|^2\nabla u - \nabla u) & \text{in } \Omega\times[0,T], \\ u(\cdot,0) = u_0(\cdot) & \text{in } \Omega, \end{cases} \tag{1.1}$$

where $\Omega$ is a smooth domain, $\varepsilon$ is a positive constant, and the unknown function $u$ represents the epitaxy surface height of the thin film. Moreover, we suppose $u$ satisfies a certain periodic boundary condition or Neumann boundary conditions $\partial_{\mathbf{n}} u|_{\partial\Omega} = 0$ and $\partial_{\mathbf{n}}\Delta u|_{\partial\Omega} = 0$, where $\mathbf{n}$ is the outward normal on the boundary. The MBE equation (1.1) can be derived via an $L^2$-gradient flow of the effective free energy functional [11, 20]

$$E(u) := \int_\Omega \left(\frac{\varepsilon}{2}|\Delta u|^2 + \frac{1}{4}(|\nabla u|^2 - 1)^2\right) d\Omega, \tag{1.2}$$

of which the first term represents the surface diffusion effect [11] and the second term describes the Ehrlich-Schwoebel effect [22]. Thanks to the flux free condition at the boundary, it is trivial to show that the energy decay property

$$\frac{dE(u)}{dt} = -\|u_t\|_0^2 \le 0, \quad \forall t > 0,$$

and the total mass conservation property

$$\frac{d}{dt}\int_\Omega u d\Omega = 0,$$

always hold for the solution of the MBE equation (1.1).

During the past several decades, the numerical solution for (1.1) (see e.g., [4, 6, 8–10, 12–14, 18, 21, 24, 25, 27, 28, 32–35, 37, 38, 41, 44, 47, 48, 51]) has been intensively investigated based on variants of temporal discretization and spatial discretization techniques.

On temporal-discretization, two popular approaches can guarantee the energy decay property of the numerical solution. The basic idea of the first approach is so-called *convex splitting* which splits the nonlinear term to the convex part which will be treated implicitly and the concave part which will be treated explicitly, see [5, 41, 44, 47]. The unconditional energy decay property and the unique solvability of the numerical solution of this approach could be easily derived. However, such methods lead to a nonlinear algebraic system that requires high computational cost. The second approach is the so-called *linear stabilization approach* which treats the nonlinear term only explicitly and guarantees the energy stability by adding a linear artificial penalty term, see [38–40, 49]. Such a method